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生物物理

SEIBUTSU BUTSURI

SUPPLEMENT 1-2
Vol.57

第55回年会予稿集

2017.9.19（火）～ 21（木）

熊本大学 黒髪北地区

主催　一般社団法人　日本生物物理学会

The Biophysical Society of Japan
一般社団法人　日本生物物理学会　http://www.biophys.jp

第 55 回日本生物物理学会年会

The 55th Annual Meeting of the Biophysical Society of Japan

目次

Contents

The 55th Annual Meeting of the Biophysical Society of Japan (BSJ2017)

第55回日本生物物理学会年会（2017年度）

会 期 Date

2017年 9月19日（火）－ 21日(木)
September 19 (Tue) - 21 (Thu), 2017

会 場 Venue

熊本大学 黒髪北地区
(〒860-8555 熊本市中央区黒髪2丁目40番1号)
Kurokami North Campus, Kumamoto University
(2-40-1 Kurokami, Chuo-ku, Kumamoto-shi, 860-8555 JAPAN)

年会実行委員長 Chair

山縣 ゆり子（熊本大学大学院生命科学研究部）
Yuriko Yamagata (Kumamoto University)

Website http://www.aeplan.co.jp/bsj2017/
※会期後は日本生物物理学会にデータが移行されますので、学会ホームページよりご覧ください。

抄録本文（Abstract）...
オンライン講演予稿集は、こちらからダウンロードいただけます。

http://www.biophys.jp/dl/pro/55th_proceedings.pdf
ID:ambsj55 Password:kumamoto2017
※スマートフォン・タブレット端末向けのプログラム検索・要旨閲覧アプリは、2017年9月15日(金)に公開予定です。

編集・発行：第55回日本生物物理学会年会実行委員会
E-mail : bp_nenkai55@kumamoto-u.ac.jp
発行日 : 表4（裏表紙）記載

The 55th Annual Meeting of the Biophysical Society of Japan (BSJ2017)

第55回日本生物物理学会年会（2017年度）

開催にあたって

第55回年会　実行委員長

山縣 ゆり子

（熊本大学大学院生命科学研究部）

一般社団法人日本生物物理学会第55回年会を、熊本大学黒髪北キャンパスにて2017年9月19日～22日の日程で開催いたします。熊本での開催は学会創立以来、初めてのことです。ご存知のように、昨年4月の熊本地震の後、第55回年会の熊本開催について実行委員の中でもいろいろな意見がありましたが、周りの方々の「ぜひ開催して下さい」という声に押され準備を進めてまいりました。暑い時期の熊本の地で、会場も復旧事業中で参加者にはご不便をおかけすることも多いかと思いますが、サイエンスに熱い年会として議論や交流を楽しんでいただければと願っております。

熊本年会では、すっかり恒例となりましたが、すべての発表は英語で行われます。シンポジウムの募集に際しては、一般会員から生物物理分野の様々な視点、特に、最先端の融合的研究に関する多数の応募と大型プロジェクトを組織している研究者による積極的な企画をしていただいたのに加え、学会本部にも日印、日台の2つの二国間交流シンポジウムを企画していただき、計44シンポジウムを開催します。

一般発表は、ポスター発表と口頭発表とし、応募者の希望を反映し、それぞれ、633件と215件の発表が行われます。13回目を迎える若手奨励賞に加えて、昨年創設された若手招待講演賞と学生発表賞が2回目を迎えます。本年の学生発表賞は、優秀な口頭発表に授与されます。

さらに、男女共同参画・若手支援シンポジウムとキャリア支援説明会、第4回総会シンポジウム や第6回BPPB論文賞受賞講演会なども年会におけるイベントとして定着してきました。また、科研費説明会では、平成30年度から実施される科研費制度改革に関する最新の情報を提供いたします。協賛企業による展示会やランチョンセミナーにおいては、最新の計測機器や研究を支援するシステムや製品等の情報が紹介されます。

全体として、生物物理学分野の研究手法の進展とそれに伴う原子から集団といったそれぞれの研究対象の質的深化に加え、国際的な環境で、20代からの若い世代の活躍を含め、学会が着実に前進していることが実感させられる年会になると期待しています。

最後に、熊本では熊本の食、人、歴史、自然などに親しんでいただくなかで、地震の爪痕や復旧・復興状況をご覧になりましたら、防災・減災を考える機会にしていただければ幸いです。

第55回日本生物物理学会年会実行委員会
-Organizers-

年会実行委員長
山縣ゆり子　(熊本大学大学院生命科学研究部)

Chair
Yuriko Yamagata　(Kumamoto University)

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野坂通子	(佐世保工業高等専門学校物質工学科)	Michiko Nosaka	(National Institute of Technology, Sasebo College)
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森本雄祐	(九州工業大学大学院情報工学研究院)	Yusuke Morimoto	(Kyushu Institute of Technology)
安永卓生	(九州工業大学大学院情報工学研究院)	Takuo Yasunaga	(Kyushu Institute of Technology)
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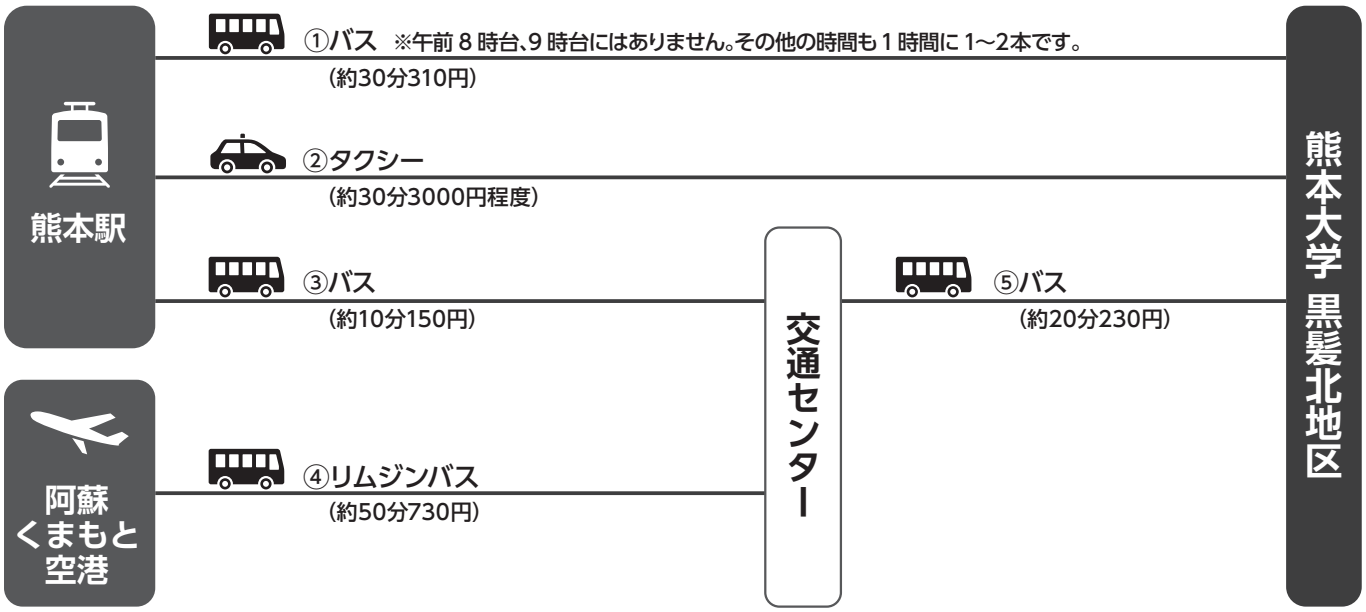
吉田紀生	(九州大学大学院理学研究院)	Norio Yoshida	(Kyushu University)
吉永壮佐	(熊本大学大学院生命科学研究部)	Sosuke Yoshinaga	(Kumamoto University)

※50音順。敬称略。

アクセス図 / 会場周辺図



①JR 熊本駅→熊本大学：熊本大学まで直通のバス
（所要約30分、310円）
※午前8時台、9時台にはありません。その他の時間も1時間に1〜2本です。

②タクシー（所要約 30分、3,000円程度）

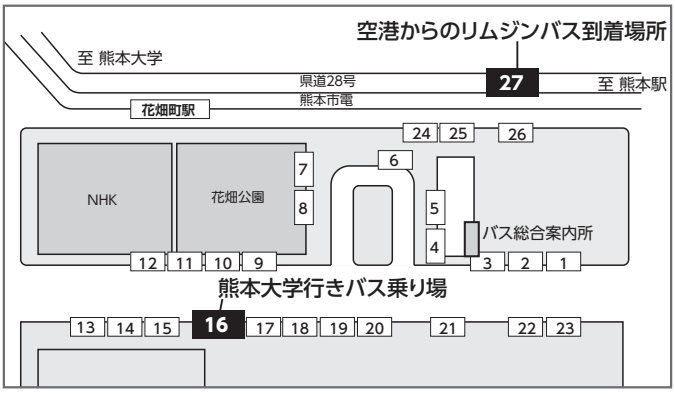
③JR 熊本駅→交通センター：熊本駅東口のバス乗り場からバス
（所要約10分、150円）

④阿蘇くまもと空港→交通センター：リムジンバス
（所要約50分、730円）

⑤交通センター→熊本大学：16番バス乗り場（右図参照）から「子1、子7、子8、子10、子17、子20」系統（熊本大学前経由）で「熊本大学前」下車（所要約20分、230円）

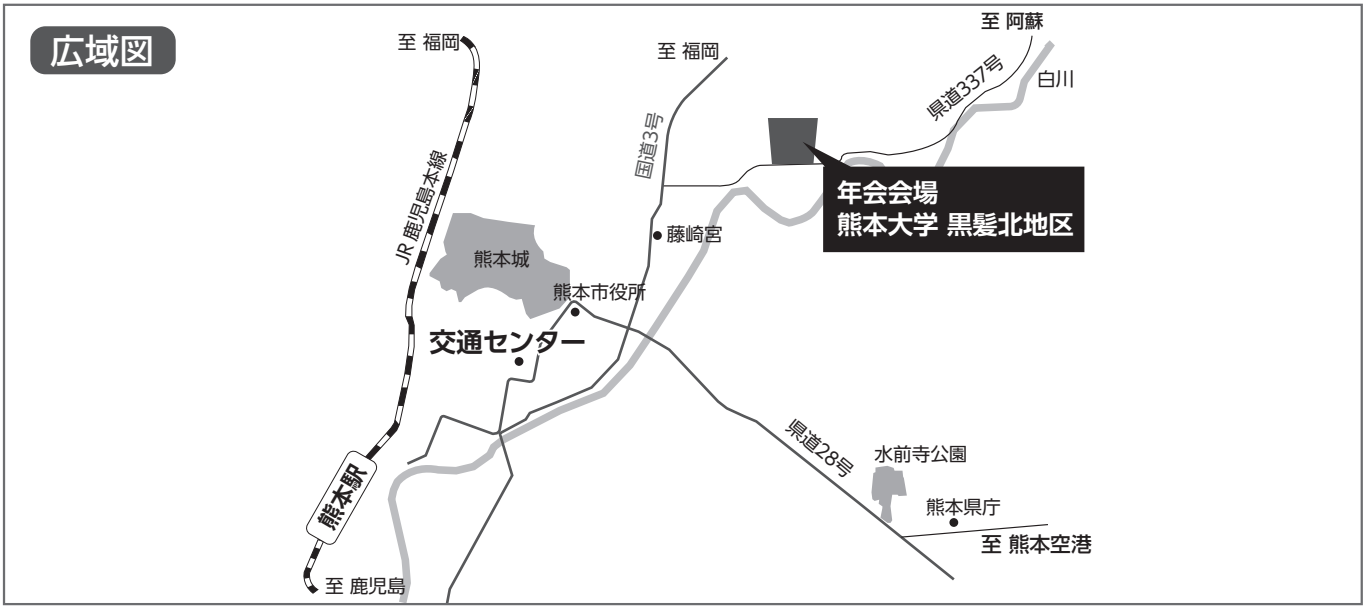
※渋滞等で所要時間が長くなることがあります。ご留意ください。

交通センターバス乗り場

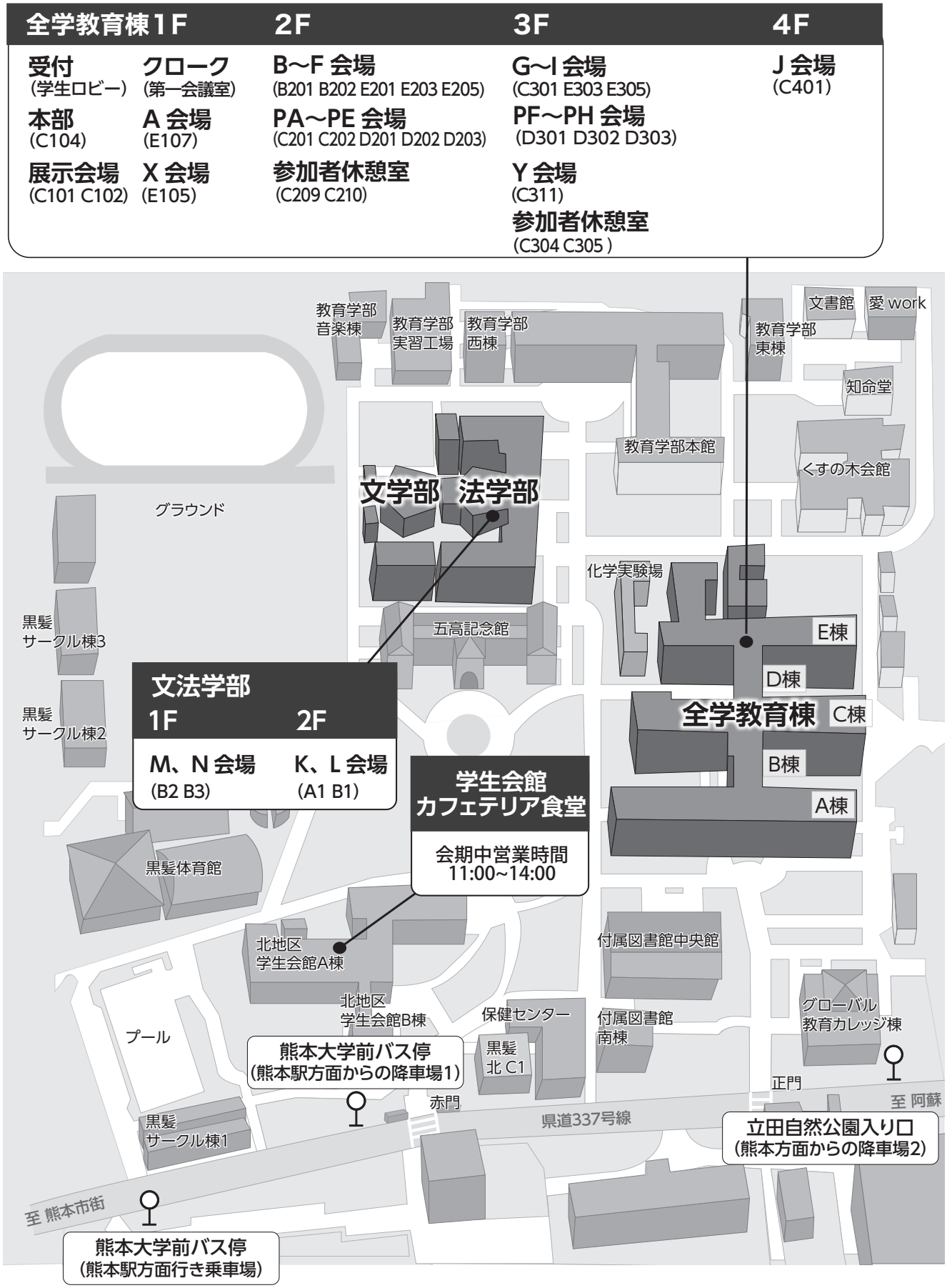


※熊本大学へのバス増便を予定しております。
詳細は年会HPをご覧ください。

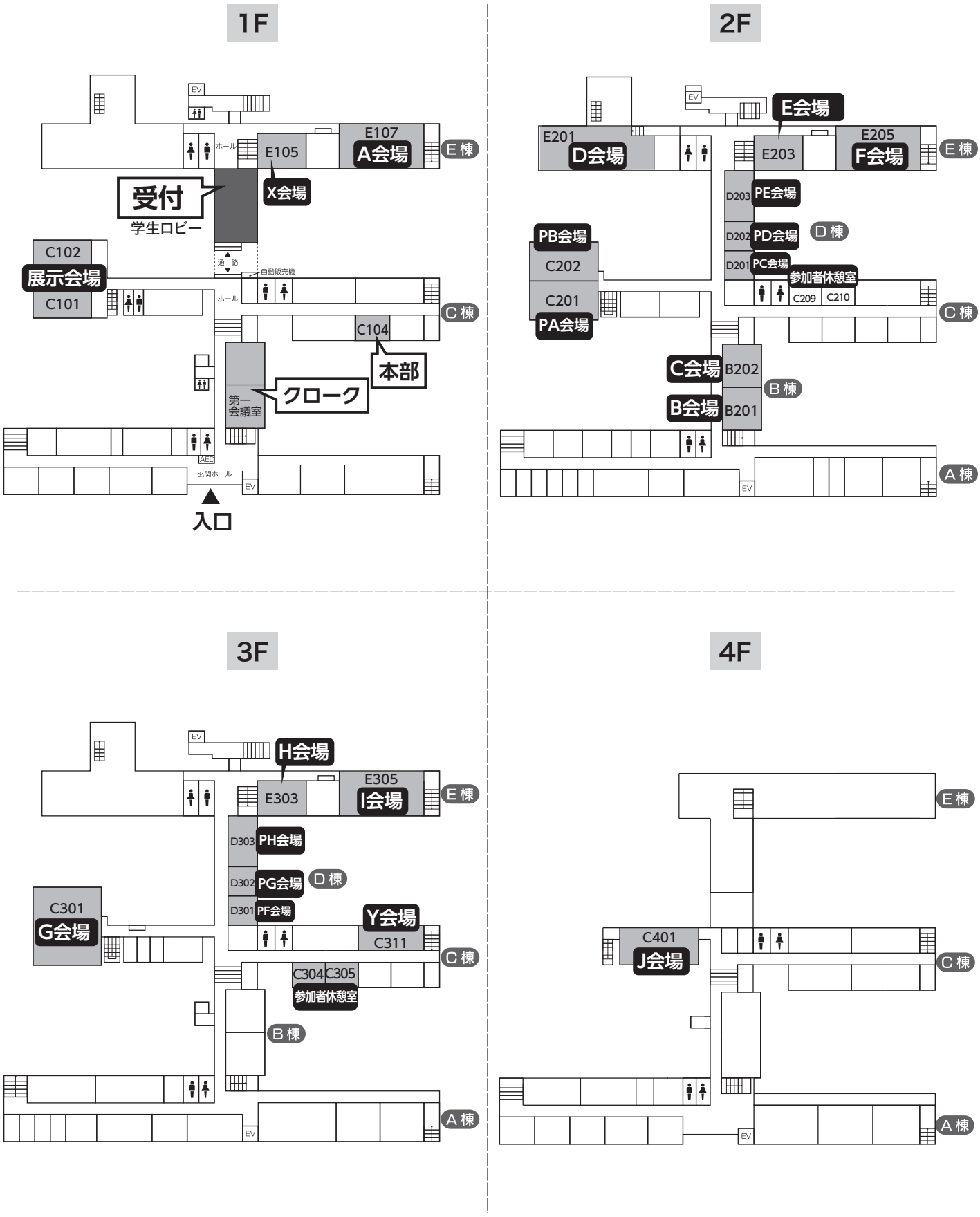
※上記以外のルートやバスの時刻表等は熊本大学の HP http://www.kumamoto-u.ac.jp/campusjouhou/access をご覧ください。



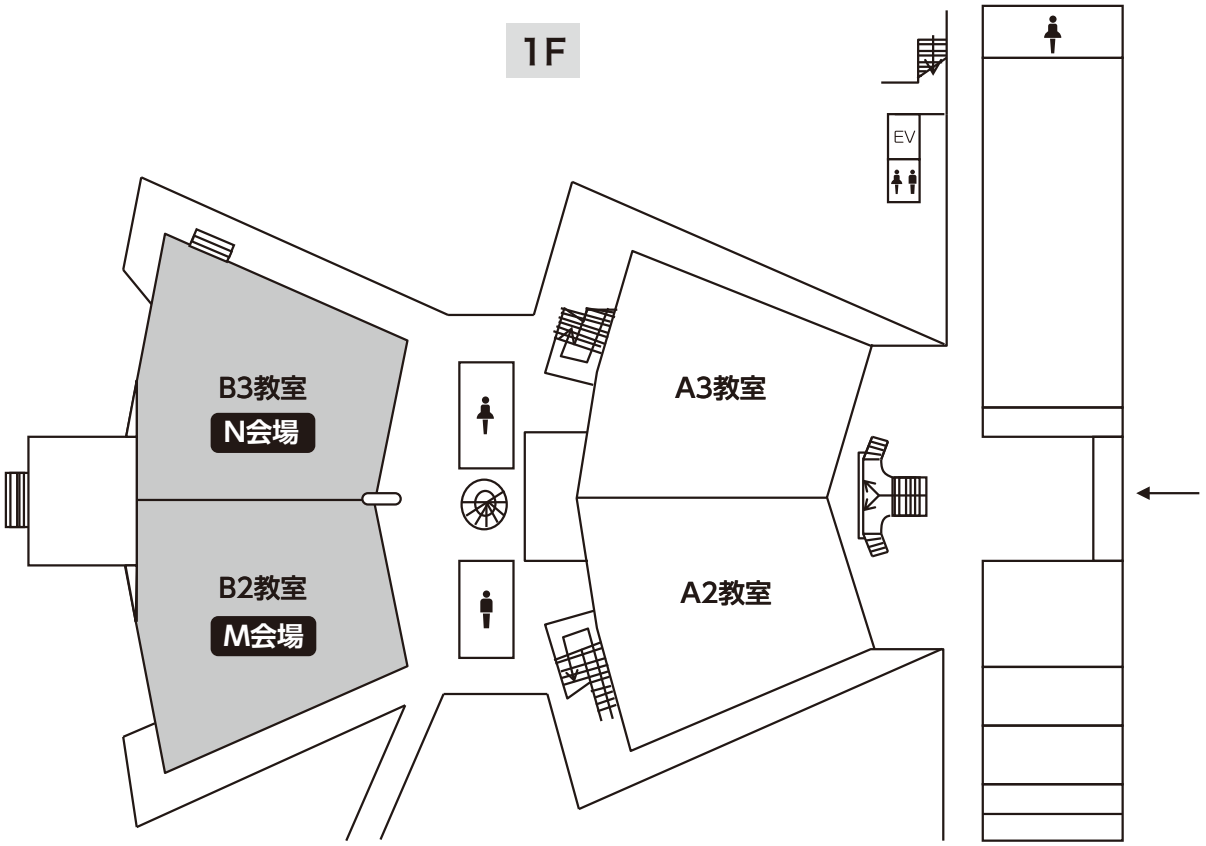
熊本大学 黒髪北地区マップ

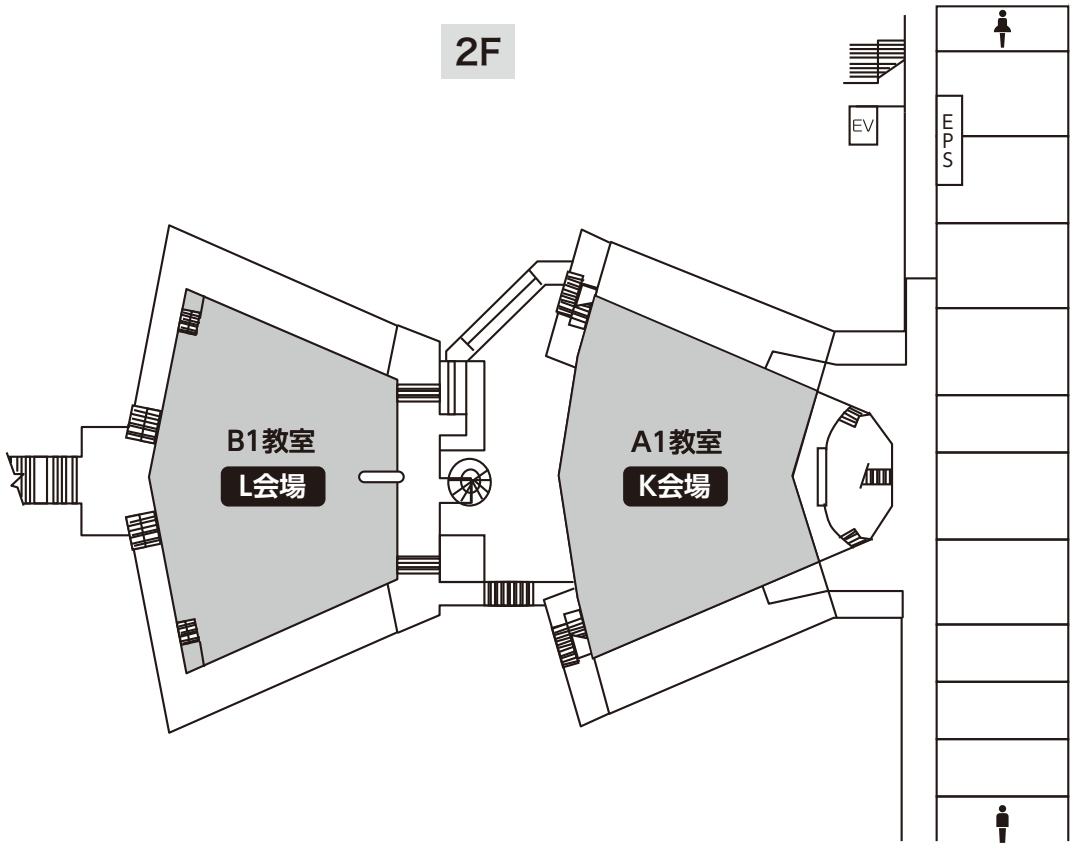


全学教育棟

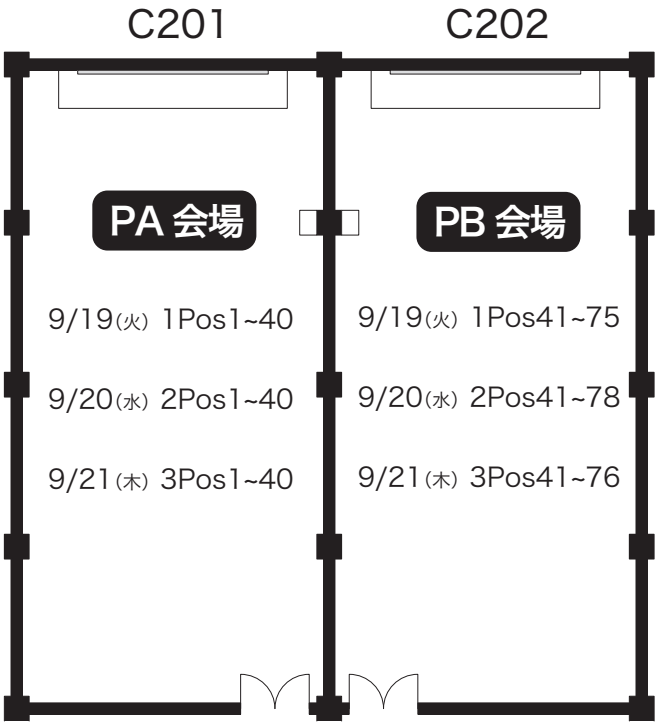

1F
EV
ホール
E105
E107
A会場
E棟
受付
学生ロビー
X会場
C102
展示会場
C101
通路
自動販売機
ホール
C棟
C104
本部
第一
会議室
クローク
AED
玄関ホール
EV
入口
2F
EV
E会場
E201
D会場
E203
E205
F会場
E棟
D203
PE会場
D202
PD会場
D棟
D201
PC会場
参加者休憩室
PB会場
C202
C201
PA会場
C209
C210
C棟
C会場
B202
B棟
B会場
B201
A棟
EV
3F
EV
H会場
E303
E305
I会場
E棟
D303
PH会場
D302
PG会場
D棟
D301
PF会場
C301
G会場
Y会場
C311
C棟
C304
C305
参加者休憩室
B棟
A棟
EV
4F
E棟
C401
J会場
C棟
A棟
EV

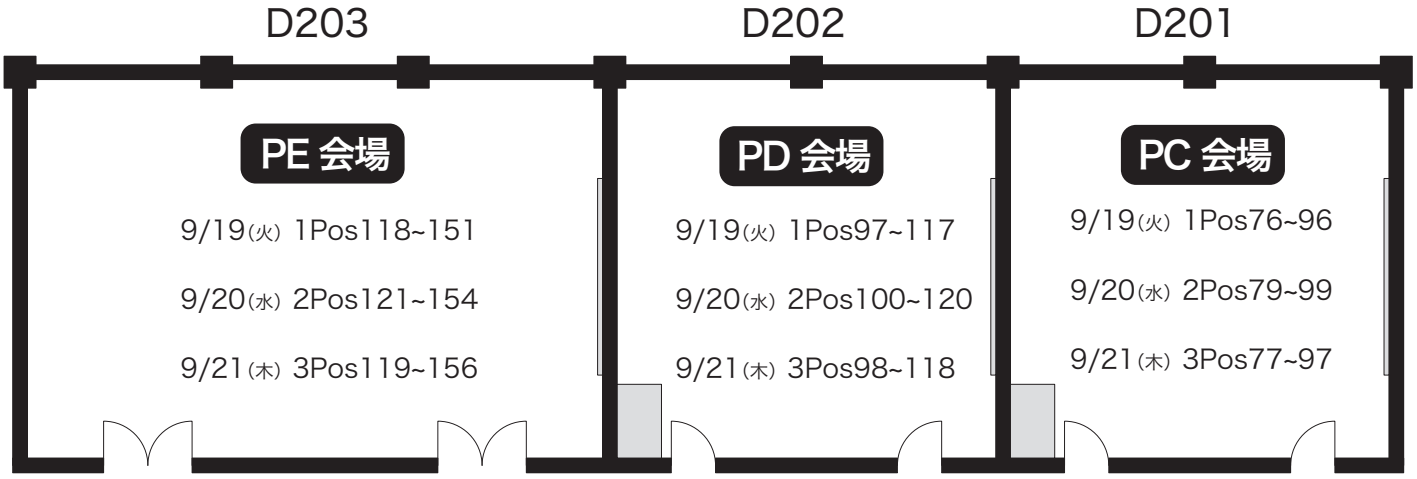
文法学部

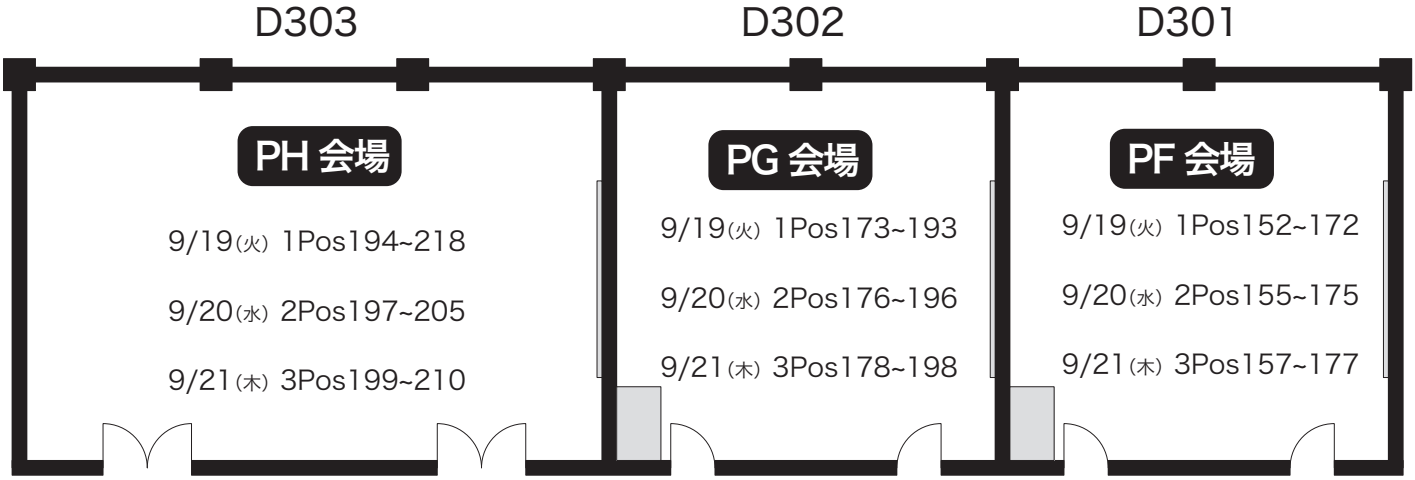




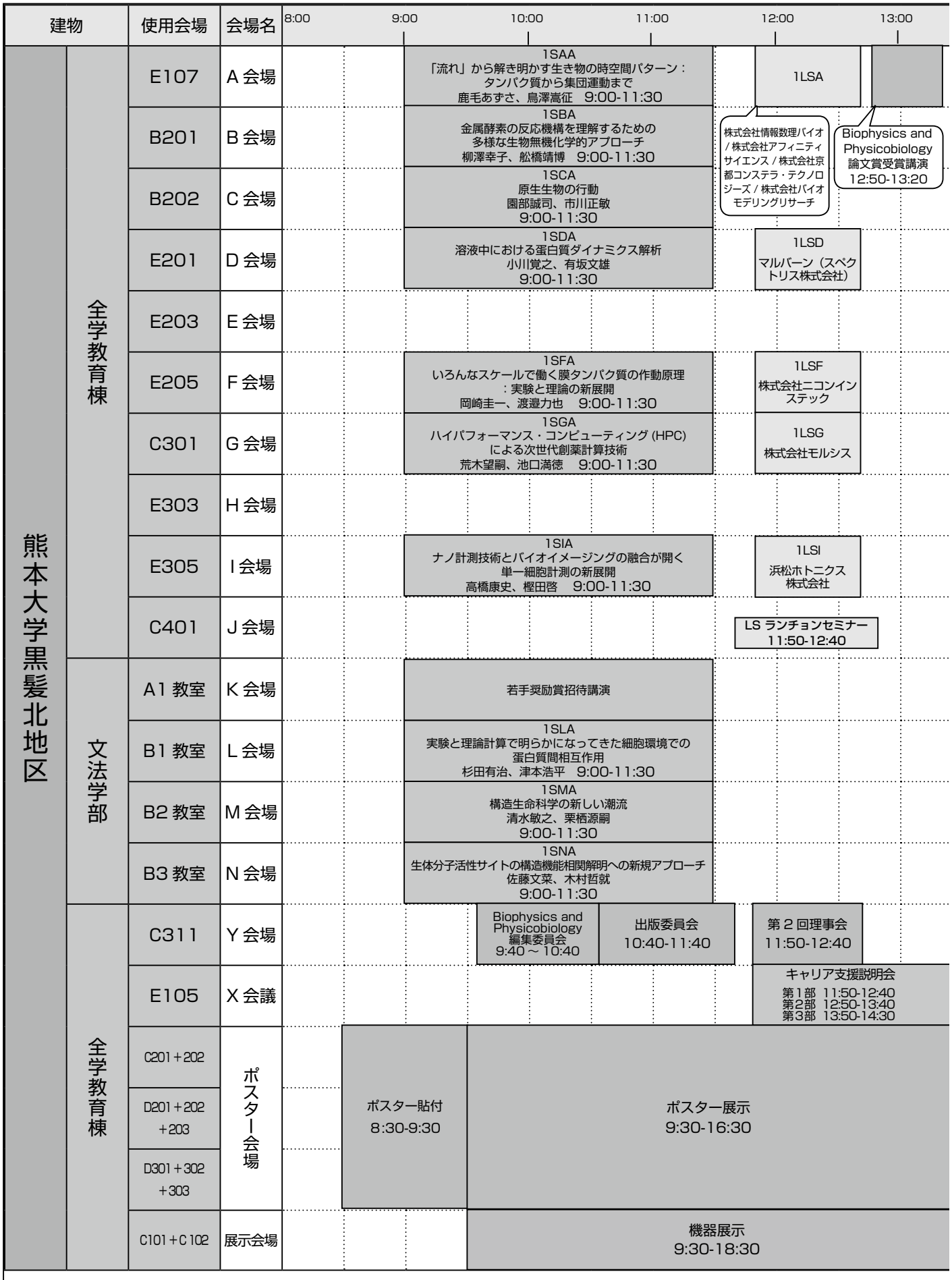
ポスター会場

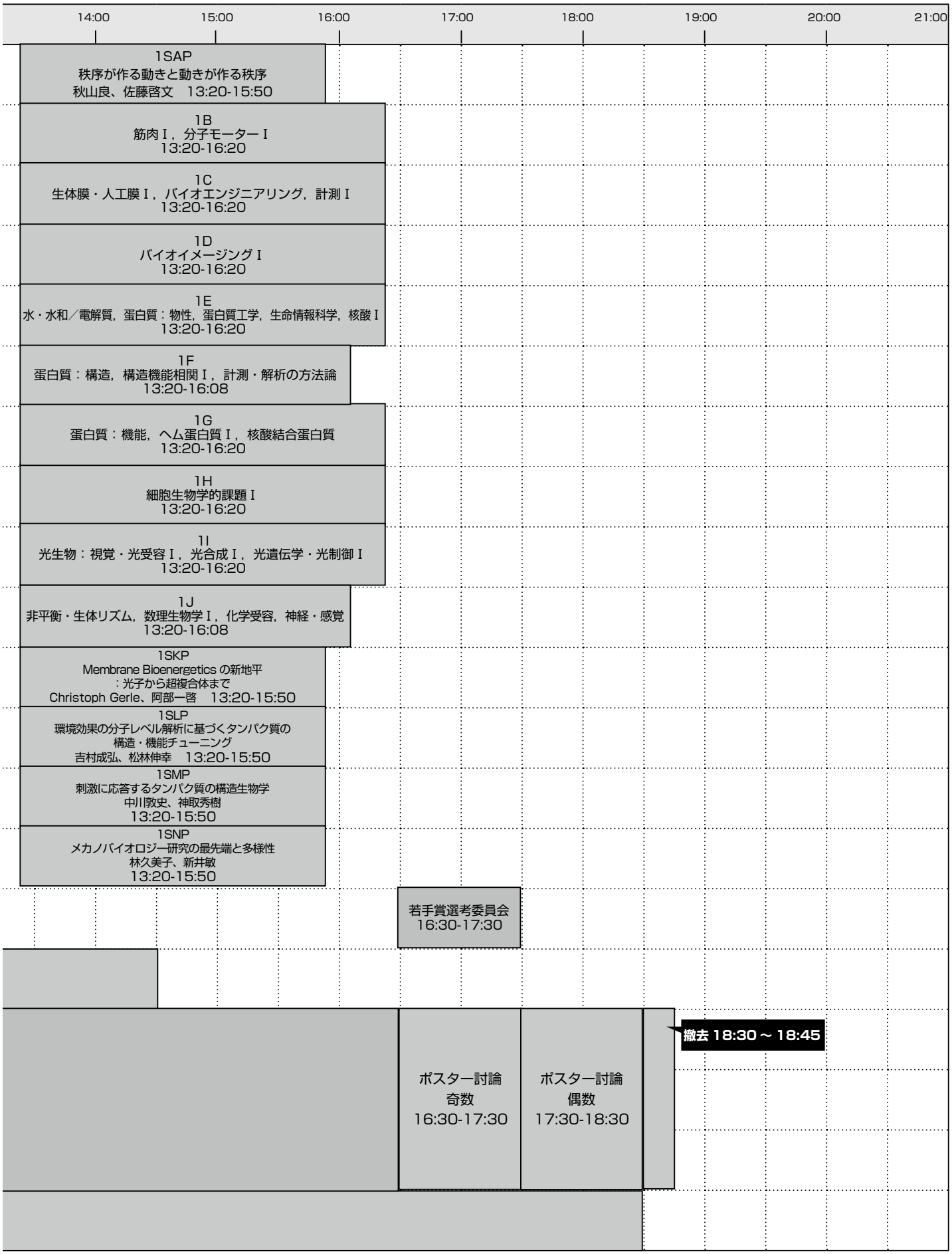

C201
C202
PA 会場
9/19(火) 1Pos1~40
9/20(水) 2Pos1~40
9/21(木) 3Pos1~40
PB 会場
9/19(火) 1Pos41~75
9/20(水) 2Pos41~78
9/21(木) 3Pos41~76


D203
D202
D201
PE 会場
9/19(火) 1Pos118~151
9/20(水) 2Pos121~154
9/21(木) 3Pos119~156
PD 会場
9/19(火) 1Pos97~117
9/20(水) 2Pos100~120
9/21(木) 3Pos98~118
PC 会場
9/19(火) 1Pos76~96
9/20(水) 2Pos79~99
9/21(木) 3Pos77~97

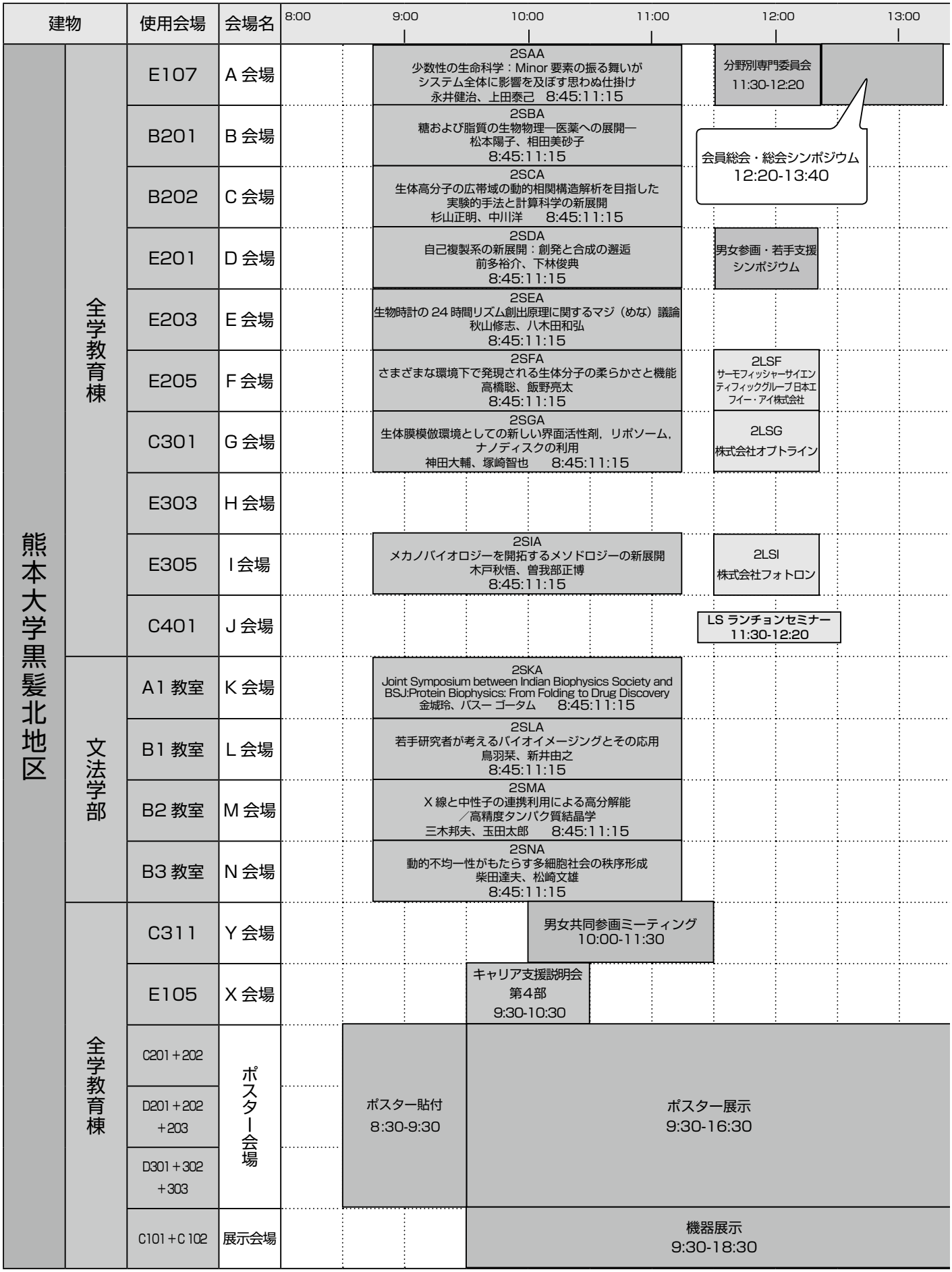

D303
D302
D301
PH 会場
9/19(火) 1Pos194~218
9/20(水) 2Pos197~205
9/21(木) 3Pos199~210
PG 会場
9/19(火) 1Pos173~193
9/20(水) 2Pos176~196
9/21(木) 3Pos178~198
PF 会場
9/19(火) 1Pos152~172
9/20(水) 2Pos155~175
9/21(木) 3Pos157~177

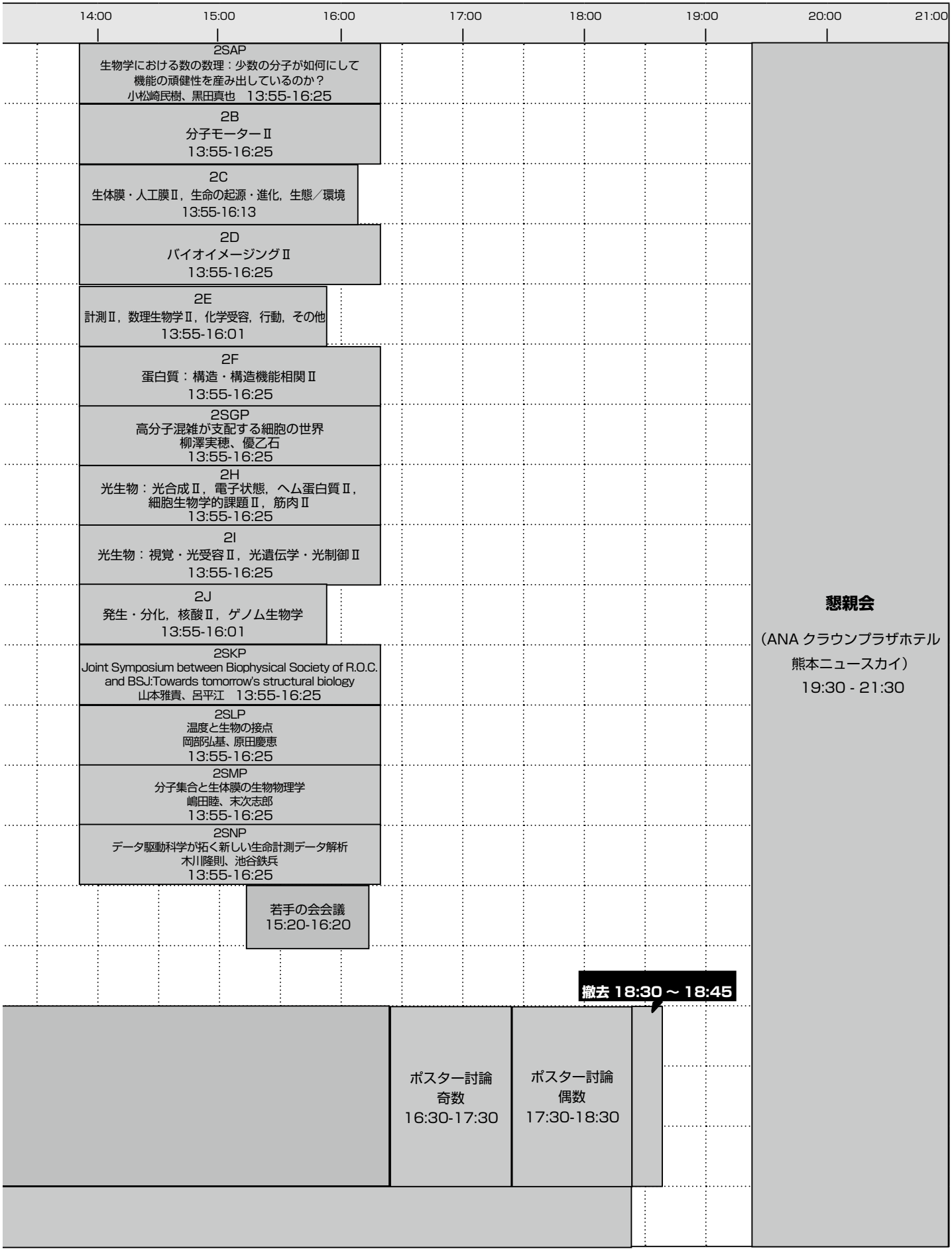
2017年9月19日（火）：年会1日目



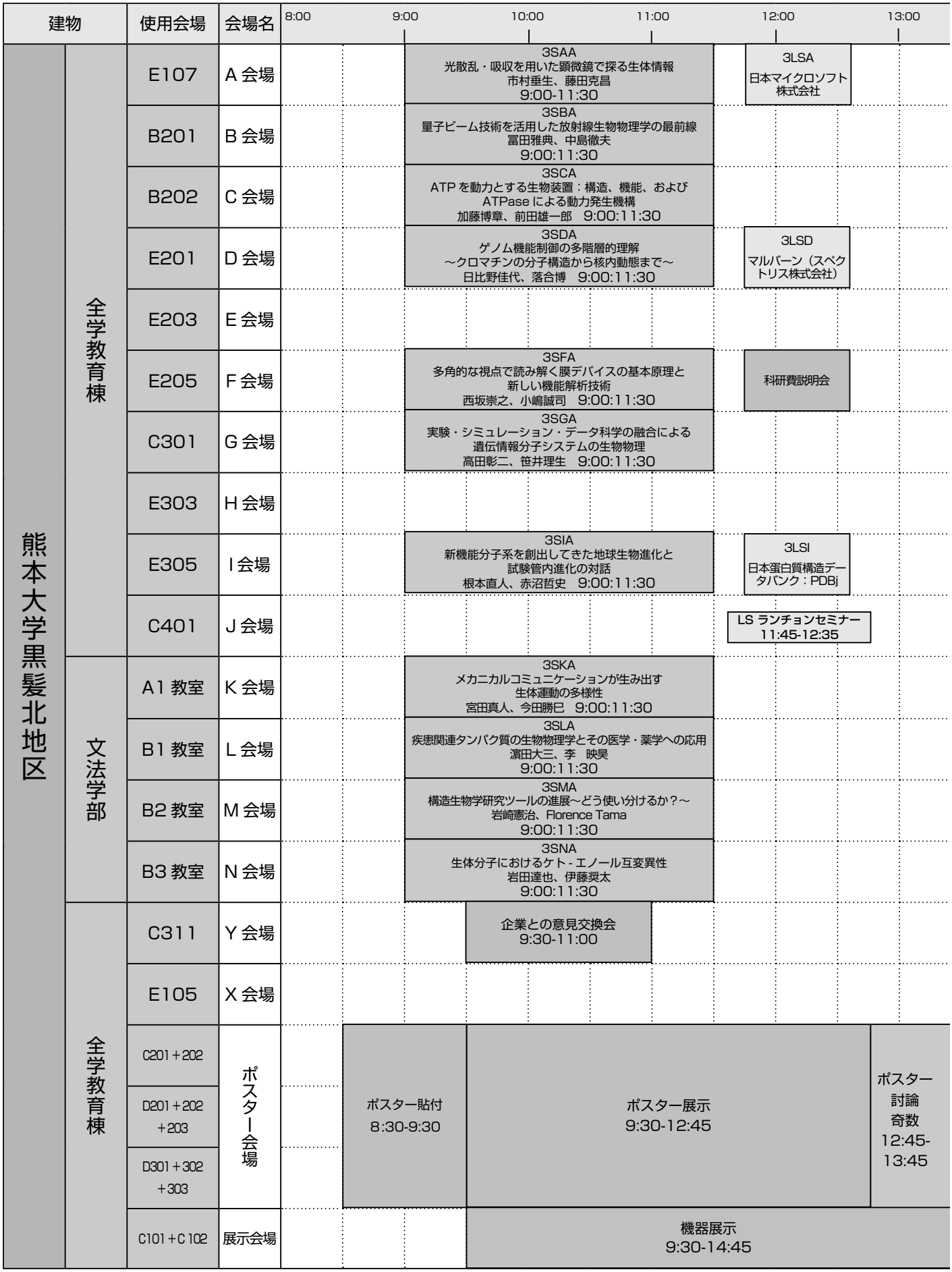

14:00
15:00
16:00
17:00
18:00
19:00
20:00
21:00
1SAP
秩序が作る動きと動きが作る秩序
秋山良、佐藤啓文　13:20-15:50
1B
筋肉Ⅰ，分子モーターⅠ
13:20-16:20
1C
生体膜・人工膜Ⅰ，バイオエンジニアリング，計測Ⅰ
13:20-16:20
1D
バイオイメージングⅠ
13:20-16:20
1E
水・水和／電解質，蛋白質：物性，蛋白質工学，生命情報科学，核酸Ⅰ
13:20-16:20
1F
蛋白質：構造，構造機能相関Ⅰ，計測・解析の方法論
13:20-16:08
1G
蛋白質：機能，ヘム蛋白質Ⅰ，核酸結合蛋白質
13:20-16:20
1H
細胞生物学的課題Ⅰ
13:20-16:20
1I
光生物：視覚・光受容Ⅰ，光合成Ⅰ，光遺伝学・光制御Ⅰ
13:20-16:20
1J
非平衡・生体リズム，数理生物学Ⅰ，化学受容，神経・感覚
13:20-16:08
1SKP
Membrane Bioenergetics の新地平
：光子から超複合体まで
Christoph Gerle、阿部一啓　13:20-15:50
1SLP
環境効果の分子レベル解析に基づくタンパク質の
構造・機能チューニング
吉村成弘、松林伸幸　13:20-15:50
1SMP
刺激に応答するタンパク質の構造生物学
中川敦史、神取秀樹
13:20-15:50
1SNP
メカノバイオロジー研究の最先端と多様性
林久美子、新井敏
13:20-15:50
若手賞選考委員会
16:30-17:30
ポスター討論
奇数
16:30-17:30
ポスター討論
偶数
17:30-18:30
撤去 18:30 ～ 18:45

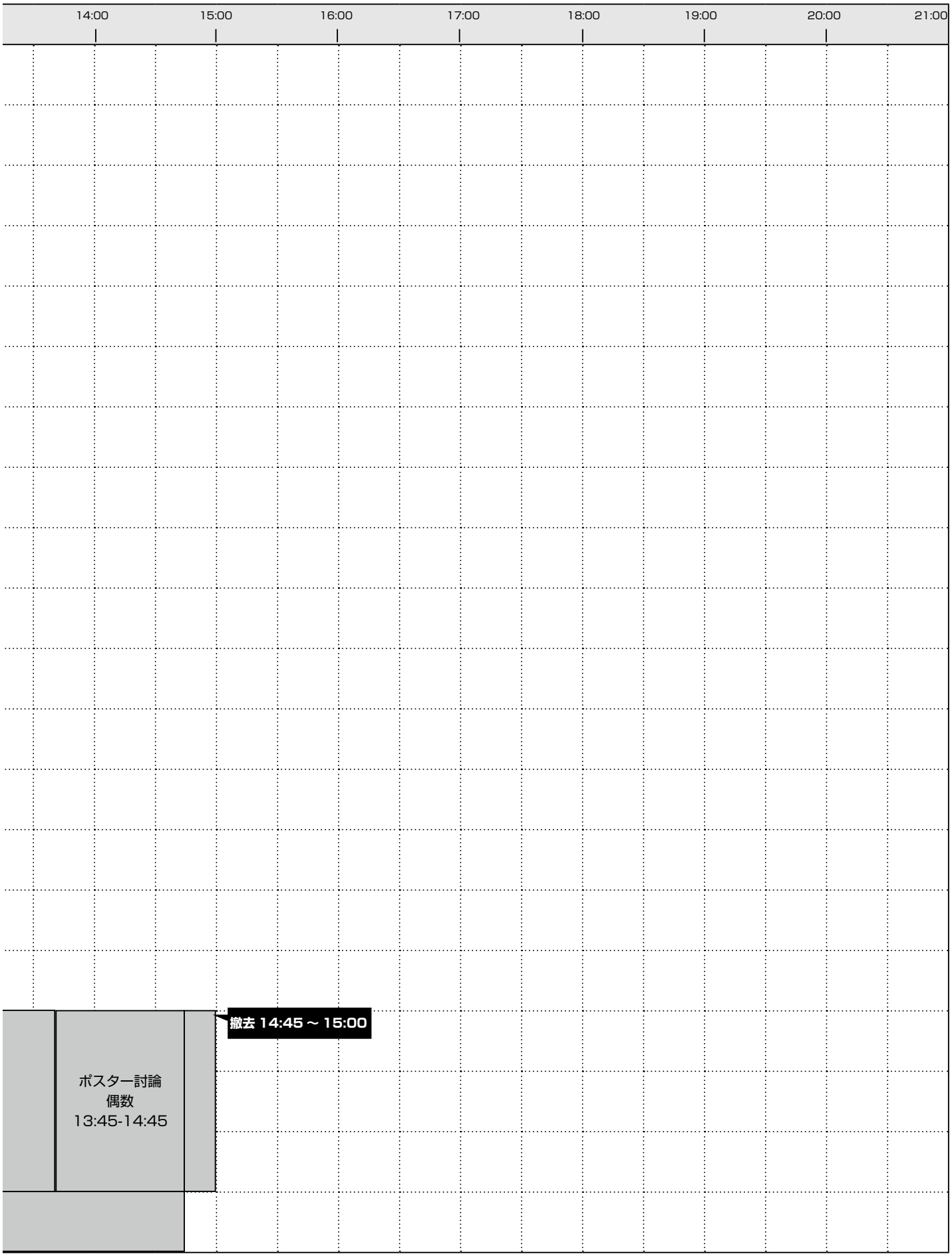
2017年9月20日（水）：年会２日目




14:00
15:00
16:00
17:00
18:00
19:00
20:00
21:00
2SAP
生物学における数の数理：少数の分子が如何にして機能の頑健性を産み出しているのか？
小松崎民樹、黒田真也　13:55-16:25
2B
分子モーターⅡ
13:55-16:25
2C
生体膜・人工膜Ⅱ，生命の起源・進化，生態／環境
13:55-16:13
2D
バイオイメージングⅡ
13:55-16:25
2E
計測Ⅱ，数理生物学Ⅱ，化学受容，行動，その他
13:55-16:01
2F
蛋白質：構造・構造機能相関Ⅱ
13:55-16:25
2SGP
高分子混雑が支配する細胞の世界
柳澤実穂、優乙石
13:55-16:25
2H
光生物：光合成Ⅱ，電子状態，ヘム蛋白質Ⅱ，細胞生物学的課題Ⅱ，筋肉Ⅱ
13:55-16:25
2I
光生物：視覚・光受容Ⅱ，光遺伝学・光制御Ⅱ
13:55-16:25
2J
発生・分化，核酸Ⅱ，ゲノム生物学
13:55-16:01
2SKP
Joint Symposium between Biophysical Society of R.O.C. and BSJ:Towards tomorrow's structural biology
山本雅貴、呂平江　13:55-16:25
2SLP
温度と生物の接点
岡部弘基、原田慶恵
13:55-16:25
2SMP
分子集合と生体膜の生物物理学
嶋田睦、末次志郎
13:55-16:25
2SNP
データ駆動科学が拓く新しい生命計測データ解析
木川隆則、池谷鉄兵
13:55-16:25
若手の会会議
15:20-16:20
撤去 18:30 ～ 18:45
ポスター討論
奇数
16:30-17:30
ポスター討論
偶数
17:30-18:30
懇親会
（ANA クラウンプラザホテル熊本ニュースカイ）
19:30 - 21:30

2017年9月21日（木）：年会3日目




14:00
15:00
16:00
17:00
18:00
19:00
20:00
21:00
撤去 14:45 ~ 15:00
ポスター討論
偶数
13:45-14:45

参加者へのご案内

1. 年会受付と参加登録

◇ 年会受付

場　　所: 全学教育棟 1F 学生ロビー(「熊本大学 黒髪北地区マップ 全学教育棟」7 ページを参照)
受付時間: 9 月 19 日(火)・20 日(水) 8:30 – 17:00、9 月 21 日(木) 8:30 – 14:00

◆事前登録

事前登録が完了された方は、日本生物物理学会会員・非会員共に参加証および領収証、プログラム集冊子が事前送付されますので、会場での受付は不要です。当日は必ず参加証をお持ちください。
但し、海外からの参加者は、年会受付にて参加証とプログラム集冊子をお受け取りください。

※参加証ホルダーを当日配布しますので、会場内では必ず参加証をご着用ください。
配付場所: 受付、各講演会場前等

注意 1) 事前登録は年会参加登録費(参加費)の振込後に完了します。振込がない場合、オンライン登録は無効となります。当日受付で当日参加費をお支払いください。
注意 2) 日本生物物理学会会員は年度会費を納めていない場合、参加証が送付されません。年度会費未納者・新規入会受付デスクにて年度会費をお支払いください。
注意 3) 参加費・年度会費ともに振込済みで、参加証が事前送付されていない場合は、総合受付デスクまでお越しください。
注意 4) 非会員のシンポジウム招待講演者については、会員である必要はなく、また、登録費は免除されます。懇親会に無料でご招待します。
注意 5) 海外の機関に所属する非会員については、ご入会いただかずに一般発表をしていただけます。

◆当日登録

事前登録が完了していない方は当日登録をしていただきます。
当日受付にお越しの上、参加費を現金でお支払いください。

◇ 当日年会諸費用 (一覧表)

当日参加	会員				非会員		
	正会員	シニア会員	大学院生	学部学生	一般	大学院生	学部学生
当日参加費	¥9,000	¥5,000	¥5,000	¥0	¥12,000	¥6,000	¥0
懇親会費	¥8,000	¥5,000	¥5,000	¥3,000	¥8,000	¥5,000	¥3,000

・参加のみの学部学生は参加費無料です。当日受付で学生証を提示してください。
参加証とプログラム集冊子をお渡しします。ただし、懇親会は有料です。

・若手奨励賞招待講演者、Biophysics and Physicobiology 論文賞受賞講演者、Biophysics and Physicobiology Editors' Choice Award 受賞代表者は、懇親会に無料でご招待します。
既に懇親会参加費を振り込まれている場合は、総合受付デスクで返金します。

◇ 参加証（名札）

参加証は会場内では必ずご着用ください。参加証のない方のご入場は固くお断りいたします。
事前送付された参加証は必ず会場にお持ちください（参加証ホルダーは受付、各講演会場前付近で配布いたします）。

◇ 領収書の発行

参加証とともに領収書をお渡しいたしますが、別の形式の領収書が必要な場合、お渡しした領収書と引き換えに総合受付デスクにて発行いたします。

◇ プログラム集冊子/オンライン予稿集【8 月 18 日（金）公開予定】

プログラム集冊子（前付・プログラム）は日本生物物理学会会員・事前登録が完了された非会員に事前に送付いたします（プログラム集冊子は総合受付デスクでも当日販売（3,500 円/税込）を行います）。なお予稿本文はプログラム集冊子には掲載されません。予稿本文は、オンライン予稿集をダウンロードして閲覧いただくことになります。

オンライン予稿集：
http://www.biophys.jp/dl/pro/55th_proceedings.pdf
ダウンロード ID：ambsj55
パスワード：kumamoto2017

プログラム（タイトル、発表者、所属）と予稿集は、年会ホームページにて公開します。
年会終了後は、半年ほど経て日本生物物理学会ホームページの年会の記録および J-Stage にて予稿集の pdf ファイルが公開されます。
日本生物物理学会ホームページの年会の記録 （http://www.biophys.jp/ann/ann02.html）
J-Stage の生物物理のページ （http://www.jstage.jst.go.jp/browse/biophys/-char/ja）

◇ プログラム検索（ウェブ版）【8 月 10 日（木）公開予定】

年会ホームページより「プログラム検索」を公開します。項目［演題タイトル（和文・英文）、発表者名（共著者含む）（漢字、カナ、ローマ字）、発表形式］から、演題番号、発表日、会場を検索・表示します。

◇ プログラム検索・予稿閲覧アプリ（無料）【9 月 15 日（金）公開予定】

スマートフォン（iPhone/Android）やタブレット（iPad/iPod Touch/Android）端末に対応した予稿閲覧アプリをご利用いただけます（演題検索、タイムテーブル一覧表示、ブックマーク登録等）。
App Store、Google Play よりダウンロードしてください（無料）。年会ホームページにもアプリ提供サイト（App Store, Google Play）を掲載しております。

アプリケーション名：第 55 回日本生物物理学会年会
検索ワード：bsj2017、生物物理、日本生物物理学会
アプリケーションの予稿閲覧パスワード：kumamoto2017

◇ 年度会費の支払いと入会の手続き

日本生物物理学会の年度会費が未納の場合は、年会受付の年度会費未納者・新規入会受付デスクでお支払いください。また、日本生物物理学会への新規入会も受け付けます。

2. 会場内のサービス・施設

◇ クローク

場　　所: 全学教育棟 1F 第一会議室(「熊本大学 黒髪北地区マップ 全学教育棟」7 ページを参照)

利用時間: 9 月 19 日(火) 8:30 - 18:45
20 日(水) 8:30 - 18:45
21 日(木) 8:30 - 15:00

※貴重品や傘、またコンピュータなどについては、破損、紛失などの責任は負いかねますので、各自でお持ちください。

※懇親会への移動など会場を去られる際は荷物をお引き取りください。

◇ 昼食

ランチョンセミナー(1～3 日目)、キャリア支援説明会(1日目)、男女共同参画・若手支援シンポジウム(2日目)、科研費説明会(3 日目)でお弁当とお茶が無料で提供されます。当日の午前中に整理券を配布いたします。整理券のご利用方法は 20 ページ「ランチョンセミナー」をご参照ください。
この他、分野別専門委員会(次ページ参照)を開催し、お弁当とお茶が無料で提供されます(整理券なし・数量に限りがあります)。積極的にご参加ください。
また会期中、以下の学生食堂をご利用いただけます。
なお、熊本大学黒髪北地区周辺のグルメマップを年会受付付近で配布しますので自由にお取りください。

■学生会館カフェテリア食堂
場所: 北地区学生会館 A 棟 (「熊本大学 黒髪北地区マップ」6 ページを参照)
営業時間:11:00～14:00

◇ 呼び出し

会場内での呼び出しは、緊急の場合を除いて行いません。参加者間の連絡用として、年会受付付近に伝言板を設置しますので、ご利用ください。

◇ 駐車場

会場には参加者用駐車場はございません。会場へは公共交通機関をご利用ください。

◇ 宿泊

宿泊に関しては年会ホームページ「宿泊案内」をご参照ください。

◇ インターネット

会場全体において Wi-Fi として国際無線 LAN ローミング基盤(eduroam)がご利用いただけます。既にご自身が所属する教育・研究機関で発行した eduroam の ID をお持ちの方は、別途申請することなく eduroam に接続することが可能です (Wi-Fi アクセス名: eduroam)。eduroam の ID をお持ちでない方には、年会期間のみ有効の熊本大学全学無線 LAN システム利用の ID と接続パスワードを年会受付で配布します。

※建物の構造や電波、アクセス状況によっては接続できない場合もあります。無線 LAN システム利用の ID は 1 人につき 1 つのみ発行いたします。
※講演中のインターネットご利用はご遠慮ください。

◇ 託児所

年会期間中は、託児所を設置いたします。詳しくは年会ホームページをご覧ください。

3. 年会行事・プログラム

◇ 会員総会・総会シンポジウム

一般社団法人日本生物物理学会第 4 回会員総会を年会 2 日目、9 月 20 日(水)12:20 - 13:40 に A 会場(全学教育棟 1F E107)で開催いたしますのでご出席ください。また、総会シンポジウムを開催します。
詳しくは 7. 開催通知 24 ページをご覧ください。

◇ 若手奨励賞招待講演

日本生物物理学会若手奨励賞及び若手招待講演賞の選考会である講演会(若手奨励賞招待講演)を、年会 1 日目 9 月 19 日(火)9:00 - 11:30 に K 会場(文法学部 2F A1 教室)で開催します。

◇ 学生発表賞

日本生物物理学会学生発表賞の選考会である一般口頭発表(9 月 19 日(火)13:20 -)を開催します。

◇ Biophysics and Physicobiology 論文賞受賞講演

Biophysics and Physicobiology 論文賞受賞の講演会を、年会 1 日目 9 月 19 日(火)12:50 - 13:20 に A 会場(全学教育棟 1F E107)で開催します。

◇ 分野別専門委員会

日時: 9 月 20 日(水)11:30 - 12:20
会場: A 会場(全学教育棟 1F E107)
対象: 分野別専門委員
昼食: 委員の皆様にはお弁当とお茶を提供いたします(整理券なし)。

◇ 懇親会

日時: 9 月 20 日(水)19:30 - 21:30 (年会会場から貸切バスで移動、発車時刻の予定 18:45 - 19:00)
会場: ANA クラウンプラザホテル熊本ニュースカイ 2 階「ストリングス」(市電「祇園橋」下車、徒歩 5 分)
(〒860-8575 熊本市中央区東阿弥陀寺町 2 番地) Tel: 096-354-2111
※懇親会の当日参加も受け付けいたします(受付場所: 総合受付デスク、または懇親会会場前)。

◇ 男女共同参画・若手支援シンポジウム

日時: 9 月 20 日(水)11:30 - 12:20
会場: D 会場(全学教育棟 2F E201)
昼食: お弁当とお茶が無料で提供されます(整理券を配布いたします。次ページ「ランチョンセミナー」の項を参照)。

◇ キャリア支援説明会

日時: 9 月 19 日(火)第1部 11:50-12:40、第2部 12:50-13:40、第3部 13:50-14:30
9 月 20 日(水)第4部 9:30-10:30
会場: X会場(全学教育棟 1F E105)
対象: 就職を考えておられる学生や研究者など ※詳細は 49 ページをご参照下さい。

昼食: 第1部のみ、お弁当とお茶が無料で提供されます(学生・院生を優先して整理券を配布いたします。下記「ランチョンセミナー」の項を参照)。

◇ 科研費説明会

日時: 9 月 21 日(木)11:45 - 12:35
会場: F会場(全学教育棟 2F E205)
昼食: お弁当とお茶が無料で提供されます(整理券を配布いたします。下記「ランチョンセミナー」参照)。

◇ ランチョンセミナー

昼食(お弁当とお茶、無料)をとりながらの共催企業によるセミナーにご参加ください。なお、お弁当の数に限りがあるため当日の以下の時間帯に整理券を配布いたします。セミナー開始前に、会場入り口で整理券と引き換えにお弁当を受け取り、ご入場ください(整理券の発券方法は下記参照)。

◆整理券の発券について

ランチョンセミナー整理券を下記のように配布いたします。
時間: 9月19日(火)～21日(木)8:30 - 10:30
場所: 全学教育棟 1F 学生ロビー付近
※整理券はランチョンセミナーの共催企業、団体よりご提供いただく昼食の引換券になります。
当日開催されるセミナー分のみ発券いたします。券は枚数が無くなり次第終了となります。

◆整理券の注意事項

整理券は各日、セミナー開始後、無効となります。
午前のプログラム終了後、ランチョンセミナー開始時間までにご来場ください。
セミナー開始までにご来場されない場合、整理券は無効となり、お弁当は整理券をお持ちでない参加者に提供されますことをご了承ください。

◆ランチョンセミナー受講時のお願い

ランチョンセミナーは企業、団体等の共催によるセミナーです。参加される場合は最後までご聴講ください。また、共催者のアンケートには、できるだけ所属・氏名を記載して回答くださるよう、ご協力をお願いします。

◇ 機器・試薬・書籍等附設展示会

機器、試薬、ソフトウエア、書籍などの附設展示会を全学教育棟 1 階 C101+C102 で行います。

◇ 市民講演会

テーマ: 「エンジョイ！サイエンス ～生命を観る・守る最前線～」 詳細は 45 ページをご参照ください。
会 場: くまもと県民交流館パレア 9 階会議室 1
(熊本市中央区手取本町 8 番 9 号 テトリアくまもとビル
市電「水道町」電停、もしくは「通町筋」バス停下車すぐ)
参加費: 無料 (どなたでも自由に参加できます)

4. 禁止事項

◇ 撮影・録音

会場内でのカメラ、ビデオ、携帯電話などによる撮影や講演音声の録音などを禁止します。
一部、理事会の承認を得て、録画を行う場合があります。

◇ 喫煙・飲食

会場内は終日禁煙です。講演会場内での飲食はランチョンセミナー、キャリア支援説明会、男女共同参画・若手支援シンポジウム、科研費説明会、各種委員会など食事が提供される場合を除いて禁止します。

◇ 携帯電話

シンポジウム、ポスター発表等の会場内での携帯電話による通話を禁止します。講演会場内では電源をオフにするかマナーモードに設定し、呼び出し音が鳴らないようご注意ください。

5. 年会についての問い合わせ

◇ **会期中**　年会本部 （会期中のみ通じます） Tel: 050-3482-9415

◇ **会期外**　年会実行委員会 E-mail: bp_nenkai55@kumamoto-u.ac.jp

参加登録・演題登録 システムサポートデスク

〒602-8048 京都市上京区下立売通小川東入る
中西印刷株式会社内
E-mail: bsj2017sys-sprt@e-naf.jp

年会実行委員会サポート

〒532-0003 大阪市淀川区宮原 2-14-14 新大阪グランドビル 6F
株式会社エー・イー企画 Tel:06-6350-7163 FAX:06-6350-7164
実行委員会サポート E-mail: jbp2017@aeplan.co.jp
広 告・展 示 関 連 E-mail: e_jbp55@aeplan.co.jp

6. 発表者へのご案内

◇ 使用言語

すべての発表は原則として英語をお使いください。

◇ 映写機器

会場にはパソコンを用意いたしません。ご自身のノートパソコンを必ずお持ちください。
発表に使用できる映写機器は、液晶プロジェクターのみです。音声出力には対応しません。
会場に備え付けの液晶プロジェクターにより、図等をスクリーンに映写して発表します。
使用ソフトはパワーポイント（米国マイクロソフト社）を標準とします。画像解像度は 1024×768 ピクセル（XGA）です。この環境下で発表データを作成ください。これより大きい画面サイズでデータを作成すると、スクリーン映写時に画面をはみ出す等の不具合が起こる可能性がある旨ご理解ください。

注意 1） 会場スタッフがパソコンを会場に備え付けられた切り替え装置（セレクター）に接続いたします。
注意 2） 切り替え装置に繋がるパソコンの映像出力端子は、「ミニ D-sub15 ピン端子（メス）」のみです。
端子の形状が異なる場合（Macintosh 等）、変換アダプターをお持ちください。
注意 3） 発表に使用するパワーポイントファイルが入った USB メモリーを念のためにお持ちください。
注意 4） バッテリー切れに備え、必ず電源アダプターをお持ちください。
注意 5） 発表中にスクリーンセーバーや省電力モードにならないよう、設定してください。

◇ シンポジウム、若手奨励賞招待講演のオーガナイザーの方へ

受付: セッション開始の 15 分前までに各会場の「進行席」までお越しの上、係りの者に来場された旨をお伝えください。

進行: 一任いたしますので、講演者の講演時間を厳守し、円滑な運営にご協力ください。事前に事務局に連絡した各講演者の講演時間等に変更が生じた場合は、会場内の進行スタッフにご指示ください。

◇ シンポジウム、若手奨励賞招待講演の講演者の方へ

受付: セッション開始の 15 分前までに各会場の「PC 受付」にお越しください。
発表スライドをご確認いただいた後、会場スタッフがパソコンをPC切り替え装置に接続いたします。※スライドチェック用の試写室はございません。

講演時間: シンポジウムの時間配分はオーガナイザーに一任しております。
若手奨励賞招待講演の講演時間は、発表 10 分、討論 3 分、パソコンの交換に 2 分です。

◇ 一般口頭発表の座長の方へ

受付: 担当セッション開始の 15 分前までに各会場の「進行席」までお越しの上、係りの者に来場された旨をお伝えください。

進行: 多くの講演者の発表を滞りなく進めるために、時間厳守でお願いします。
会場には時間を計測するスタッフを配置しています。

◇ 一般口頭発表の講演者の方へ

受付: セッション開始の 15 分前までに指定された会場の「PC受付」までお越しください。会場スタッフがパソコンを切り替え装置(セレクター)に接続いたします。※スライドチェック用の試写室はございません。

講演時間: 発表 8 分、質疑応答 3 分 30 秒、交代時間 30 秒

◇ ポスター発表の方へ

ポスターの貼付・展示、説明・討論、撤去:

		9 月 19 日(火)	9 月 20 日(水)	9 月 21 日(木)
貼付・展示		8:30 – 16:30	8:30 – 16:30	8:30 – 12:45
説明・討論	奇数番号	16:30 – 17:30	16:30 – 17:30	12:45 – 13:45
	偶数番号	17:30 – 18:30	17:30 – 18:30	13:45 – 14:45
撤去		18:45 までに撤去	18:45 までに撤去	15:00 までに撤去

1. ポスターは日替わりで貼り替えてください。
2. ポスターボードの大きさは、幅 90 cm、高さ 210 cm。貼付に必要な押しピンは会場に用意します。
3. 撤去時間を過ぎて残ったポスターは年会事務局にて破棄しますので、ご了承ください。

◇ ポスター発表要項

ポスターは英語で作成してください。
ただし、タイトル、所属、著者名は、可能であれば日本語の併記もお願いいたします。
発表代表者の氏名には左肩に小さな○印を付けてください。

◇ 発表形式と演題番号（各予稿左上の番号）の見方

発表形式は、シンポジウム発表（Symposium Speech）、若手奨励賞招待講演（“Early Career Award in Biophysics” Candidate Presentations）、一般口頭発表（Oral Presentation）、ポスター発表（Poster Presentation）、があります。

シンポジウム発表：（例）1SAA-03
1 文字目は発表日（1:9 月 19 日（火）、2:9 月 20 日（水）、3:9 月 21 日（木））、2 文字目は Symposium（S）、3 文字目は会場名（A 会場）、4 文字目は午前・午後（AM,PM）、最後の 2 桁の数字は発表順です。

若手奨励賞招待講演：（例）1YK1045
1 文字目は発表日（1:9 月 19 日（火））、2 文字目は Young（Y）、3 文字目は会場名（K 会場）、最後の 4 桁の数字は講演開始時刻です。

一般口頭発表（例）1B1320
1 文字目は発表日（1:9 月 19 日（火）、2:9 月 20 日（水）、3:9 月 21 日（木））、2 文字目は会場名（B 会場）、最後の 4 桁の数字は講演時間開始です。学生発表賞に応募した発表には演題番号の右側に「*」がついております。

ポスター発表：（例）1Pos001
1 文字目は発表日（1:9 月 19 日（火）、2:9 月 20 日（水）、3:9 月 21 日（木））、2 文字目は Poster（Pos）、最後の 3 桁の数字はパネル番号を示します。

7. 一般社団法人日本生物物理学会第 4 回会員総会開催通知

日時: 9 月 20 日(土)12:20 – 13:40

会場: A 会場(全学教育棟 1F E107)

一般社団法人日本生物物理学会第 4 回会員総会を開催いたします。主な議題は下記の通りです。是非ご出席ください。

議長: 会長 神取 秀樹

総会議題

(1)報告事項

平成 28 年度決算報告ならびに監査結果報告

平成 29 年度会計ならびに事業の中間報告と今後の計画

次期年会について

(2)第 4 回会員総会シンポジウム:国際化と IUPAB

概要:46 ページをご覧ください。

8. 理事会、会員総会、各種委員会の案内

委員会等	開催日程		会場
ホームページ編集委員会	9 月 18 日 (月)	14:00 – 16:00	全学教育棟 C311(Y 会場)
生物物理編集委員会		16:30 – 18:30	全学教育棟 C311(Y 会場)
Biophysics and Physicobiology 編集委員会	9 月 19 日 (火)	9:40 – 10:40	全学教育棟 C311(Y 会場)
出版委員会		10:40 – 11:40	全学教育棟 C311(Y 会場)
平成 29 年度第 2 回理事会 (旧運営委員会)		11:50 – 12:40	全学教育棟 C311(Y 会場)
若手奨励賞選考委員会		16:30 – 17:30	全学教育棟 C311(Y 会場)
男女共同参画・若手支援委員会	9 月 20 日 (水)	10:00 – 11:30	全学教育棟 C311(Y 会場)
分野別専門委員会		11:30 – 12:20	全学教育棟 E107(A 会場)
会員総会・総会シンポジウム(総会)		12:20 – 13:40	全学教育棟 E107(A 会場)
若手の会会議		15:20 – 16:20	全学教育棟 C311(Y 会場)
企業との意見交換会	9 月 21 日 (木)	9:30 – 11:00	全学教育棟 C311(Y 会場)

( )は法人化前の名称

謝 辞

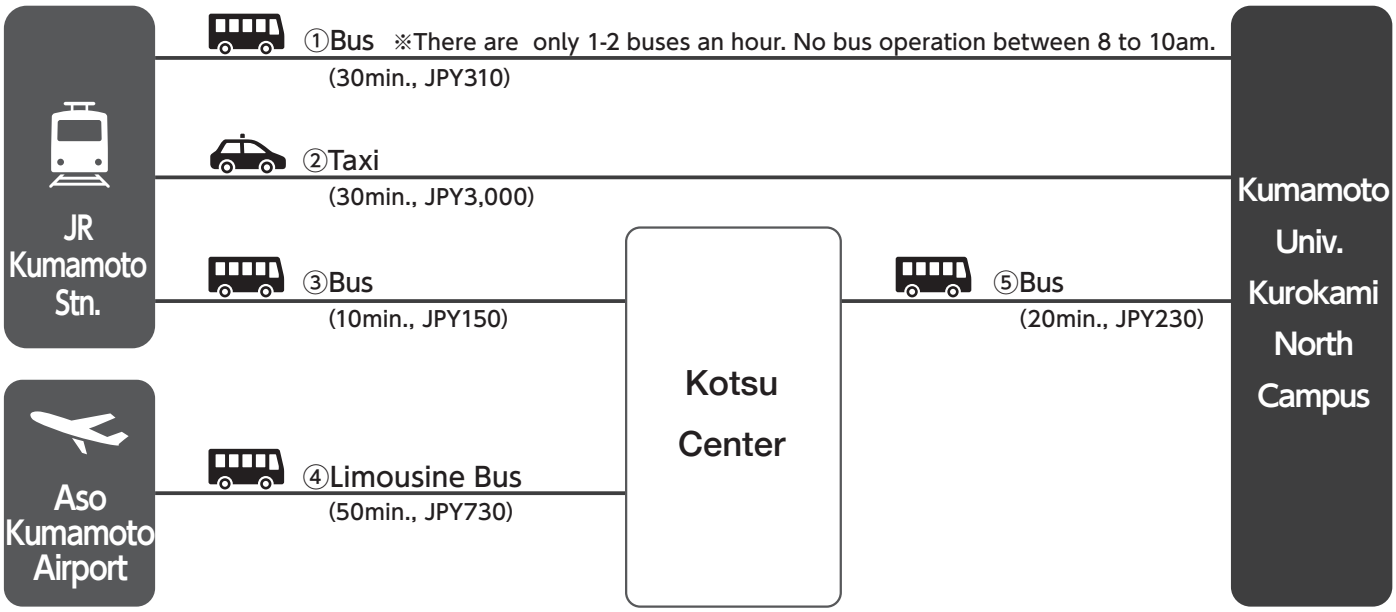
本年会の開催・運営に当たり、以下の団体よりご協力・ご援助いただきました。
関係者一同より御礼申し上げます。

助成(敬称略)
熊本国際観光コンベンション協会
熊本大学薬学部同窓会

共催/協賛(敬称略)
AMED 革新的先端研究開発支援事業(AMED－CREST/PRIME)
「メカノバイオロジー機構の解明による革新的医療機器及び医療技術の創出」
CREST「構造生命」/さきがけ「構造生命科学」領域
新学術領域研究 温度を基軸とした生命現象の統合的理解(温度生物学)
新学術領域研究 スパースモデリングの深化と高次元データ駆動科学の創成
新学術領域研究 3D 活性サイト科学
新学術領域研究 生命分子システムにおける動的秩序形成と高次機能発現
新学術領域研究 動的構造生命科学を拓く新発想測定技術
－タンパク質が動作する姿を活写する－
新学術領域研究 理論と実験の協奏による柔らかな分子系の機能の科学
ポスト「京」重点課題1 生体分子システムの機能制御による革新的創薬基盤の構築
文部科学省 光・量子融合連携研究開発プログラム
「中性子と放射光の連携利用によるタンパク質反応プロセスの解明」

第 55 回日本生物物理学会年会
実行委員長 山縣 ゆり子

Access Information / Area Map



①Direct Bus: JR Kumamoto Stn. → Kumamoto Univ.
(30min., JPY3,000)
※There are only 1-2 buses an hour. No bus operation between 8 to 10am.

②Taxi (30min., JPY3,000)

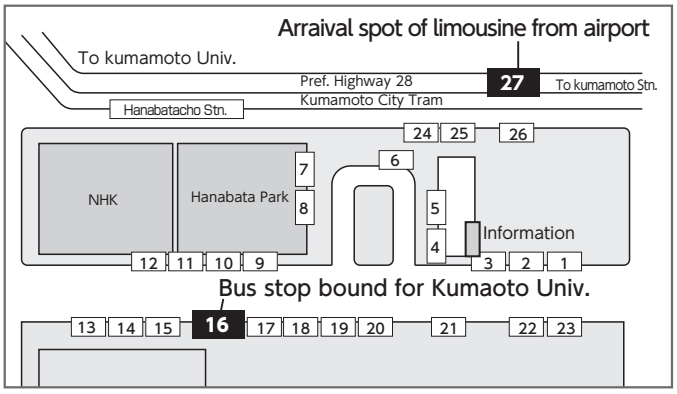
③Bus: JR Kumamoto Stn. East Exit → Kotsu Center
(10min., JPY150)

④Limousine Bus: Aso Kumamoto Airport → Kotsu Center
(50min., JPY730)

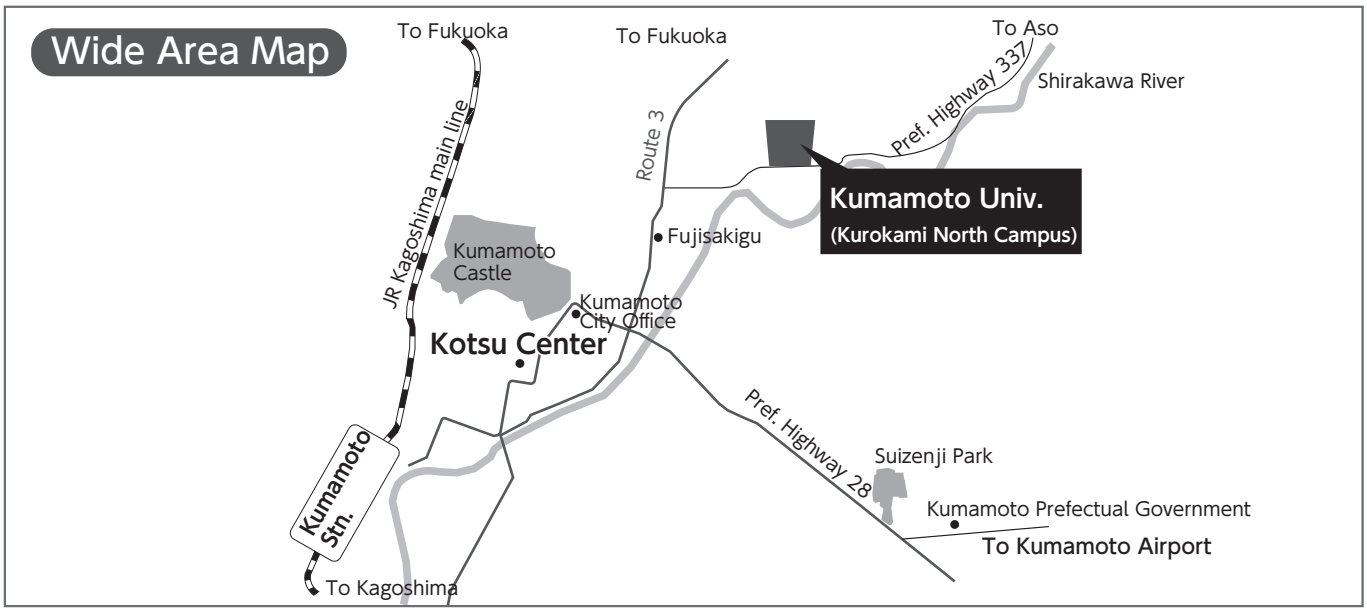
⑤Bus: No.16 bus stop, Kotsu Center (refer to the right map)→ Kumamoto Univ. Get off at 'Kumamoto Daigaku Mae". (20min., JPY230)

※Please be aware that traveling time will be longer due to traffic or other conditions.

Kotsu Center Bus Terminal



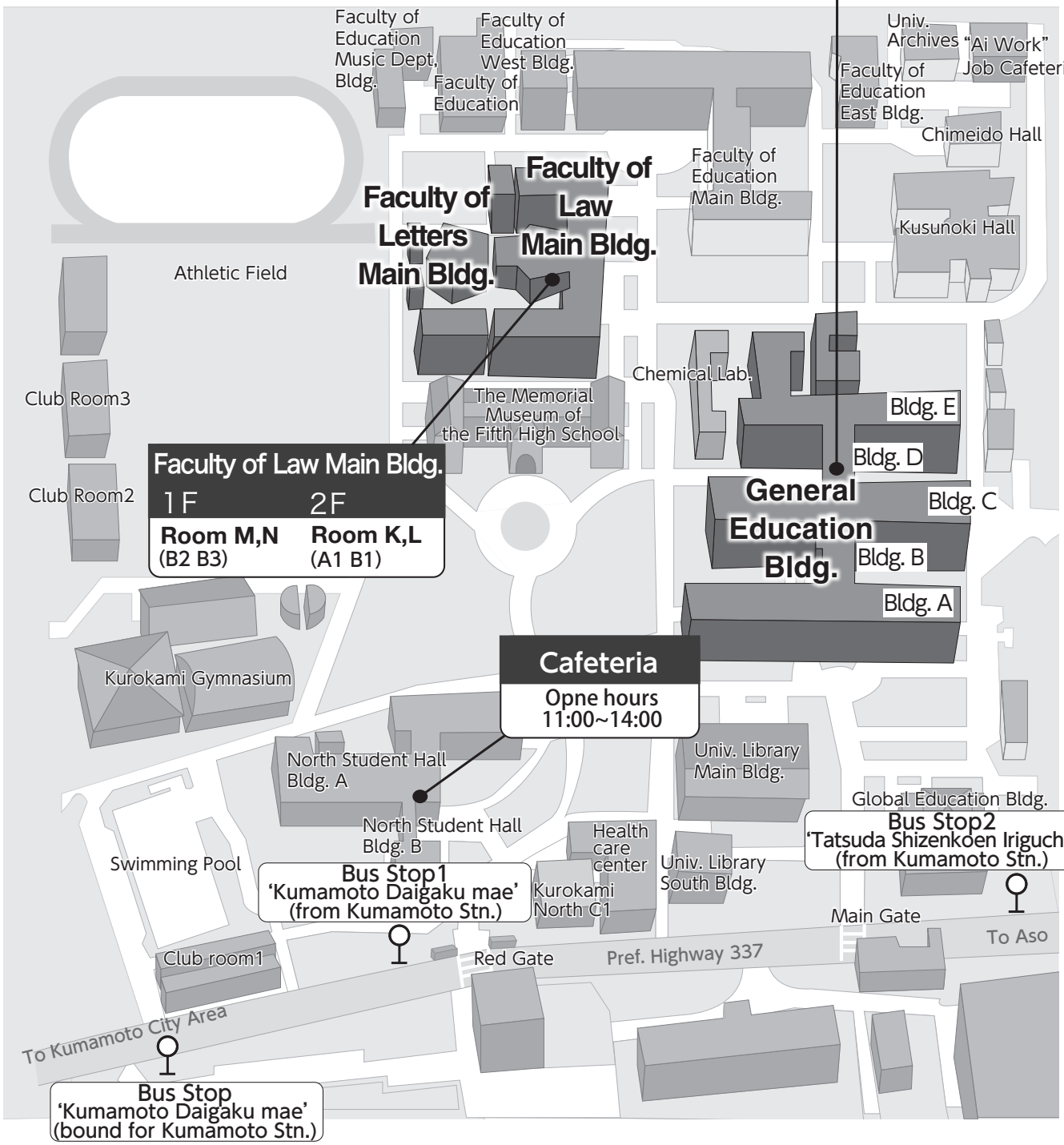
※Additional bus services bound for Kumamoto Univ. will be provided. Please see the meeting website for more information.



Kumamoto Univ. Kurokami North Campus

General Education Bldg.

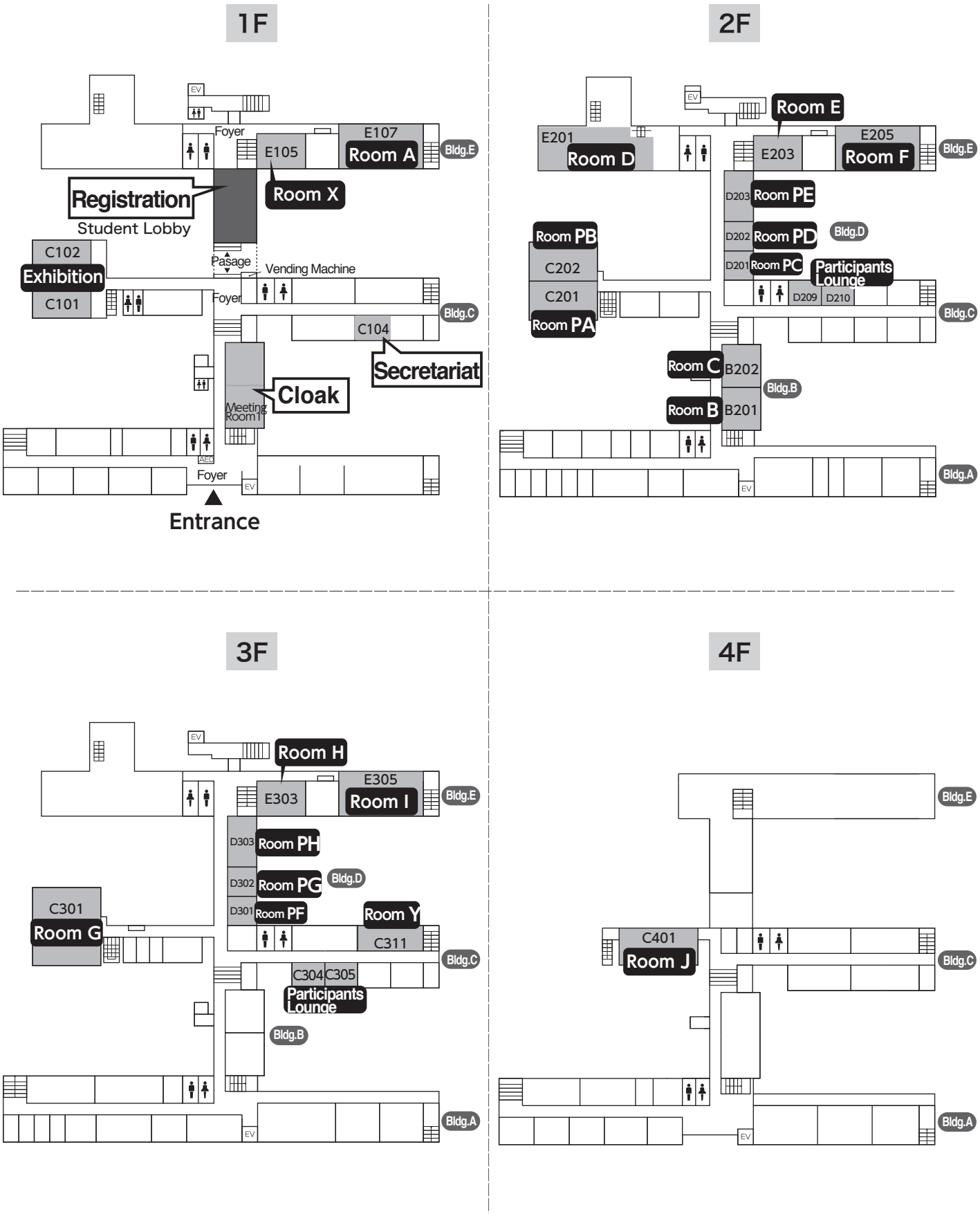
1F	2F	3F	4F
Registration (Student Lobby) **Secretariat** (C104) **Exhibition** (C101 C102) **Room X** (E105) **Cloak** (Meeting Room1) **Room A** (E107)	**Room B-F** (B201 B202 E201 E203 E205) **Room PA~PE** (C201 C202 D201 D202 D203) **Participants Lounge** (C209 C210)	**Room G-I** (C301 E303 E305) **Room PF~PH** (D301 D302 D303) **Room Y** (C311) **Participants Lounge** (C304 C305)	**Room J** (C401)



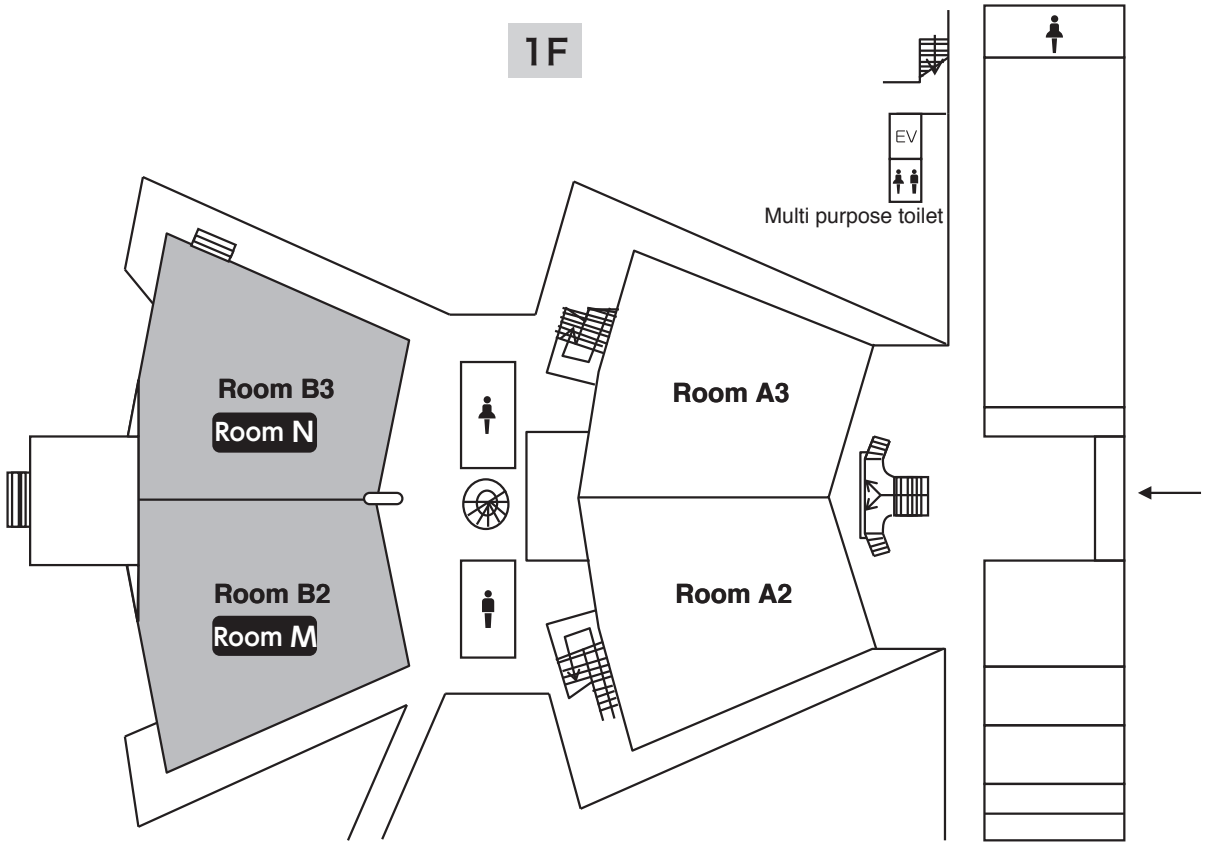
Faculty of Law Main Bldg.

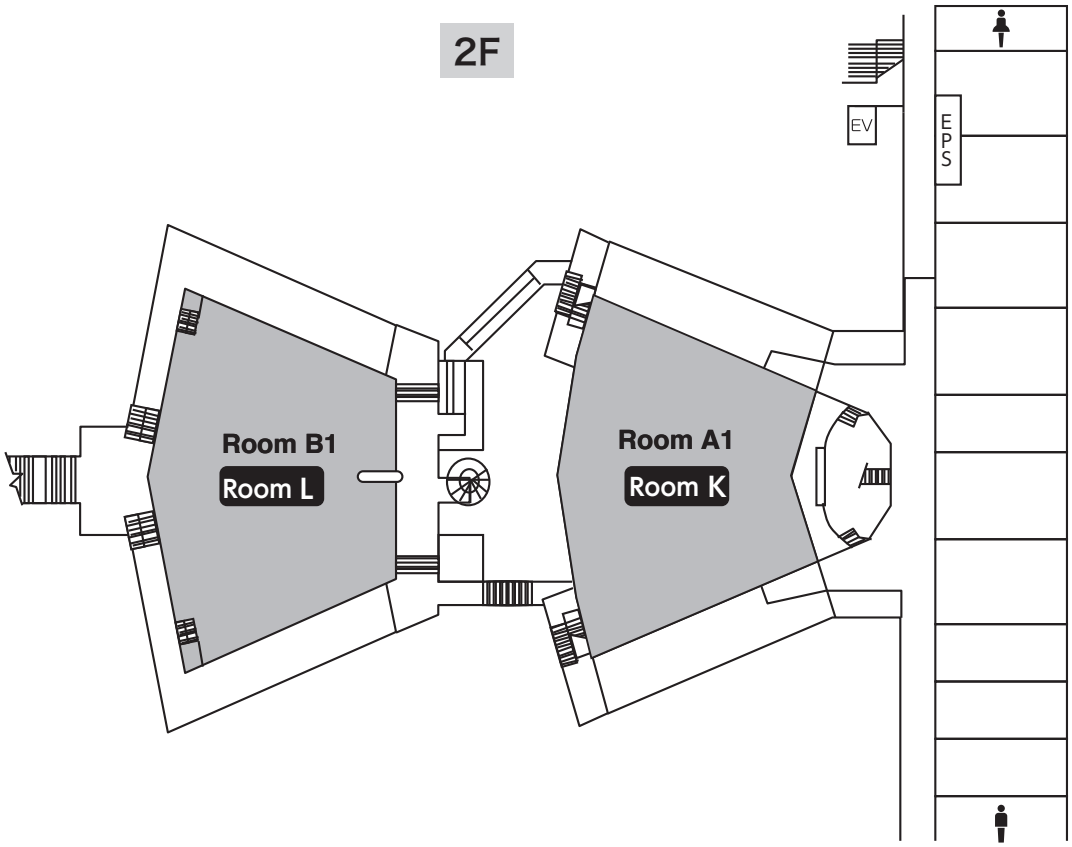
1F	2F
Room M,N (B2 B3)	**Room K,L** (A1 B1)

General Education Building

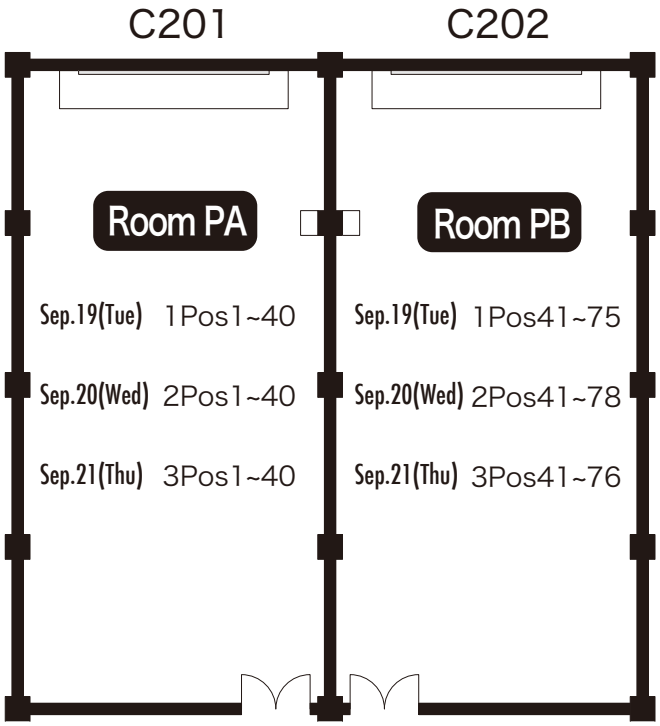


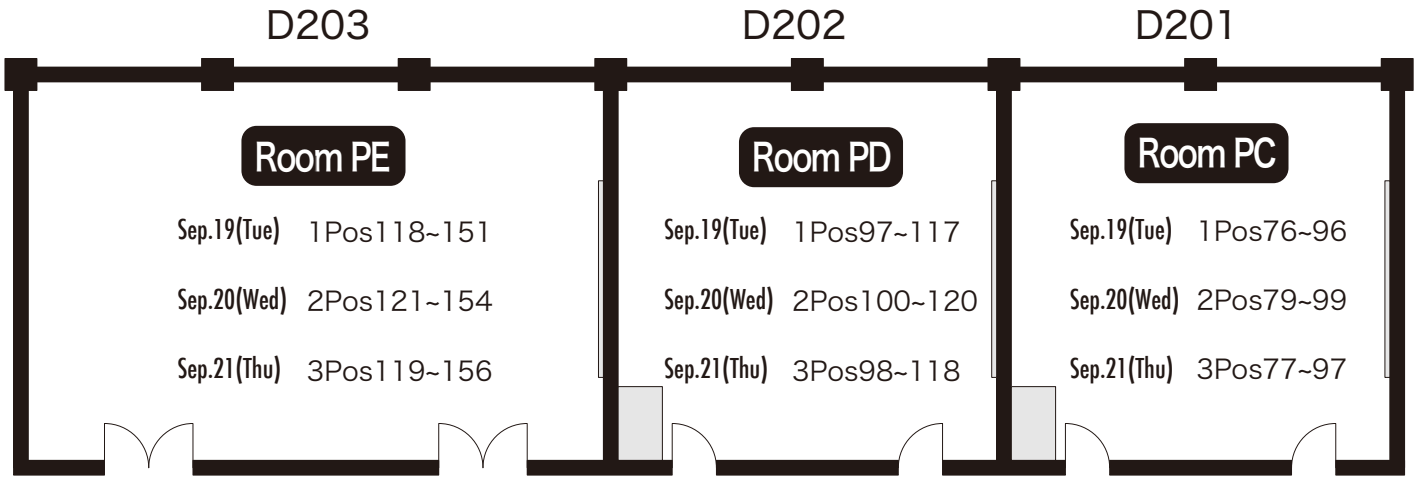
Faculty of Law Main Building

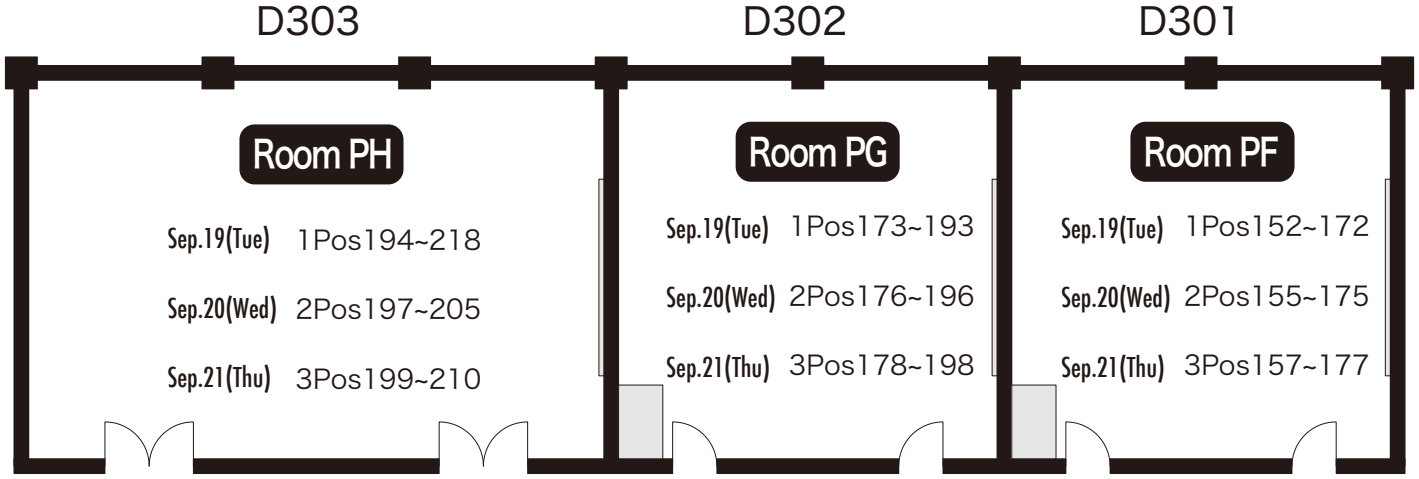




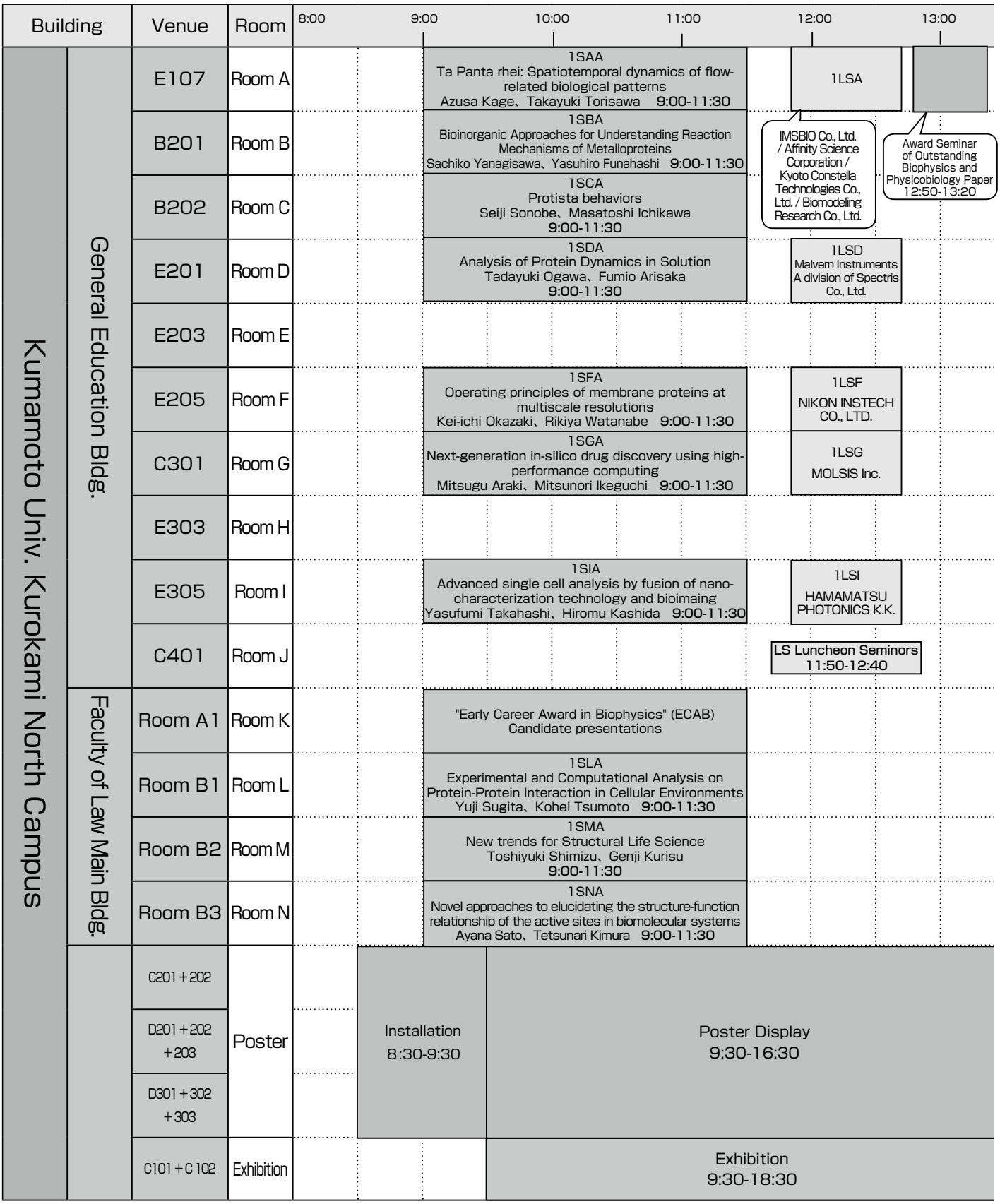
Poster Place

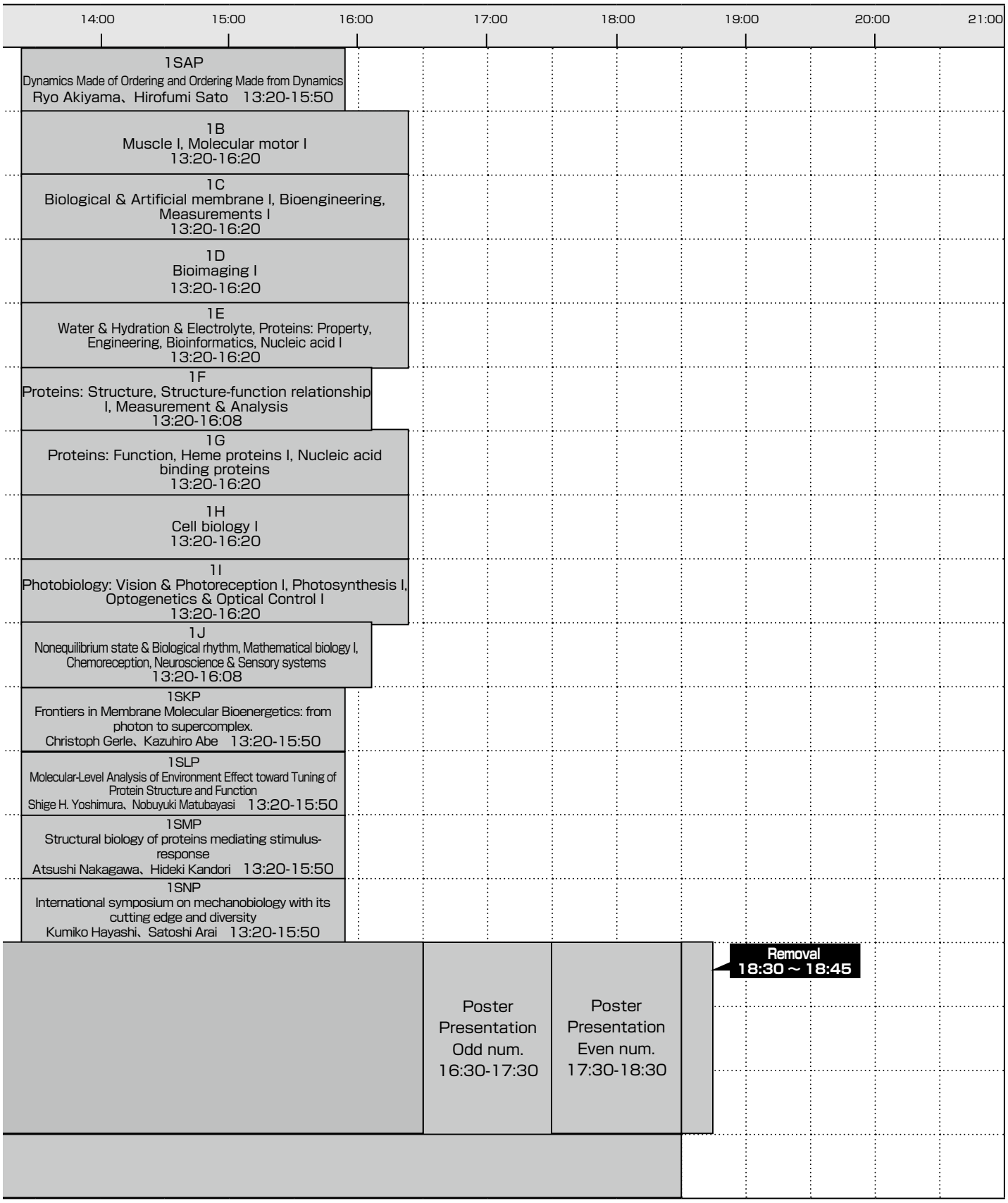




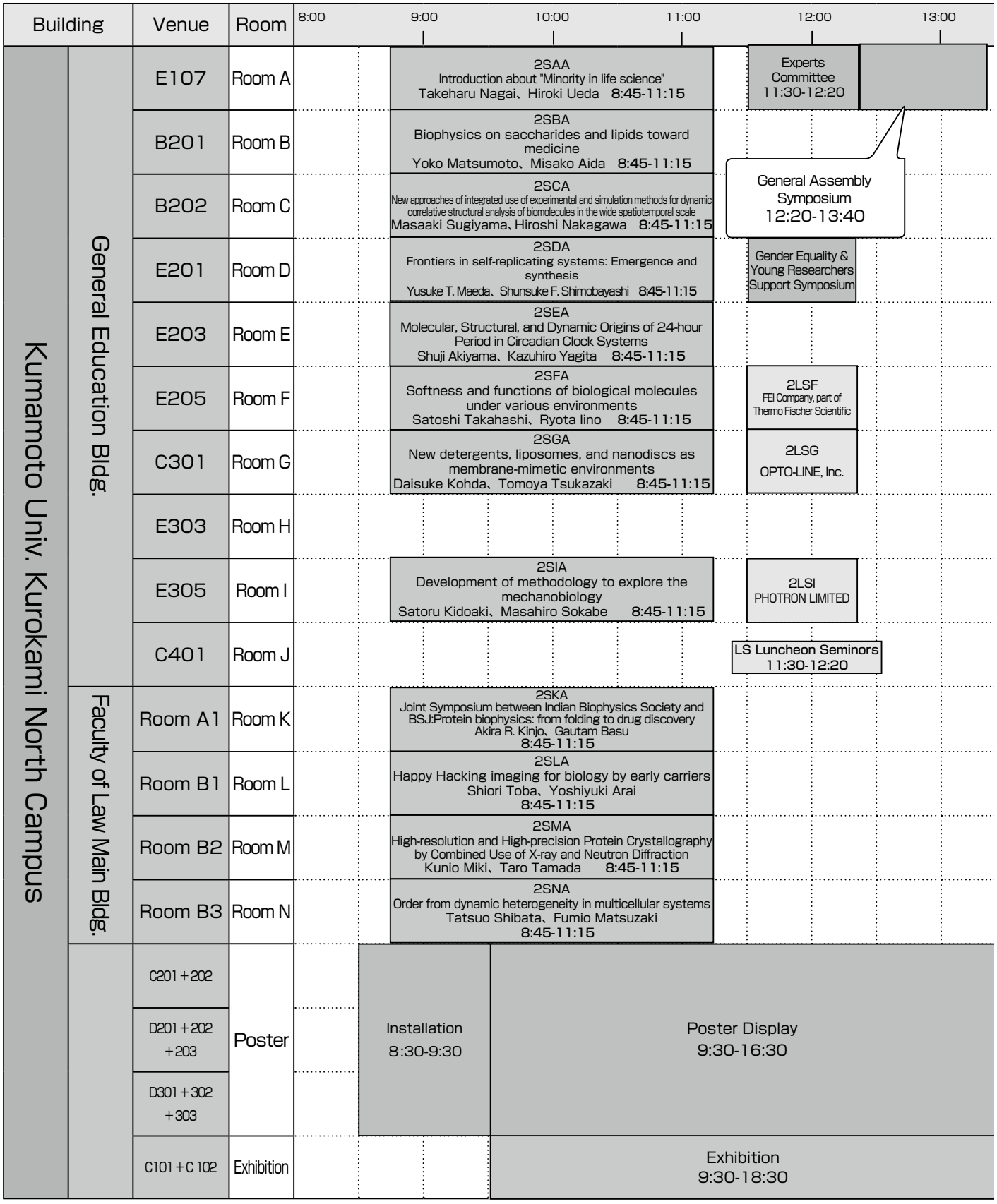


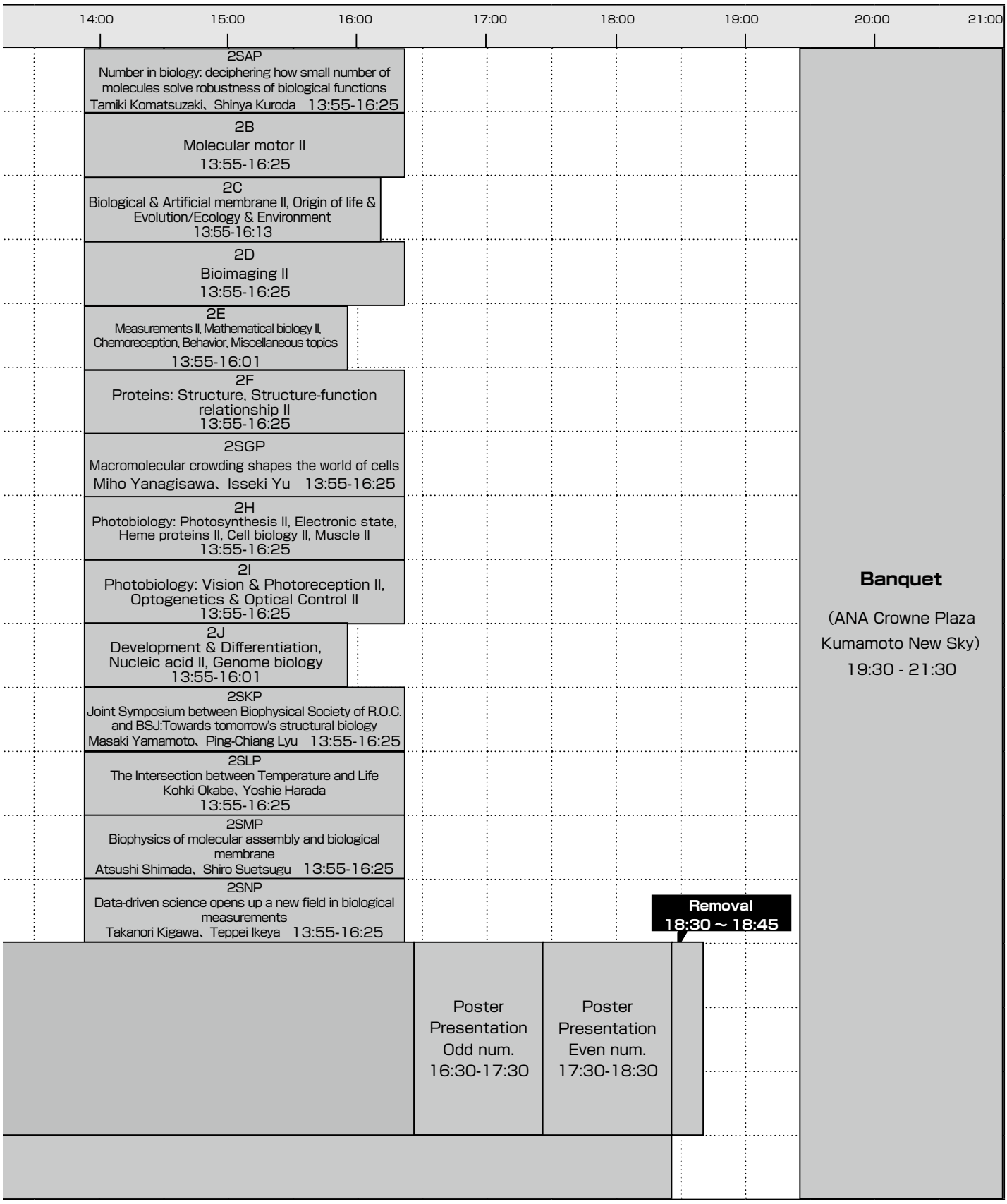
September 19 (Tue.) Day1



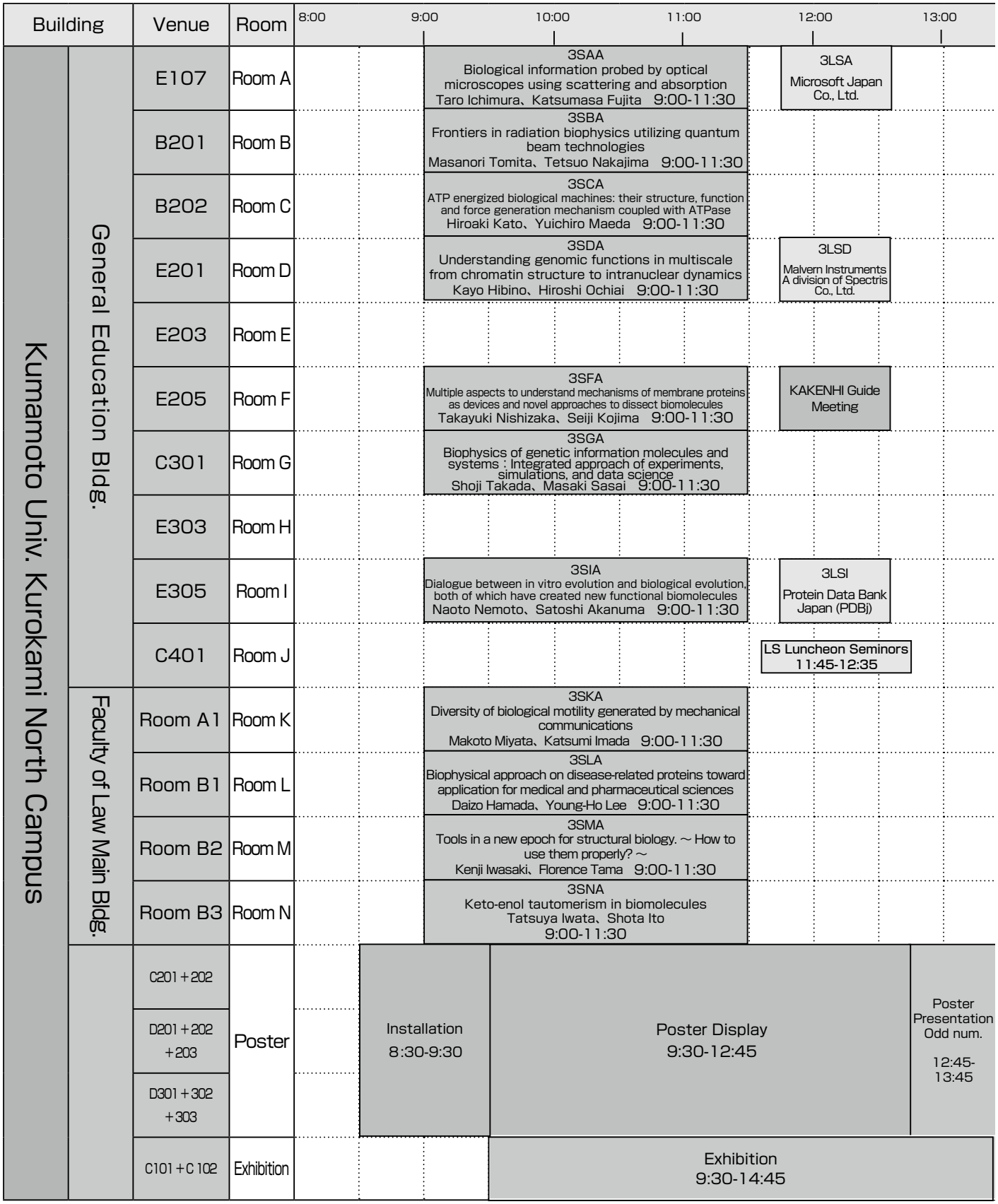

14:00
15:00
16:00
17:00
18:00
19:00
20:00
21:00
1SAP
Dynamics Made of Ordering and Ordering Made from Dynamics
Ryo Akiyama、Hirofumi Sato 13:20-15:50
1B
Muscle I, Molecular motor I
13:20-16:20
1C
Biological & Artificial membrane I, Bioengineering, Measurements I
13:20-16:20
1D
Bioimaging I
13:20-16:20
1E
Water & Hydration & Electrolyte, Proteins: Property, Engineering, Bioinformatics, Nucleic acid I
13:20-16:20
1F
Proteins: Structure, Structure-function relationship I, Measurement & Analysis
13:20-16:08
1G
Proteins: Function, Heme proteins I, Nucleic acid binding proteins
13:20-16:20
1H
Cell biology I
13:20-16:20
1I
Photobiology: Vision & Photoreception I, Photosynthesis I, Optogenetics & Optical Control I
13:20-16:20
1J
Nonequilibrium state & Biological rhythm, Mathematical biology I, Chemoreception, Neuroscience & Sensory systems
13:20-16:08
1SKP
Frontiers in Membrane Molecular Bioenergetics: from photon to supercomplex.
Christoph Gerle、Kazuhiro Abe 13:20-15:50
1SLP
Molecular-Level Analysis of Environment Effect toward Tuning of Protein Structure and Function
Shige H. Yoshimura、Nobuyuki Matubayasi 13:20-15:50
1SMP
Structural biology of proteins mediating stimulus-response
Atsushi Nakagawa、Hideki Kandori 13:20-15:50
1SNP
International symposium on mechanobiology with its cutting edge and diversity
Kumiko Hayashi、Satoshi Arai 13:20-15:50
Poster Presentation Odd num. 16:30-17:30
Poster Presentation Even num. 17:30-18:30
Removal 18:30 ~ 18:45

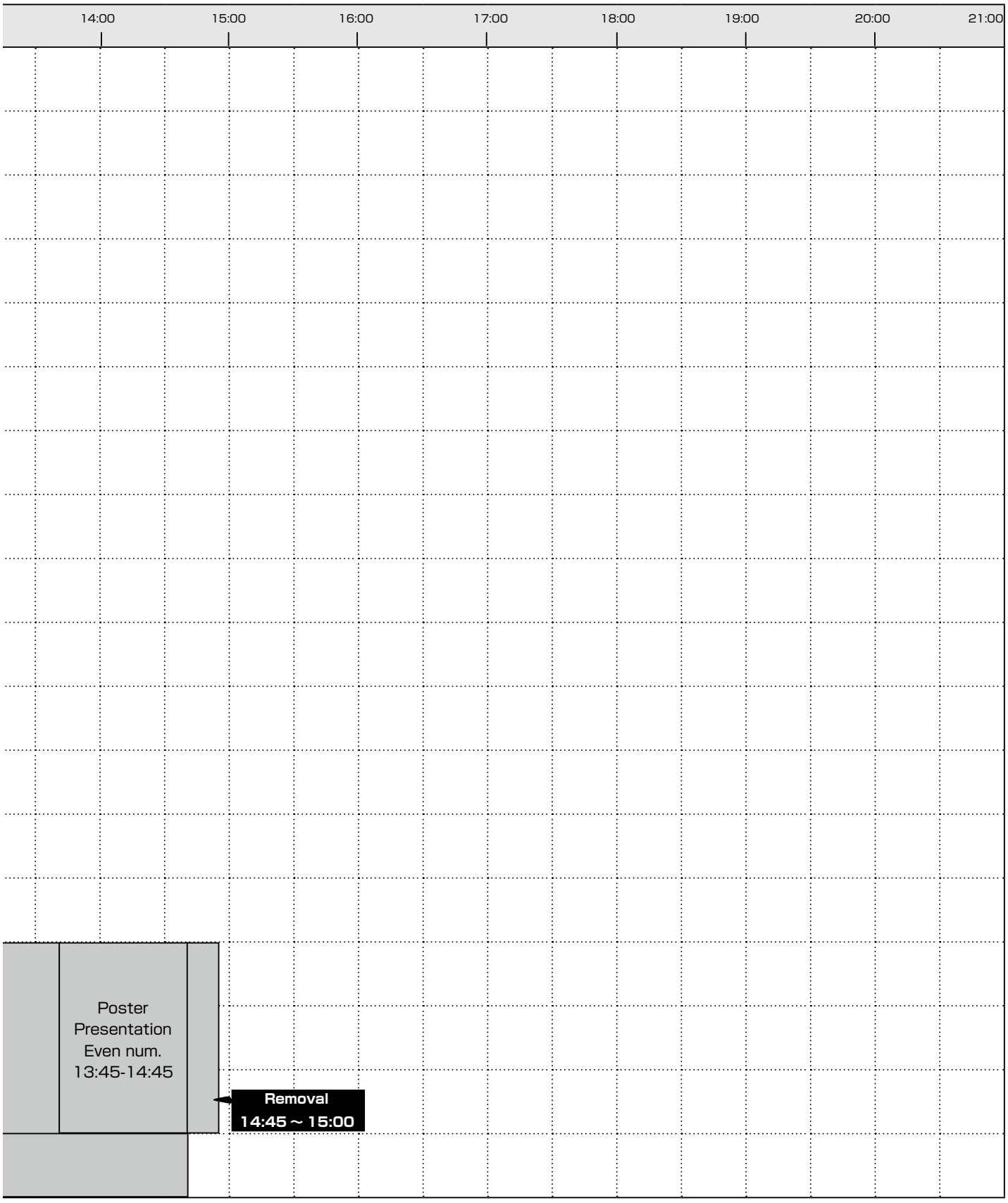
September 20 (Wed.) Day2




14:00
15:00
16:00
17:00
18:00
19:00
20:00
21:00
2SAP
Number in biology: deciphering how small number of molecules solve robustness of biological functions
Tamiki Komatsuzaki、Shinya Kuroda 13:55-16:25
2B
Molecular motor II
13:55-16:25
2C
Biological & Artificial membrane II, Origin of life & Evolution/Ecology & Environment
13:55-16:13
2D
Bioimaging II
13:55-16:25
2E
Measurements II, Mathematical biology II, Chemoreception, Behavior, Miscellaneous topics
13:55-16:01
2F
Proteins: Structure, Structure-function relationship II
13:55-16:25
2SGP
Macromolecular crowding shapes the world of cells
Miho Yanagisawa、Isseki Yu 13:55-16:25
2H
Photobiology: Photosynthesis II, Electronic state, Heme proteins II, Cell biology II, Muscle II
13:55-16:25
2I
Photobiology: Vision & Photoreception II, Optogenetics & Optical Control II
13:55-16:25
2J
Development & Differentiation, Nucleic acid II, Genome biology
13:55-16:01
2SKP
Joint Symposium between Biophysical Society of R.O.C. and BSJ:Towards tomorrow's structural biology
Masaki Yamamoto、Ping-Chiang Lyu 13:55-16:25
2SLP
The Intersection between Temperature and Life
Kohki Okabe、Yoshie Harada
13:55-16:25
2SMP
Biophysics of molecular assembly and biological membrane
Atsushi Shimada、Shiro Suetsugu 13:55-16:25
2SNP
Data-driven science opens up a new field in biological measurements
Takanori Kigawa、Teppei Ikeya 13:55-16:25
Removal
18:30 ~ 18:45
Poster Presentation Odd num.
16:30-17:30
Poster Presentation Even num.
17:30-18:30
Banquet
(ANA Crowne Plaza Kumamoto New Sky)
19:30 - 21:30

September 21 (Thu.) Day 3




14:00
15:00
16:00
17:00
18:00
19:00
20:00
21:00
Poster
Presentation
Even num.
13:45-14:45
Removal
14:45 ~ 15:00

Information for Participants and Presenters

1. Registration

◇ Registration desk

Location：Student Lobby, 1F, General Education Building (Refer to the page 29.)
Open Hours： Sep. 19(Tue) / 20(Wed) 8：30 – 17：00, Sep. 21(Thu) 8：30 – 14：00

◆Advance registration

For participants who have completed advance registration with full payment of the registration fee by the deadline, there is no need to stop by the registration desk. A name badge, a receipt and a program booklet have already been sent to these participants.

*Participants from overseas: Receive a name badge and a program booklet at the registration desk.
*Please wear your name badge throughout the meeting. Without it, you cannot enter the meeting site.
(Name badge holders will be provided at a place near the registration desk and in front of each lecture room.)

Note 1) Advance registration is completed only after the payment is done. In case your payment cannot be confirmed by the deadline, your registration is automatically cancelled. In this case, please register on-site at the registration desk.
Note 2) Name badges have not been sent to those who have not paid the BSJ annual membership fee. Please complete the payment at the BSJ desk of the meeting site.
Note 3) If you have already paid both registration and BSJ annual membership fees but not received a name badge, please visit the registration desk.
Note 4) For non-members who are invited to talk at a symposium, the membership is not required and your registration fee is waived. You are invited for free to the banquet.
Note 5) Attendees who belong to institutions outside of Japan can make a presentation without a membership.

◆On-site registration

Those who have not completed advance registration are required to register on-site at the registration desk. Only cash payment is acceptable.

◇ On-site registration fees

	BSJ Member				Non-Member		
	Regular	Senior	Student	Undergraduate student	Regular	Student	Undergraduate student
Registration fee	¥9,000	¥5,000	¥5,000	¥0	¥12,000	¥6,000	¥0
Banquet fee	¥8,000	¥5,000	¥5,000	¥3,000	¥8,000	¥5,000	¥3,000

・For undergraduate students, the registration fee is waived. You are required to present your student ID at the registration desk to receive a name badge and a program booklet. But the banquet fee is charged if you attend the banquet.

・The “Early Career Award in Biophysics” Candidate presenters, the Biophysics and Physicobiology Outstanding Paper Award presenter and the representative of Biophysics and Physicobiology Editors’ Choice awardee are invited for free to the banquet. If you have already paid the banquet fee, you can get a full refund at the registration desk.

◇ Name badge

Please be sure to wear your name badge throughout the meeting. Entry without the badge is NOT acceptable. Remember to bring your name badge that was sent in advance. (Name badge holders will be provided at a place near the registration desk and in front of each lecture room.)

◇ Receipt

A receipt is attached to the name badge. If you need another receipt form, it will be issued in exchange for the one attached to your name badge.

◇ Program booklet / Abstract online system【Release date: Aug. 18 (Fri)】

A program booklet (a part of front matters, and program) will be sent in advance to BSJ members and non-members with advance registration. The abstracts will be released only on the online system. No printed abstract booklet will be issued. On the online system, you can browse, search and download abstracts.

Program booklets can be purchased at the meeting site: JPY3,500/booklet.

Abstract online system:
http://www.biophys.jp/dl/pro/55th_proceedings.pdf
Download ID: ambsj55
PW: kumamoto2017

The program (presentation title, presenter's name and affiliation) and the online abstracts will be released on the BSJ55 web site. A half year later after the meeting, the abstracts will be posted on the J-Stage web site which is linked from the BSJ web site.

BSJ web site: http://www.biophys.jp/ann/ann02.html

J-Stage web site: http://www.jstage.jst.go.jp/browse/biophys/-char/ja

◇ Program search system (Web version)【Release date: Aug. 10 (Thu)】

Program search system will be released on the BSJ55 web site.

◇ Free app to search and browse Program & Abstracts【Release date: Sep. 15 (Fri)】

A free app for smart phones (iPhone /Android) and tablets (iPad /iPod Touch /Android) can be downloaded from App Store or Google Play.

App name：The 55th Annual Meeting of the Biophysical Society of Japan
Search word： bsj2017
PW of the abstracts browsing system：kumamoto2017

◇ BSJ membership (payment of the annual membership fee, and admission procedures)

For those who have not yet paid their annual membership fee, you can pay at the BSJ desk. For non-members, you are welcome to sign up at the BSJ desk to become a new member. For non-members who are invited to talk at a symposium or belong to institutions outside of Japan, the BSJ membership is not required.

2. Services & Facilities

◇ Cloakroom

Location： Meeting Room 1, 1F, General Education Building (Refer to the page 29.)

Open Hours： Sep. 19(Tue) 8:30 - 18:45
20(Wed) 8:30 - 18:45
21(Thu) 8:30 - 15:00

*Valuables or computers cannot be checked into the cloak since the society/meeting does not hold any responsibility for loss or damage of your items.
*Please pick your items up when you leave the meeting venue.

◇ Lunch

Free lunch:

Free lunch will be provided at luncheon seminars (day 1-3), Gender Equality & Young Researchers Support Symposium (day 2), and KAKENHI Guide Meeting (day 3). Lunch tickets will be distributed in the morning of day 1-3. Please refer to luncheon seminar page.
Also a limited number of free lunch without lunch tickets will be provided at Experts Committee (day 2).

◆Cafeteria

A Cafeteria is available as follows:
Location: North Student Hall Bldg. A
Open hours: 11:00 - 14:00
＊Please take freely "Restaurant map of Kumamoto Univ. North Campus area" that will be provided around the registration desk.

◇ Paging service・bulletin board

No paging service is available to call an individual except for an emergency. Please use a bulletin board near the registration desk in order to contact with other participants.

◇ Parking

Parking lot is not available for participants.

◇ Accommodation

Please refer to "Accommodation" page of the BSJ2017 web site.

◇ Internet

Eduroam as Wi-Fi is available at the meeting site. You can access internet with your ID of eduroam (Wi-Fi network name: eduroam). If you don't have an eduroam ID, please receive an ID and password to use the university wireless LAN service at the registration desk.
* Wi-Fi condition can be unstable or disconnected due to construction of a building, conditions of reception or access. One wireless LAN ID will be provided per person.
* Using internet in the lecture room is not accepted.

◇ Child Care Service

Child care service is available during the meeting. Further information is announced on the BSJ2017 web site.

3. Programs & Events

*Several programs and events (committee meetings, general assembly meeting and its associated symposium, and lecture for public) are omitted here.

◇ "Early Career Award in Biophysics" Candidate presentations

Date & Time: Sep. 19 (Tue) 9:00 - 11:30
Place: Room K (Room A1 2F, Faculty of Law Main Building)

◇ Student Presentation Award

This award will be selected from among oral presentations on Sep. 19 (Tue) PM.

◇ Lecture by Biophysics and Physicobiology Outstanding Paper Awardees

Date & Time: Sep. 19 (Tue) 12:50 – 13:20
Place: Room A (E107 1F, General Education Building)

◇ Banquet

Date & Time: Sep. 20 (Wed) 19:30 – 21:30
Free shuttle buses will be provided from the meeting venue. Departure time: 18:45 - 19:00
Place: Strings, 2F, ANA Crowne Plaza Kumamoto New Sky
(a 5-minute walk from Gionbashi station of city tram)
Address: 2 Higashiamidaji-machi, Chuo-ku, Kumomoto-city / Tel: 096-354-2111
*On-site registration is available at the registration desk or the banquet reception desk.

◇ Luncheon seminar

Lunch tickets will be distributed at the luncheon seminar desk, as shown below.

◆Distribution of lunch tickets

Luncheon seminar desk
Hours: Sep. 19, 20, & 21 8:30 – 10:30
*The desk will be closed when all the tickets are distributed.
Location: Student Lobby, 1F, General Education Building
*Only tickets for the seminars on the day are provided on a first-come-first-served basis.
*Lunches are provided by courtesy of companies and groups co-sponsoring luncheon seminars.

◆Attention

Please note that the lunch tickets will become invalid when you do not come before the starting time of the seminars and that the resulting remaining lunches will be provided to those who are attending the seminars without lunch tickets.

◆Request

We kindly ask you to attend till the last.Also, please enter your affiliation and name in the questionnaire provided at the luncheon seminar as possible as you can.

◇ Exhibition

Instruments, reagents, software, books, etc. are displayed at the exhibition hall (C101+C102 1F, General Education building).

4. Prohibited Items

◇ Photography & recording

Photography and recording with camera, video, mobile phone and any device is NOT allowed at the meeting site. Please note that some recording may be performed after obtaining the board meeting's approval.

◇ Smoking, drinking & eating

Smoking is NOT allowed at the meeting site. Drinking and eating is NOT allowed inside lecture rooms except for luncheon seminars and other seminars/meetings in which meals are served.

◇ Mobile phone use

Talking on a mobile phone in the lecture/presentation rooms is NOT allowed. Please set your mobile phone on the silent mode or off, and make sure it will not make noises during lectures/presentations.

5. Contact

◇ During the meeting

Secretariat (Tel: 050-3482-9415 *phone number reachable during the meeting)

◇ Before or after the meeting

The organizing committee of the BSJ55
bp_nenkai55@kumamoto-u.ac.jp
Registration and abstract submission support desk
Nakanishi Printing Company
Ogawa-higashiiru, Shimodachiuri-dori, Kamigyo-ku, Kyoto 602-8048
bsj2017sys-sprt@e-naf.jp
Support team, exhibition and advertisement secretariat
A & E planning Co., Ltd.
Shin-Osaka Grand Bldg. 6F, 2-14-14, Miyahara, Yodogawa-ku, Osaka 532-0003
Tel: 06-6350-7163 / Fax: 06-6350-7164
Support team: jbp2017@aeplan.co.jp
Exhibition and Advertisement secretariat: e_jbp55@aeplan.co.jp

6. Information for Presenters

◇ Language

Prepare your slides in English and give your presentation in English.

◇ Projector

Please bring a laptop with you for your presentation. A projector is equipped in each lecture room.
A sound output is not accepted.

1) Please prepare your presentation file in Microsoft PowerPoint.
2) The output resolution should be XGA (1024 x 768). The higher resolutions would possibly lose some information.
3) Our staff will connect your laptop to a switcher.
4) The output connector of your laptop should be “miniD-sub15pin”. If your connector is a different type (for example, that of Macintosh computer), please bring a conversion adaptor.
5) Bring your PowerPoint file in a USB memory.
6) Bring your AC adaptor in case that your battery would die.
7) Deactivate the screen-saver and power saving mode of your laptop.

◇ For organizers of symposia & “Early Career Award in Biophysics” (ECAB) Candidate presentations

Please come to the assigned room by 15 minutes before the start of the session, and then tell our staff of your arrival. Keep the time schedule and make smooth progress in the program. As a time keeper, our staff will help you.

◇ For speakers of symposia or ECAB Candidate presentations

Please come to the “PC Desk” in the assigned room by 15 minutes before the start of the session.
Our staff will connect your computer to a switcher.
*Please note that there is no preview room.

◆ Time allocation:

Symposium: Time allocation will be controlled by chairpersons.
ECAB Candidate Presentation: Presentation 10min. + Discussion 3min + Laptop change 2min.

◇ For chairpersons of oral presentation.

Please come to the assigned room at least 15 min before the start of the session, and then inform our staff of your arrival. Keep the time schedule and make smooth progress of the session. As a time keeper, our staff will help you.

◇ For speakers of oral presentation.

Please come to the PC Desk in the assigned room by 15 min before your presentation. Our staff will connect your laptop to a switcher. * Please note that there is no preview room.

◆ Time allocation: Presentation 8min.+ Discussion 3min. & 30sec. + Laptop change 30sec.

◇ For poster presenters

		Day 1, Sep. 19	Day 2, Sep. 20	Day 3, Sep. 21
Setup, Display		8:45 – 16:30	8:30 – 16:30	8:45 – 12:45
Presentation Discussion	Odd Numbers	16:30 – 17:30	16:30 – 17:30	12:45 – 13:45
	Even Numbers	17:30 – 18:30	17:30 – 18:30	13:45 – 14:45
Removal		until 18:45	until 18:45	until 15:00

*Periods of poster display: Posters will be replaced every day for the next day's poster presentations.
*Panel size: 90cm wide x 210cm high. Push pins are available at the site.
*Removal: Any posters remaining on panels after the removal time will be discarded by the secretariat.

◇ Instructions for poster presentation

A poster must be written in English.
Put a small circle on the upper left of the presenter's name.

◇ Presentation types and how to read the presentation numbers

Presentation types are Symposium Speech, "Early Career Award in Biophysics" Candidate Presentations, Oral Presentation, and Poster Presentations.

Speech at symposium: (Ex.) 1SAA-03

Presentation day (1, Sep. 19; 2, Sep. 20; 3, Sep. 21) + Symposium (S) + Session room (Room A) + AM (A) / PM (P) + Order of the talk

"Early Career Award in Biophysics" Candidate Presentations: (Ex.) 1YK1045

Presentation day (1, Sep. 19) + Young Scientists (Y) + Session room (Room K) + Starting time of the talk

Oral Presentation (Ex.) 1B1320

Presentation day (1, Sep. 19; 2, Sep. 20; 3, Sep. 21) + Session room (Room B) + Starting time of the talk
For presentations which are eligible for consideration for Student Presentation Award, "*" is attached on the right side of a presentation number.

Poster presentations: (Ex.) 1Pos001

Presentation day (1, Sep. 19; 2, Sep. 20; 3, Sep. 21) + Poster (Pos) + Panel number

第 55 回日本生物物理学会年会　市民講演会
「エンジョイ！サイエンス ～生命を観る・守る最前線～」

日　時：9 月 18 日（月・祝） 開場 13 時 30 分，開演 14 時，終演 16 時

会　場：くまもと県民交流館パレア会議室 1
（〒 860-8554 熊本市中央区手取本町 8 番 9 号　テトリアくまもとビル 9 階，市電「水道町」電停もしくは「通町筋」バス停下車すぐ）

参加費：無料（どなたでも自由に参加できます）

主　催：第 55 回日本生物物理学会年会実行委員会

共　催：熊本大学薬学部

世話人：安永 卓生（九州工業大学大学院情報工学研究院）
山縣 ゆり子（熊本大学大学院生命科学研究部）

講演プログラム

「見えないものを観る　～からだの中の分子のはたらき～」

原田 慶恵 教授（大阪大学・蛋白質研究所）

私たちのからだをつくるたくさんの細胞。それぞれの細胞では，さまざまなタンパク質分子が働いています。ちょっと工夫をして，顕微鏡でのぞいた小さな小さなタンパク質分子たちが働く世界を紹介します。

「ウイルスは宿主細胞のクロマチン構造を変化させるか？～感染症との関わり～」

今井 由美子プロジェクトリーダー
（医薬基盤・健康・栄養研究所・感染病態制御ワクチンプロジェクト）

ヒトの DNA の総長は 2m 程ですが，ヒストンタンパク質と複合体を形成してクロマチン構造をとって，細胞の核の中に収納されています。今回，ウイルスが宿主のクロマチンの高次構造を変化させる仕組みや，感染症との関わりについてお話ししたいと思います。

講演は日本語で行われます。

第 4 回会員総会シンポジウム：国際連携と IUPAB

オーガナイザー：日本生物物理学会　理事会
日　時：9 月 20 日（水）12:45 〜 13:40（会員総会中）
会　場：A 会場（全学教育棟 E107）
司　会：神取秀樹

概要：国際純粋および応用生物物理学連合（International Union for Pure and Applied Biophysics; IUPAB）は 1961 年に創設され，日本は当初よりアクティブなメンバー（正式加盟団体は日本学術会議 IUPAB 分科会）として加盟しています。現在，約 60 の国と地域が参加し，研究者間の交流と生物物理学の振興に寄与しています。

IUPAB の重要なイベントが 3 年に一度，開催される International Biophysics Congress (IBC) です。日本は 1978 年に第 6 回大会を京都で開催，国内 1200 人，海外から 600 人の参加者が集い，その後の日本の生物物理学発展に多大な影響を及ぼしました。2014 年，オーストラリアのブリスベンで開催された IBC には，本学会は若手の旅費支援を行いました。2017 年 7 月 16 〜 20 日には第 19 回大会が英国のエジンバラで開催され，本学会は 10 名の若手に旅費支援を行いました。

今年の会員総会シンポジウムは国際連携をテーマとします。長年，IUPAB の発展にご尽力され，会長も務められた永山氏，現在，IUPAB 理事ならびに日本学術会議 IUPAB 分科会委員長を務めておられる野地氏にご講演いただいた後，エジンバラ会議の旅費支援を受けた若手にショートプレゼンテーションをしていただく予定です。

講演者・プログラム

1. 永山國昭（永山顕微鏡研究所，IUPAB 元会長）
「本学会の国際連携に関する取組み」

2. 野地博行（東大院工，IUPAB 理事，日本学術会議 IUPAB 分科会委員長）
「近年の IUPAB の活動について」

3. 第 19 回 IBC に旅費支援を受けた若手のショートプレゼンテーション

4. 総合討論

【速報】
本年７月のエジンバラ IBC 会議において，2023 年の日本開催が決まりました。
シンポジウムでは今回の招致活動についてもご紹介いただきます。

一般社団法人日本生物物理学会　第 6 回 Biophysics and Physicobiology 論文賞受賞講演会

The 6th Award Seminar for outstanding Biophysics and Physicobiology paper

オーガナイザー：日本生物物理学会 Biophysics and Physicobiology 論文賞選考委員会

Organizers: Award committee for outstanding Biophysics and Physicobiology paper

日　時：9 月 19 日（火）12:50 ～ 13:20 ／ Sept. 19 Tue.

場　所：A 会場（全学教育棟 E107）／ Room A (General Education Building E107)

形　式：講演会／ Lecture

第 6 回 Biophysics and Physicobiology 論文賞受賞者

BPPB Outstanding Paper Awardee

川端 猛，杉原 裕介，福西 快文，中村 春木

Takeshi Kawabata, Yusuke Sugihara, Yoshifumi Fukunishi, Haruki Nakamura

大阪大学 蛋白質研究所

Institute for Protein Research, Osaka University

LigandBox : 化合物の立体構造のデータベース

LigandBox: A database for 3D structures of chemical compounds

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A database for the 3D structures of available compounds is essential for the virtual screening by molecular docking. In 2013, we opened the web server for the LigandBox database containing four million available compounds, collected from the catalogues of commercial suppliers, and approved drugs and biochemical compounds. Each chemical compound in the database has several 3D conformers with hydrogen atoms and atomic charges, which are ready to be docked into receptors using docking programs. The 3D conformations were generated using our molecular simulation program package, myPresto. Various physical properties, such as aqueous solubility (LogS) have also been calculated to characterize the ADME-Tox properties of the compounds. The Web database provides two services for compound searches: a property/chemical ID search and a chemical structure search. The chemical structure search is performed by a descriptor search and a maximum common substructure (MCS) search combination, using our program *kcombu*. By specifying a query chemical structure, users can find similar compounds among the millions of compounds in the database within a few minutes. In 2017, the LigandBox stores more than 10 million compounds. Our database is expected to assist a wide range of researchers, in the fields of medical science, chemical biology, and biochemistry, who are seeking to discover active chemical compounds by the virtual screening.

男女共同参画・若手支援委員会企画シンポジウム
男女共同参画のミクロとマクロ
（Micro and macro approaches to gender equality in science）

オーガナイザー：日本生物物理学会　男女共同参画・若手支援委員会

Organizers : Promotion of Gender Equality and Young Researchers Committee

日　　時：9 月 20 日（水）11:30 ～ 12:20（ランチョンセミナーの時間帯）

会　　場：D 会場（全学教育棟 E201）

言　　語：日本語

昼　　食：お弁当とお茶を無料で提供いたします。ただし，数に限りがあります。

形　　式：問題提起プレゼンテーションとパネルディスカッション

司　　会：根岸瑠美（東大）

問題提起：高橋聡（東北大）

パネラー：豊島陽子（東大），原田慶恵（阪大），林久美子（東北大），柳澤実穂（農工大）
本間道夫（名大），由良敬（お茶大），藤原慶（慶大），豊田正嗣（埼玉大）
（当日変更可能性あり）

概要：男女共同参画を考える上で，行政政策方針や大学・研究機関・自治体などの各種制度設計について知ることが肝要であると同時に，我々研究者が直接所属する研究室や個々人の家庭内事情などは，直接自身に降りかかることであり，無視のできないものと考えられます。本シンポジウムでは，前者を男女共同参画の「マクロ」，後者を「ミクロ」と表現し，ミクロとマクロの 2 つの視点から，現在の問題とその解決策についてディスカッションすることを目的とします。

本企画シンポジウムは，問題提起プレゼンテーションと，8 名のパネラーによるパネルディスカッションの 2 部構成で行います。はじめに，高橋氏から男女共同参画学協会連絡会が実施しているアンケートの結果をもとに，問題提起として女性研究者の置かれている現状を報告していただきます。その後，各パネラーの方より自己紹介をしていただき，パネルディスカッションを実施します。第一線で活躍され各種評価等にも携わっている方，女性研究者や女子学生を指導している方，現在小さなお子さんを子育て中の方，海外での子育てを経験されている方など，男女共に幅広い立場の方にパネラーになっていただきました。ワークライフバランス，出産・子育て等のライフイベント，女性のキャリアアップの実例などについてお話を伺い，男女共同参画のために何が必要か，ミクロとマクロの両視点から参加者も含めて会場で議論したいと思います。

様々な経験を持つパネラーが一堂に会します。色々なお話が聞けると思いますので，興味のある方は是非ご参加下さい。特に，学生，若手研究者の方の参加を歓迎します。

キャリア支援説明会

オーガナイザー：日本生物物理学会 男女共同参画・若手支援委員会
日　時：9 月 19 日（火）第 1 部　11:50–12:40，第 2 部　12:50–13:40，第 3 部　13:50–14:30
9 月 20 日（水）9:30–10:30
会　場：X 会場（全学教育棟 1 階 E105）
形　式：セミナー 第 1 部のみランチョンセミナー **説明はすべて日本語で行われます。**

概要：若手研究者や学生の今後のキャリア構築の一助となるように，一昨年の年会から「キャリア支援説明会」を開催しています。本年会では，キャリアコンサルタントとして，主に大学院生やポストドクターの就職支援活動をされている（株）アカリクの山内宗和氏によるセミナーを実施します。第 1 部のみランチョンセミナーのため参加者数に限りがありますが，第 2 部以降から参加することも可能です。

プログラム：

9 月 19 日（火）

第 1 部 11:50–12:40　博士・PD の方の為の就活ガイダンス

【博士・PD 向け】中途採用（即戦力採用）の強化，ダイバーシティ（人材の多様化）の推進などが積極的に取り組まれている現在の企業採用事情。3 ～ 4 年前と比べ, 明らかにその就職事情は好転しています。しかし，その状況を活かすことができるかどうかは，就職事情の理解度と，その対策によって大きく変わってしまいます。このような状況を踏まえ，まずは専攻を問わず，博士・PD の為の就活ガイダンスを開催します。
◆現在の企業の採用活動について ◆博士・PD の就活について◆「専門性」を活かせる企業の探し方

第 2 部 12:50–13:40　先人に学ぶ，研究職以外でどんな「活きる道」があるのか

【修士・博士・PD 向け】第 1 部の「専門性」を活かせる企業の探し方の講演内容を受けて，ではどのような選択肢が博士・PD にあるのか，について，皆さんの先人達の就職実績に基づきながら,「生物物理」専攻の方に特化した内容で講演します。（求人状況によって変わる可能性がありますが，直近で企業への就職を考えている方の為に，具体的な求人の紹介も実施する予定です。）第 2 部に関しては，修士の方向けにも情報提供します。

第 3 部　13:50–14:30　質疑応答

9 月 20 日（水）

第 4 部　9:30–10:30　「専門外就職」へ向けて何をすべきか

【修士・博士・PD 向け】第 3 部の質疑応答の内容を受けて，今までの研究を継続する形で民間企業への就職をする方以外は全て「専門外就職」であるという前提で, 民間企業への就職活動を行う為には何をすべきか，について解説します。「何故研究職を辞めて●●という職種に就こうと思ったのか」,「何故アカデミックを離れて民間企業へ就職するのか」といった面接におけるネガティブな質問に対して，どうポジティブに「気持ちを持っていくのか」も大切となります。そこで書類の書き方や面接での話し方などを含め，具体的な内容に踏み込んで解説します。第 1 部のランチョンセミナーに参加できなかった方のために，第 1 部の情報も再度紹介いたします。

「科研費改革の動向」
Reorganization of KAKENHI: Current Activities of JSPS

世話人：原田慶恵（大阪大学蛋白質研究所，日本学術振興会学術システム研究センター専門研究員）

Organizer：Yoshie Harada (Institute for Protein Research, Osaka University; Program Officer, Research Center for Science Systems, JSPS)

日　時：9 月 21 日（木）11:45–12:35（ランチョンセミナーの時間帯）

会　場：F 会場（E205 教室）

昼　食：お弁当とお茶が無料で提供されます。ただし，数に限りがあります。

形　式：日本語による講演会

講師：日本学術振興会　研究助成企画課長　大鷲 正和

日本が将来にわたって卓越した研究成果を生み出し続けるために，科学技術・学術審議会において「科研費制度の抜本的改革」が提言され，現在，科研費の研究種目・枠組みの見直しや審査システムの見直しが行われています。平成 30 年度科研費（平成 29 年 9 月公募）には「審査システム改革 2018」として，審査システムの完全移行が行われる予定であり，科研費業務の大部分を担当している日本学術振興会の学術システム研究センターが中心となり，3 年余りにわたり議論を進め，審査区分と審査方式とを一体的に見直してきたところです。ついては，本年 1 月，新たな審査区分として「小区分・中区分・大区分」を設定し，それに伴い，新たな審査方式（総合審査，2 段階書面審査）について取りまとめられましたので，今回は，このシステム改革の内容を中心に，ご説明をいただきます。

若手奨励賞招待講演　Early Career Award in Biophysics Candidate Presentations

第 1 日目（9 月 19 日（火））／Day 1（Sep. 19 Tue.）

9:00～11:30　K 会場（文法学部 2 階 A1 教室）／Room K (Room A1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

1YK　日本生物物理学会若手奨励賞選考会
Early Research in Biophysics Award Candidate Presentations

オーガナイザー：男女共同参画・若手支援委員会
Organizer: Promotion of Gender Equality and Young Researchers Committee

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Since 2005, Biophysical Society of Japan (BSJ) has granted "Early Career Award in Biophysics" to young BSJ members for their excellent presentations that show great potential to contribute to the progress of biophysics. In this 13th year, we received 39 highly qualified applications. After the first round of competitive screening based on submitted documents, the following ten applicants were selected as the young invited speakers. In this symposium, each speaker will make 10-minute presentation followed by 3-minute discussion as the second round of screening. Up to five winners will be selected and announced at the banquet held in the evening of the second day. We welcome all the BSJ members to attend this symposium to foresee the future of biophysics in Japan through the speakers and their researches.

09:00　小田 茂和　1J1556
1YK0900　神経グロビンによる知覚変化の情報処理機構
Information processing mechanism underlying a perceptual change by a neuroglobin
○小田 茂和[1], 豊島 有[2], デゥボノ マリオ[3]（[1]岡崎統合バイオサイエンスセンター 定量生物学研究部門（基礎生物学研究所）, [2]東京大学 大学院理学系研究科生物科学専攻, [3]MRC分子生物学研究所）
Shigekazu Oda[1], Yu Toyoshima[2], Mario De Bono[3] ([1]*Okazaki Institute for Integrative Science, Division of Quantitative Biology (National Institute for Basic Biology)*, [2]*Department of Biological Sciences, Graduate School of Science, University of Tokyo*, [3]*MRC Laboratory of Molecular Biology*)

09:15　金城 純一　3Pos191
1YK0915　光第二高調波顕微鏡によるタンパク質構造解析
Optical second-harmonic generation microscope as a tool for protein structure analysis
○金城 純一[1], 岡田 康志[1,2], 島 知弘[2], 辻井 美香[3], 今田 勝巳[3], 市村 垂生[1], 渡邉 朋信[1]（[1]理研QBiC, [2]東大・院理, [3]阪大・院理）
Junichi Kaneshiro[1], Yasushi Okada[1,2], Tomohiro Shima[2], Mika Tsujii[3], Katsumi Imada[3], Taro Ichimura[1], Tomonobu M. Watanabe[1] ([1]*RIKEN QBiC*, [2]*Grad. Sch. Sci. Univ. Tokyo*, [3]*Grad. Sch. Sci. Osaka Univ.*)

09:30　小島 慧一　2I1537
1YK0930　暗所視を司る錐体視物質の低い熱雑音の進化的獲得
Evolutionary acquisition of low thermal noise of cone pigments for scotopic vision
○小島 慧一[1,2], 松谷 優樹[2], 柳川 正隆[3], 山下 高廣[2], 今元 泰[2], 久冨 修[4], 山野 由美子[5], 和田 昭盛[5], 七田 芳則[2,6]（[1]岡山大学大学院医歯薬学総合研究科, [2]京都大学大学院理学研究科, [3]理研・細胞情報, [4]大阪大学大学院理学研究科, [5]神戸薬科大学, [6]立命館大学・総研機構）
Keiichi Kojima[1,2], Yuki Matsutani[2], Masataka Yanagawa[3], Takahiro Yamashita[2], Yasushi Imamoto[2], Osamu Hisatomi[4], Yumiko Yamano[5], Akimori Wada[5], Yoshinori Shichida[2,6] ([1]*Grad. Sch. of Med. Dent. Pharm. Sci., Okayama Univ*, [2]*Grad. Sch. Sci., Kyoto Univ.*, [3]*Cell. Info. Lab., RIKEN*, [4]*Grad. Sch. Sci., Osaka Univ.*, [5]*Kobe Pharm. Univ.*, [6]*Ritsumeikan Univ.*)

09:45　近藤 徹　2H1419
1YK0945　単一分子分光で明らかになった光合成光保護機構
Photosynthetic photoprotection mechanism revealed by single-molecule spectroscopy
○近藤 徹[1,2], ピノーラ アルベルタ[3], チェン ウェイジア[1], ダロスト ルカ[3], バッシ ロベルト[3], シュラウコーエン ガブリエラ[1,2]（[1]マサチューセッツ工科大学, [2]Mit-Harvard エキシトン工学センター, [3]ヴェローナ大学）
Toru Kondo[1,2], Alberta Pinnola[3], Wei Jia Chen[1], Luca Dall'Osto[3], Roberto Bassi[3], Gabriela Schlau-Cohen[1,2] ([1]*Mit*, [2]*Mit-Harvard Center for Excitonics*, [3]*Univ. Verona*)

10:00　田代 陽介　1C1408

1YK1000　細菌の膜小胞取り込みに寄与する表面電位と膜弛緩性

Contribution of surface potentials and membrane looseness on bacterial uptake of membrane vesicles

○田代 陽介, 髙木 航太郎, 長谷川 雄将, 二又 裕之（静大院・総合科技）

Yosuke Tashiro, Kotaro Takaki, Yusuke Hasegawa, Hiroyuki Futamata (*Grad. Sch. Intgr. Sci. Technol., Shizuoka Univ.*)

10:15　中根 大介　1B1608

1YK1015　シアノバクテリアは光の向きを認識して IV 型線毛を非対称に分布する

Asymmetric distribution of type IV pili triggered by directional light in unicellular cyanobacteria

○中根 大介, 西坂 崇之（学習院大 物理）

Daisuke Nakane, Takayuki Nishizaka (*Dept. Phys., Gakushuin Univ.*)

10:30　新津 藍　1E1514

1YK1030　再設計法と新規設計法による膜貫通アルファヘリックスペプチドバレルの開発

Redesign and de novo design of transmembrane alpha-helical peptide barrels

○新津 藍[1,2], Mahendran Kozhinjampara[3], Andrew R. Thomson[4], Hagan Beyley[3], 杉田 有治[1], Derek N. Woolfson[2]（[1]理研・和光, [2]ブリストル大学, [3]オックスフォード大学, [4]グラスゴー大学）

Ai Niitsu[1,2], Kozhinjampara R. Mahendran[3], Andrew R. Thomson[4], Hagan Beyley[3], Yuji Sugita[1], Derek N. Woolfson[2] ([1]*Wako Inst, RIKEN*, [2]*Univ. Bristol*, [3]*Univ. Oxford*, [4]*Univ. Glasgow*)

10:45　平島 剛志　2J1355

1YK1045　細胞の異方的なメカノレスポンスが発生過程の精巣上体細管の径を維持する

Anisotropic Cellular Mechanoresponse Maintains the Radial Size of Developing Epididymal Tubules

○平島 剛志[1], 安達 泰治[2]（[1]京都大学大学院医学研究科 基礎病態学講座 病態生物医学分野, [2]京都大学 ウイルス・再生医科学研究所）

Tsuyoshi Hirashima[1], Taiji Adachi[2] ([1]*Grad Sch Med, Kyoto Univ*, [2]*Inst Front Life Med Sci, Kyoto Univ*)

11:00　森 俊文　1G1344

1YK1100　Pin1 の酵素反応におけるタンパク質ダイナミクスの重要性

Crucial role of enzyme dynamics in the catalytic reaction mechanism of Pin1

○森 俊文[1,2], 斉藤 真司[1,2]（[1]分子研, [2]総研大）

Toshifumi Mori[1,2], Shinji Saito[1,2] ([1]*IMS*, [2]*SOKENDAI*)

11:15　森本 雄祐　1Pos091

1YK1115　細胞内シグナル伝達における膜電位の役割

Role of membrane potential in intracellular signal transduction

○森本 雄祐[1,2,3], 上田 昌宏[2,3]（[1]九工大・生命情報, [2]理研・生命システム, [3]阪大・生命機能）

Yusuke V. Morimoto[1,2,3], Masahiro Ueda[2,3] ([1]*Dept. of Biosci. Bioinfo., Kyushu Inst. Tech.*, [2]*RIKEN, QBiC*, [3]*Grad. Sch. Frontier Biosci., Osaka Univ.*)

シンポジウム　Symposium

第 1 日目（9 月 19 日（火））／Day 1（Sep. 19 Tue.）

9:00～11:30　A 会場（全学教育棟 1 階 E107）／Room A (Room E107, General Education Bldg. 1F)

1SAA　「流れ」から解き明かす生き物の時空間パターン：タンパク質から集団運動まで
Ta Panta rhei: Spatiotemporal dynamics of flow-related biological patterns

オーガナイザー：鹿毛 あずさ（東北大学），鳥澤 嵩征（情報通信研究機構）
Organizers: Azusa Kage (Tohoku University), Takayuki Torisawa (NICT)

"Everything flows": this statement by an ancient Greek philosopher now sheds light on a new direction of biophysical studies. In recent years, a wide variety of studies have emerged focusing on the diverse flow-related phenomena in biological systems, the components of which were cytoskeletal proteins, cilia, or cells. In this session, we would like to discuss the growing and interdisciplinary field of flow-related spatiotemporal dynamics ranging from a theory on a single element to an experiment on collective behavior of real cells with the promising young investigators with diverse backgrounds.

1SAA-1　Spatiotemporal dynamics of flow-related biological patterns: Overview
Takayuki Torisawa (*Advanced ICT Inst., NICT*)

1SAA-2　Multiscale dynamics of red blood cells in flow
Stephanie Nix, Yukitaka Ishimoto (*Akita Pref. U.*)

1SAA-3　細胞表層シートを用いた繊毛虫ゾウリムシ繊毛運動の解析
Analysis on the ciliary movements in *Paramecium* using the ciliated cortical sheet
○久冨 理[1,2], 堀 学[3]（[1]富山大・院・理工, [2]山梨大・院・医, [3]山口大・理）
Osamu Kutomi[1,2], Manabu Hori[3] ([1]*Grad. Sch. Sci. and Eng., Univ. Toyama*, [2]*Grad. Sch. Med., Univ. Yamanashi*, [3]*Fac. Sci., Yamaguchi Univ*)

1SAA-4　Emergent collective motion of the unicellular green alga *Chlamydomonas*: 2-body swimming and beyond
Azusa Kage[1], Takayuki Torisawa[2], Ken H. Nagai[3] ([1]*Sch. Eng., Tohoku Univ.*, [2]*Advanced ICT Inst., NICT*, [3]*Sch. Materials Sci., JAIST*)

1SAA-5　遊泳バクテリアで捉える自己駆動粒子の集団運動における普遍性
Universality in collective motion of self-propelled elements captured through swimming bacteria
○西口 大貴[1,2,3], 永井 健[4], Chaté Hugues[1,5], 佐野 雅己[1]（[1]CEA-Saclay, [2]東大理, [3]パスツール研究所, [4]北陸先端大, [5]北京計算科学中心）
Daiki Nishiguchi[1,2,3], Ken H. Nagai[4], Hugues Chate[1,5], Masaki Sano[1] ([1]*CEA-Saclay*, [2]*Dept. of Phys., The Univ. of Tokyo*, [3]*Pasteur Institute*, [4]*JAIST*, [5]*Beijin CSRC*)

1SAA-6　The impact of flow and environmental sensing on bacterial biofilm degradation
Knut Drescher[1, 2] ([1]*Max Planck Institute for Terrestrial Microbiology, 35043 Marburg, Germany*, [2]*Department of Physics, Philipps University Marburg, 35032 Marburg, Germany*)

9:00～11:30　B 会場（全学教育棟 2 階 B201）／Room B (Room B201, General Education Bldg. 2F)

1SBA　金属酵素の反応機構を理解するための多様な生物無機化学的アプローチ
Bioinorganic Approaches for Understanding Reaction Mechanisms of Metalloproteins

オーガナイザー：舩橋 靖博（大阪大学），柳澤 幸子（兵庫県立大学）
Organizers: Yasuhiro Funahashi (Osaka University), Sachiko Yanagisawa (University of Hyogo)

Elucidation of enzymatic reaction mechanisms is one of the most important subjects in biophysics. For understanding the essential mechanistic points, we should find correlation between structures and dynamics in the active site and protein environments, and furthermore, we should know chemical properties of the catalytic center. In this symposium, we focus on iron-containing proteins to understand enzymatic reactions using methods of structural biology, spectroscopy, coordination chemistry, and theoretical calculation. These bioinorganic approaches must lead us to get to the bottom of the biophysical phenomena.

はじめに
Opening Remarks

1SBA-1 ヘムタンパク質の電子論
Electronic Theory of Hemoprotein Chemistry
○山本 泰彦（筑波大・数理物質系化学域）
Yasuhiko Yamamoto (*Department of Chemistry, University of Tsukuba*)

1SBA-2 核共鳴非弾性散乱分光により解き明かす鉄蛋白質活性点の構造化学とダイナミックス
Nuclear resonance vibrational spectroscopic studies of the geometric structure and dynamics of iron-containing biomolecules
○太田 雄大（兵県大・院生命理学）
Takehiro Ohta (*Grad. Sch. Sci., Univ. Hyogo*)

1SBA-3 Mononuclear Nonheme Iron(IV)-Oxo Complexes with Tripodal Ligands in Oxidation Reactions
Mi Sook Seo, Wonwoo Nam (*Ewha Womans University*)

1SBA-4 X 線自由電子レーザーを用いた時間分解結晶構造解析：酵素反応への応用
Time-resolved crystallography using X-ray free electron laser: application to enzymatic reaction
○當舎 武彦（理研SPring-8）
Takehiko Tosha (*RIKEN, SPring-8*)

1SBA-5 QM/MM 計算で解明した鉄含有酵素の反応機構
Reaction mechanisms of iron-containing proteins elucidated using QM/MM calculations
○庄司 光男[1], 山崎 笙太郎[2], 栢沼 愛[1], 重田 育照[1]（[1]筑波大学計算科学研究センター, [2]筑波大学数理物質科学研究科）
Mitsuo Shoji[1], Sotaro Yamasaki[2], Megumi Kayanuma[1], Yasuteru Shigeta[1] ([1]*CCS, Univ. Tsukuba*, [2]*Grad. Sch. Of Pure & App. Sci., Univ. Tsukuba*)

おわりに
Closing Remarks

9:00〜11:30　C 会場（全学教育棟 2 階 B202）／Room C (Room B202, General Education Bldg. 2F)

1SCA　原生生物の行動
Protista behaviors

オーガナイザー：園部 誠司（兵庫県立大学），市川 正敏（京都大学）
Organizers: Seiji Sonobe (University of Hyogo), Masatoshi Ichikawa (Kyoto University)

The organisms belong to Protista have survived through their evolutions in various environments, and their fast growth and diversities make them win the cruel struggle for existence. Furthermore, recent progress has discovered unique behaviors of single cell organisms deeply connected to their life strategy. In this symposium, we will present some interesting topics on the behaviors of protists to discuss on their strange but clever responses to survive.

はじめに
Opening Remarks

1SCA-1 細胞運動における自発的シグナル生成の仕組み
A mechanism of spontaneous signal generation in cell migration
○松岡 里実[1,2], 福島 誠也[1,2], 上田 昌宏[1,2]（[1]理化学研究所生命システム研究センター, [2]大阪大学大学院生命機能研究科）
Satomi Matsuoka[1,2], Seiya Fukushima[1,2], Masahiro Ueda[1,2] ([1]*RIKEN, Quantitative Biology Center (QBiC)*, [2]*Osaka University, Graduate School of Frontier Biosciences*)

1SCA-2 連続光照射時のオオアメーバの運動
Behavior of *Amoeba proteus* on constant photo-irradiation
○西上 幸範（京都大学大学院理学研究科物理学）
Yukinori Nishigami (*Department of Physics, Graduate School of Science, Kyoto University*)

1SCA-3 繊毛虫の学習能力の再考
Rethinking the learning capacity of ciliates
○國田 樹（琉球大学工学部）
Itsuki Kunita (*University of The Ryukyus*)

1SCA-4 ロクロクビムシのプロボーシスの伸縮運動
Extension and Contraction of the Proboscis of a Ciliate, *Lacrymaria olor*
○梁瀬 隆二（兵県大・院生命理学）
Ryuji Yanase (*Grad. Sch. Sci., Univ. Hyogo*)

1SCA-5 壁面付近における繊毛虫の遊泳運動
Swimming behavior of a ciliate near a wall
○大村 拓也, 市川 正敏（京都大学大学院理学研究科）
Takuya Ohmura, Masatoshi Ichikawa (*Grad. Sch. of Sci, Kyoto Univ.*)

1SCA-6 ラビリンチュラ類の外質ネットによる栄養摂取
Nutrition of thraustochytrids (Labyrinthulea) by their ectoplasmic nets
○本多 大輔[1], 浜本 洋子[2], 岩田 いづみ[2]（[1]甲南大学　理工学部, [2]甲南大学　自然科学研究科）
Daiske Honda[1], Yoko Hamamoto[2], Izumi Iwata[2] ([1]*Faculty of Science and Engineering, Konan University*, [2]*Graduate School of Natural Science, Konan University*)

おわりに
Closing Remarks

9:00～11:30　D 会場（全学教育棟 2 階 E201）／Room D (Room E201, General Education Bldg. 2F)

1SDA　溶液中における蛋白質ダイナミクス解析
Analysis of Protein Dynamics in Solution

オーガナイザー：小川 覚之（東京大学），有坂 文雄（東京工業大学）
Organizers: Tadayuki Ogawa (The University of Tokyo), Fumio Arisaka (Tokyo Institute of Technology)

Accurate description of protein behavior in solution is required in various fields such as biophysics, structural biology, and antibody drugs. This symposium focuses on the protein analysis in solution by using multiple independent methods; liquid chromatography, dynamic light scattering, small angle X-ray scattering, analytical ultracentrifuge, calorimetry, and atomic force microscope. Fusion and integration of multiple methods will foster our deeper understanding of the protein dynamics in solution.

1SDA-1 高速原子間力顕微鏡を用いた回転軸の無い腸内連鎖球菌由来 V_1-ATPase の回転運動の解析
Analysis of Rotational Dynamics of Rotorless *Enterococcus hirae* V_1-ATPase using High-Speed Atomic Force Microscopy
○今村 元紀[1], 中本 和哉[2], 丸山 慎太郎[2], 河合 文啓[3], 飯野 亮太[3], 内橋 貴之[4], 村田 武士[2], 安藤 敏夫[1]（[1]金沢大・バイオ AFM FRC, [2]千葉大・院理, [3]岡崎統合バイオ/分子研, [4]名古屋大・院理）
Motonori Imamura[1], Kazuya Nakamoto[2], Shintaro Maruyama[2], Fumihiro Kawai[3], Ryota Iino[3], Takayuki Uchihashi[4], Takeshi Murata[2], Toshio Ando[1] ([1]*Bio-AFM FRC, Kanazawa Univ.*, [2]*Grad. Sch. Sci., Chiba Univ.*, [3]*Okazaki Inst. Integ. Biosci., IMS, NINS*, [4]*Grad Sch. Sci., Nagoya Univ.*)

1SDA-2 超遠心分析によるバイオおよびナノ粒子の溶液挙動の解析
Solution behavior of bio- and nano-particles as analyzed by analytical ultracentrifugation
○有坂 文雄（東京工業大学）
Fumio Arisaka (*Tokyo Institute of Technolgy*)

1SDA-3 Elucidation of structural dynamics of protein with binding to drugs based on kinetic and thermodynamic analysis
Satoru Nagatoishi[1,2], Kouhei Tsumoto[1,2] ([1]*The Institute of Medical Science, The University of Tokyo*, [2]*School of Engineering, The University of Tokyo*)

1SDA-4 SEC-SAXS によるタンパク質複合体の溶液構造解析
Solution structure analysis of the protein complex using SEC-SAXS
○清水 伸隆（高エネ機構・物構研・放射光）
Nobutaka Shimizu (*PF, IMSS, KEK*)

1SDA-5 高温における可逆的かつ迅速な蛋白質非天然状態の会合体形成
Reversible and rapid oligomerization of non-native proteins at high temperature
○城所 俊一（長岡技科大・生物機能）
Shun-ichi Kidokoro (*Dept. Bioeng., Nagaoka Univ. Tech.*)

1SDA-6 ピロリ菌 CagA がんタンパク質の構造多型が極性制御因子 PAR1 b 結合に及ぼす影響
Impact of structural polymorphism of the H. pylori CagA oncoprotein on binding to polarity regulating kinase PAR1b
○西川 裕子[1], 林 剛留[1], 有坂 文雄[2], 千田 俊哉[3], 畠山 昌則[1]（[1]東大・院医, [2]日大・生物, [3]物構研・高エネ研）
Hiroko Nishikawa[1], Takeru Hayashi[1], Fumio Arisaka[2], Toshiya Senda[3], Masanori Hatakeyama[1] ([1]*Grad. Sch. Med., Univ. Tokyo*, [2]*Coll. Biores. Sci., Nihon Univ.*, [3]*Inst. of Mater. Struct. Sci., KEK*)

1SDA-7 Solution-based Analyses on Microtubule Depolymerization via Depolymerizing Machine
Tadayuki Ogawa[1], Shinya Saijo[2], Nobutaka Shimizu[2], Xuguang Jiang[1], Nobutaka Hirokawa[1] ([1]*Univ. Tokyo*, [2]*KEK-PF*)

9:00〜11:30　F 会場（全学教育棟 2 階 E205）／Room F (Room E205, General Education Bldg. 2F)

1SFA　いろんなスケールで働く膜タンパク質の作動原理：実験と理論の新展開
Operating principles of membrane proteins at multiscale resolutions

オーガナイザー：岡崎 圭一（分子科学研究所），渡邉 力也（東京大学）
Organizers: Kei-ichi Okazaki (IMS), Rikiya Watanabe (The University of Tokyo)

Recent developments of both experiment and theory enable us to clarify operating principles of membrane proteins such as channel, transporter and motor. These membrane proteins show diverse functions and work at multiscale resolutions. In this symposium, we cover state-of-the-art experimental and theoretical techniques from time resolved, single-molecule experiments to quantum chemical calculation, coarse-grained and atomistic MD simulations. We aim to clarify mechanisms from a complementary approach of experiment and theory.

1SFA-1 脂質二重膜がカリウムチャネル開閉に及ぼす多様な影響
Specific and non-specific actions of membrane lipids on the gating of the potassium channel
○岩本 真幸, 老木 成稔（福井・医・分子生理）
Masayuki Iwamoto, Shigetoshi Oiki (*Dept. Mol. Physiol. & Biophys., Univ. Fukui Facult. Med. Sci.*)

1SFA-2 遷移パスシミュレーションによる Na^+/H^+ antiporter の輸送メカニズム
Transport mechanism of Na^+/H^+ antiporter from transition-path simulations
○岡崎 圭一[1], Hummer Gerhard[2]（[1]分子研, [2]MPI of Biophysics）
Kei-ichi Okazaki[1], Gerhard Hummer[2] ([1]*IMS*, [2]*MPI of Biophysics*)

1SFA-3 高速原子間力顕微鏡によるナノディスクに埋め込まれた膜タンパク質のダイナミクス観察
High-speed AFM imaging of membrane proteins in lipid nanodiscs
○柴田 幹大（金沢大・新学術創成）
Mikihiro Shibata (*InFiniti, Kanazawa Univ.*)

1SFA-4 X 線自由電子レーザーで捉えたバクテリオロドプシン構造変化の三次元動画
A three-dimensional movie of structural changes in bacteriorhodopsin captured by X-ray free electron lasers
○南後 恵理子[1,2], 岩田 想[1,2]（[1]理研 放射光セ, [2]京大医）
Eriko Nango[1,2], So Iwata[1,2] ([1]*RSC*, [2]*Kyoto Univ. Med.*)

1SFA-5 分子シミュレーションで探る膜輸送体・受容体の分子機能
Atomistically deciphering functional processes of membrane transporter and receptor with molecular simulations
○林 重彦（京都大学大学院理学研究科化学専攻）
Shigehiko Hayashi (*Dept. of Chem., Grad. Sch. of Science, Kyoto Univ.*)

1SFA-6 バナナ状たんぱく質の集合による膜チューブ形成
Membrane tubulation induced by assembly of banana-shaped protein rods
○野口 博司（東大物性研）
Hiroshi Noguchi (*ISSP, Univ. Tokyo*)

9:00～11:30　G 会場（全学教育棟 3 階 C301）／Room G (Room C301, General Education Bldg. 3F)

1SGA　ポスト「京」重点課題 1 生体分子システムの機能制御による革新的創薬基盤の構築 共催 ハイパフォーマンス・コンピューティング(HPC)による次世代創薬計算技術
Next-generation in-silico drug discovery using high-performance computing

オーガナイザー：荒木 望嗣（京都大学），池口 満徳（横浜市立大学）
Organizers: Mitsugu Araki (Kyoto University), Mitsunori Ikeguchi (Yokohama City University)

Utilization of high performance computing (HPC) in the medical field is accelerating from the K computer to post K computer. Fundamental molecular-simulation techniques previously developed in the field of biophysics are now practically applied to the drug development process. In this symposium, next-generation in-silico drug discovery involving experimental collaboration and machine learning will be discussed with young researchers in "Priority issue 1 on Post-K computer" (Building Innovative Drug Discovery Infrastructure Through Functional Control of Biomolecular Systems).

1SGA-1 Development of GENESIS for high performance computing of biomolecular simulations
Jaewoon Jung[1,2], Chigusa Kobayashi[1], Yuji Sugita[1,2,3] ([1]*RIKEN AICS*, [2]*RIKEN TMS*, [3]*RIKEN QBiC*)

1SGA-2 エネルギー表示溶液理論を用いた蛋白質－蛋白質複合体構造予測
Protein-protein complex structure prediction using the solution theory in the energy representation
○竹村 和浩[1], 松林 伸幸[2], 北尾 彰朗[1]（[1]東大・分生研, [2]阪大・基礎工）
Kazuhiro Takemura[1], Nobuyuki Matubayasi[2], Akio Kitao[1] ([1]*IMCB, Univ. of Tokyo*, [2]*Grad. Sch. Eng. Sci, Osaka Univ.*)

1SGA-3 分子動力学シミュレーションと小角 X 線散乱実験を組み合わせた蛋白質の動的構造変化の解析
Protein dynamics revealed by a combination analysis of molecular dynamics simulations and small-angle x-ray scattering experiments
○浴本 亨, 池口 満徳（横浜市大）
Toru Ekimoto, Mitsunori Ikeguchi (*Yokohama City Univ.*)

1SGA-4 Molecular dynamics simulations for the study of thermodynamic properties in streptavidin mutant-biotin analog systems
Keiko Shinoda, Hideaki Fujitani (*RCAST, The Univ. Of Tokyo*)

1SGA-5 創薬ビッグデータ統合システムの開発とゲノム医療への応用
Development of Next-generation computational infrastructure for drug discovery and practical application to genomic medicine
○荒木 望嗣[1,2], 奥野 恭史[1]（[1]京都大・院医, [2]理研・AICS）
Mitsugu Araki[1,2], Yasushi Okuno[1] ([1]*Grad. Sch. Med., Kyoto Univ.*, [2]*RIKEN, AICS*)

1SGA-6 機械学習による MD 計算に基づく結合ポーズ推定の高速化
Acceleration of MD-based Binding-Pose Prediction with Ligands and Proteins by Machine Learning
○寺山 慧[1], 岩田 浩明[2], 荒木 望嗣[4], 奥野 恭史[3,4], 津田 宏治[1,5,6]（[1]東大・新領域, [2]先端医療振興財団, [3]京大・医, [4]理研・計算科学研究機構, [5]理研・革新知能統合研究センター, [6]物質・材料研究機構）
Kei Terayama[1], Hiroaki Iwata[2], Mitsugu Araki[4], Yasushi Okuno[3,4], Koji Tsuda[1,5,6] ([1]*Grad. Sch. Frontier Sci., Univ. Tokyo*, [2]*Found. for Biomedical Researcha and Innovation*, [3]*Grad. Sch. Med., Kyoto Univ.*, [4]*AICS, RIKEN*, [5]*AIP, RIKEN*, [6]*Center for Material Research By Info. Integration, NIMS*)

9:00〜11:30　I 会場（全学教育棟 3 階 E305）／Room I (Room E305, General Education Bldg. 3F)

1SIA　ナノ計測技術とバイオイメージングの融合が開く単一細胞計測の新展開
Advanced single cell analysis by fusion of nano-characterization technology and bioimaing

オーガナイザー：高橋 康史（金沢大学），樫田 啓（名古屋大学）
Organizers: Yasufumi Takahashi (Kanazawa University), Hiromu Kashida (Nagoya University)

A combination of diverse interdisciplinary approaches in nanotechnology, engineering, chemistry, optics, chemical biology starts providing a new technologies for single-cell analysis. The symposium will focus on such newly developed single-cell analysis techniques, of which recent progresses will be presented by several young scientists in this field.

1SIA-1　DNA を利用した色素間エネルギー移動の詳細な解析
Analysis of energy transfer between dyes by using DNA scaffold
○樫田 啓[1,2]（[1]名大・院工, [2]JSTさきがけ）
Hiromu Kashida[1,2] ([1]*Grad. Sch. Eng., Nagoya Univ.*, [2]*PRESTO, JST*)

1SIA-2　生きた脳で RNA の観測ができたら
in vivo RNA labelling reveals dynamic regulation of ribonucleic foci in living neurons
大本 育実[1], 梅嶋 宏樹[1], 原田 慶恵[1], 韓 Yong-Woon[1], 岡本 晃充[2], ○王 丹[1]（[1]京大iCeMS, [2]東大先端研）
Ikumi Oomoto[1], Hiroki Umeshima[1], Yoshie Harada[1], Yong-Woon Han[1], Akimitsu Okamoto[2], **Ohtan Wang**[1] ([1]*Kyoto University, iCeMS*, [2]*Research Center for Advanced Science and Technology, University of Tokyo*)

1SIA-3　CUBIC: 細胞・細胞回路の網羅的解析を目的としたセロミクスパイプライン
CUBIC: a Cell-omics pipeline for comprehensive cell and cell circuit analysis
○洲崎 悦生[1,2,3]（[1]東大医・システムズ薬理学, [2]さきがけ・JST, [3]理研・QBiC・合成生物学）
Etsuo A. Susaki[1,2,3] ([1]*Dept. Syst. Pharmacol., UTokyo Grad. Sch. Med.*, [2]*PRESTO, JST*, [3]*Lab. Synthetic Biol., RIKEN QBiC*)

1SIA-4　細胞内カルシウムシグナル解読への新しいアプローチ
A new approach to decoding of Ca^{2+} signals in a single cell
○坂内 博子[1,2], 丹羽 史尋[3], 櫻木 繁雄[4], 御子柴 克彦[2] ([1]JSTさきがけ, [2]理化学研究所 BSI, [3]パリ高等師範学校, [4]東北大・院生命科学）
Hiroko Bannai[1,2], Fumihiro Niwa[3], Shigeo Sakuragi[4], Katsuhiko Mikoshiba[2] ([1]*JST PRESTO*, [2]*RIKEN BSI*, [3]*IBENS*, [4]*Tohoku Univ, Grad. Sch. Life Sci.*)

1SIA-5　アクチン線維が負の張力センサーとして働く仕組みを分子イメージングから解明する試み
Analysis of fluctuations of a single actin filament that works as a tension sensor
○辰巳 仁史（金沢工業大学・バイオ・化学部・応用バイオ学科）
Hitoshi Tatsumi (*Department of Applied Bioscience, Kanazawa Institute of Technology (KIT)*)

1SIA-6　ゴーストサイトメトリー
Ghost Cytometry
○太田 禎生[1, 2]（[1] 東京大学大学院工学系研究科応用化学専攻, [2]科学技術振興機構さきがけ）
Sadao Ota[1, 2] ([1]*Applied Chemistry Department, University of Tokyo*, [2]*JST, PRESTO*)

9:00〜11:30　L 会場（文法学部 2 階 B1 教室）／Room L (Room B1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

1SLA　実験と理論計算で明らかになってきた細胞環境での蛋白質間相互作用
Experimental and Computational Analysis on Protein-Protein Interaction in Cellular Environments

オーガナイザー：杉田 有治（理化学研究所），津本 浩平（東京大学）
Organizers: Yuji Sugita (RIKEN), Kohei Tsumoto (The University of Tokyo)

Understanding of protein-protein interactions in cellular environments is one of the essential research issues in biophysics. To understand them, not only X-ray structures of macromolecules but also various experimental and computational methods are necessary. In particular, recent advance of computer simulations allows us to simulate multiple proteins, nucleic acids, and metabolites simultaneously. We discuss about how to combine those computational studies with experimental measurements.

1SLA-1　Specific and non-specific protein-protein interactions in cellular environments
Yuji Sugita (*RIKEN*)

1SLA-2　Atomistic modeling of protein liquid-liquid phase separation
Sanbo Qin, **Huan-Xiang Zhou** (*Florida State University*)

1SLA-3　Nonspecific protein-protein interactions in dense protein solutions and near membranes
Michael Feig[1,2] ([1]*MSU*, [2]*QBiC*)

休憩
Break

1SLA-4　網羅的変異解析による VemP 翻訳伸長停止モチーフの同定と解析
Identification and characterization of a translation arrest motif in VemP by systematic mutational analysis
○森 博幸, 坂下 宗平, 伊藤 淳, 石井 英治, 秋山 芳展（京大 ウイルス・再生研）
Hiroyuki Mori, Sohei Sakashita, Jun Ito, Eiji Ishii, Yoshinori Akiyama (*Inst. Front. Life Med. Sci., Kyoto Univ.*)

1SLA-5　細胞内での一酸化窒素の動態
NO Dynamics in Cellular System
○城 宜嗣（兵庫県立大大学院生命理学研究科）
Yoshitsugu Shiro (*Univ. Hyogo*)

9:00〜11:30　M 会場（文法学部 1 階 B2 教室）／Room M (Room B2, Faculty of Letters, Faculty of Law Main Bldg. 1F)

1SMA　CREST「構造生命」/さきがけ「構造生命科学」領域 共催
構造生命科学の新しい潮流
New trends for Structural Life Science

オーガナイザー：清水 敏之（東京大学），栗栖 源嗣（大阪大学）
Organizers: Toshiyuki Shimizu (The University of Tokyo), Genji Kurisu (Osaka University)

“Structural life science” aims to integrate cutting-edge life science areas with structural biology for innovation in life science. Structural research of proteins, which play key roles in biological events, have provided a remarkable achievement so far, and the next important step is to determine the dynamics of such proteins and to study the functional mechanisms. In this symposium, the up-and-coming researchers will give presentation using various methods targeting membrane proteins.

はじめに
Opening Remarks
Toshiyuki Shimizu

1SMA-1 Ｖ１モーターの構造形成の分子機構
Molecular mechanism of the structural formation of V1 rotary motor
○村田 武士[1,2]（[1]千葉大・理学, [2]JST・さきがけ）
Takeshi Murata[1,2] ([1]*Grad. Sch. Sci., Chiba Univ.*, [2]*PRESTO, JST*)

1SMA-2 蛋白質膜透過駆動モーター SecDF
Protein Translocation Motor SecDF
○塚崎 智也[1], 古川 新[1], 吉海江 国仁[1], 森 貴治[2], 森 博幸[3], 森本 雄祐[4], 菅野 泰功[1], 岩木 薫大[1], 南野 徹[5], 杉田 有治[2], 田中 良樹[1]（[1]奈良先端大・バイオ, [2]理研, [3]京大・ウイルス・再生医科学研, [4]九工大・情報工学, [5]阪大・生命機能）
Tomoya Tsukazaki[1], Arata Furukawa[1], Kunihito Yoshikaie[1], Takaharu Mori[2], Hiroyuki Mori[3], Yusuke V. Morimoto[4], Yasunori Sugano[1], Shigehiro Iwaki[1], Tohru Minamino[5], Yuji Sugita[2], Yoshiki Tanaka[1] ([1]*Grad. Sch. of Biol. Sci., NAIST*, [2]*RIKEN*, [3]*Inst. for Front. Life and Med. Sci., Kyoto Univ.*, [4]*Grad. Sch. of Comp. Sci. and Sys. Eng., Kyushu Inst. of Tech.*, [5]*Grad. Sch. of Front. Biosci., Osaka Univ.*)

1SMA-3 Functional dynamics of membrane proteins revealed by NMR
Takumi Ueda, Ichio Shimada (*Grad. Sch. Pharm. Sci. The Univ. of Tokyo*)

1SMA-4 Combining XFEL crystallography and single-crystal spectroscopy for studying reaction dynamics of respiratory metalloenzymes
Minoru Kubo (*RIKEN SPring-8 Center*)

1SMA-5 Structural basis of muscle force generation and regulatory mechanism by CryoEM
Takashi Fujii (*RIKEN, QBiC*)

おわりに
Closing Remarks
Genji Kurisu

9:00～11:30　N 会場（文法学部 1 階 B3 教室）／Room N (Room B3, Faculty of Letters, Faculty of Law Main Bldg. 1F)

1SNA　新学術領域研究「3D 活性サイト科学」共催
生体分子活性サイトの構造機能相関解明への新規アプローチ
Novel approaches to elucidating the structure-function relationship of the active sites in biomolecular systems

オーガナイザー：佐藤 文菜（自治医科大学），木村 哲就（神戸大学）
Organizers: Ayana Sato-Tomita (Jichi Medical University), Tetsunari Kimura (Kobe University)

Subtle changes in the active-site structures and/or the electronic states of biomolecules, such as proteins, are key dynamics to perform their functions with high-selectivity and high-efficiency, besides conformational changes in the macroscopic scale. In this symposium, we introduce a number of state-of-the-art approaches that can characterize the active-sites in bimolecular systems with high spatial and temporal resolution, namely, X-ray fluorescence holography, time-resolved or damage-free XFEL crystallography, diffracted X-ray tracking, time-resolved spectroscopy, ENDOR, and computer simulation, and discuss their structure-dynamics-function relationships.

はじめに
Opening Remarks
Ayana Sato-Tomita

1SNA-1 蛍光 X 線ホログラフィーによるヘムタンパク質の金属周辺構造観測
First X-ray fluorescence holographic imaging of iron environments in heme proteins
○佐藤 文菜[1], 柴山 修哉[1], 八方 直久[2], 林 好一[3], 佐々木 裕次[4]（[1]自治医大・生物物理, [2]広島市大・情報科学, [3]名工大・物理工学, [4]東大・新領域）
Ayana Sato-Tomita[1], Naoya Shibayama[1], Naohisa Happo[2], Kouichi Hayashi[3], Yuji Sasaki[4] ([1]*Div. Biophys., Jichi. Med. Univ.*, [2]*Grad. Sch. Info. Sci., Hiroshima City Univ.*, [3]*Dep. Phys. Sci. Eng., NITech*, [4]*Grad. Sch. Frontier Sci., Univ. Tokyo*)

1SNA-2 High resolution and time-resolved X-ray crystallographic study on enzymatic reaction of human MTH1
Teruya Nakamura[1,2], Shaimaa Waz[2], Keisuke Hirata[2], Mami Chirifu[2], Shinji Ikemizu[2], Yuriko Yamagata[2] ([1]*Priority Organization for Innovation and Excellence, Kumamoto Univ.*, [2]*Grad. Sch. of Pharmaceut. Sci., Kumamoto Univ.*)

1SNA-3 時間分解分光法による ABC トランスポーターの輸送と ATP 加水分解過程の直接観察
Direct observation of allocate-transport and ATP-hydrolysis for the ABC transport by time-resolved spectroscopy
○木村 哲就[1,2], 林 沙英[1], 城 宜嗣[3], 杉本 宏[4], 池本 夕佳[5]（[1]神戸大・院理, [2]K-CONNEX, [3]兵県大・院生命理, [4]理研・SPring-8, [5]JASRI）
Tetsunari Kimura[1,2], Sae Hayashi[1], Yoshitsugu Shiro[3], Hiroshi Sugimoto[4], Yuka Ikemoto[5] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*K-CONNEX*, [3]*Grad. Sch. Life Sci., Univ. of Hyogo*, [4]*SPring-8, RIKEN*, [5]*JASRI*)

1SNA-4 生物学的プロトントンネリング機構解明へ～新規 ENDOR 解析法によるタンパク質構造精密解析～
Substrate Positioning of Soybean Lipoxygenase For H-Atom Abstraction by ENDOR 'Crystallography'
○堀谷 正樹（佐大・農）
Masaki Horitani (*Saga Univ., Dept of Appl Biochem & Food Sci*)

1SNA-5 生自然殺害細胞内 X 線 1 分子計測
X-ray single molecular observations in living Natural killer cells
○張 宰源[1,3], 倉持 昌弘[1,3], 一柳 光平[2], 佐々木 裕次[1,3]（[1]東京大学 新領域創成科学研究科, [2]高エネルギー加速器研究機構, [3]産総研-東大 先端オペランド計測技術オープンイノベーションラボラトリ）
Jae-Won Chang[1,3], Masahiro Kuramochi[1,3], Kouhei Ichiyanagi[2], Yuji Sasaki[1,3] ([1]*Graduate School of Frontier Science, The University of Tokyo*, [2]*KEK*, [3]*OPERANDO-OIL*)

1SNA-6 SACLA と SPring-8 により可視化された亜硝酸還元酵素のレドックス依存的な構造変化
Redox-dependent structural change in nitrite reductase visualized by SPring-8 and SACLA
○溝端 栄一（大阪大・院工）
Eiichi Mizohata (*Grad. Sch. Eng., Osaka Univ.*)

1SNA-7 Energetics of proton transfer in proteins
Hiroshi Ishikita (*The University of Tokyo, RCAST*)

おわりに
Closing Remarks
Tetsunari Kimura

13:20～15:50　A 会場（全学教育棟 1 階 E107）／Room A (Room E107, General Education Bldg. 1F)

1SAP　新学術領域研究「生命分子システムにおける動的秩序形成と高次機能発現」共催
秩序が作る動きと動きが作る秩序
Dynamical ordering of biomolecular systems for creation of integrated functions: Dynamics Made of Ordering and Ordering Made from Dynamics

オーガナイザー：秋山 良（九州大学），佐藤 啓文（京都大学）
Organizers: Ryo Akiyama (Kyushu Univeristy), Hirofumi Sato (Kyoto University)

Dynamic ordering should have two aspects. First one is dynamics made of ordering. An ordered structure is constructed from molecules, and the dynamical structural change occurs due to some non-equilibrium phenomena such as chemical reactions. Second one is ordering made from dynamics. Dynamical motions cause effective attractions between units in a system and the attractions construct ordering structures. Both aspects have common frameworks like van der Waals picture on gas-liquid transition. This symposium aims for mutual development in both.

はじめに
Opening Remarks

1SAP-1 時間発展する超分子集合体
Time-dependent evolution of a metastable supramolecular assembly
○杉安 和憲（物材機構）
Kazunori Sugiyasu (*NIMS*)

1SAP-2 分子の集合・離脱が駆動する神経軸索ガイダンスの分子メカニクス
Molecular Mechanics for Axon Navigation in the Brain
○稲垣 直之（奈良先端大・バイオ）
Naoyuki Inagaki (*Nara Inst Sci Technol*)

1SAP-3 How can we control swarming of self-propeled biomolecular motors
Akira Kakugo[1,2], Jakia Jannat Keya[1], Arif Md. Rashedul Kabir[2] ([1]*Graduate School of Chemical Sciences and Engineering, Hokkaido University*, [2]*Faculty of Science, Hokkaido University*)

1SAP-4 アクトミオシン細胞骨格におけるモーター誘起応力の理論
Theory on motor-induced stress in an isotropic actin-myosin network
○平岩 徹也（東京大学理学系研究科）
Tetsuya Hiraiwa (*Department of Physics, The University of Tokyo*)

1SAP-5 ロタキサン連結高分子系超分子における組織化制御
Dynamical Ordering of Supramolecular Architecture Comprising Rotaxane-Linked Polymers
○高田 十志和（東工大・物質理工）
Toshikazu Takata (*Dept. of Chem. Sci. and Eng., Tokyo Inst. of Tech.*)

1SAP-6 基板上で自発的に運動・増殖する細胞のためのミニマル粒子モデル
A particle-based minimal model for crawling and proliferating cells on substrate
○山本 量一[1], シュニーダー サイモン[2], モリーナ ジョン[1] ([1]京都大学大学院工学研究科 化学工学専攻, [2]京都大学 福井謙一記念研究センター）
Ryoichi Yamamoto[1], Simon Schnyder[2], John J. Molina[1] ([1]*Department of Chemical Engineering, Kyoto University*, [2]*Fukui Institute for Fundamental Chemistry, Kyoto University*)

13:20～15:50　K 会場（文法学部 2 階 A1 教室）／Room K (Room A1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

1SKP　Membrane Molecular Bioenergetics の新地平：光子から超複合体まで
Frontiers in Membrane Molecular Bioenergetics: from photon to supercomplex

オーガナイザー：ゲーレ クリストフ（大阪大学），阿部 一啓（名古屋大学）
Organizers: Christoph Gerle (Osaka University), Kazuhiro Abe (Nagoya University)

Recent methodological breakthroughs in single particle cryo-EM, free electron X-ray laser crystallography, in vitro mimetic membrane syststems and theoretical approaches are rapidly reshaping our view of molecular bioenergetics. In this symposium young researchers at the very forefront of structural, functional and theoretical investigation of membrane bioenergetics will present their latest discoveries. Various fields of bioenergetics will be covered ranging from the photosynthetics light reactions over electron transport chain mediated proton motive force generation and up to the synthesis of ATP by rotary ATP synthases.

1SKP-1 光化学系 I-フェレドキシン電子伝達複合体の X 線構造および NMR 解析
X-ray structure and NMR analysis of the electron transfer complex between Photosystem I and Ferredoxin
○田中 秀明[1,2], 河合 寿子[1], 武藤 梨沙[1], ピエール セティフ[3], ノヴァチク マーク[4], レグナー マティアス[4], 池上 貴久[5], 栗栖 源嗣[1,2]（[1]大阪大学蛋白質研究所, [2]JST-CREST, [3]CEA Saclay, [4]Ruhr-University Bochum, [5]横市大・生命医科学）
Hideaki Tanaka[1,2], Hisako Kawai[1], Risa Mutton[1], Setif Pierre[3], Marc Nowaczyk[4], Matthias Rogner[4], Takahisa Ikegami[5], Genji Kurisu[1,2] ([1]*IPR, Osaka Univ.*, [2]*JST-CREST*, [3]*CEA Saclay*, [4]*Ruhr-University Bochum*, [5]*Grad. Sch. of Medical Life Science, Yokohama City Univ.*)

1SKP-2 分子構造に基づく理論解析による光合成膜蛋白質における反応機構の解明
Theoretical investigation based on molecular structures reveals reaction mechanisms in photosynthetic membrane proteins
○斉藤 圭亮（東京大学 先端科学技術研究センター）
Keisuke Saito (*RCAST, The University of Tokyo*)

1SKP-3 The Regulatory Functions and movements of quinones: It's Insane in the Membrane!
Duncan McMillan[1], Yoshio Nakatani[2], Lars Jeuken[3], Julia Butt[4], Gregory Cook[2], Hiroyuki Noji[5] ([1]*Department of Biotechnology, Delft University of Technology*, [2]*Department of Microbiology and Immunology, University of Otago*, [3]*School of Biomedical Sciences, University of Leeds*, [4]*School of Chemistry, and School of Biological Sciences, University of East Anglia*, [5]*Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo*)

1SKP-4 X 線自由電子レーザーを用いた、チトクロム酸化酵素からの一酸化炭素解離に伴う構造変化の時分割結晶構造解析
A nanosecond time-resolved XFEL analysis of structural changes associated with CO release from Cytochrome *c* Oxidase
○島田 敦広[1], 久保 稔[2], 馬場 清喜[3], 吾郷 日出夫[2], 月原 冨武[4], 吉川 信也[5]（[1]岐阜大 応生, [2]理研 SPring-8, [3]高輝度研, [4]阪大 蛋白研, [5]兵県大 ピコ研）
Atsuhiro Shimada[1], Minoru Kubo[2], Seiki Baba[3], Hideo Ago[2], Tomitake Tsukihara[4], Shinya Yoshikawa[5] ([1]*Fac. Appl. Biol. Sci., Gifu Univ.*, [2]*RIKEN, SPring-8 Center*, [3]*JASRI*, [4]*Inst. for Protein Res., Osaka Univ.*, [5]*Picobiol. Inst., Univ. Hyogo*)

1SKP-5 好熱菌由来 V 型 ATP 合成酵素の単粒子解析
Single-particle analysis of V-type ATPase/synthase from *Thermus thermophilus* by cryo-EM
○中西 温子[1], 岸川 淳一[1], 光岡 薫[2], 横山 謙[1]（[1]京産大・総生・生命システム, [2]阪大・超高圧電顕センター）
Atsuko Nakanishi[1], Jun-ichi Kishikawa[1], Kaoru Mitsuoka[2], Ken Yokoyama[1] ([1]*Dept. of Life Sci. Kyoto Sangyo Univ.*, [2]*Res. Ctr. UVHEM. Univ. Osaka*)

1SKP-6 Cryo-EM structures of the autoinhibited E. coli ATP synthase in three rotational states
Meghna Sobti[1], Callum Smits[1], Andrew Wong[2], Robert Ishmukhametov[3], Daniela Stock[1,4], Sara Sandin[2], **Alastair Stewart**[1,4]
([1]*VCCRI, Sydney, Australia*, [2]*SBS, NTU, Singapore*, [3]*Physics, University of Oxford, UK*, [4]*Medicine, UNSW, Australia*)

13:20〜15:50　L 会場（文法学部 2 階 B1 教室）／Room L (Room B1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

1SLP　環境効果の分子レベル解析に基づくタンパク質の構造・機能チューニング
Molecular-Level Analysis of Environment Effect toward Tuning of Protein Structure and Function

オーガナイザー：松林 伸幸（大阪大学），吉村 成弘（京都大学）
Organizers: Nobuyuki Matubayasi (Osaka University), Shige H. Yoshimura (Kyoto University)

In a living cell, proteins are folded, interact, and function in a multi-component environment. This implies that the structure and function of protein could be modulated by changing its surroundings. The present symposium focuses on understanding how protein structure and function are affected by its environments, with recent topics from solution chemistry, structural biology, protein engineering, and cell biology. The technical application of such environment-based protein tuning, which is distinct from genetic engineering, will also be discussed.

1SLP-1 タンパク質構造・配置に対する混合溶媒効果の全原子自由エネルギー計算による解析
Mixed-solvent effect on protein configuration studied by all-atom computation of free energy
○松林 伸幸（大阪大学 大学院基礎工学研究科 化学工学領域）
Nobuyuki Matubayasi (*Division of Chemical Engineering, Grad Sch Eng Sci, Osaka Univ*)

1SLP-2 好アルカリ性細菌の高アルカリ性環境適応に関与するメゾレベルでの場としての細胞表層酸性高分子役割の解明
Elucidation of the role of cell surface acidic polymers as a place at meso level from alkaliphilic bacteria
○伊藤 政博（東洋大 生命科）
Masahiro Ito (*Faculty of Life Sciences, Toyo Univ.*)

1SLP-3 リン脂質二重膜の構造変化に伴う水和状態の変化：テラヘルツ分光法による研究から
Changes in the hydration states of phospholipid bilayers accompanying bilayer structural changes: From the studies by THz spectroscopy
○菱田 真史（筑波大・数物）
Mafumi Hishida (*Dept. Chem., Univ. Tsukuba*)

1SLP-4 蛋白質―脂質相互作用と小孔形成毒素
Protein-lipid interactions in a pore-forming toxin
○津本 浩平[1], カアベイロ ホセ[2]（[1]東大・院工，医科研, [2]九大・薬学）
Kouhei Tsumoto[1], Jose Caaveiro[2] ([1]*Grad. Sch. Eng. and Inst. Med. Sci., Univ. Tokyo*, [2]*Grad. Sch. Pharm., Kyushu Univ.*)

1SLP-5 タンパク質構造への分子環境の効果：抗原抗体界面の分子動力学計算による研究
Molecular environment effects on the protein structure: Molecular dynamics studies on the antigen-antibody interface
○山下 雄史（東大先端研）
Takefumi Yamashita (*RCAST, Univ. Tokyo*)

1SLP-6 NMR analysis of proteins in living cells
Hidehito Tochio (*Dept. Biophys., Grad. Schl. Sci., Kyoto Univ.*)

13:20〜15:50　M 会場（文法学部 1 階 B2 教室）／Room M (Room B2, Faculty of Letters, Faculty of Law Main Bldg. 1F)

1SMP　刺激に応答するタンパク質の構造生物学
Structural biology of proteins mediating stimulus-response

オーガナイザー：中川 敦史（大阪大学），神取 秀樹（名古屋工業大学）
Organizers: Atsushi Nakagawa (Osaka University), Hideki Kandori (Nagoya Institute of Technology)

Living organisms receive and response to stimuli from their environment. These processes are essential for living systems and many proteins work in this process. In this symposium, we will discuss the stimulus-response mechanism of living systems based on the molecular mechanisms of the proteins that function in gas-sensing, photo-sensing, mechano-sensing, voltage-sensing, and redox-sensing.

1SMP-1 Structural basis for the heme-dependent transcriptional regulation
Shigetoshi Aono[1,2] ([1]*Okazaki Int. Integ. Biosci.*, [2]*Inst. Mol. Sci.*)

1SMP-2 光活性化アデニル酸シクラーゼの構造と機能
Structure and function of photoactivated adenylyl cyclase
大木 規央[2], 朴 三用[2], ○伊関 峰生[1]（[1]東邦大・薬, [2]横浜市大・院生命医科学）
Mio Ohki[2], Sam-Yong Park[2], **Mineo Iseki**[1] ([1]*Facul. Pharm. Sci., Toho Univ.*, [2]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

1SMP-3 細菌機械受容チャネル MscL のメカノゲーティングに対する計算科学的アプローチ
Computational Approach to Mechano-Gating of the Bacterial Mechanosensitive Channel MscL
○澤田 康之[1], 曽我部 正博[2]（[1]名古屋経済大学人間生活科学部管理栄養学科, [2]名大院・医・メカノバイオロジーラボ）
Yasuyuki Sawada[1], Masahiro Sokabe[2] ([1]*Dept Nutrition Fac Human Life Science Nagoya Univ Economics*, [2]*Mechanobiology Lab Nagoya Univ Grad Sch Med*)

1SMP-4 電位依存性ホスファターゼ VSP のカップリング機構に関する構造生物学的研究
Structural analysis of voltage-sensing phosphatase (VSP) on the electrochemical coupling
○成田 宏隆[1,3], 神田 直樹[1], 岡村 康司[2], 中川 敦史[1,3]（[1]阪大・蛋白研, [2]阪大・院医, [3]CREST, JST）
Hirotaka Narita[1,3], Naoki Kanda[1], Yasushi Okamura[2], Atsushi Nakagawa[1,3] ([1]*Inst. Protein Res., Osaka Univ.*, [2]*Grad. Sch. of Med., Osaka Univ.*, [3]*CREST, JST*)

1SMP-5 電位依存性プロトンチャネル VSOP/Hv1 の電場中での動態の解析
Molecular dynamics study of kinetics of the voltage-gated proton channel VSOP/Hv1 under electric fields
○近藤 寛子[1], 米澤 康滋[2], 宮下 尚之[3], 岩城 雅代[4], 竹下 浩平[5], 藤原 祐一郎[6], 城田 松之[7,8,9], 木下 賢吾[8,9,10], 岡村 康司[6], 中川 敦史[5], 神取 秀樹[4], 鷹野 優[1]（[1]広市大・院・情報, [2]近畿大・先端研, [3]近畿大・生物理工, [4]名工大・院・工, [5]阪大・蛋白研, [6]阪大・院・医, [7]東北大・院・医, [8]東北大・メガバンク, [9]東北大・院・情報, [10]東北大・加齢研）
Hiroko X. Kondo[1], Yasushige Yonezawa[2], Naoyuki Miyashita[3], Masayo Iwaki[4], Kohei Takeshita[5], Yuichiro Fujiwara[6], Matsuyuki Shirota[7,8,9], Kengo Kinoshita[8,9,10], Yasushi Okamura[6], Atsushi Nakagawa[5], Hideki Kandori[4], Yu Takano[1] ([1]*GSIS, Hiroshima City Univ*, [2]*Iat, Kindai Univ*, [3]*Bost, Kindai Univ*, [4]*Grad Sch Eng, Nagoya Inst Tech*, [5]*IPR, Osaka Univ*, [6]*Grad Sch Med, Osaka Univ*, [7]*Grad Sch Med, Tohoku Univ*, [8]*ToMMo, Tohoku Univ*, [9]*GSIS, Tohoku Univ*, [10]*IDAC, Tohoku Univ*)

1SMP-6 Structural basis of redox-dependent regulation of SERCA2b
Michio Inoue[1], Nanami Sakuta[1], Satoshi Watanabe[1], Ryou Ushioda[2], Yoshiki Tanaka[3], Tomoya Tsukazaki[3], Kazuhiro Nagata[2], **Kenji Inaba**[1] ([1]*Tohoku Univ*, [2]*Kyoto Sangyo Univ*, [3]*NAIST*)

13:20〜15:50　N 会場（文法学部 1 階 B3 教室）／Room N (Room B3, Faculty of Letters, Faculty of Law Main Bldg. 1F)

1SNP　協賛　AMED 革新的先端研究開発支援事業（AMED－CREST/PRIME）
「メカノバイオロジー機構の解明による革新的医療機器及び医療技術の創出」

メカノバイオロジーを開拓するメソドロジーの新展開

International symposium on mechanobiology with its cutting edge and diversity

オーガナイザー：新井 敏（早稲田大学），林 久美子（東北大学）

Organizers: Satoshi Arai (Waseda University), Kumiko Hayashi (Tohoku University)

The main-stream of mechanobiology unveils the mechanism of how cells sense and respond to the mechanical stimulus at molecular level. Furthermore, recent studies on mechanobiology spread to the broaden area by researchers who interpret the concept of “mechano” differently. This symposium proposed here will focus on the current topics in the main-stream and also covers topics regarding the mechanobiology with diversity. In particular, speakers include those who are less familiar with biophysical meeting.

1SNP-1　オルガネラサイズの熱源を作り細胞機能を温熱制御する試み
Thermal Control of Cellular Functions Using Organelle-sized Heat Spots
○新井 敏（早大・理工研）
Satoshi Arai (*Res. Inst. Sci. Eng., Waseda Univ.*)

1SNP-2　Nanostructured Smart Materials for the Remote Manipulation of Cell Behavior
Attilio Marino[1], Gianni Ciofani[1,2] ([1]*Smart Bio-Int., IIT, Italy*, [2]*Dept. Mech. Aero. Eng., Politec. Torino, Italy*)

1SNP-3　A molecular mechanism of gene regulation by matrix mechanics -A moving story of FHL2 and Force-
Naotaka Nakazawa[1], Aneesh Sathe[2], G.V. Shivashankar[2,3,4], Michael Sheetz[2,3,5] ([1]*iCeMS, Kyoto Univ.*, [2]*Mechanobiology Institute, National Univ. of Singapore*, [3]*Dept. of Biol. Sci., National Univ. of Singapore*, [4]*iFOM, Italy*, [5]*Dept. of Biol. Sci., Columbia Univ.*)

1SNP-4　Curvature-propagated mechanochemical waves in subcellular pattern formation
Min Wu, Maohan Su, Cheesan Tong, Shengping Xiao (*National Univ. Singapore*)

1SNP-5　メカノトランスダクションと心筋リプログラミング、心臓再生
Mechano-transduction and Direct Cardiac Reprogramming for Heart Regeneration
○家田 真樹（慶應義塾大学医学部循環器内科）
Masaki Ieda (*Department of Cardiology, Keio University School of Medicine*)

1SNP-6　臓器内部における末梢神経のメカノセンシング動態
Mechanosensing dynamics of peripheral nerves inside organs
○神谷 厚範（国循センター・研究所）
Atsunori Kamiya (*NCVC*)

1SNP-7　ゆらぎを利用した低侵襲な力測定による神経細胞オルガネラ輸送の解明
Non-invasive force measurement using fluctuation for organelle transport in neurons
○林 久美子（東北大工）
Kumiko Hayashi (*Sch. Eng., Tohoku Univ.*)

第 2 日目（9 月 20 日（水））／Day 2（Sep. 20 Wed.）

8:45〜11:15　A 会場（全学教育棟 1 階 E107）／Room A (Room E107, General Education Bldg. 1F)

2SAA　少数性の生命科学：Minor 要素の振る舞いがシステム全体に影響を及ぼす思わぬ仕掛け
Introduction about “Minority in life science”

オーガナイザー：永井 健治（大阪大学），上田 泰己（東京大学/理化学研究所）
Organizers: Takeharu Nagai (Osaka University), Hiroki Ueda (The Univ. of Tokyo/RIKEN)

If we carefully observe the cell population that at first glance looks uniform and homogeneous, we may find small number of heterogeneous cells with a different nature. Moreover, this minority cells would sometimes significantly alter the behavior of the whole cell population. In this symposium, we would like to discuss not only analytical methods for sensitive detection or visualization of such minority cells, but also the theories regarding principle or mechanism how the minority cells are generated and exert biological roles.

2SAA-1　Development of techniques for imaging physiological functions toward visualization of singularity caused by minority elements
○永井 健治（阪大 産研）
Takeharu Nagai (*The Institute of Scientific and Industrial Research, Osaka University*)

2SAA-2　細胞集団に螺旋信号波をもたらす臨界現象
Critical transition controls the self-organized spiral nuclearion
○堀川 一樹（徳島大 医歯薬）
Kazuki Horikawa (*Tokushima Univ. Biomedical Sci.*)

2SAA-3　Minor 要素の人為的な活性制御を可能とする受容体の配位ケミカルジェネティクス
Coordination chemical genetics of receptors for artificially regulating minority events
○清中 茂樹（京大工）
Shigeki Kiyonaka (*Grad. Sch. Eng., Kyoto Univ.*)

2SAA-4　Small cells bur large impacts, revealed by extensive 2P / 8K-CMOS singularity imaging
○西村 智（自治医大）
Satoshi Nishimura (*Jichi Med Univ*)

2SAA-5　High speed Raman imaging for chemical profiling of cells and tissues
○藤田 克昌（阪大）
Katsumasa Fujita (*Osaka Univ*)

2SAA-6　How can one quantify singularity in cells from Single Cell Raman Imaging?
○小松崎 民樹[1,2]（[1]北大電子研, [2]北大 生命科学院）
Tamiki Komatsuzaki[1,2] ([1]*Hokkaido Univ., RIES, MSC*, [2]*Hokkaido Univ., Grad. School of Life Science*)

2SAA-7　マイノリティ細胞による自己免疫疾患発症制御機構の解明
Regulation of autoimmunity by minority cells
○岡崎 拓（徳島大学先端酵素学研究所）
Taku Okazaki (*Institute of Advanced Medical Sciences, Tokushima University*)

2SAA-8　点描画解析プラットフォームを用いた確率的全脳マッピング
Probabilistic Mapping of Mouse Brains with Scalable and Pointillistic Analytical Platform
○村上 達哉[1], 真野 智之[2,3], 犀川 周[3], 堀口 修平[4], 馬場 孝輔[5], 望月 秀樹[5], 田井中 一貴[6], 上田 泰己[1]（[1]東大・医, [2]プリンストン大, [3]東大・新領域, [4]阪大・基礎工, [5]阪大・医, [6]新潟大・脳研）
Tatsuya Murakami[1], Tomoyuki Mano[2,3], Shu Saikawa[3], Shuhei Horiguchi[4], Kousuke Baba[5], Mochizuki Hideki[5], Kazuki Tainaka[6], Hiroki Ueda[1] ([1]*Med., Univ. Tokyo*, [2]*Dept. Chem., Princeton Univ.*, [3]*Univ. Tokyo*, [4]*Osaka Univ.*, [5]*Med., Osaka Univ.*, [6]*Niigata Univ.*)

8:45〜11:15　B 会場（全学教育棟 2 階 B201）／Room B (Room B201, General Education Bldg. 2F)

2SBA　糖および脂質の生物物理―医薬への展開―
Biophysics on saccharides and lipids toward medicine

オーガナイザー：松本 陽子（崇城大学），相田 美砂子（広島大学）
Organizers: Yoko Matsumoto (Sojo University), Misako Aida (Hiroshima University)

Saccharides play important roles in adhering to cells, transmitting information, and recognizing molecules in the cell membranes composed of lipids through receptors. Recently, lipid vesicles including saccharides have been generated and effective for inhibiting the growth of tumor cells. Therefore, saccharides and lipids are good targets to create a novel therapeutic system. In this symposium, we introduce biophysical and therapeutic studies related to characteristics of saccharides and lipids and discuss the development for medicine.

2SBA-1　トレハロースリポソームによるがん治療効果とアポトーシス
Therapeutic effects of trehalose liposomes against carcinoma along with apoptosis
○松本 陽子（崇城大院・応用生命）
Yoko Matsumoto (*Grad. Life, Univ. Sojo*)

2SBA-2　天然糖トレハロースによる空間認知記憶の改善とオートファジーの関与
Trehalose intake improves spatial memory through autophagy activation in the brain of mice
○丹治 邦和, 三木 康生, 森 文秋, 若林 孝一（弘前大院・医・脳神経病理）
Kunikazu Tanji, Yasuo Miki, Fumiaki Mori, Koichi Wakabayashi (*Dept. of Neuropathol., Inst. of Brain Sci., Hirosaki Univ. Graduate Sch. of Med.*)

2SBA-3　肺がん転移促進タンパク質 CERS6 およびそれを分子標的とした薬剤戦略
Targeting ceramide synthase 6-dependent metastasis-prone phenotype in lung cancer cells
○鈴木 元（名大院・医・分子腫瘍）
Motoshi Suzuki (*Nagoya Univ Grad Sch Med, Mol Carcinog*)

2SBA-4　脂質代謝酵素 PLA2 ファミリーによるリポクオリティ制御の新機軸
Novel insights into the lipoquality control by the PLA2 family
○村上 誠[1,2,3]（[1]東京大学大学院医学系研究科 疾患生命工学センター 健康環境医工学部門, [2]公益財団法人東京都医学総合研究所, [3]日本医療研究開発機構CREST）
Makoto Murakami[1,2,3] ([1]*Center for Disease Biology and Integrative Medicine, Faculty of Medicine, The University of Tokyo*, [2]*Tokyo Metropolitan Institute of Medical Science*, [3]*AMED-CREST*)

2SBA-5　実在形質膜をモデル化した脂質二重層膜の分子動力学計算
Molecular dynamics study of lipid bilayers modeling real plasma membranes
安藤 嘉倫, ○岡崎 進（名大院・工）
Yoshimichi Andoh, **Susumu Okazaki** (*Nagoya University*)

2SBA-6　広帯域分光を用いた二糖周辺の水の水素結合ネットワーク評価
Characterization of the hydrogen-bond network of water around sucrose and trehalose investigated with broadband spectroscopy
○白神 慧一郎[1], 小川 雄一[2], 中村 昌人[3], 味戸 克裕[3], 田島 卓郎[3]（[1]理研・IMS, [2]京大・農, [3]NTT・先端集積デバイス研）
Keiichiro Shiraga[1], Yuichi Ogawa[2], Masahito Nakamura[3], Katsuhiro Ajito[3], Takuro Tajima[3] ([1]*RIKEN Center for IMS*, [2]*Grad. Sch. Agri., Kyoto Univ.*, [3]*Device Technology Labs., NTT*)

2SBA-7　グルコースとトレハロースの水溶液中における構造と水和に関する ab initio QM/MM-MD 法による研究
Ab initio QM/MM-MD study on conformation and hydration of glucose and trehalose in aqueous solution
○相田 美砂子（広島大院・理）
Misako Aida (*Grad. Sch. Sci., Hiroshima Univ*)

8:45〜11:15　C 会場（全学教育棟 2 階 B202）／Room C (Room B202, General Education Bldg. 2F)

2SCA　生体高分子の広い時空間での動的相関構造解析を目指した実験的手法と計算科学の新展開
New approaches of integrated use of experimental and simulation methods for dynamic correlative structural analysis of biomolecules in the wide spatiotemporal scale

オーガナイザー：杉山 正明（京都大学），中川 洋（日本原子力研究開発機構）
Organizers: Masaaki Sugiyama (Kyoto University), Hiroshi Nakagawa (Japan Atomic Energy Agency)

Biomacromolecules are functionalized by modulating their structure and assemble state in a physiological solution. This functional dynamics is subjected to the wide space-time from 10-12 m to 10-6 m and 10-12 sec to 10-6 sec and therefore it is crucially important to have analysis methods crossover this wide space-time range. In this symposium, we would like to approach to the structure and dynamics related to wide hierarchy with marriage of experimental methods, represented by quantum beam scattering techniques and NMR, and computational science.

2SCA-1　このシンポジウムの狙いについて
Introduction of hybrid/integrative structural biology
○杉山 正明（京大原子炉）
Masaaki Sugiyama (*KURRI*)

2SCA-2　モデル膜の熱揺らぎと機械的性質に及ぼすペプチドの効果
Effects of incorporating small peptide on collective thermal fluctuations and elastic and viscous properties in model lipid bilayers
○長尾 道弘[1,2], Kelley Elizabeth[1], Butler Paul[1]（[1]米国標準技術研究所, [2]インディアナ大）
Michihiro Nagao[1,2], Elizabeth Kelley[1], Paul Butler[1] ([1]*NIST*, [2]*Indiana U.*)

2SCA-3　Protein dynamics as studied by neutron spin echo and MD simulation
Rintaro Inoue[1], Takashi Oda[2], Tomotaka Oroguchi[3], Mitsunori Ikeguchi[2], Masaaki Sugiyama[1], Mamoru Sato[2] ([1]*Research Reactor Institute, Kyoto University*, [2]*Yokohama City University*, [3]*Keio University*)

2SCA-4　Protein Structural Fluctuations Investigated by X-ray Solution Scattering and Molecular Dynamics Simulation
Tomotaka Oroguchi[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*)

2SCA-5　統合的な構造物学アプローチによるに糖タンパク質および糖鎖の構造ダイナミクスの解析
Integrative structural biology approaches for understanding conformational dynamics of oligosaccharides and glycoproteins
○矢木 宏和[1], 谷中 冴子[2], 與語 理那[1,2], 鈴木 達哉[2], 山口 拓実[3], 杉山 正明[4], 加藤 晃一[1,2]（[1]名市大・院薬, [2]自然科学研究機構・岡崎統合バイオ、分子研, [3]北陸先端・マテリアル, [4]京大・原子炉実験所）
Hirokazu Yagi[1], Saeko Yanaka[2], Rina Yogo[1,2], Tatsuya Suzuki[2], Takumi Yamaguchi[3], Masaaki Sugiyama[4], Koichi Kato[1,2] ([1]*Grad. Sch. of Pharm. Sci., Nagoya City Univ.*, [2]*Okazaki Inst. for Integra. Biosci. and Inst. for Mol. Sci., Nat. Inst. of Nat. Sci.*, [3]*Sch. Of Materials Sci., JAIST*, [4]*Research Reactor Institute, Kyoto University*)

2SCA-6　分子シミュレーションの動的解析手法によるタンパク質のダイナミクスの研究
Investigating protein dynamics by using dynamical analysis methods of molecular simulations
○光武 亜代理（慶應義塾大学理工学部物理学科）
Ayori Mitsutake (*Dept. Phys, Keio Univ.*)

2SCA-7　中性子散乱と計算機科学の融合による蛋白質のドメインダイナミクスの解析
Analysis of protein domain dynamics by integrating of neutron scattering and computer science
○中川 洋[1,2]（[1]日本原子力研究開発機構・原子力科学研究部門・物質科学研究センター・階層構造研究グループ, [2]JST, さきがけ）
Hiroshi Nakagawa[1,2] ([1]*Japan Atomic Energy Agency, Materials Science Research Center*, [2]*JST, PRESTO*)

8:45〜11:15　D 会場（全学教育棟 2 階 E201）／Room D (Room E201, General Education Bldg. 2F)

2SDA　自己複製系の新展開：創発と合成の邂逅
Frontiers in self-replicating systems: Emergence and synthesis

オーガナイザー：前多 裕介（九州大学），下林 俊典（海洋研究開発機構）
Organizers: Yusuke Maeda T. (Kyushu Univeristy), Shunsuke Shimobayashi F. (JAMSTEC)

Living cells produce themselves so that a major conceptual question in biology is self-reproduction. One may understand it for self-replication of biopolymers following von Neumann logic, which implies a memory. But, how does self-reproduction operate without apparent memory? In this symposium, recent developments of mechanical aspects for self-reproduction will be shown from physics, mathematics, and synthetic biology. Self-replication and functional expression of information coding polymers of DNA and RNA are particularly focused in both experiment and theory.

2SDA-1　Emergence of genetic information in information-polymer soup
Shoichi Toyabe (*Grad. Sch. Eng., Tohoku Univ.*)

2SDA-2　自己複製する鋳型高分子系において複雑な配列が選択される条件
Conditions for selecting complex sequences in mathematical model of self-replicating template polymer system
○松原 嘉哉, 金子 邦彦（東大・総文）
Yoshiya Matsubara, Kunihiko Kaneko (*Grad. Sch. Arts and Sci., The Univ. of Tokyo*)

2SDA-3　染色体複製サイクルの繰り返しによる環状 DNA の試験管内自律増殖
Autonomous propagation of circular DNA molecules in vitro through a continuous repetition of a chromosome replication cycle
○末次 正幸, 高田 啓（立教大・理・生命理）
Masayuki Su'etsugu, Hiraku Takada (*Col. of Sci., Rikkyo Univ.*)

2SDA-4　Emergence of DNA-encapsulating liposomes from a DNA− Lipid blend film
Shunsuke Shimobayashi (*Department of Mathematical Science and Advanced Technology, Japan Agency for Marine-Earth Science and Technology*)

2SDA-5　オンチップ人工細胞：無細胞系の遺伝子発現と幾何形状による制御
Artificial-cells-on-a-chip: cell-free gene expression in microwells with various geometries
○イズリ ジャン[1], 坂本 遼太[1], ノワロー ヴィンセント[2], 前多 裕介[1]（[1]九州大学理学研究院物理学部門, [2]ミネソタ大・物理）
Ziane Izri[1], Ryota Sakamoto[1], Vincent Noireaux[2], Yusuke Maeda[1] ([1]*Dept. Phys., Kyushu Univ.*, [2]*Dept. Phys., Univ. Minnesota*)

2SDA-6　細胞内外で機能する合成 RNA-タンパク質複合体の設計と構築
Synthetic RNA-protein nanostructured devices that function in vitro and in cells
○齊藤 博英, 大野 博久（京都大学）
Hirohide Saito, Hirohisa Ohno (*Kyoto Univ.*)

8:45〜11:15　E 会場（全学教育棟 2 階 E203）／Room E (Room E203, General Education Bldg. 2F)

2SEA　生物時計の 24 時間リズム創出原理に関するマジ（めな）議論
Molecular, Structural, and Dynamic Origins of 24-hour Period in Circadian Clock Systems

オーガナイザー：秋山 修志（分子科学研究所），八木田 和弘（京都府立医科大学）
Organizers: Shuji Akiyama (IMS), Kazuhiro Yagita (Kyoto Prefectural University of Medicine)

Circadian clocks reveal a self-sustained oscillation with an approximately 24 h period. In these days, there is a growing number of researches approaching origins of slow yet ordered dynamics from the viewpoints of biophysics, chemical biology, structural biology, and bioinformatics. The accumulated evidence offers an ideal opportunity to revisit a fundamental question in chronobiology: what determines the temperature-compensated 24 h period? In this symposium, we will present the current understanding of the clock systems in prokaryotes and eukaryotes and discuss emerging ideas.

はじめに
Opening Remarks

2SEA-1 シアノバクテリアのタンパク質時計が教えてくれること
Lessons from Cyanobacterial Circadian Clock System
○秋山 修志[1,2,3]（[1]分子研 協奏分子システム研究センター, [2]総研大, [3]理研・放射光科学総合研究センター）
Shuji Akiyama[1,2,3] ([1]*CIMoS, IMS, NINS*, [2]*SOKENDAI*, [3]*RIKEN SPring-8 Center*)

2SEA-2 天然変性タンパク質とリン酸化
Protein intrinsic disorder and phosphorylation
○太田 元規（名大・情報）
Motonori Ota (*Sch. Info. Nagoya U.*)

2SEA-3 Chemical and structural biology approaches to understand molecular mechanism underlying 24-hour period of mammalian circadian clock
Tsuyoshi Hirota (*Institute of Transformative Bio-molecules, Nagoya University*)

2SEA-4 Flexible time: turning of circadian period through the loop region of CRYPTOCHROME protein
Koji Ode[1,2], Hiroki Ueda[1,2] ([1]*Dept. Sys. Pharm., Grad. Sch. Med., The Univ. Tokyo*, [2]*Lab. Syn. Biol., QBiC, RIKEN*)

2SEA-5 哺乳類の発生過程における 24 時間周期の形成機構
Appearance of 24 hour rhythms during the developmental process in mammals
○八木田 和弘（京都府立医科大学 統合生理学）
Kazuhiro Yagita (*Kyoto Prefectural University of Medicine*)

おわりに
Closing Remarks

8:45～11:15　F 会場（全学教育棟 2 階 E205）／Room F (Room E205, General Education Bldg. 2F)

2SFA　新学術領域研究「理論と実験の協奏による柔らかな分子系の機能の科学」共催
さまざまな環境下で発現される生体分子の柔らかさと機能
Softness and functions of biological molecules under various environments

オーガナイザー：高橋 聡（東北大学），飯野 亮太（自然科学研究機構）
Organizers: Satoshi Takahashi (Tohoku University), Ryota Iino (NINS)

Biological systems express their functions through the coordinated dynamics of soft biological macromolecules in various environments. In this symposium, we ask young investigators to present their recent investigations based on molecular dynamics simulations, in cell NMR, high speed AFM and advanced optical microscopies and to discuss the current understanding and future perspectives of their target biological systems.

2SFA-1 細胞内クラウディング環境下の蛋白質のフォールディング・ダイナミクスを NMR で観測する
NMR approaches to investigate protein folding and dynamics in the crowded intracellular environment
○伊藤 隆（首都大・理工・分子物質化学）
Yutaka Ito (*Dept. Chemistry, Tokyo Metropolitan Univ.*)

2SFA-2 長時間分子シミュレーショントラジェクトリの解析から探るタンパク質の不均一なダイナミクス
Deciphering the heterogeneous dynamics of proteins from the analysis of millisecond-long molecular dynamics simulations
○森 俊文[1,2], 斉藤 真司[1,2]（[1]分子研, [2]総研大）
Toshifumi Mori[1,2], Shinji Saito[1,2] ([1]*IMS*, [2]*SOKENDAI*)

2SFA-3 Ultrahigh-speed single-particle tracking by interferometric scattering (iSCAT) microscopy
Chia-Lung Hsieh (*Institute of Atomic and Molecular Sciences, Academia Sinica*)

2SFA-4 ラマン散乱顕微鏡とアルキン標識による生物活性小分子のイメージングとスクリーニング
Raman scattering microscopy and alkyne-tag for imaging and screening of bio-active small molecules
○安藤 潤[1,2,3,4], 藤田 克昌[1,2], 袖岡 幹子[2,3]（[1]大阪大学・応用物理学専攻, [2]AMED-CREST, AMED, [3]理研, [4]分子科学研究所）
Jun Ando[1,2,3,4], Katsumasa Fujita[1,2], Mikiko Sodeoka[2,3] ([1]*Dept. of Applied Physics, Osaka Univ.*, [2]*AMED-CREST, AMED*, [3]*RIKEN*, [4]*Institute for Molecular Science*)

2SFA-5 High-Speed AFM Observation of Domain Flexibility Related to Enzymatic Function of CRISPR-Cas9
Takayuki Uchihashi[1], Mikihiro Shibata[2,3], Hiroshi Nishimasu[4,5], Noriyuki Kodera[3,5], Seiichi Hirano[4], Toshio Ando[3,6], Osamu Nureki[4] ([1]*Dept. Phys., Nagoya Univ.*, [2]*ISFS, Kanazawa Univ.*, [3]*Bio-AFM FRC, Kanazawa Univ.*, [4]*Dept. Biol., Univ. Tokyo*, [5]*JST-PRESTO*, [6]*JST-CREST*)

2SFA-6 高速 1 分子イメージング解析で明らかとなったリニア分子モーター、回転分子モーターの化学力学共役機構
Chemo-mechanical coupling mechanisms of linear and rotary molecular motors revealed by high-speed single-molecule imaging analysis
○飯野 亮太[1,2,3]（[1]自然科学研究機構 岡崎統合バイオサイエンスセンター, [2]自然科学研究機構 分子科学研究所, [3]総合研究大学院大学）
Ryota Iino[1,2,3] ([1]*OIIB, NINS*, [2]*IMS, NINS*, [3]*SOKENDAI*)

8:45〜11:15　G 会場（全学教育棟 3 階 C301）／Room G (Room C301, General Education Bldg. 3F)

2SGA　新学術領域研究「動的構造生命科学を拓く新発想測定技術」共催
生体膜模倣環境としての新しい界面活性剤，リポソーム，ナノディスクの利用
New detergents, liposomes, and nanodiscs as membrane-mimetic environments

オーガナイザー：塚崎 智也（奈良先端科学技術大学院大学），神田 大輔（九州大学）
Organizers: Tomoya Tsukazaki (NAIST), Daisuke Kohda (Kyushu University)

The solubilization with detergents and reconstitution into lipid bilayers is a critical process in membrane protein studies. Intensive talks on the basics and the applications of new detergents, liposomes, and nanodiscs for proper treatment of membrane proteins will be given to view a present and future status of the membrane-memetic technology.

2SGA-1 リポソーム・ナノディスクの膜環境と脂質ダイナミクス
Structure and Dynamics of Lipids in Liposomes and Nanodiscs
○中野 実（富山大学大学院 医学薬学研究部）
Minoru Nakano (*Graduate School of Medicine and Pharmaceutical Sciences, University of Toyama*)

2SGA-2 脂質ナノディスク形成のための膜活性ポリマーのデザイン
Molecular design of membrane-active polymers for lipid nanodisc formation
○安原 主馬, 井上 雅也, 荒木田 臣, 菊池 純一（奈良先端科学技術大学院大学 物質創成科学研究科）
Kazuma Yasuhara, Masaya Inoue, Jin Arakida, Jun-ichi Kikuchi (*Graduate School of Materials Science, Nara Institute of Science and Technology*)

2SGA-3 脂質ータンパク協同性による上皮成長因子受容体の膜近傍ドメイン二量体形成機構
Lipid-protein cooperativity in the regulation of juxtamembrane domain dimer formation in epidermal growth factor receptor
○前田 亮[1], 佐藤 毅[2], 岡本 憲二[1], 佐甲 靖志[1]（[1]理研・佐甲細胞情報, [2]京都薬科大学）
Ryo Maeda[1], Takeshi Sato[2], Kenji Okamoto[1], Yasushi Sako[1] ([1]*Cellular Informatics Lab., RIKEN*, [2]*Kyoto Pharmaceutical Univ.*)

2SGA-4 High-speed AFM observation of membrane protein embedded in Nanodisc
Takamitsu Haruyama[1], Yasunori Sugano[1], Yoshiki Tanaka[1], Hiroki Konno[2], Tomoya Tsukazaki[1] ([1]*Grad. Sch. of Biol. Sci., NAIST*, [2]*Bio-AFM FRC, Inst. of Sci. & Eng., Kanazawa Univ.*)

2SGA-5 GraDeR: 遊離界面活性剤無膜タンパク質の調整方法
GraDeR: micelle free membrane protein preparation
○Gerle Christoph（阪大・タンパク研）
Christoph Gerle (*IPR, Osaka Univ.*)

2SGA-6 リポソーム中の膜タンパク質機能構造を捉えるクライオ電子顕微鏡単粒子解析法
CryoEM single particle analysis for functional structure of membrane proteins in liposomes
○重松 秀樹（理研ライフサイエンス技術基盤研究センター）
Hideki Shigematsu (*RIKEN CLST*)

8:45〜11:15　I 会場（全学教育棟 3 階 E305）／Room I (Room E305, General Education Bldg. 3F)
2SIA　協賛　AMED 革新的先端研究開発支援事業（AMED－CREST/PRIME）
「メカノバイオロジー機構の解明による革新的医療機器及び医療技術の創出」
メカノバイオロジーを開拓するメソドロジーの新展開
Development of methodology to explore the mechanobiology

オーガナイザー：木戸秋 悟（九州大学），曽我部 正博（名古屋大学）
Organizers: Satoru Kidoaki (Kyushu University), Masahiro Sokabe (Nagoya University)

For the development of mechanobiology, an integrated approach from multifaceted technical fields has been essential. The frontier of mechanobiology has been developed by combining various methodologies such as molecular biological techniques, sophisticated imaging probe and microscope technology, mechanical loading device, microfluidics, design of surface chemistry and viscoelasticity of materials, computational technique, etc. This session is dedicated to discuss the latest trends on the methodology to explore the mechanobioly, and not only on the methodologies but also on the basic mechanobioligic findings based on the methodlogies.

2SIA-1 メカノバイオロジー: これまでの成果とこれからの課題
Mechanobiology: Past achievements and future issues
○曽我部 正博（名大院・ 医・ メカノバイオロジー・ラボ）
Masahiro Sokabe (*Mechanobiology Lab, Nagoya Univ Grad Sch Med*)

2SIA-2 Mechanobio-materials manipulating motility and functions of stem cells
Satoru Kidoaki (*IMCE, Kyushu Univ.*)

2SIA-3 メカノバイオロジーのための形状記憶型動的培養基盤
Shape Memory-based Dynamic Culture Platforms for Mechanobiology
○宇都 甲一郎（若手国際セ・物材研）
Koichiro Uto (*ICYS, NIMS*)

2SIA-4 遺伝子発現制御に対するアクチンの役割を理解するための微細構造化細胞培養基材の開発
Microtopographical cell culture substrate to understand the role of actin cytoskeleton for regulation of gene expression
山崎 雅史[1], ○三好 洋美[1,2]（[1]首都大院・システムデザイン, [2]AMED・PRIME）
Masashi Yamazaki[1], **Hiromi Miyoshi**[1,2] ([1]*Grad. Sch. System Design, Tokyo Metropolitan Univ.*, [2]*PRIME, AMED*)

2SIA-5 Live-cell imaging of actin dynamics in cortex and lamellipodium by high-speed atomic force microscopy
Yoshitsuna Itagaki[1], Yanshu Zhan[1], Aiko Yoshida[1], Nobuaki Sakai[2], Yoshitsugu Uekusa[2], Masahiro Kumeta[1], **Shige H. Yoshimura**[1] ([1]*Grad. Schl. Biostudies, Kyoto U.*, [2]*R&D Group, Olympus Corp.*)

2SIA-6 細胞の力学：単一細胞から多細胞へ
Cell Mechanics: from single cell to multi-cellular dynamics
谷本 博一[1,2], 川口 喬吾[1,3], 上道 雅仁[1], ○佐野 雅己[1]（[1]東大院理・物理, [2]ジャックモノー研, [3]ハーバード大、システム生物）
Hirokazu Tanimoto[1,2], Kyogo Kawaguchi[1,3], Masahito Uwamichi[1], **Masaki Sano**[1] ([1]*Dept. Phys. Univ. Tokyo*, [2]*Inst. Jacques Monod*, [3]*Sys. Bio. Harvard Univ.*)

8:45〜11:15　K 会場（文法学部 2 階 A1 教室）／Room K (Room A1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

2SKA　Joint Symposium between Indian Biophysics Society and BSJ: Protein Biophysics: From Folding to Drug Discovery

オーガナイザー：金城 玲（大阪大学），バスー ゴータム（Bose Institute）
Organizers: Akira R. Kinjo (Osaka University), Gautam Basu (Bose Institute)

Computational approaches such as modeling, simulation and statistical analysis are becoming ever more crucial not only to make sense of the massive amount of biological data but to predict systems' behaviors and thereby to generate hypotheses that may drive further experimental studies. In this symposium, focusing on molecular aspects of biophysical systems, speakers from India and Japan will present some of their recent studies ranging from protein structure and folding to evolution and drug discovery using computational methods.

2SKA-1　配列空間における蛋白質フォールディング
Protein folding in the sequence space
○金城 玲（大阪大学蛋白質研究所）
Akira R. Kinjo (*Inst. Protein Res., Osaka Univ.*)

2SKA-2　Toward a Quantitative Description of Microscopic Pathway Heterogeneity in Protein Folding
Athi N. Naganathan (*IIT Madras*)

2SKA-3　Structural features of the urea denatured apomyoglobin using molecular modeling and experimental data
Yasutaka Seki (*Molecular Biophysics, Kochi Medical School, Kochi University*)

2SKA-4　Structural Proteome to Targetability Estimation: Novel Concepts in Drug Discovery
Nagasuma Chandra (*Indian Inst. Sci.*)

2SKA-5　Data integration and statistical/*ab initio* modelling towards rational drug discovery
Kenji Mizuguchi (*NIBIOHN*)

2SKA-6　Cis proline-specific protein structure and dynamics
Gautam Basu (*Bose Inst.*)

8:45〜11:15　L 会場（文法学部 2 階 B1 教室）／Room L (Room B1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

2SLA　若手研究者が考えるバイオイメージングとその応用
Happy Hacking imaging for biology by early carriers

オーガナイザー：鳥羽 栞（弘前医療福祉大学），新井 由之（大阪大学）
Organizers: Shiori Toba (Hirosaki University of Health and Welfare), Yoshiyuki Arai (Osaka University)

Optical microscopy enables us to visualize the dynamic behavior of living samples. In this session, we will present the recent imaging technologies, including superresolution, adaptive optics, digital holography, and image processing. We hope to discuss recent developments and the significant findings based on our observation. We believe this symposium will encourage the further applications to increase the experimental output and stimulating the scientist in your field.

2SLA-1　超解像光学顕微鏡法 PALM によって明らかになった軸索輸送における非定型微小管
Opening talk: visualizing unconventional biological component using super-resolution photo-activated localization microscopy
○鳥羽 栞[1,2]（[1]大阪市立大・医, [2]現所属：弘前医療福祉大）
Shiori Toba[1,2] ([1]*Osaka City Univ. Grad. Sch. of Medicine*, [2]*Present Address: Hirosaki Univ. of Health and Welfare*)

2SLA-2　新規光技術を用いた二光子励起顕微鏡の機能向上
Improvements of two-photon excitation microscopy by utilizing novel optical technologies
○大友 康平[1,2]（[1]北大・電子研, [2]北大・院・情報）
Kohei Otomo[1,2] ([1]*RIES, Hokkaido Univ.*, [2]*Grad. Sch. IST, Hokkaido Univ.*)

2SLA-3 補償光学：光の乱れの補正による深部生細胞イメージング
Adaptive optics: Towards deep imaging of living cells by active correction of optical disturbance
○玉田 洋介（基生研・生物進化）
Yosuke Tamada (*Div. Evol. Biol., Natl. Inst. Basic Biol.*)

2SLA-4 SIM/STORM イメージングの使命と将来の展望
Missions and the future of SIM/STORM super-resolution microscopy
○友杉 亘（株式会社ニコン）
Wataru Tomosugi (*Nikon Corporation*)

2SLA-5 能動学習を用いた生物画像の効率的自動分類
Efficient Automatic Classification of Biomedical Images Using Active Learning Algorithm
○朽名 夏麿[1,2], 島原 佑基[1,2], 馳澤 盛一郎[1,2]（[1]エルピクセル(株), [2]東大・院新領）
Natsumaro Kutsuna[1,2], Yuki Shimahara[1,2], Seiichiro Hasezawa[1,2] ([1]*Lpixel Inc.*, [2]*Grad. Sch. Front. Sci., Univ. Tokyo*)

2SLA-6 ディジタルホログラフィとバイオイメージングへの応用可能性
Digital holography and its applicability to biology
○田原 樹[1,2]（[1]関西大・システム理工, [2]JST さきがけ）
Tatsuki Tahara[1,2] ([1]*Kansai University*, [2]*PRESTO, JST*)

2SLA-7 Closing remarks: Advanced bioimaging techniques for biophysics
Yoshiyuki Arai (*ISIR, Osaka Univ*)

8:45〜11:15　M 会場（文法学部 1 階 B2 教室）／Room M (Room B2, Faculty of Letters, Faculty of Law Main Bldg. 1F)

2SMA　文部科学省 光・量子融合連携研究開発プログラム「中性子と放射光の連携利用によるタンパク質反応プロセスの解明」共催
X 線と中性子の連携利用による高分解能／高精度タンパク質結晶学
High-resolution and High-precision Protein Crystallography by Combined Use of X-ray and Neutron Diffraction

オーガナイザー：玉田 太郎（量子科学技術研究開発機構），三木 邦夫（京都大学）
Organizers: Taro Tamada (National Institutes for Quantum and Radiological Science and Technology), Kunio Miki (Kyoto University)

Recent development of synchrotron facility enables us to perform protein crystal structure analyses at ultra-high resolution. As a consequence of charge-density analysis based on ultra-high resolution structures we can obtain information of outer-electron distribution of protein molecules. On the other hand, we can now discuss detailed reaction mechanism from exact hydrogen positions visualized by neutron crystallography. It is time now to utilize X-ray and neutron diffraction jointly to obtain deep information on protein structures. In this symposium, we show most recent results in this field and discuss its current methodological problems and its future view.

2SMA-1 はじめに
Introduction
○三木 邦夫（京都大学大学院理学研究科）
Kunio Miki (*Graduate School of Science, Kyoto University*)

2SMA-2 緑色蛍光タンパク質の X 線および中性子線解析
X-ray and neutron diffraction analyses of green fluorescent protein
○竹田 一旗（京都大学大学院理学研究科生物構造化学研究室）
Kazuki Takeda (*Grad. Sch. Sci., Kyoto Univ.*)

2SMA-3 Experimental environments for high-resolution diffraction data collection at SPring-8
Takashi Kumasaka, Kazuya Hasegawa (*Protein Crystal Analysis Division, Japan Synchrotron Radiation Research Institute (JASRI)*)

2SMA-4 電子伝達タンパク質の高分解能中性子結晶構造解析
High-resolution neutron crystal structural studies of electron transfer proteins
○玉田 太郎（量研・量子ビーム）
Taro Tamada (*QuBS, QST*)

2SMA-5 Challenging to visualize ammonia transposition in a channel of amidotransferase GatCAB using neutron macromolecular crystallography

Min Yao[1,2], Long Li[2] ([1]*Faculty of Advanced Life Science, Hokkaido University*, [2]*Graduate School of Life Science, Hokkaido University*)

2SMA-6 Neutron protein crystallography with single-crystal neutron diffractometer iBIX at pulsed neutron source MLF, J-PARC

Katsuhiro Kusaka[1], Taro Yamada[1], Naomine Yano[1], Takaaki Hosoya[1], Takashi Ohhara[2], Ichiro Tanaka[1], Masaki Katagiri[1] ([1]*Frontier Research Center of Applied Atomic Sciences, Ibaraki University*, [2]*J-PARC Center, JAEA*)

8:45～11:15　N 会場（文法学部 1 階 B3 教室）／Room N (Room B3, Faculty of Letters, Faculty of Law Main Bldg. 1F)

2SNA　動的不均一性がもたらす多細胞社会の秩序形成
Order from dynamic heterogeneity in multicellular systems

オーガナイザー：柴田 達夫（理化学研究所），松崎 文雄（理化学研究所）
Organizers: Tatsuo Shibata (RIKEN), Fumio Matsuzaki (RIKEN)

Recent technological advances in single cell transcriptome analysis and imaging of living tissues and organs have started to provide the view that apparently homogeneous cell populations contain in fact remarkable heterogeneities. From this finding, the question naturally arises as to how the ordered form and function of tissues and organs is created and maintained from a population of cells with disordered and stochastic characteristics. In this symposium, we will discuss the underlying principles that bridge this gap, based on the recent analysis of state transitions and linage tracing of cells in populations in vivo and in vitro.

2SNA-1 形態形成における確率過程
Stochastic process in multicellular morphogenesis

○柴田 達夫（理研QBiC）
Tatsuo Shibata (*RIKEN QBiC*)

2SNA-2 Molecular mechanism to generate heterogeneous gene expression in mouse ES cell population

Hitoshi Niwa (*IMEG, Kumamoto University*)

2SNA-3 マウス着床前発生において細胞はどのように分化するか？
How do cells differentiate during preimplantation mouse development ?

○藤森 俊彦（基生研・初期発生）
Toshihiko Fujimori (*Div. of Embryology, NIBB*)

2SNA-4 組織恒常性を支える幹細胞の動的不均一性をマウス精子形成に学ぶ
Dynamical heterogeneity of the stem cell pool underlying the homeostatic sperm production in mice

○吉田 松生（基礎生物学研究所）
Shosei Yoshida (*National Institute for Basic Biology*)

2SNA-5 機械学習によるデータ駆動型サイエンス：現状と展望
Machine learning for data-driven scientific discovery: state-of-the-art and future perspective

○吉田 亮（統数研）
Ryo Yoshida (*Inst. Stat. Math.*)

2SNA-6 脳発生過程における神経幹細胞の動的多様性
Dynamic heterogeneity of neural stem cells in brain development

○松崎 文雄（理化学研究所　多細胞システム形成研究センター）
Fumio Matsuzaki (*RIKEN Center for Developmental Biology*)

13:55〜16:25　A 会場（全学教育棟 1 階 E107）／Room A (Room E107, General Education Bldg. 1F)

2SAP　生物学における数の数理：少数の分子が如何にして機能の頑健性を産み出しているのか？
Number in biology: deciphering how small number of molecules solve robustness of biological functions

オーガナイザー：小松崎 民樹（北海道大学），黒田 真也（東京大学）

Organizers: Tamiki Komatsuzaki (Hokkaido University), Shinya Kuroda (The University of Tokyo)

All live systems are composed of a sequence of chemical reactions and quite often in systems biology people have expressed molecules by "concentration valuable", but actually molecules are discrete objects, so that the number of molecules should be expressed. Moreover, the numbers of molecules in single cells are countably very small at the order of 1 to 1000 compared to Avogadro number. Naive intuition suggests that large number fluctuation in reactions is not well desired to promote signal transduction cascades robustly. Likewise, the open question in biology is to elucidate the numbers of each actors/actresses in biology and how our live system solves biological functions under the existence of such apparent conflicts.

はじめに
Opening Remarks
Tamiki Komatsuzaki

2SAP-1　生命システムにおける状態・形・少数性の問題
State, Shape, and Small-Number Issues in Biological Systems
○冨樫 祐一（広島大・理）
Yuichi Togashi (*Grad. Sch. Sci., Hiroshima Univ.*)

2SAP-2　Collective motion switches directionality of molecular motor along filament
Nen Saito (*Grad. Sch. Sci., Univ. Tokyo*)

2SAP-3　Information thermodynamic study of biochemical clock
Sosuke Ito[1], Pieter Rein Ten Wolde[2] ([1]*Hokkaido University, RIES*, [2]*FOM Institute AMOLF*)

2SAP-4　シロイヌナズナ遺伝子発現揺らぎの新規モデル分布
Novel statistical model of fluctuating gene expression levels of Arabidopsis thaliana
○粟津 暁紀[1], 永野 惇[2]（[1]広大理, [2]龍谷大農）
Akinori Awazu[1], Atsushi Nagano[2] ([1]*Dept. of Math. and Life Sci., Hiroshima Univ.*, [2]*Faculty of Agriculture, Ryukoku Univ.*)

2SAP-5　E-Cell System: from a single molecule to a whole cell
Kazunari Kaizu, Masaki Watabe, Kouichi Takahashi (*RIKEN Quantitative Biology Center (QBiC)*)

2SAP-6　スパインにおける小体積効果：Robust, Sensitive で Efficient な情報伝達
Small-Volume Effect Enables Robust, Sensitive, and Efficient Information Transfer in the Spine
○藤井 雅史（東大・院理）
Masashi Fujii (*Grad. Sch. Sci., Univ. Tokyo*)

2SAP-7　A quantitative view of the biosphere: from the most abundant taxa to the most abundant proteins
Yinon Bar-On, Rob Phillips, Ron Milo (*Weizmann Inst. Sci.*)

おわりに
Closing Remarks
Shinya Kuroda

13:55〜16:25　G 会場（全学教育棟 3 階 C301）／Room G (Room C301, General Education Bldg. 3F)

2SGP　高分子混雑が支配する細胞の世界
Macromolecular crowding shapes the world of cells

オーガナイザー：柳澤 実穂（東京農工大学），優 乙石（理化学研究所）
Organizers: Miho Yanagisawa (Tokyo University of Agriculture and Technology), Isseki Yu (RIKEN)

Biopolymers such as proteins are present in very high concentrations in cells, which greatly affect the dynamics, structure, and function of them. Although these effects, so-called "macromolecular crowding" has been attracting attention, molecular-level mechanisms are still unknown due to its complexity. At this symposium, we focus on the characteristics of the cellular environment and/or cell-mimicking conditions dominated by macromolecular crowding. Combining experimental, theoretical, and computational approaches, we discuss the influence of macromolecular crowding on diffusion, structural stability, and biological reactivity of DNA or proteins.

2SGP-1　はじめに：高分子混雑の世界
Introduction: the world of macromolecular crowding
○柳澤 実穂（東京農工大学大学院工学研究院先端物理工学部門）
Miho Yanagisawa (*Tokyo Univ. Agri. Technol.*)

2SGP-2　回転および並進拡散計測による細胞内分子クラウディング状態の評価
Evaluation of molecular crowding based on the rotational and translational diffusion measurement in living cells
○山本 条太郎（北大・院先端生命）
Johtaro Yamamoto (*Fac. Adv. Life Sci.*)

2SGP-3　混雑化で生み出される人工細胞内の Min システム反応拡散波
A localization wave of proteins reconstituted in artificial cells with crowding environments
○藤原 慶（慶應大・生命情報）
Kei Fujiwara (*Dep. Biosci. and Info., Keio University*)

2SGP-4　Brownian motion in dense DNA solutions
Yoshihiro Murayama (*Tokyo Univ. of Agri. and Tech.*)

2SGP-5　不均一な環境下での異常拡散
Anomalous diffusion in heterogeneous environments
○秋元 琢磨（東京理科大学理工学部物理学科）
Takuma Akimoto (*Tokyo University of Science*)

2SGP-6　高分子混雑環境下での蛋白質 NMR 緩和解析
NMR relaxation analysis of the protein under macromolecular crowding environment
○岡村 英保[1], 木川 隆則[1,2]（[1]理研 生命システム研究センター, [2]東工大 情報理工学院）
Hideyasu Okamura[1], Takanori Kigawa[1,2] ([1]*RIKEN QBiC*, [2]*Department of Computer Science, Tokyo Institute of Technology*)

2SGP-7　細胞混雑中の蛋白質と代謝物のダイナミクス: 全原子分子動力学法による理論的研究
Dynamics of Proteins and Metabolites in Cellular Crowding Environment: Theoretical Study with All-atom Molecular Dynamics Simulation
○優 乙石[1,2], ワン ポーホン[2], ファイグ マイケル[3], 杉田 有治[1,2]（[1]理研 iTHES, [2]理研 杉田理論分子科学研究室, [3]ミシガン州立大）
Isseki Yu[1,2], Po-Hung Wang[2], Michael Feig[3], Yuji Sugita[1,2] ([1]*RIKEN iTHES*, [2]*RIKEN Theoretical Molecular Science Lab.*, [3]*Michigan State University*)

13:55〜16:25　K 会場（文法学部 2 階 A1 教室）／Room K (Room A1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

2SKP　Joint Symposium between Biophysical Society of R.O.C. and BSJ: Towards tomorrow's structural biology

オーガナイザー：山本 雅貴（理化学研究所），呂 平江（National Tsing Hua University）
Organizers: Masaki Yamamoto (RIKEN), Ping-Chiang Lyu (National Tsing Hua University)

Biological functions are realized by networks of proteins in the cell. Structural biology is developing in order to elucidate its function based on the three-dimensional structure of individual proteins and currently giving the high-impact results globally. This symposium is held for information exchange and cooperation between the biophysical society of Taiwan R.O.C. and the biophysical society of Japan with an overview of the current state of structural biology and its future.

2SKP-1　タンパク質微小結晶構造解析の将来に向けて
Towards the next generation protein micro-crystallography at SPring-8 and SACLA
○山本 雅貴（理化学研究所 放射光科学総合研究センター）
Masaki Yamamoto (*RIKEN RSC*)

2SKP-2　Structure and function of the polymyxin-resistance-associated response regulator PmrA
Chwan-Deng Hsiao (*Institute of Molecular Biology, Academia Sinica*)

2SKP-3　二重殻構造を持つイネ萎縮ウイルスの構造構築機構
Structure assembly mechanism of a double-shelled virus, Rice dwarf virus
東浦 彰史, 中道 優介, 堤 研太, 宮崎 直幸, 岩崎 憲治, ○中川 敦史（阪大・蛋白研）
Akifumi Higashiuira, Yusuke Nakamichi, Kenta Tsutsumi, Naoyuki Miyazaki, Kenji Iwasaki, **Atsushi Nakagawa** (*Inst. Protein Res., Osaka Univ.*)

2SKP-4　A structural proteomic approach to understand cobra venom actions beyond neurotoxicity of the bitten victims
Wen-Guey Wu (*Institute of Bioinformatics and Structural Biology, National Tsing Hua University, Taiwan*)

2SKP-5　統合構造生物学と生理学のための最新 NMR
Advanced NMR for Integrated Structural Biology and Physiology
○児嶋 長次郎[1,2]（[1]横浜国大・工, [2]阪大・蛋白研）
Chojiro Kojima[1,2] ([1]*Grad. Sch. Eng., Yokohama Nat. Univ.*, [2]*Inst. Protein Res., Osaka Univ.*)

2SKP-6　Circular permutation: Database, Prediction and Design
Ping-Chiang Lyu (*Institute of Bioinformatics and Structural Biology, National Tsing Hua University*)

13:55〜16:25　L 会場（文法学部 2 階 B1 教室）／Room L (Room B1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

2SLP　新学術領域研究「温度を基軸とした生命現象の統合的理解（温度生物学）」共催
温度と生物の接点
The Intersection between Temperature and Life

オーガナイザー：岡部 弘基（東京大学），原田 慶恵（大阪大学）
Organizers: Kohki Okabe (The University of Tokyo), Yoshie Yarada (Osaka University)

In recent years, temperature has attracted great attention in the search for deeper understanding of cell functions. Despite the universality of temperature as a physical parameter, the fundamental principles of how temperature facilitates life activities are still a mystery. In this symposium, through the introduction of the challenges thermal biology faces when exploring the mechanisms of thermal sensation and response in various organisms, we will discuss the unaddressed issues and future prospects of this innovative multidisciplinary science.

2SLP-1　細胞における温度動態：観察と意義
Thermal dynamics in individual cells: observation and significance
○森 泰生（京都大学大学院工学研究科）
Yasuo Mori (*Kyoto Univ., Grad. Sch. Engineering*)

2SLP-2 マウス体内時計の温度応答
Temperature-responses of the circadian clock oscillation in mice
○深田 吉孝（東大院理・生物科学・深田研究室）
Yoshitaka Fukada (*Dept. Biological Sciences, School of Science, The Univ. Tokyo*)

2SLP-3 16S rRNA 遺伝子の GC 含量と原核生物の生育温度との関係
Relationship between guanine-plus-cytosine content of 16S rRNA genes and growth temperature of the prokaryotic hosts
佐藤 悠[1], ○木村 浩之[2]（[1]静岡大・創造院, [2]静岡大・グリーン研）
Yu Sato[1], **Hiroyuki Kimura**[2] ([1]*Grad. Sch. Sci. Technol., Shizuoka Univ.*, [2]*Res. Inst. Green Sci. Technol., Shizuoka Univ.*)

2SLP-4 細胞内微小空間における温度と分子の相互作用
Interaction between temperature and molecules in intracellular microenvironments
○岡部 弘基[1,2], 船津 高志[1]（[1]東京大学大学院薬学系研究科, [2]JST さきがけ）
Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Graduate School of Pharmaceutical Sciences, The University of Tokyo*, [2]*JST, PRESTO*)

2SLP-5 温度応答性超分子を用いたがん集積システムの開発
Development of a tumor-accumulation system using temperature-responsive supramolecule
○唐澤 悟[1,2,3], 荒木 健[3], 臼井 一晃[3], 村山 周平[4], 青木 伊知男[4]（[1]昭和薬大, [2]JSTさきがけ, [3]九大院薬, [4]量子研）
Satoru Karasawa[1,2,3], Takeru Araki[3], Kazuteru Usui[3], Shuhei Murayama[4], Ichio Aoki[4] ([1]*Univ. Showa*, [2]*JST PRESTO*, [3]*Grad. Sch. Pharm. Univ. Kyushu*, [4]*Ins. QST*)

13:55〜16:25　M 会場（文法学部 1 階 B2 教室）／Room M (Room B2, Faculty of Letters, Faculty of Law Main Bldg. 1F)

2SMP　分子集合と生体膜の生物物理学
Biophysics of molecular assembly and biological membrane

オーガナイザー：末次 志郎（奈良先端科学技術大学院大学），嶋田 睦（九州大学）
Organizers: Shiro Suetsugu (NAIST), Atsushi Shimada (Kyushu University)

Biological membranes mediate the assemblies of proteins and other biomolecules to assist their physiological functions. Conversely, the membrane-associated assemblies of biomolecules could affect the three-dimensional configuration of the membrane and assist its function. In this symposium, we will discuss recent discoveries on these membrane-associated molecular assemblies involved in various cellular mechanisms. We will also discuss how biophysical techniques could contribute to these discoveries and provide an opportunity to consider the future of the expanding interdisciplinary field between biophysics and cell biology.

2SMP-1 エンドサイトーシス関連細胞質タンパク質の構造から迫るクラスリン重合機構
Insights into clathrin assembly from the structures of cytosolic endocytic proteins
○嶋田 睦[1,2]（[1]九大・生医研, [2]理研・播磨）
Atsushi Shimada[1,2] ([1]*Med. Inst. Bioreg., Kyushu Univ.*, [2]*RIKEN SPring-8 Center*)

2SMP-2 Dynamic remodeling of Dynamin complexes during membrane fission
Tetsuya Takeda[1], Daiki Ishikuro[2], Huiran Yang[1], Toshiya Kozai[2], Kaho Seyama[1], Yusuke Kumagai[2], Hiroshi Yamada[1], Takayuki Uchihashi[4], Toshio Ando[2,3], Kohji Takei[1] ([1]*Grad. Sch. Med. Dent. Pharm. Sci., Okayama Univ.*, [2]*Coll. Sci. Eng., Kanazawa Univ.*, [3]*Bio AFM, Kanazawa Univ.*, [4]*Dept. Phys., Nagoya Univ.*)

2SMP-3 エンドサイトーシス型受容体 ApoER2 のリガンド結合状態の結晶構造
Crystal structure of the endocytic receptor ApoER2 in the ligand-bound state
○禾 晃和（横市大・院生命医科）
Terukazu Nogi (*Grad. Sch. Med. Lif. Sci., Yokohama City Univ.*)

2SMP-4 Mechanisms of *trans*-synaptic adhesion for inducing synapse formation
Shuya Fukai (*IMCB, Univ. Tokyo*)

2SMP-5 The spatial distribution of the BAR domain proteins on the membrane
Shiro Suetsugu (*NAIST*)

2SMP-6 Molecular mechanisms involved in the reassembly of the actin cortex in membrane blebs
Junichi Ikenouchi (*Dept. Biol., Facl. Sci., Kyushu Univ.*)

2SMP-7 Role of plasma membrane tension in cell migration and invasion
Kazuya Tsujita (*Biosignal Research Center, Kobe University*)

2SMP-8 Actin polymerization in contact with the plasma membrane may be a Brownian ratchet-based information collector
Naoki Watanabe[1,2], Kazuma Koseki[2], Daisuke Taniguchi[2] ([1]*Kyoto Univ. Grad. Sch. Biostudies*, [2]*Kyoto Univ. Grad. Sch. Med.*)

13:55～16:25　N 会場（文法学部 1 階 B3 教室）／Room N (Room B3, Faculty of Letters, Faculty of Law Main Bldg. 1F)

2SNP　新学術領域研究「スパースモデリングの深化と高次元データ駆動科学の創成」共催
データ駆動科学が拓く新しい生命計測データ解析
Data-driven science opens up a new field in biological measurements

オーガナイザー：木川 隆則（理化学研究所），池谷 鉄兵（首都大学東京）
Organizers: Takanori Kigawa (RIKEN), Teppei Ikeya (Tokyo Metropolitan University)

Methods used in data-driven science, such as sparse modeling and machine learning, enable us to extract the maximum amount of information from experimental measurement data. In this symposium, the leading scientists in information science will introduce the basic theory and the state-of-the-art methods, and those in biology as well as non-biology fields will present the practical applications using these technologies. In addition, the future perspectives of biological measurement and observation methods developed by data-driven approaches will be discussed.

はじめに
Opening Remarks
○池谷 鉄兵（首都大学東京）
Teppei Ikeya (*Tokyo Metropolitan University*)

2SNP-1 スパースモデリングに基づく計測データ解析
Measurement data analysis based on sparse modeling
○田中 利幸（京都大学大学院情報学研究科）
Toshiyuki Tanaka (*Graduate School of Informatics, Kyoto University*)

2SNP-2 位相的データ解析とその応用
Topological Data Analysis and its Applications
○福水 健次（統数研）
Kenji Fukumizu (*ISM*)

2SNP-3 ディープラーニングを用いた医用 CT 画像のテクスチャ識別
Texture classification on Medical CT image using Deep Learning
○庄野 逸（電気通信大学）
Hayaru Shouno (*University of Electro Communications*)

2SNP-4 シミュレーション／データ両駆動型データ同化の創出へ
Towards a generation of the simulation-/data-driven data assimilation
○長尾 大道[1,2]（[1]東大地震研, [2]東大情報理工）
Hiromichi Nagao[1,2] ([1]*ERI, UTokyo*, [2]*IST, UTokyo*)

2SNP-5 低感度 NMR スペクトルから情報を得るための安定同位体標識法の in-cell NMR への応用
How to cope with noisy NMR spectra; application of a novel isotope labeling strategy to in-cell NMR
○葛西 卓磨[1,2], 樋口 佳恵[1], 猪股 晃介[1], 木川 隆則[1,3]（[1]理研・生命システム, [2]JST・さきがけ, [3]東工大・情報理工）
Takuma Kasai[1,2], Kae Higuchi[1], Kohsuke Inomata[1], Takanori Kigawa[1,3] ([1]*RIKEN QBiC*, [2]*PRESTO, JST*, [3]*Sch. Comput., Tokyo Inst. Tech.*)

2SNP-6 統計的画像処理による超解像顕微鏡法
Super-resolution imaging by statistical image data processing
○岡田 康志[1,2]（[1]理研・生命システム研究センター, [2]東大･理･物理）
Yasushi Okada[1,2] ([1]*Quantitative Biology Center, RIKEN*, [2]*Dept. Physics, Univ. Tokyo*)

おわりに
Closing Remarks
○木川 隆則（理化学研究所）
Takanori Kigawa (*RIKEN*)

第 3 日目（9 月 21 日（木））／Day 3（Sep. 21 Thu.）

9:00～11:30　A 会場（全学教育棟 1 階 E107）／Room A (Room E107, General Education Bldg. 1F)
3SAA　光散乱・吸収を用いた顕微鏡で探る生体情報
Biological information probed by optical microscopes using scattering and absorption

オーガナイザー：市村 垂生（理化学研究所），藤田 克昌（大阪大学）
Organizers: Taro Ichimura (RIKEN), Katsumasa Fujita (Osaka University)

Light is scattered and absorbed by molecules in various interaction processes, which includes elastic, inelastic, nonlinear, and photothermal effects, depending on molecular species and excitation schemes. By detecting and analyzing the optical responses, one can directly probe molecular structure, alignment, concentration, and surrounding environment without fluorescent labeling. In this symposium, several types of advanced microscopes using light scattering and absorption will be introduced. Biological information probed by the microscopes will be discussed to explore their biological application.

はじめに
Opening Remarks
○藤田 克昌（大阪大学）
Katsumasa Fujita (*Osaka University*)

3SAA-1　散乱光で細胞・分子の状態を測る
Light scattering microscopes to quantify the cellular and molecular states
○市村 垂生, 金城 純一, Germond Arno, 渡邉 朋信（理研・QBiC）
Taro Ichimura, Junichi Kaneshiro, Arno Germond, Tomonobu Watanabe (*RIKEN QBiC*)

3SAA-2　光第二高調波イメージングの細胞生物学研究への応用
Application of SHG imaging to cell biology
○塗谷 睦生[1,2]（[1]慶應義塾大学医学部薬理学教室, [2]横浜国立大学環境情報研究院）
Mutsuo Nuriya[1,2] ([1]*Department of Pharmacology, Keio University School of Medicine*, [2]*Graduate School of Environment and Information Sciences, Yokohama National University*)

3SAA-3　Quantitative and multimodal phase imaging for analysis of cellular characteristics
Nicolas Pavillon, **Nicholas Smith** (*Osaka Univ, IFReC*)

3SAA-4　非ラベル分子の画像化のための位相敏感広帯域 CARS 分光
Phase-sensitive multiplex-CARS spectroscopy for label-free molecular imaging
○鈴木 隆行[1], 小原 祐樹[2], 三沢 和彦[2]（[1]明治大・院理工, [2]農工大・院工）
Takayuki Suzuki[1], Yuki Obara[2], Kazuhiko Misawa[2] ([1]*Grad. Sch. Sci., Meiji Univ.*, [2]*Grad. Sch. Eng., Tokyo Univ. of A&T*)

3SAA-5　誘導ラマン散乱顕微法による高速代謝物イメージング
High-speed imaging of metabolites with stimulated Raman scattering microscopy
○小関 泰之（東京大学大学院工学系研究科電気系工学専攻）
Yasuyuki Ozeki (*Department of Electrical Engineering and Information Systems, University of Tokyo*)

3SAA-6　光熱変換顕微法による生物組織の高感度・高分解光吸収イメージング
Photothermal microscopy for high sensitivity and high resolution absorption contrast imaging of biological tissues
○宮崎 淳（和歌山大学システム工学部）
Jun Miyazaki (*Fac. Sys. Eng., Wakayama Univ.*)

おわりに
Closing Remarks
○市村 垂生（理化学研究所）
Taro Ichimura (*RIKEN*)

9:00～11:30　B 会場（全学教育棟 2 階 B201）／Room B (Room B201, General Education Bldg. 2F)

3SBA　量子ビーム技術を活用した放射線生物物理学の最前線
Frontiers in radiation biophysics utilizing quantum beam technologies

オーガナイザー：冨田 雅典（電力中央研究所），中島 徹夫（量子科学技術研究開発機構）
Organizers: Masanori Tomita (Central Research Institute of Electric Power Industry), Tetsuo Nakajima (National Institute of Radiological Sciences)

Nowadays the quantum beam technology progresses remarkably. Energy and targeted irradiation region of quantum beams, including high-energy charged particles, synchrotron radiations and microbeams, can be controlled with high accuracy. These advances have led us to elucidate the long-term issues in radiation biophysics, i.e., distribution of DNA damage, intra- and inter-cellular communications, inter-tissue signaling, different effects due to radiation qualities etc. In this symposium, we introduce recent progresses of radiation biophysics using quantum beam technology and discuss the application of our results to studies of radiation effects and radiotherapy.

3SBA-1　高 LET 重イオン線によってヒト正常線維芽細胞に誘導されるバイスタンダーシグナル伝達と細胞死の機構解明
High-LET heavy-ion-induced bystander signalling and cell death in normal human fibroblasts
○冨田 雅典（電中研・原技研・放射線安全）
Masanori Tomita (*Radiat. Safety Res. Cent., CRIEPI*)

3SBA-2　高 LET 放射線による DNA 酸化損傷の生成とその分布観察
Observation of DNA oxidative damage induced by high LET radiation
○伊藤 敦（東海大・工）
Atsushi Ito (*Sch. Eng. Tokai Univ.*)

3SBA-3　Analysis of the modification of cell death by energy deposition to a local site in a cell
Munetoshi Maeda (*Proton Medic. Res. Gr., WERC*)

3SBA-4　Computational analysis of bystander signaling in cellular population irradiated with microbeam
Yuya Hattori[1], Akinari Yokoya[2], Daisuke Kurabayashi[1], Ritsuko Watanabe[2] ([1]*Dept. of Sys. & Ctrl. Eng., Sch. of Eng., Tokyo Tech.*, [2]*Quantum Beam Science Research Directorate, QST*)

3SBA-5　マイクロビーム照射とシミュレーションを用いた線虫の筋運動に対する放射線影響の解析
Analyses of radiation effects on muscular movements in *Caenorhabditis elegans* using microbeam irradiation and simulation-based approach
○鈴木 芳代[1], 服部 佑哉[2], 坂下 哲哉[1], 横田 裕一郎[1], 小林 泰彦[1], 舟山 知夫[1]（[1]量研 高崎研 放射線生物応用, [2]東工大 工学院 システム制御系）
Michiyo Suzuki[1], Yuya Hattori[2], Tetsuya Sakashita[1], Yuichiro Yokota[1], Yasuhiko Kobayashi[1], Tomoo Funayama[1] ([1]*Dept. of Radiat. Appl. Biol. Res., QST-Takasaki*, [2]*Dept. of Sys. & Ctrl. Eng., Sch. of Eng., Tokyo Tech*)

3SBA-6　メダカ胚で観察された重イオン局所照射によって誘発される照射野以外への影響
Abscopal activation of microglia in embryonic fish brain following targeted irradiation with heavy-ion microbeam
○保田 隆子[1], 尾田 正二[1], 舟山 知夫[2], 三谷 啓志[1]（[1]東京大 新領域, [2]量研機構 高崎量子応用研 放射線生）
Takako Yasuda[1], Shoji Oda[1], Tomoo Funayama[2], Hiroshi Mitani[1] ([1]*Grad. Sch. Frontier Sci., Univ. Tokyo*, [2]*TARRI, QuBS, QST*)

3SBA-7　生物影響からみた光子放射線と粒子放射線の違いー評価と防護ー
Differences between photon and particle radiations in terms of their biological effects: Evaluation and protection
○中島 徹夫（量研機構・放医研・放射線影響）
Tetsuo Nakajima (*Dept of Radiation Effects Research, NIRS, QST*)

9:00〜11:30　C 会場（全学教育棟 2 階 B202）／Room C (Room B202, General Education Bldg. 2F)

3SCA　ATP をエネルギー源とする生物装置の構造、機能、および ATPase による動力発生機構
ATP energized biological machines: their structure, function and force generation mechanism coupled with ATPase

オーガナイザー：加藤 博章（京都大学），前田 雄一郎（名古屋大学）
Organizers: Hiroaki Kato (Kyoto University), Yuichiro Maeda (Nagoya University)

ATP is the energy source of organism and the cleavage of one of the phosphoanhydride bonds generates force that drives biologically important processes. This symposium focuses force generation mechanism of biomolecules such as a proton pump, dynein motor, ATP binding cassette transporter, circadian clock, KaiC, and filamentous actin. The speakers we invited have been studying the structure and mechanism of each machine at the research frontier. We try to find their common mechanistic behavior underlying force generation mechanism by ATP hydrolysis.

はじめに
Opening Remarks

3SCA-1　F 型結晶構造から明らかとなったアクチン重合と ATP 加水分解機構
ATPase mechanism and dynamic assembly of actin revealed by the F-form crystal structures
○武田 修一[1], 成田 哲博[1], 小田 俊朗[2], 田中 康太郎[1], 小池 亮太郎[3], 太田 元規[3], 藤原 郁子[4], 渡邉 信久[5], 前田 雄一郎[1]
([1]名大・院生命理学, [2]東海学院大, [3]名大・院情報科学, [4]名工大・材料科学フロンティア研究院, [5]名大・シンクロトロン）
Shuichi Takeda[1], Akihiro Narita[1], Toshiro Oda[2], Kotaro Tanaka[1], Ryotaro Koike[3], Motonori Ota[3], Ikuko Fujiwara[4], Nobuhisa Watanabe[5], Yuichiro Maeda[1] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*Univ. Tokaigakuin*, [3]*Grad. Sch. of Info. Sci., Univ. Nagoya*, [4]*FRIMS., NITech*, [5]*SRRC., Univ. Nagoya*)

3SCA-2　Struture and mechanism of dynein motors
Takahide Kon (*Dept. of Biol. Sci., Grad. Sch. of Sci., Osaka Univ.*)

3SCA-3　回転分子モーターの分子動力学シミュレーション
Molecular dynamics simulations of molecular rotary motors
○池口 満徳（横浜市立大学）
Mitsunori Ikeguchi (*Yokohama City Univ.*)

3SCA-4　Design of circadian clock of cyanobacteria by dual ATPases in KaiC
Takao Kondo (*Nagoya Univ*)

3SCA-5　ABC トランスポーターは ATP 結合と加水分解のエネルギーを多剤排出にどのように利用するのか
How ATP binding cassette (ABC) transporter harnesses the energy of ATP binding and hydrolysis to multidrug export
○加藤 博章[1,2]（[1]京大・院薬, [2]理研・播磨）
Hiroaki Kato[1,2] ([1]*Grad. Sch. Pharm. Sci., Kyoto Univ.*, [2]*RIKEN/SPring-8*)

おわりに
Closing Remarks
Yuichiro Maeda

9:00〜11:30　D 会場（全学教育棟 2 階 E201）／Room D (Room E201, General Education Bldg. 2F)

3SDA　ゲノム機能制御の多階層的理解 〜クロマチンの分子構造から核内動態まで〜
Understanding genomic functions in multiscale from chromatin structure to intranuclear dynamics

オーガナイザー：日比野 佳代（国立遺伝学研究所/総合研究大学院大学），落合 博（広島大学）
Organizers: Kayo Hibino (NIG / SOKENDAI), Hiroshi Ochiai (Hiroshima University)

The structure and dynamics of chromatin have been suggested to be closely related to the nuclear functions and disease. However, it is not fully understood how they regulate the function in the nucleus. Recent technologies related to live imaging, genome editing, and higher-order genomic structural analysis are clarifying how genomic DNA behaves dynamically in the nucleus. Based on these cutting-edge research results, we will discuss the relationship among the structure, dynamics of chromatin, and nuclear function from the molecule to the entire nuclear level.

3SDA-1　Structural analysis of the centromere specific nucleosome
Hiroaki Tachiwana[1,2], Midori Suzuki[3], Yoshimasa Takizawa[4], Matthias Wolf[4], Hitoshi Kurumizaka[2] ([1]*Japanese Foundation for Cancer Research, Cancer Institute*, [2]*Faculty of Science & Engineering, Waseda University*, [3]*Graduate School of Advanced Science & Engineering, Waseda University*, [4]*Okinawa Institute of Science and Technology Graduate University*)

3SDA-2　単一ヌクレオソームイメージングが明かすクロマチンダイナミクスと転写
Single nucleosome imaging reveals global chromatin stabilization upon transcription
○日比野 佳代[1,2], 永島 崚甫[2], 前島 一博[1,2]（[1]遺伝研, [2]総研大）
Kayo Hibino[1,2], Ryosuke Nagashima[2], Kazuhiro Maeshima[1,2] ([1]*NIG*, [2]*SOKENDAI*)

3SDA-3　Relationship between kinetics of higher-order genomic structure and transcriptional activity
Hiroshi Ochiai[1,2] ([1]*PRESTO, JST*, [2]*Grad. Sch. Sci., Hiroshima Univ.*)

3SDA-4　Transcription dynamics in living Drosophila embryos
Takashi Fukaya, Tyler Heist, Michael Levine (*Lewis-Sigler Institute for Integrative Genomics, Princeton University*)

3SDA-5　リボソーム RNA 遺伝子の核内動態： DNA 複製阻害タンパク質 Fob1 と DNA 損傷チェックポイントタンパク質に依存した核膜孔との結合
Fob1-dependent binding of ribosomal RNA genes to the nuclear periphery in budding yeast
○堀籠 智洋[1], 鵜之沢 英理[1,2,3], 大木 孝将[1], 小林 武彦[1,2,3]（[1]東京大学・分生研, [2]遺伝研, [3]総研大）
Chihiro Horigome[1], Eri Unozawa[1,2,3], Takamasa Ooki[1], Takehiko Kobayashi[1,2,3] ([1]*Inst. Mol. Cell. Biosci., Univ. Tokyo*, [2]*NIG*, [3]*SOKENDAI*)

3SDA-6　３次元ゲノム構造の多階層的理解〜ヌクレオソームレベルから全染色体レベルまで〜
Understanding 3D genome structure in mulitiscale from the nucleosome to whole choromosome level
○谷口 雄一（理化学研究所生命システム研究センター）
Yuichi Taniguchi (*Quantitative Biology Center, RIKEN*)

3SDA-7　キャプチャー Hi-C を用いたゲノム間相互作用解析
Genome wide interaction analysis using Capture Hi-C
○堤 修一[1], 岡部 篤史[2], 油谷 浩幸[1]（[1]ゲノムサイエンス, 東大・先端研, [2]分子腫瘍, 千葉大・院・医学研究院）
Shuichi Tsutsumi[1], Atsushi Okabe[2], Hiroyuki Aburatani[1] ([1]*Genome Sci. Div., RCAST, Univ. Tokyo*, [2]*Mol. Onc., Grad. Sch. of Med., Univ. Chiba*)

3SDA-8　Bridging the gap between the dynamics and organization of chromatin domains by mathematical modeling
Soya Shinkai[1,2], Tadasu Nozaki[3], Kazuhiro Maeshima[3], Yuichi Togashi[2] ([1]*RIKEN QBiC*, [2]*RcMcD, Hiroshima Univ.*, [3]*Natl. Inst. of Genet.*)

9:00〜11:30　F 会場（全学教育棟 2 階 E205）／Room F (Room E205, General Education Bldg. 2F)

3SFA　多角的な視点で読み解く膜デバイスの基本原理と新しい機能解析技術
Multiple aspects to understand mechanisms of membrane proteins as devices and novel approaches to dissect biomolecules

オーガナイザー：西坂 崇之（学習院大学），小嶋 誠司（名古屋大学）
Organizers: Takayuki Nishizaka (Gakushuin University), Seiji Kojima (Nagoya University)

How far is the elucidation of the basic principle of membrane proteins approaching the goal? In this symposium, we would like to address this question with the audience by introducing latest results based on various innovative methods. Topics include new developments of structural biology, computational simulation, advanced optical microscopies and microfabrications. These original researches from a multilateral perspective will reveal mechanisms of diverse membrane devices such as membrane receptors, pumps and transporters, which help us to look at the direction of biophysics ten years ahead.

はじめに
Opening Remarks
Takayuki Nishizaka

3SFA-1 Single-Molecule Detection of Biomolecules and Protein Conformational Dynamics
Takayuki Nishizaka[1], Shoko Fujimura[2], Yoshiro Sohma[2,3], Daisuke Nakane[1] ([1]*Dept. Phys., Gakushuin Univ.*, [2]*Sch. of Med, Keio Univ.*, [3]*Sch. of Pharm, IUHW*)

3SFA-2 小胞型ヌクレオチドトランスポーターのアロステリック制御
Allosteric regulation of vesicular nucleotide transporter
○表 弘志（岡山大学大学院医歯薬）
Hiorshi Omote (*Okayama University Grad. School of Med., Dent. and Pharm. Sci.*)

3SFA-3 Single molecule analysis of membrane transport proteins using artificial cell-membrane microsystems
Rikiya Watanabe (*Department of Applied Chemistry, The University of Tokyo*)

3SFA-4 ギャップ結合チャネルのクライオ電子顕微鏡単粒子解析
Single particle cryo-EM of a gap junction channel
○大嶋 篤典[1,2]（[1]名古屋大学細胞生理学研究センター, [2]名大・院・創薬）
Atsunori Oshima[1,2] ([1]*CeSPI, Nagoya Univ.*, [2]*Dept. Pha., Nagoya Univ.*)

3SFA-5 Ca^{2+}-ATPase の E1/E2 転移における大規模構造変化の分子動力学法シミュレーション
Molecular dynamics simulations for conformational changes on E1/E2 transition of Ca^{2+}-ATPase
○小林 千草[1], 松永 康佑[1,2], Jung Jaewoon[1,3], 杉田 有治[1,3,4]（[1]理研, AICS, [2]JST, さきがけ, [3]理研, 杉田理論分子科学, [4]理研, QBiC）
Chigusa Kobayashi[1], Yasuhiro Matsunaga[1,2], Jaewoon Jung[1,3], Yuji Sugita[1,3,4] ([1]*RIKEN, AICS*, [2]*JST, PRESTO*, [3]*RIKEN, TMS*, [4]*RIKEN, QBiC*)

3SFA-6 Mechanics of Single Protein Molecules
Matthias Rief (*Technischen Universität München, Physik-Department*)

9:00〜11:30　G 会場（全学教育棟 3 階 C301）／Room G (Room C301, General Education Bldg. 3F)

3SGA　実験・シミュレーション・データ科学の融合による遺伝情報分子システムの生物物理
Biophysics of genetic information molecules and systems: Integrated approach of experiments, simulations, and data science

オーガナイザー：高田 彰二（京都大学），笹井 理生（名古屋大学）
Organizers: Shoji Takada (Kyoto University), Masaki Sasai (Nagoya University)

Genome contains not only gene sequence information but also information on which, when, and how genes are expressed. To understand genetic information molecules, we need to know proteins working therein, 3D chromatin structures, and transcriptions. Towards that goal, we integrate experiments with physical simulations and data science. In this symposium, we discuss biophysical challenges for genetic information molecules by experiments, simulations, data science, and their collaboration.

3SGA-1　分子シミュレーションによるヌクレオソームと転写因子の動態研究
Dynamics of nucleosomes and transcription factors studied by molecular simulations
○高田 彰二（京大院理・生物物理）
Shoji Takada (*Biophys. Sci. Kyoto Univ*)

3SGA-2　methyl CpG 結合ドメインタンパク質の分子基盤研究
Structural biochemistry of methyl CpG binding domain containing proteins
○有吉 眞理子（阪大・院・生命機能）
Mariko Ariyoshi (*Grad. Sch. Frotier Bio.*)

3SGA-3　高速 AFM による天然変性タンパク質の構造動態解析
Structural dynamics analysis of intrinsically disordered proteins by high-speed AFM
○古寺 哲幸[1], 能代 大輔[1,2], Dora Sujit[1], 安藤 敏夫[1,2]（[1]金沢大・バイオAFM, [2]CREST・JST）
Noriyuki Kodera[1], Daisuke Noshiro[1,2], Sujit Dora[1], Toshio Ando[1,2] ([1]*Bio-AFM FRC, Kanazawa Univ.*, [2]*CREST, JST*)

3SGA-4　Chromosome association of noncoding RNA during homologous chromosome pairing in fission yeast meiosis
Da-Qiao Ding[2], Tokuko Haraguchi[1,2], **Yasushi Hiraoka**[1,2] ([1]*Graduate School of Frontier Biosciences, Osaka University*, [2]*National Institute of Information and Communications Technology*)

3SGA-5　シーケンシングと分子動力学計算の組み合わせによるクロマチン 3D 構造解析
3D chromatin structure revealed by the combination of sequencing analysis and molecular dynamics simulation
○大野 雅恵[1], 安藤 格士[2], 谷口 雄一[1]（[1]理研・QBiC, [2]東理大・基礎工・電子応用）
Masae Ohno[1], Tadashi Ando[2], Yuichi Taniguchi[1] ([1]*QBiC, RIKEN*, [2]*Dept. of Appl. Elec., Tokyo Univ. of Science*)

3SGA-6　高解像度 Hi-C データを活用した遺伝子発現制御の理解
Understanding gene regulation by using high-resolution Hi-C data
○須山 幹太（九州大学生体防御医学研究所）
Mikita Suyama (*Medical Institute of Bioregulation, Kyushu University*)

3SGA-7　The phase-separation principle of human genome architecture
Shin Fujishiro, Masaki Sasai (*Dept. Comp. Sci. & Eng., Nagoya Univ.*)

9:00〜11:30　I 会場（全学教育棟 3 階 E305）／Room I (Room E305, General Education Bldg. 3F)

3SIA　新機能分子系を創出してきた地球生物進化と試験管内進化の対話
Dialogue between in vitro evolution and biological evolution, both of which have created new functional biomolecules

オーガナイザー：根本 直人（埼玉大学），赤沼 哲史（早稲田大学）
Organizers: Naoto Nemoto (Saitama University), Satoshi Akanuma (Waseda University)

Unlike biological evolution in organisms, in vitro evolutionary molecular engineering has focused on single molecules as the targets of evolution to understand the basic principle of molecular evolution. The research field has now created functional molecules so called 'NEO-biomolecules'. The next step of artificial evolution is to evolve systems involving more than one molecule, such as ribosomes. In this symposium, we will discuss the relationship between evolutions of single molecules and complex systems, to accelerate the progress of both fields.

3SIA-1　Biobit の可能世界
Possible world of Biobit
○伏見 譲（JST先端計測）
Yuzuru Husimi (*Japan Science and Technology Agency*)

3SIA-2　VHH ファージライブラリーからの有用な抗体の迅速単離と試験管内抗体進化
Rapid isolation of valuable antibodies from VHH phage display libraries and in vitro antibody evolution
○村上 明一[1], 吉田 麻衣子[1,2], 塚原 成俊[3], 東 隆親[2], 岸本 英博[1]（[1]琉球大学大学院医学研究科 寄生虫・免疫病因病態学講座, [2]株式会社抗体工学研究センター, [3]イノベックスサイエンス株式会社）
Akikazu Murakami[1], Maiko Yoshida[1,2], Narutoshi Tsukahara[3], Takachika Azuma[2], Hidehiro Kishimoto[1] ([1]*Grad. Sch of Med., U-Ryukyus*, [2]*Antibody Engineering Research Center Inc.*, [3]*Innovex Science Co., Ltd.*)

3SIA-3　網羅的配列解析による抗体ファージライブラリーからの抗原特異的抗体の効率的な選別
Efficient selection of antigen-specific antibodies from phage library using high throughput sequencing
○伊東 祐二（鹿児島大学大学院理工学研究科生命化学専攻）
Yuji Ito (*Grad. Sch. Sci. and Eng., Kagoshima Univ.*)

3SIA-4　アミノ酸の種類が制限された cDNA ディスプレイライブラリからのポリメラーゼリボザイムに対するコファクターペプチドの試験管内淘汰
In Vitro selection of cofactor peptides of polymerase ribozyme form a cDNA display library composing of limited set of amino acids
○熊地 重文（(株）Epsilon Molecular Engineering）
Shigefumi Kumachi (*Epsilon Molecular Engineering Inc.*)

3SIA-5　Evolutionary Engineering and Characterization of Membrane Proteins Using Liposome Display
Tomoaki Matsuura (*Dep. Biotechnol, Grad. Sch. Eng., Osaka Univ.*)

3SIA-6　Rapid adaptation of RNA bacteriophage to environmental changes
Akiko Kashiwagi (*Fac. Agr and LifSci, Hirosaki Univ.*)

3SIA-7　バクテリア 16S rRNA の進化中立性の実験的検証
Comparative RNA function analysis reveals primarily neutral evolvability of bacterial 16S rRNA genes
○宮崎 健太郎[1,2]（[1]産総研 生物プロセス, [2]東大院 新領域）
Kentaro Miyazaki[1,2] ([1]*AIST*, [2]*Univ Tokyo*)

3SIA-8　Evolution and function of OEC-family proteins in chloroplasts
Kentaro Ifuku (*Grad. Sch. Biostudies, Kyoto Univ.*)

3SIA-9　進化分子工学と極限環境生物
Evolutionary Engineering and Extremophiles
○大島 泰郎（共和化工(株)環境微生物学研究所）
Tairo Oshima (*Inst. Environ. Microbiol., Kyowa-Kako*)

9:00〜11:30　K 会場（文法学部 2 階 A1 教室）／Room K (Room A1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

3SKA　メカニカルコミュニケーションが生み出す生体運動の多様性
Diversity of biological motility generated by mechanical communications

オーガナイザー：宮田 真人（大阪市立大学），今田 勝巳（大阪大学）
Organizers: Makoto Miyata (Osaka City University), Katsumi Imada (Osaka University)

While living organisms commonly utilize the energy produced by hydrolysis of nucleotide or electrochemical potential across cell membrane for their motility, they have developed various power transmission mechanisms unique to each individual. In this symposium, we will discuss molecular mechanism of power transmission that produces diversity of the biological motility, namely 'mechanical communication', from various viewpoints including structure, theory, molecular and cellular biology, and dynamics.

はじめに
Opening Remarks
Makoto Miyata

3SKA-1　ハプト藻に存在するハプトネマの急速コイリング運動における微小管ダイナミクス
Microtubule dynamics for rapid coiling movement of haptonema in the haptophyte algae
○野村 真未[1], 阿閉 耕平[1], 広瀬 恵子[2], 柴 小菊[1], 稲葉 一男[1]（[1]筑波大学 下田臨海実験センター, [2]産業技術総合研究所 バイオメディカル研究部門）
Mami Nomura[1], Kohei Atsuji[1], Keiko Hirose[2], Kogiku Shiba[1], Kazuo Inaba[1] ([1]*Shimoda Marine Research Center, University of Tshukuba*, [2]*Biomedical Research Institute, National Institute of Advanced Industrial Science and Technology*)

3SKA-2　螺旋形細菌レプトスピラの遊泳と滑走のメカニズム
Swimming and gliding mechanisms of the spirochete *Leptospira*
○中村 修一（東北大・院工）
Shuichi Nakamura (*Grad. Sch. Eng., Tohoku Univ.*)

3SKA-3　Structure, mechanics, and shape dynamics of Spiroplasma
Hirofumi Wada (*Department of Physical Sciences, Ritsumeikan University*)

3SKA-4　Mechano-electrical communications in actin filament
Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

3SKA-5　Hypervariation in primary and quaternary structures of ParMs, prokaryotic actin-like polymerizing motors
Robert C. Robinson[1,2] ([1]*Institute of Molecular and Cell Biology*, [2]*RIIS, Okayama Univ.*)

3SKA-6　クライオ電子顕微鏡で解き明かす細菌べん毛モーター回転子の立体構造と回転対称性
Structure and rotational symmetry of the rotor of the bacterial flagellar motor revealed by electron cryomicroscopy
○川本 晃大[1], 宮田 知子[1], 木下 実紀[1], 南野 徹[1], 加藤 貴之[1], 難波 啓一[1,2]（[1]阪大院・生命機能, [2]理研・QBiC）
Akihiro Kawamoto[1], Tomoko Miyata[1], Miki Kinoshita[1], Tohru Minamino[1], Takayuki Kato[1], Keiichi Namba[1,2] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ*, [2]*QBiC., RIKEN*)

3SKA-7　べん毛軸構造蛋白質の構造と集合体形成
Structure and assembly of bacterial flagellar axial proteins
○今田 勝巳（阪大・院理）
Katsumi Imada (*Grad. Sch. Sci., Osaka Univ.*)

9:00〜11:30　L 会場（文法学部 2 階 B1 教室）／Room L (Room B1, Faculty of Letters, Faculty of Law Main Bldg. 2F)

3SLA　疾患関連タンパク質の生物物理学とその医学・薬学への応用
Biophysical approach on disease-related proteins toward application for medical and pharmaceutical sciences

オーガナイザー：濵田 大三（神戸大学），李 映昊（大阪大学）
Organizers: Daizo Hamada (Kobe University), Young-Ho Lee (Osaka University)

Biophysical approaches have been widely applied to medical and pharmaceutical researches on disease-related proteins. Despite of extensive endeavors, much remains to be learnt about how biophysical application is effectively used to understand the underlying molecular mechanisms of disease onset and progression, and to develop the methodologies for the prevention and cure of diseases. In this symposium, we invite several qualified researchers and discuss the state-of-the-art biophysical method and perspective of the biophysics for medical and pharmaceutical researches.

3SLA-1　AL アミロイドーシスにおけるアミロイド形成の引金 - 診断と阻害戦略への展望
Triggers of amyloid formation in AL amyloidosis - perspective for development of diagnosis and inhibition strategy
○濵田 大三[1,2,3]（[1]神戸大・工, [2]神戸大 統合研究拠点 応用構造科学, [3]理研 SPring-8）
Daizo Hamada[1,2,3] ([1]*Grad Sch Eng, Kobe Univ*, [2]*CASS, Kobe Univ*, [3]*RIKEN SPring-8*)

3SLA-2　Ras がん遺伝子産物を分子標的としたがん治療薬のインシリコ創薬
In silico discovery of anti-cancer drugs targeting the Ras oncoproteins
○片岡 徹（神戸大・院医）
Tohru Kataoka (*Grad Sch Med, Kobe Univ.*)

3SLA-3　Computational approach for understanding protein-aggregation diseases
Sihyun Ham (*Dept of Chem, Sookmyung Women's Univ.*)

3SLA-4　動的構造解析による多剤耐性転写制御因子の非特異的かつ高親和性な結合メカニズムの解明
Promiscuous high-affinity recognition of a multidrug resistance transcriptional regulator revealed by structural dynamics analyses
○竹内 恒[1], 今井 美咲[1,2], 徳永 裕二[1], 嶋田 一夫[3]（[1]産総研・創薬分子, [2]バイオ産業情報化コンソ, [3]東京大・院薬系）
Koh Takeuchi[1], Misaki Imai[1,2], Yuji Tokunaga[1], Ichio Shimada[3] ([1]*AIST, Molprof*, [2]*JBIC*, [3]*The Univ of Tokyo, Grad Sch Pharma Sci*)

3SLA-5　熱測定によるアミロイド疾患の診断を目指した研究
Calorimetric approach for investigating disease-related amyloidogenesis
○李 映昊（大阪大・蛋白質研究所）
Young-Ho Lee (*Inst of Protein Res, Osaka Univ.*)

9:00〜11:30　M 会場（文法学部 1 階 B2 教室）／Room M (Room B2, Faculty of Letters, Faculty of Law Main Bldg. 1F)

3SMA　構造生物学研究ツールの進展〜どう使い分けるか？
Tools in a new epoch for structural biology. ~How to use them properly?~

オーガナイザー：岩崎 憲治（大阪大学），タマ フロハンス（名古屋大学/理化学研究所）
Organizers: Kenji Iwasaki (Osaka University), Florence Tama (Nagoya University/RIKEN)

While X-ray crystallography is a longstanding, powerful tool in structural biology, cryo-electron microscopy and X-ray free electron laser have recently reported vivid results which would not be obtainable by conventional methods. Furthermore, integration of these experimental data work computational methods such as molecular dynamics, can provide information on dynamics and conformational states of biological molecules. In this symposium, studies illustrating these methods, integration of these methods to gain insights into structure and dynamics will be presented.

3SMA-1　原子分解能をめざしたクライオ電子顕微鏡の技術開発
Towards atomic resolution structural analysis by electron cryomicroscopy
○難波 啓一（阪大・生命機能）
Keiichi Namba (*Grad Schl Frontier Biosci, Osaka Univ*)

3SMA-2 近原子分解能クライオ電子顕微鏡単粒子解析に向けたデータ測定及び画像処理条件の最適化
Studies on Data Acquisition Conditions and Image Processing for Near-atomic Resolution Cryo-EM Single Particle Analysis
○横山 武司（理研CLST）
Takeshi Yokoyama (*CLST., RIKEN*)

3SMA-3 SACLA を用いたタンパク質の時間分割構造解析
Time-resolved x-ray crystallography at SACLA
○岩田 想[1,2]（[1]京大院・医, [2]理研・放射光科学総合研究センター）
So Iwata[1,2] ([1]*Grad. Sch. Med., Univ. Kyoto*, [2]*SPring-8 Center, RIKEN*)

3SMA-4 XFEL によって明らかになった光化学系 II 水分解触媒の中間体構造と反応機構
Structure of an intermediate S-state of photosystem II and the mechanism of water-splitting revealed by XFEL
○沈 建仁（岡山大学異分野基礎科学研究所）
Jian-Ren Shen (*Res. Inst. for Interdiscip. Sci., Okayama Univ.*)

3SMA-5 Computational tools to characterize structure and dynamics of biomolecular systems from single molecule experiments
Florence Tama[1,2,3] ([1]*RIKEN AICS*, [2]*Nagoya University, Physics*, [3]*ITbM-WPI*)

3SMA-6 電子顕微鏡法のための画像解析と構造決定法の紹介
Image analysis and structural reconstruction for electron microscopy
○安永 卓生（九工大・情報工・生命情報工）
Takuo Yasunaga (*Dept. of Biosci. Bioinfo., Sch. of Comp. Sci. Sys. Eng., Kyutech*)

9:00～11:30　N 会場（文法学部 1 階 B3 教室）／Room N (Room B3, Faculty of Letters, Faculty of Law Main Bldg. 1F)

3SNA　生体分子におけるケト-エノール互変異性
Keto-enol tautomerism in biomolecules

オーガナイザー：岩田 達也（東邦大学），伊藤 奨太（名古屋工業大学）
Organizers: Tatsuya Iwata (Toho University), Shota Ito (Nagoya Institute of Technology)

Keto (R–C(=O)CH–R'R'') and enol (R–C(OH)=C–R'R'') forms are tautomers of each other, and the equilibrium is called as keto-enol tautomerism. In general, the keto form is more stable than its enol tautomer in simple compounds. However, keto-enol tautomerism is utilized for the regulation of proper reactions in biomolecules. Therefore, response regulation mechanism by keto-enol tautomerism reaction on biomolecules is one of the interesting topic in biophysics. Researches on keto-enol tautomerism of biomolecules will be presented and variety and reaction mechanisms will be discussed.

はじめに
Opening Remarks

3SNA-1 Keto-enol tautomerism of Gln on BLUF domain
Shota Ito (*Nagoya Inst. Tech.*)

3SNA-2 核酸分子におけるケト-エノール互変異性
Keto-enol tautomerism in nucleic acids
○紙谷 浩之（広島大・院医歯薬保（薬））
Hiroyuki Kamiya (*Grad. Sch. Biomed. Hlth. Sci., Hiroshima Univ.*)

3SNA-3 タンパク質環境における互変異性に関する計算科学的研究
Computational Studies on tautomerism in protein environment
○重田 育照[1], 神谷 克政[2], 庄司 光男[1]（[1]筑波大学計算科学研究センター, [2]神奈川工科大学基礎・教育センター）
Yasuteru Shigeta[1], Katsumasa Kamiya[2], Mitsuo Shoji[1] ([1]*Center for Computational Sciences, University of Tsukuba*, [2]*Center for Basic Education and Integrated Learning*)

3SNA-4 植物の葉の香りを決めるケトエノール互変
Keto-enol tautomerism determining plant leaf fragrance
○山内 靖雄（神戸大学大学院農学研究科）
Yasuo Yamauchi (*Grad. Sch. Agr. Sci., Kobe Univ.*)

3SNA-5 Keto-enol tautomerism of curcumin upon binding to amyloid fibrils
Daijiro Yanagisawa (*Mol. Neurosci. Res. Ctr, Shiga Univ. Med. Sci.*)

口頭発表　Oral Presentation

第 1 日目（9 月 19 日（火））／Day 1（Sep. 19 Tue.）

13:20〜16:20　B 会場（全学教育棟 2 階 B201）／Room B (Room B201, General Education Bldg. 2F)
1B　筋肉Ⅰ，分子モーターⅠ / Muscle I, Molecular motor I

1B1320　ウサギ骨格筋線維の X 線赤道反射に対するミオシン阻害剤の効果
Effects of myosin inhibitors on the X-ray equatorial reflections of rabbit skeletal muscle
○岩本 裕之（SPring-8･JASRI）
Hiroyuki Iwamoto (*SPring-8 JASRI*)

1B1332　ミオシン分子の巧みな集団運動によって心筋細胞の高速振動周期は一定に調節される
Constant beating frequency of sarcomeres in cardiomyocytes regulated ingeniously by collective motion of myosin molecules
○新谷 正嶺[1,2], 鷲尾 巧[3], 樋口 秀男[1]（[1]東大・理学・物理, [2]日本学術振興会・学振PD, [3]東大・新領域・人環）
Seine Shintani[1,2], Takumi Washio[3], Hideo Higuchi[1] ([1]*Dept. of Phys., Univ. of Tokyo*, [2]*JSPS Research Fellow*, [3]*Dept. Human and Eng. Env., Univ. of Tokyo*)

1B1344*　心筋ミオシンの自発的振動の解明
spontaneous oscillation of cardiac myosins
○黄 勇太, 樋口 秀男, 茅 元司（東京大・院理）
Yongtae Hwang, Hideo Higuchi, Motoshi Kaya (*Univ. of Tokyo Dep. Science*)

1B1356*　アクチンの切断は動的ネットワークの収縮を誘起する
The fragmentation of actin filaments induces the contraction of the active network
○松田 恭平, 小林 琢也, 須河 光弘, 豊島 陽子, 矢島 潤一郎（東京大学大学院 総合文化研究科）
Kyohei Matsuda, Takuya Kobayashi, Mitsuhiro Sugawa, Yoko Y. Toyoshima, Junichiro Yajima (*Graduate School of Arts and Sciences, The University of Tokyo*)

1B1408*　細胞質ダイニンのマルチスケールシミュレーション：全原子から連続体へ
Multiscale Simulations of Cytoplasmic Dynein: From All-atom to Continuum Mechanics
○飯田 慎仁[1,3], Hanson Benjamin[3], 神谷 成敏[2], 栗栖 源嗣[1], 昆 隆英[3], 中村 春木[1], Harris Sarah[4]（[1]阪大・蛋白研, [2]兵県大院・シミュレーション, [3]阪大院・理, [4]Sch. Phys. Astro., Univ. Leeds）
Shinji Iida[1,3], Benjamin Hanson[3], Narutoshi Kamiya[2], Genji Kurisu[1], Takahide Kon[3], Haruki Nakamura[1], Sarah Harris[4] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sch. SS., Univ. Hyogo*, [3]*Grad. Sch. Sci., Osaka Univ.*, [4]*Sch. Phys. Astro., Univ. Leeds*)

休憩（Coffee Break）　14:20–14:26

1B1426*　キネシンネックリンカーによる発生力は小さい
Neck linker of kinesin is low force generator
○近藤 雄一, 樋口 秀男（東京大学）
Yuichi Kondo, Hideo Higuchi (*Grad. Sch. Sci., Univ. of Tokyo*)

1B1438*　N 末端側 β バレルヘッドバンドが V_1-ATPase の非対称性を産み及び協同性を付与する
An N-terminal β-barrel head-band gives rise to the asymmetrical motor structure of V_1-ATPase and promotes cooperativity
○丸山 慎太郎[1], 鈴木 花野[1], 佐々木 輝[1], 水谷 健二[2], 斎藤 靖子[3], ヤクシジ ファビアナ・リカ[1], 石塚（桂） 芳子[4], 白水 美香子[4], 横山 茂之[5], 山登 一郎[1,3], 村田 武士[1,6]（[1]千葉大・院理, [2]横浜市大・院生命医科学, [3]東京理科大・院生命理工, [4]理研・ライフサイエンス技術基盤研究センター, [5]理研・構造生物学研究室, [6]JST・さきがけ）
Shintaro Maruyama[1], Kano Suzuki[1], Hikaru Sasaki[1], Kenji Mizutani[2], Yasuko Saito[3], Fabiana Lica Yakushiji[1], Yoshiko Ishiduka-Katsura[4], Mikako Shirouzu[4], Shigeyuki Yokoyama[5], Ichiro Yamato[1,3], Takeshi Murata[1,6] ([1]*Grad. Sch. Sci., Univ. Chiba*, [2]*Grad. Sch. Med. Life. Sci., Univ. Yokohama City*, [3]*Grad. Bio. Sci. & Tech., Tokyo Univ. of Science*, [4]*DSSB, RIKEN*, [5]*Struct. Biol. Lab., RIKEN*, [6]*JST, PRESTO*)

1B1450*　結晶構造との対応付けを目指したミトコンドリア F_1-ATPase の回転解析
Single-molecule analysis of bovine mitochondrial F_1-ATPase for direct assignment of crystal structures and rotational pausing states
○小林 稜平, 上野 博史, 鈴木 俊治, 原 舞雪, 野地 博行（東大・院工・応化）
Ryohei Kobayashi, Hiroshi Ueno, Toshiharu Suzuki, Mayu Hara, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

1B1502*　腸内連鎖球菌由来の回転分子モーター V_1-ATPase のサブステップと化学力学共役機構
Substeps and chemo-mechanical coupling scheme of rotary molecular motor *Enterococcus hirae* V_1-ATPase
○飯田 龍也[1,2,3], 皆川 慶嘉[4], 上野 博史[4], 河合 文啓[3], 村田 武士[5], 飯野 亮太[1,2,3]（[1]総合研究大学院大学, [2]分子科学研究所, [3]岡崎統合バイオサイエンスセンター, [4]東京大学, [5]千葉大学）
Tatsuya Iida[1,2,3], Yoshihiro Minagawa[4], Hiroshi Ueno[4], Fumihiro Kawai[3], Takeshi Murata[5], Ryota Iino[1,2,3] ([1]*SOKENDAI (The Grad. Univ. for Adv. Stud.)*, [2]*Inst. for Mol. Sci.*, [3]*Okazaki Inst. for Integr. Biosci.*, [4]*The Univ. Tokyo*, [5]*Chiba Univ.*)

1B1514* DNA ナノチューブに沿って一方向に移動する生体分子モーターの設計
Engineered biomolecular motor that directly moves along DNA nanotubes
○指宿 良太[1], 大岩 和弘[1,2], 小嶋 寛明[2], 古田 健也[2]（[1]兵県大 院生命理学, [2]未来ICT研 情報通信研究機構）
Ryota Ibusuki[1], Kazuhiro Oiwa[1,2], Hiroaki Kojima[2], Ken'ya Furuta[2] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Adv ICT Res Inst, NICT.*)

休憩（Coffee Break） 15:26–15:32

1B1532* 電圧駆動型モータータンパク質プレスチンの細胞外ループが、作動電圧域を調節する
Characteristic extracellular loops of prestin modulate its voltage operating point
○桑原 誠[1], 和佐野 浩一郎[2], 高橋 里枝[2], 小森 智貴[1], 上村 想太郎[1], 島 知弘[1], 本間 和明[2]（[1]東大・理・生物科学, [2]ノースウェスタン大・医）
Makoto Kuwabara[1], Koichiro Wasano[2], Satoe Takahashi[2], Tomotaka Komori[1], Sotaro Uemura[1], Tomohiro Shima[1], Kazuaki Homma[2] ([1]*Dep. of Biol. Sci., Grad Sch. of Sci., The Univ. of Tokyo*, [2]*Feinberg Sch. of Med., Northwestern Univ.*)

1B1544* Motor evolved from F-ATPase for *Mycoplasma mobile* gliding
Takuma Toyonaga[1], Takayuki Kato[2], Akihiro Kawamoto[2], Keiichi Namba[2,3], Makoto Miyata[1,4] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Grad. Sch. Front. Biosci., Osaka Univ.*, [3]*QBiC, RIKEN*, [4]*OCARINA, Osaka City Univ.*)

1B1556* 拡散係数の増大を用いた F_1-ATPase の遷移率の解析
Analyzing the Transition Rate of F_1-ATPase from Enhanced Diffusion
○品川 遼太, 佐々木 一夫（東北大・院工学）
Ryota Shinagawa, Kazuo Sasaki (*Grad. Sch. Eng., Univ. Tohoku*)

1B1608 シアノバクテリアは光の向きを認識して IV 型線毛を非対称に分布する
Asymmetric distribution of type IV pili triggered by directional light in unicellular cyanobacteria
○中根 大介, 西坂 崇之（学習院大 物理）
Daisuke Nakane, Takayuki Nishizaka (*Dept. Phys., Gakushuin Univ.*)

13:20〜16:20 C 会場（全学教育棟 2 階 B202）／Room C (Room B202, General Education Bldg. 2F)
1C 生体膜・人工膜Ⅰ, バイオエンジニアリング, 計測Ⅰ / Biological & Artificial membrane I, Bioengineering, Measurements I

1C1320 分子拡散に対するミクロ空間に閉じ込めと高分子混雑の相乗効果
A synergistic effect of macromolecular crowding and biomimetic confinement on molecular diffusion
○渡辺 千穂, 柳澤 実穂（農工大院工）
Chiho Watanabe, Miho Yanagisawa (*Grad. Sch. Eng., Tokyo Univ. Agri. Tech.*)

1C1332* DNA 人工細胞骨格によるリポソームの力学的補強
DNA cytoskeleton for stabilizing artificial cells and the mechanical reinforcement
○黒川 知加子[1], 藤原 慶[2], 森田 雅宗[5], 川又 生吹[4], 川岸 由[4], 酒井 淳[1], 村山 能宏[1], 野村M 慎一郎[4], 村田 智[4], 瀧ノ上 正浩[3], 柳澤 実穂[1]（[1]東京農工大学大学院工学研究院先端物理工学部門, [2]慶應義塾大学理工学部生命情報学科, [3]東京工業大学情報理工学院情報工学系, [4]東北大学大学院工学研究科バイオロボティクス専攻, [5]産業技術総合研究所バイオメディカル研究部門）
Chikako Kurokawa[1], Kei Fujiwara[2], Masamune Morita[5], Ibuki Kawamata[4], Yui Kawagishi[4], Atsushi Sakai[1], Yoshihiro Murayama[1], Shin-ichiro Nomura. M[4], Satoshi Murata[4], Masahiro Takinoue[3], Miho Yanagisawa[1] ([1]*Department of Applied Physics, Tokyo University of Agriculture and Technology*, [2]*Department of Bioscience and Informatics, Keio University*, [3]*Department of Computer Science, Tokyo Institute of Technology*, [4]*Department of Robotics, Tohoku University*, [5]*Advanced Industrial Science and Technology, Biomedical Research Institute*)

1C1344* 選択的抗がん作用をもつトレハロース脂質含有リポソームの物性の計算化学的解析
Molecular dynamics analysis of physical properties of mixed liposomes containing trehalose surfactant with selective anticancer effect
○加々宮 崇（東工大 バイオセンター）
Takashi Kagamiya (*Center for Biol. Res. & Inform., Tokyo Tech*)

1C1356* 電子線による高精細バーチャル電極ディスプレイを用いた膜ドメインと膜形態の動的制御
Dynamic Control of Membrane Domains and Morphology Using an Electron-beam Induced Fine Virtual Cathode Display
○宮廻 裕樹, 星野 隆行（東京大学大学院情報理工学系研究科）
Hiroki Miyazako, Takayuki Hoshino (*IST, UTokyo*)

1C1408 細菌の膜小胞取り込みに寄与する表面電位と膜弛緩性
Contribution of surface potentials and membrane looseness on bacterial uptake of membrane vesicles
○田代 陽介, 髙木 航太郎, 長谷川 雄将, 二又 裕之（静大院・総合科技）
Yosuke Tashiro, Kotaro Takaki, Yusuke Hasegawa, Hiroyuki Futamata (*Grad. Sch. Intgr. Sci. Technol., Shizuoka Univ.*)

休憩（Coffee Break） 14:20–14:26

1C1426 高速原子間力顕微鏡（高速 AFM）による細菌が生産する膜小胞の物性解析
Physical heterogeneity of bacterial membrane vesicles revealed by high-speed AFM
○菊池 洋輔[1], 清川 達則[2], 森永 花菜[2], 諏佐 勇磨[2], 安田 まり奈[2], 奥脇 響[3], 相馬 隆光[3], 尾花 望[3], 豊福 雅典[3], 野村 暢彦[3], 古寺 哲幸[1], 安藤 敏夫[1], 福森 義宏[4], 田岡 東[1]（[1]金沢大・理工, [2]筑波大・院生命, [3]筑波大・生命, [4]金沢大・理事）
Yousuke Kikuchi[1], Tatunori Kiyokawa[2], Kana Morinaga[2], Yuuma Susa[2], Marina Yasuda[2], Hibiki Okuwaki[3], Ryukou Souma[3], Nozomu Obana[3], Masanori Toyohuku[3], Nobuhiko Nomura[3], Noriyuki Kodera[1], Toshio Ando[1], Yoshihiro Fukumori[4], Azuma Taoka[1] ([1]*Col. of Sci. and Eng., Kanazawa Univ.*, [2]*Grad. Life and Env. Sci., Tsukuba Univ.*, [3]*Life and Env. Sci., Tsukuba Univ.*, [4]*Vice President, Kanazawa Univ.*)

1C1438 肺サーファクタントタンパク質 B の N 末端セグメントにより起こる脂質単分子膜の崩壊現象
Collapse in lipid monolayers induced by N-terminal segments of lung surfactant protein B
○日比野 政裕[1,2], 長塚 秀幸[1], 藤岡 美穂[2], 王 灝伊[2]（[1]室蘭工大・院環境創生, [2]室蘭工大・応理）
Masahiro Hibino[1,2], Hideyuki Nagatsuka[1], Miho Fujioka[2], Haoyi Wang[2] ([1]*Div. Sustain. Environ. Eng., Muroran Inst. Tech.*, [2]*Dept. Appl. Sci., Muroran Inst. Tech.*)

1C1450 ラクトフェリシン B 由来の抗菌活性を持つヘキサペプチドの大腸菌細胞質への侵入
Entry of Antimicrobial Hexapeptide Derived from Lactoferricin B into Single cells of *E. coli* without Damaging their Membranes
○モニルザマン エムディー[1], イスラム エムディ ザヒドゥル[1], シャーミン サブリナ[1], 道羅 英夫[2], 山崎 昌一[1,3,4]（[1]静大・創造院, [2]静大・グリーン研, [3]静大・電研, [4]静大・院理）
Md. Moniruzzaman[1], Md. Zahidul Islam[1], Sabrina Sharmin[1], Hideo Dohra[2], Masahito Yamazaki[1,3,4] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Res. Inst. Green Sci. Tech., Shizuoka Univ.*, [3]*Res. Inst. Ele., Shizuoka Univ.*, [4]*Grad. Sch. Sci., Shizuoka Univ.*)

1C1502* 外側と内側の単分子膜の脂質の充填がマガイニン２の脂質膜中のポア形成に影響を与える
Effect of Asymmetric Packing of Lipids in Outer and Inner Monolayer on Magainin 2-Induced Pore Formation in Lipid Bilayer
○ハーサン モイヌル[1], カラール モハマド アブ サエム[1], レバツニー ビクター[1,2], 山崎 昌[1,3,4]（[1]静大・創造院, [2]ロシア科学アカデミー, [3]静大・電研, [4]静大・院理）
Moynul Hasan[1], Mohammad Abu Sayem Karal[1], Victor Levadny[1,2], Masahito Yamazaki[1,3,4] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Rus. Acad. Sci.*, [3]*Res. Inst. Ele., Shizuoka Univ.*, [4]*Grad. Sch. Sci., Shizuoka Univ.*)

1C1514 Formation mechanism of “lipid raft” in cell membranes
Shunsuke Shimobayashi[1], Masatoshi Ichikawa[2], Takashi Taniguchi[3] ([1]*Department of Mathematical Science and Advanced Technology, Japan Agency for Marine-Earth Science and Technology*, [2]*Department of Physics, Graduate School of Science, Kyoto University*, [3]*Department of Chemical Engineering, Graduate School of Engineering, Kyoto University*)

休憩（Coffee Break） 15:26–15:32

1C1532* パターン化人工膜を用いた光シグナル伝達中における脂質ラフトの機能解析
Role of lipid rafts in phototransduction studied with a micropatterned model membrane
○谷本 泰士[1], 小嶋 佐妃子[1], 粟津 暁紀[2], 林 文夫[3], 森垣 憲一[1,4]（[1]神戸大・農, [2]広島大・理, [3]神戸大・理, [4]神戸大・バイオシグナル）
Yasushi Tanimoto[1], Sakiko Kojima[1], Akinori Awazu[2], Fumio Hayashi[3], Kenichi Morigaki[1,4] ([1]*Grad. Sch. Agri, Univ Kobe*, [2]*Math. and Life Sci. Hiroshima Univ.*, [3]*Grad. Sch. Sci, Univ Kobe*, [4]*Biosignal Research Center, Univ Kobe*)

1C1544 パターン化人工膜を利用した NAP-22 の膜結合と凝集挙動解析
Membrane binding and aggregation of neuronal acidic protein of 22kDa (NAP-22) studied with a patterned model membrane
○小嶋 佐妃子[1], 谷本 泰士[1], 林 文夫[3], 前川 昌平[3], 森垣 憲一[1,2]（[1]神戸大・院農, [2]神戸大・バイオシグナル, [3]神戸大・院理）
Sakiko Kojima[1], Yasushi Tanimoto[1], Fumio Hayashi[3], Shohei Maekawa[3], Kenichi Morigaki[1,2] ([1]*Grad. Sch. Agri., Univ. Kobe*, [2]*Biosignal Research Center, Univ. Kobe*, [3]*Grad. Sch. Sci., Univ. Kobe*)

1C1556* Two-in-one biohybrid microfluidic system for detection and elimination of staphylococcus
Huisoo Jang[1,3], Sun Min Kim[2,3], Tae-Joon Jeon[1,3] ([1]*Department of Biological Engineering, Inha University, Incheon, Korea*, [2]*Department of Mechanical Engineering, Inha University, Incheon, Korea*, [3]*Biohybrid Systems Research Center (BSRC), Inha University, Incheon, Korea*)

1C1608* DNA Hairpin Based Spore Detection through α-Hemolysin Nanopores
Hyunil Ryu[1,2], Joongjin Park[1,3], Min-Cheol Lim[3], Jiwook Shim[4], Sun Min Kim[1,5], Young-Rok Kim[3], Tae-Joon Jeon[1,2] ([1]*Department of Biological Engineering, Inha University*, [2]*Biohybrid Systems Research Center (BSRC), Inha University*, [3]*Institute of Life Sciences and Resources & Department of Food Science and Biotechnology, Kyung Hee University*, [4]*Department of Biomedical Engineering, Rowan University*, [5]*Department of Mechanical Engineering, Inha University*)

13:20～16:20　D 会場（全学教育棟 2 階 E201）／Room D (Room E201, General Education Bldg. 2F)
1D　バイオイメージングⅠ / Bioimaging I

1D1320* ハナガサクラゲ由来の耐酸性・単量体型 GFP
Acid-tolerant monomeric GFP derived from jellyfish Olindias formosa
○篠田 肇[1], Ma Yuanqing[1], 中島 良介[2], 櫻井 啓介[2], 松田 知己[1,2], 永井 健治[1,2]（[1]阪大・工, [2]阪大・産研）
Hajime Shinoda[1], Yuanqing Ma[1], Ryosuke Nakashima[2], Keisuke Sakurai[2], Tomoki Matsuda[1,2], Takeharu Nagai[1,2] ([1]*Grad. Sch. Eng., Univ. Osaka*, [2]*ISIR, Univ. Osaka*)

1D1332* 複数の自由行動マウスにおける脳活動計測が可能な化学発光膜電位指示薬の開発
Development of a chemiluminescent voltage indicator applicable to a brain activity recording in freely-behaving multiple mice
○稲垣 成矩[1], 揚妻 正和[2], 筒井 秀和[3,4], 大原 慎也[5], 新井 由之[6], 神野 有香[4], 白 貴蓉[6], 飯島 敏夫[5], Daniels Matthew[7], 岡村 康司[1,4], 松田 知己[6], 永井 健治[1,6]（[1]阪大・生命, [2]基盤神経・生理研, [3]北陸先端大・マテリアル, [4]阪大・医学, [5]東北大・生命, [6]阪大・産研, [7]Div of Card Med, Univ of Oxford）
Shigenori Inagaki[1], Masakazu Agetsuma[2], Hidekazu Tsutsui[3,4], Shinya Ohara[5], Yoshiyuki Arai[6], Yuka Jinno[4], Guirong Bai[6], Toshio Ijima[5], Matthew Daniels[7], Yasushi Okamura[1,4], Tomoki Matsuda[6], Takeharu Nagai[1,6] ([1]*FBS, Osaka Univ*, [2]*Dep of Dev Physiol, NIPS*, [3]*Dep of Mat Science, JAIST*, [4]*Grad Sch of Med, Osaka Univ*, [5]*Grad Sch of Life Sci, Tohoku Univ*, [6]*ISIR, Osaka Univ*, [7]*Div of Card Med, Univ of Oxford*)

1D1344* 細胞内グルタチオンの求核付加・解離平衡に基づく超解像蛍光イメージングプローブの開発
Development of spontaneously blinking fluorophores based on nucleophilic addition of intracellular glutathione for superresolution imaging
○両角 明彦[1,4], 神谷 真子[2,5], 宇野 真之介[1], 梅澤 啓太郎[1], 吉原 利忠[3], 飛田 成史[3], 浦野 泰照[1,2,4]（[1]東大院薬, [2]東大院医, [3]群馬大院理工, [4]AMED CREST, [5]JST さきがけ）
Akihico Morozumi[1,4], Mako Kamiya[2,5], Shin-nosuke Uno[1], Keitaro Umezawa[1], Toshitada Yoshihara[3], Seiji Tobita[3], Yasuteru Urano[1,2,4] ([1]*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*, [2]*Grad. Sch. of Med., The Univ. of Tokyo*, [3]*Grad. Sch. Sci. Tech., Gunma Univ.*, [4]*AMED CREST*, [5]*JST PRESTO*)

1D1356* 新規微分干渉顕微法を用いた生細胞ヘテロクロマチンにおける物質密度のイメージング
Density imaging of heterochromatin in live cells using orientation-independent-DIC microscopy
○今井 亮輔[1,2], 野崎 慎[1], 谷 知己[3], 海津 一成[4], 日比野 佳代[1,2], 井手 聖[1,2], 田村 佐知子[1], 高橋 恒一[4], Shribak Michael[3], 前島 一博[1,2]（[1]遺伝研・構造遺伝学研究センター, [2]総研大・生命科学研究科・遺伝学専攻, [3]Marine Biological Lab., Woods Hole, USA, [4]理研・生命システム研究センター）
Ryosuke Imai[1,2], Tadasu Nozaki[1], Tomomi Tani[3], Kazunari Kaizu[4], Kayo Hibino[1,2], Satoru Ide[1,2], Sachiko Tamura[1], Koichi Takahashi[4], Michael Shribak[3], Kazuhiro Maeshima[1,2] ([1]*Struct. Biol. Center, Natl. Inst. of Genet.*, [2]*Dept. of Genet., Sch. of Life Sci., SOKENDAI*, [3]*Marine Biological Lab., Woods Hole, USA*, [4]*Quant. Biol. Center, RIKEN*)

1D1408* Development of Bioluminescent Low Affinity Ca2+ Indicators Applicable to Analyze Ca2+ Dynamics in Endoplasmic Reticulum
Nadim Hossain Md[1], Kazushi Suzuki[1,2], Megumi Iwano[2], Tomoki Matsuda[1,2], Takeharu Nagai[1,2] ([1]*Graduate School of Engineering, Osaka University*, [2]*The Institute of Scientific & Industrial Research (ISIR), Osaka University*)

休憩（Coffee Break） 14:20–14:26

1D1426 Single-cell quantitative analysis of ATP concentration by fluorescence lifetime imaging microscopy
Hideki Itoh[1], Satoshi Arai[2], Thankiah Sudhaharan[1], Tetsuya Kitaguchi[3], E. Birgitte Lane[1] ([1]*Inst. of Med. Biol. (Imb), Agcy. for Sci., Tech. and Res. (A*STAR), Singapore*, [2]*Res. Inst. Sci. Eng., Waseda Univ., Japan*, [3]*WASEDA Biosci. Inst. Singapore (WABIOS), Singapore*)

1D1438 熱産生する褐色脂肪細胞における Ca^{2+} を伴う 3 相のミトコンドリア pH 変化
Triphasic mitochondrial pH changes associated with Ca^{2+} for heat production in stimulated brown adipocytes
○鈴木 団[1,2]（[1]JSTさきがけ, [2]早稲田大・理工研）
Madoka Suzuki[1,2] ([1]*PRESTO, JST*, [2]*Res. Inst. Sci. & Eng., Waseda Univ.*)

1D1450* ヒト 2 型自然リンパ球の 1 細胞実時間イメージングによる 2 型サイトカイン応答観察に基づいた新規アレルギー診断の可能性
Potentiality for novel allergy diagnosis by real-time single-cell secretion imaging of human type 2 innate lymphoid cells
○宮田 楓[1], 白崎 善隆[1,2], 鈴木 信勇[1], 馬塲 里英[3], 加畑 宏樹[3], 山岸 舞[1,2], 小原 收[2], 福永 興壱[3], 茂呂 和世[2], 上村 想太郎[1]（[1]東京大学 大学院理学系研究科, [2]理化学研究所 統合生命医科学研究センター, [3]慶応大学 呼吸器内科）
Kaede Miyata[1], Yoshitaka Shirasaki[1,2], Nobutake Suzuki[1], Rie Baba[3], Hiroki Kabata[3], Mai Yamagishi[1,2], Osamu Ohara[2], Koichi Fukunaga[3], Kazuyo Moro[2], Sotaro Uemura[1] ([1]*Graduate School of Tokyo*, [2]*Institute of Physical and Chemical Research, IMS.*, [3]*Division of Pulmonary Medicine, Keio University*)

1D1502* 生理的条件下の細胞形態変化に伴う ATP レベル変動の定量的解析
Spatiotemporal quantification of native ATP dynamics during changes in cellular morphology
○鈴木 李夏, 堀田 耕司, 岡 浩太郎（慶應義塾大学大学院理工学研究科）
Rika Suzuki, Kohji Hotta, Kotaro Oka (*Grad. Sch. Sci and Tech., Keio Univ.*)

1D1514* 独立成分解析（ICA）を利用したマウス全脳の匂い BOLD 応答検出
Detection of the odor BOLD response in the mouse whole brain, using independent component analysis (ICA)
○舩津 大嗣, 林 芙優, 吉永 壮佐, 杠 直哉, 草薙 俊輔, 武田 光広, 寺沢 宏明（熊本大・院生命科学）
Hirotsugu Funatsu, Fuyu Hayashi, Sosuke Yoshinaga, Naoya Yuzuriha, Shunsuke Kusanagi, Mitsuhiro Takeda, Hiroaki Terasawa (*Fac. Life Sci. Kumamoto Univ.*)

休憩（Coffee Break） 15:26–15:32

1D1532* 過渡的刺激に対する２型自然リンパ球（ILC2）の確率的な分泌応答
Stochastic Secretion Response to Transient Stimulus of Type-2 Innate Lymphoid Cells (ILC2)
○依田 和樹, 鈴木 信勇, 上村 想太郎, 白崎 善隆（東大・院・理・生物科学）
Kazuki Yoda, Nobutake Suzuki, Sotaro Uemura, Yoshitaka Shirasaki (*Grad. Sch. Sci., Univ. Tokyo*)

1D1544* 一粒子輝度イメージングによるグルココルチコイド受容体二量体の生細胞内時空間分布解析
Shot noise free number and brightness analysis visualizes spatio-temporal distribution of glucocorticoid receptor dimer in living cells
○福島 綾介[1], 山本 条太郎[2], 金城 政孝[2]（[1]北大・生命科学院, [2]北大・先端生命）
Ryosuke Fukushima[1], Jotaro Yamamoto[2], Masataka Kinjo[2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

1D1556* 顕微ラマン分光法によるバクテリア一細胞の代謝活性測定
Single bacterial cell analysis of metabolic activity by Raman microspectroscopy
○加藤 陽太[1], 上野 博史[1], 野地 博行[1,2]（[1]東大・院工, [2]JST・ImPACT）
Yota Kato[1], Hiroshi Ueno[1], Hiroyuki Noji[1,2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*ImPACT, JST*)

1D1608* 高速 AFM が大腸がん細胞における核膜孔の選択的なゲートの喪失を明らかにした
Loss of Nuclear Pore Selective Barrier Revealed by High-Speed Atomic Force Microscopy in Colorectal Cancer Cells
○モハメド マフムード シャバン[1,2,3,4], 小林 亜紀子[1,2,3,4], 田岡 東[4], 中山 隆宏[2], 菊池 洋輔[4], 羽澤 勝治[1,2,3,4], みなもと としなり[5], 福森 義宏[4], 古寺 哲幸[2], 内橋 貴之[2], 安藤 敏夫[2], ウォング リチャード[1,2,3,4]（[1]金沢大学 セルバイオノミクスユニット, [2]金沢大学 バイオAFMフロンティア研究センター, [3]金沢大学 理工研究域 分子細胞生物学研究室, [4]金沢大学 理工研究域, [5]金沢大学がん研究所の翻訳・臨床腫瘍学部門）
Mahmoud Shaaban Mohamed[1,2,3,4], Akiko Kobayashi[1,2,3,4], Azuma Taoka[4], Takahiro Watanabe-Nakayama[2], Yosuke Kikuchi[4], Masaharu Hazawa[1,2,3,4], Toshinari Minamoto[5], Yoshihiro Fukumori[4], Noriyuki Kodera[2], Takayuki Uchihashi[2], Toshio Ando[2], Richard Wong[1,2,3,4] ([1]*Cell-Bionomics Research Unit, Kanazawa Univ.*, [2]*Bio-AFM Frontier Research Center, Kanazawa Univ.*, [3]*Lab of Mol. Cell Biol. Institute of Science and Engineering, Kanazawa Univ.*, [4]*Institute of Science and Engineering, Kanazawa Univ.*, [5]*Division of Translational and Clinical Oncology, Cancer Res. Inst., Kanazawa Univ.*)

13:20～16:20　E 会場（全学教育棟 2 階 E203）／Room E (Room E203, General Education Bldg. 2F)
1E　水・水和／電解質，蛋白質： 物性，蛋白質工学，生命情報科学，核酸Ⅰ /
Water & Hydration & Electrolyte, Proteins: Property, Engineering, Bioinformatics, Nucleic acid I

1E1320* 水-タンパク質間相互作用のための連続体モデルによる分散力エネルギー計算
Continuum-model-based Dispersion Energy Calculation for Protein-Water Interaction
○パーキン 暖, 水原 志暢, 高野 光則（早大・物理応物）
Dan Parkin, Yukinobu Mizuhara, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

1E1332 気液界面におけるタンパク質の変性
Protein Unfolding at the Air-Water Interface
○矢野 陽子[1], 荒川 悦雄[2], フォグリ ウォルフガング[2], 亀沢 知夏[2], 松下 正[3]（[1]近畿大学理工学部物理学コース, [2]東京学芸大学基礎自然科学講座物理科学分野, [3]高エネルギー加速器研究機構物質構造化学研究所）
Yohko Yano[1], Etsuo Arakawa[2], Wolfgang Voegeli[2], Chika Kamezawa[2], Tadashi Matsushita[3] ([1]*Department of Physics, Kindai University*, [2]*Department of Physics, Tokyo Gakugei University*, [3]*Photon Factory, Institute of Materials Structure Science, KEK*)

1E1344 Unexpected heterogeneity and slow dynamics of simple poly-alanine peptides detected by single molecule fluorescence spectroscopy
Supawich Kamonprasertsuk[1,2], Hiroyuki Oikawa[1,2], Satoshi Takahashi[1,2] ([1]*Institute for Multidisciplinary Research for Advanced Materials, Tohoku University*, [2]*Department of Chemistry, Graduate School and Faculty of Science, Tohoku University*)

1E1356 二次元蛍光寿命相関分光法によるシトクロム *c* のフォールディング過程の部位選択的な観測
Site-selective observation of folding dynamics of cytochrome *c* by two-dimensional fluorescence lifetime correlation spectroscopy
○坂口 美幸[1], 山中 優[2], 廣田 俊[2], 石井 邦彦[1,3], 田原 太平[1,3]（[1]理研・田原分子分光, [2]奈良先端大・物質創成, [3]理研・光量子工学領域）
Miyuki Sakaguchi[1], Masaru Yamanaka[2], Shun Hirota[2], Kunihiko Ishii[1,3], Tahei Tahara[1,3] ([1]*Msl, RIKEN*, [2]*Grad. Sch. Mat. Sci., NAIST*, [3]*RAP, RIKEN*)

1E1408* Oct4 の 2 つの DNA 結合サブドメインを結ぶ linker 領域の構造多様性
Structural variety of the linker connecting two DNA-binding subdomains of Oct4
○速水 智教[1,2], 高田 彰二[3], 笠原 浩太[4], 中村 春木[1], 肥後 順一[1]（[1]阪大・蛋白研, [2]阪大・院生命機能, [3]京大・院理学・生物物理, [4]立命館大・生命・生情）
Tomonori Hayami[1,2], Shoji Takada[3], Kota Kasahara[4], Haruki Nakamura[1], Junichi Higo[1] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sch. Fro. Bio., Osaka Univ.*, [3]*Dept. Biophys., Grad. Sch. Sci., Kyoto Univ.*, [4]*Dept. Bioinfo., Col. Life Sci., Ritsumeikan Univ.*)

休憩（Coffee Break） 14:20–14:26

1E1426* フィブリノーゲンによるアミロイド線維形成阻害機構の解明
Investigation of inhibition mechanism of fibrinogen in the amyloid fibrillation
○赤井 大気, 山本 直樹, 茶谷 絵理（神戸大・院・理）
Taiki Akai, Naoki Yamamoto, Eri Chatani (*Grad. Sch. of Sci., Kobe Univ.*)

1E1438* プリオンアプタマーはアルツハイマー病に関与するプリオン蛋白質と Aβ オリゴマーの複合体の形成を阻害する
An anti-prion aptamer inhibits the formation of prion protein-amyloid β oligomer complex that is related to Alzheimer's disease
○飯田 真美子[1,2], 真嶋 司[1,2], 山置 佑大[1], 永田 崇[1,2], 片平 正人[1,2]（[1]京都大学 エネルギー理工学研究所, [2]京都大学大学院 エネルギー科学研究科）
Mamiko Iida[1,2], Tsukasa Mashima[1,2], Yudai Yamaoki[1], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Inst. of Adv. Energy, Kyoto Univ.*, [2]*Grad. Sch. of Energy Sci., Kyoto Univ.*)

1E1450* Photo cross-linking and MS analyses of the amyloid β-peptide oligomers
Mai Kawashita[1], Shintaro Yoshida[1], Sosuke Yoshinaga[1], Mitsuhiro Takeda[1], Ayumi Tanaka[1], Takashi Hamaguchi[1], Hitomi Yamaguchi[1], Shigeto Iwamoto[1], Takashi Saito[2], Yoshihiko Takinami[3], Toshiyuki Kohno[4], Takaomi C. Saido[2], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*RIKEN, Inst. Phys. Chem. Res.*, [3]*Bruker Daltonics*, [4]*Kitasato Univ. Sch. Med.*)

1E1502 アミロイド分解能を有する人工ペプチドの設計
Designing artificial peptides that have ability to hydrolyze amyloid fibrils
○飯田 禎弘, 田村 厚夫（神戸大 院理）
Yoshihiro Iida, Atsuo Tamura (*Grad. Sch. Sci., Univ. Kobe*)

1E1514 再設計法と新規設計法による膜貫通アルファヘリックスペプチドバレルの開発
Redesign and de novo design of transmembrane alpha-helical peptide barrels
○新津 藍[1,2], Mahendran Kozhinjampara[3], Thomson Andrew R.[4], Beyley Hagan[3], 杉田 有治[1], Woolfson Derek N.[2]（[1]理研・和光, [2]ブリストル大学, [3]オックスフォード大学, [4]グラスゴー大学）
Ai Niitsu[1,2], Kozhinjampara R. Mahendran[3], Andrew R. Thomson[4], Hagan Beyley[3], Yuji Sugita[1], Derek N. Woolfson[2] ([1]*Wako Inst, RIKEN*, [2]*Univ. Bristol*, [3]*Univ. Oxford*, [4]*Univ. Glasgow*)

休憩（Coffee Break） 15:26–15:32

1E1532* Rational design of a novel affinity ligand for antibody purification by controlling the pH-sensitive antibody interaction
Yoshiki Oka[1], Taihei Sawada[1], Takahiro Watanabe[1], Hisashi Kudo[1], Manami Wada[1], Hidenobu Kawai[1], Mari Chang[2], Yuuki Hayashi[1], Munehito Arai[1,2] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Dept. Phys., Univ. Tokyo*)

1E1544 メニーコアプロセッサ向け蛋白質・リガンドドッキングエンジン sievgene_M の開発
Development of protein-ligand docking engine sievgene_M for manycore processors
○杉原 崇憲[1,2], 黒澤 隆[2,3], 中村 寛則[4], 真下 忠彰[2,5], 福西 快文[2,6], 中村 春木[2,7]（[1]（一社）バイオ産業情報化コンソーシアム, [2]次世代天然物化学技術研究組合, [3]（株）日立ソリューションズ東日本, [4]（株）バイオモデリングリサーチ, [5]（株）情報数理バイオ, [6]産総研molprof, [7]阪大蛋白研）
Takanori Sugihara[1,2], Takashi Kurosawa[2,3], Hironori Nakamura[4], Tadaaki Mashimo[2,5], Yoshifumi Fukunishi[2,6], Haruki Nakamura[2,7] ([1]*JBIC*, [2]*N2PC*, [3]*Hitachi Solutions East Japan, Ltd.*, [4]*Biomodeling Research Co., Ltd.*, [5]*IMSBIO Co., Ltd.*, [6]*AIST/molprof*, [7]*Inst. for Protein Research, Osaka Univ.*)

1E1556* Analysis of protein pockets using a fast and efficient comparison method with a reduced vector representation
Tsukasa Nakamura[1], Kentaro Tomii[1,2,3] ([1]*CBMS, GSFS, Univ. Tokyo*, [2]*AIRC, AIST*, [3]*BRD, AIST*)

1E1608* Phase transition in a single giant DNA molecule: Differences between 1-propanol and 2-propanol aqueous solutions
Yue Ma, Yuko Yoshikawa, Koichiro Sadakane, Takahiro Kenmotsu, Kenichi Yoshikawa (*Graduate School of Life and Medical Sciences, Doshisha University*)

13:20〜16:08　F 会場（全学教育棟 2 階 E205）／Room F (Room E205, General Education Bldg. 2F)
1F　蛋白質： 構造，構造機能相関Ⅰ，計測・解析の方法論 / Proteins: Structure, Structure-function relationship I, Measurement & Analysis

1F1320* 光依存性内向きプロトンポンプ *Po*XeR の X 線結晶構造解析
Crystal structure of *Po*XeR, a light-driven inward proton pump
○生田 達也, 石谷 隆一郎, 濡木 理（東大・院理・生物科学）
Tatsuya Ikuta, Ryuichiro Ishitani, Osamu Nureki (*Grad. Sch. Sci., Univ. Tokyo*)

1F1332* Crystal structure of mammalian Claudin3 in complex with a toxin
Shun Nakamura[1], Katsumasa Irie[1,2], Hiroo Tanaka[3], Atsushi Tamura[3], Sachiko Tsukita[3], Yoshinori Fujiyoshi[2] ([1]*Grad. Sch. Pharm., Univ. Nagoya*, [2]*CeSPI, Univ. Nagoya*, [3]*Grad. Sch. Med., Univ. Osaka*)

1F1344* Ca^{2+}/Zn^{2+}結合型ヒト S100A3 蛋白質四量体の X 線結晶構造解析に向けての研究
The studies for X-ray crystallographic analysis of the Ca^{2+} and Zn^{2+} bound human S100A3 protein tetramer
○井手 賢司[1], 木澤 謙司[2], 北西 健一[1], 海野 昌喜[1,3]（[1]茨城大院理工, [2]花王（株）, [3]茨城大IFRC）
Kenji Ite[1], Kenji Kizawa[2], Kenichi Kitanishi[1], Masaki Unno[1,3] ([1]*Grad. Sch. Sci. Eng., Ibaraki Univ.*, [2]*Kao Corp.*, [3]*IFRC, Ibaraki Univ.*)

1F1356* 銅輸送チャネルにおける金属結合モチーフの構造変化と、それに伴う脂質二重膜への埋没
Structural change of the metal binding motif of copper transporter induces the embedding of the motif into lipid bilayer
○岡田 毬子[1], 三浦 隆史[2], 中林 孝和[1]（[1]東北大・院薬学, [2]医療福祉大・薬学）
Mariko Okada[1], Takashi Miura[2], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [2]*Dept. of Pharm. Sci., Int'l Univ. of Health and Welfare*)

1F1408* 高速 AFM 観察で明らかにされた α7 ホモ 14 量体の α6 による解体過程
High-speed AFM reveals disassembly process homo-tetradecamer of proteasomal α7 subunit induced by interaction with α6 subunit
○小財 稔矢[1], 佐藤 匡史[2], 矢木 宏和[2], 内橋 貴之[3], 加藤 晃一[2,4,5]（[1]金沢大・院数物, [2]名市大・院薬, [3]名大・理学, [4]岡崎統合バイオ, [5]総研大）
Toshiya Kozai[1], Tadashi Satoh[2], Hirokazu Yagi[2], Takayuki Uchihashi[3], Koichi Kato[2,4,5] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*Grad. Sch. Pharm. Sci., Nagoya City Univ.*, [3]*Dept. Phys., Nagoya Univ.*, [4]*Okazaki Inst. Integ. Biosci.*, [5]*Nat. Univ., SOKENDAI*)

休憩（Coffee Break） 14:20–14:26

1F1426* コンピュータシミュレーションによるリゾチームと α ラクトアルブミンのモルテングロビュール状態の構造探索
Exploring Structures of the Molten Globule State of Lysozyme and αLactalbumin by Computer Simulations
○清水 政宏, 岡本 祐幸（名古屋大学大学院理学研究科物理学教室）
Masahiro Shimizu, Yuko Okamoto (*Dept. Phys., Sch. Sci., Univ. Nagoya*)

1F1438* 乾燥過程における G3LEA モデルペプチドの生体膜保護に関する計算化学的研究
Molecular dynamics study of the protective function of G3LEA model peptide on dried POPC bilayer
○高橋 佑太, 古田 忠臣, 櫻井 実（東京工業大学 バイオ研究基盤支援総合センター 櫻井研究室）
Yuta Takahashi, Tadaomi Furuta, Minoru Sakurai (*Center for Biol. Res. & Inform., Tokyo Tech*)

1F1450* 時計タンパク質 KaiC のリン酸化と ATP 加水分解による構造変化メカニズム
Conformational change by phosphorylation and ATP hydrolysis in the cyanobacterial circadian oscillator KaiC
○大山 克明[1], 浅井 智広[2], 寺内 一姫[1,2]（[1]立命館大学大学院 生命科学研究科, [2]立命館大学 生命科学部）
Katsuaki Oyama[1], Chihiro Azai[2], Kazuki Terauchi[1,2] ([1]*Graduate School of Life Sciences, Ritsumeikan University*, [2]*College of Life Sciences, Ritsumeikan University*)

1F1502* Computational investigation of conformational dynamics in Tom20/mitochondrial targeting signal complex
Arpita Srivastava[1], Osamu Miyashita[2], Florence Tama[1,2,3] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Adv. Inst. Comp. Sci., RIKEN*, [3]*Inst. of Transformative Bio-Molecules, Nagoya Univ.*)

1F1514* 分子動力学法による野生型・変異型エリスロポエチン受容体の動的解析
Dynamical analysis of wild type and mutant erythropoietin receptors by molecular dynamics simulations
○唐澤 直之, 光武 亜代理, 高野 宏（慶大・理工）
Naoyuki Karasawa, Ayori Mitsutake, Hiroshi Takano (*Grad. Sch. Sci. Technol., Keio Univ.*)

休憩（Coffee Break） 15:26–15:32

1F1532* 抗原ペプチドの硫酸化がペプチドー抗体間相互作用に与える影響の熱力学的解析
Thermodynamic analysis of the effect of sulfation on a peptide-antibody interaction
○宮鍋 一紘[1], 秋葉 宏樹[2], 高松 佑一郎[3], 山下 雄史[3], ホセ カアベイロ[4], 津本 浩平[1]（[1]東大院・工, [2]医薬健栄研, [3]東大・先端研, [4]九大院・薬）
Kazuhiro Miyanabe[1], Hiroki Akiba[2], Yuichiro Takamatsu[3], Takefumi Yamashita[3], Caaveiro Jose[4], Kouhei Tsumoto[1] ([1]*Sch. Eng., Univ. Tokyo*, [2]*NIBIOHN*, [3]*RCAST, Univ. Tokyo*, [4]*Grad. Sch. Pharm. Sci., Kyushu. Univ*)

1F1544* Structure-based analyses of the interaction between the chemokine receptor-regulator FROUNT and novel anti-inflammatory compounds
Soichiro Ezaki[1], Sosuke Yoshinaga[1], Norihito Ishida[1], Mitsuhiro Takeda[1], Kaori Yunoki[1], Yuya Terashima[2], Etsuko Toda[2], Kouji Matsushima[2], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*Grad. Sch. Med., Univ. Tokyo*)

1F1556 Laser processing of protein crystals for native SAD data collection
Ayaka Harada[1], Naohiro Matsugaki[1,2], Yoshiaki Kawano[3], Masaki Yamamoto[3], Toshiya Senda[1,2] ([1]*KEK, PF, Structural Biology Research Center*, [2]*The Grad. Univ. for Advanced Studies, School of High Energy Accelerator Science*, [3]*RIKEN/SPring8*)

13:20〜16:20 G 会場（全学教育棟 3 階 C301）／Room G (Room C301, General Education Bldg. 3F)
1G 蛋白質: 機能, ヘム蛋白質 I , 核酸結合蛋白質 / Proteins: Function, Heme proteins I, Nucleic acid binding proteins

1G1320 線虫 *C. elegans* の低温耐性から見た不凍タンパク質の機能解析、および生体内 X 線一分子観察
In vivo X-ray single molecule observation and functional analysis of antifreeze proteins for cold tolerance in *C. elegans*
○倉持 昌弘[1], 高梨 千晶[1], 関口 博史[2], 戸井 基道[3], 津田 栄[4], 佐々木 裕次[1]（[1]東京大学・院新領域, [2]高輝度光科学研究センター, [3]産総研・バイオメディカル, [4]産総研・生物プロセス）
Masahiro Kuramochi[1], Chiaki Takanashi[1], Hiroshi Sekiguchi[2], Motomichi Doi[3], Sakae Tsuda[4], Yuji C Sasaki[1] ([1]*Grad. Sch. Front. Sci., Univ. Tokyo*, [2]*JASRI*, [3]*Biomedical R.I., AIST*, [4]*Bioproduction R.I., AIST*)

1G1332 A mechanism of enzymatic activation of Cu/Zn-superoxide dismutase by its copper chaperone
Yoshiaki Furukawa, Mami Fukuoka (*Dept. of Chemistry, Keio Univ.*)

1G1344 Pin1 の酵素反応におけるタンパク質ダイナミクスの重要性
Crucial role of enzyme dynamics in the catalytic reaction mechanism of Pin1
○森 俊文[1,2], 斉藤 真司[1,2]（[1]分子研, [2]総研大）
Toshifumi Mori[1,2], Shinji Saito[1,2] ([1]*IMS*, [2]*SOKENDAI*)

1G1356* ラン藻由来炭化水素合成関連酵素の活性と可溶性の向上
Improving activity and solubility of cyanobacterial enzymes for hydrocarbon biosynthesis
○工藤 恒, 林 勇樹, 新井 宗仁（東大・総合文化・生命環境）
Hisashi Kudo, Yuuki Hayashi, Munehito Arai (*Dept. Life Sci., Univ. Tokyo*)

1G1408* 生細胞直接円偏光二色性測定によるシトクロム c 内多核ヘムの配置変化の追跡
Circular Dichroism Spectroscopy of Living Microbe Reveals Redox-Triggered Conformational Change of Heme Cofactors in Cytochromes c
○徳納 吉秀[1], チノタイクン パンティラー[1], 服部 伸吾[2], 橋本 和仁[3], 石井 和之[2], 岡本 章玄[3]（[1]東大院工・応用化学, [2]東大・生産技術研究所, [3]物質材料研究機構）
Yoshihide Tokunou[1], Punthira Chinotaikul[1], Shingo Hattori[2], Kazuhito Hashimoto[3], Kazuyuki Ishii[2], Akihiro Okamoto[3] ([1]*Department of Applied Chemistry, School of Engineering, The University of Tokyo*, [2]*Institute of Industrial Science, The University of Tokyo*, [3]*National Institute for Materials Science*)

休憩（Coffee Break） 14:20–14:26

1G1426* 基質 DNA の長さ、濃度、及び標的配列位置が APOBEC3F の脱アミノ活性に及ぼす影響
Influences of length and concentration of the DNA substrate, as well as the location of the target sequence, on deamination by APOBEC3F
○万 里[1,2], 永田 崇[1,2], 片平 正人[1,2]（[1]京都大学 エネルギー理工学研究所, [2]京都大学大学院 エネルギー科学研究科）
Li Wan[1,2], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Institute of Advanced Energy, University of Kyoto*, [2]*Graduate School of Energy Science, University of Kyoto*)

1G1438* (6-4)光回復酵素の光反応過程における基質特異性に関する赤外分光研究
FTIR study of photoreaction of Xenopus (6-4) photolyase on substrate specificity
○熊谷 真衣[1], 山田 大智[1], 岩田 達也[2], 山元 淳平[3], 神取 秀樹[1]（[1]名工大・院工, [2]東邦大・薬, [3]阪大・院基礎工）
Mai Kumagai[1], Daichi Yamada[1], Tatsuya Iwata[2], Junpei Yamamoto[3], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*Fac. Pharm. Sci., Toho Univ.*, [3]*Grad. Sch. Eng. Sci, Osaka Univ.*)

1G1450* 3D-RISM 計算での溶媒分布と MD から導く EcoRV の DNA 切断反応における水分子と Mg2+の役割
Role of Mg2+ ion and water in DNA hydrolysis by EcoRV, studied by 3D-RISM and MD
○大西 到[1], 砂場 俊哉[1], 本松 良太[1], 安庭 潤治[1], 丸山 豊[2], 吉田 紀生[3], 皿井 明倫[1], 平田 文男[4], 入佐 正幸[1]（[1]九州工大情報工, [2]慶応大, [3]九大理, [4]立命館・分子研）
Itaru Onishi[1], Shunya Sunaba[1], Ryota Motomatsu[1], Junji Yasuniwa[1], Yutaka Maruyama[2], Norio Yoshida[3], Akinori Sarai[1], Fumio Hitara[4], Masayuki Irisa[1] ([1]*Kyushu Inst. of Tech.*, [2]*Keio Univ.*, [3]*Kyushu Univ.*, [4]*IMS and Ritsumei Univ.*)

1G1502 An arginine side chain in the (6-4) photolyase governs formation of a robust repair-active complex with UV-damaged DNA
Junpei Yamamoto[1], Yuma Terai[1], Ryuma Sato[2], Ryuhei Harada[2], Yasuteru Shigeta[2], Shigenori Iwai[1] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*CCS, Univ. Tsukuba*)

1G1514 RecA Nucleoprotein Filament Formation on SSB-wrapped DNA Includes RecA-SSB Interaction
Hung-Yi Wu, Chih-Hao Lu, **Hung-Wen Li** (*National Taiwan University*)

休憩（Coffee Break） 15:26–15:32

1G1532 テロメア長短縮をもたらす TLS/FUS 蛋白質とテロメア DNA および TERRA のグアニン四重鎖との複合体に関する NMR 解析
NMR studies for the complex of TLS/FUS protein and G-quadruplexes of telomeric DNA and TERRA, which induces telomere shortening
○近藤 敬子[1], 真嶋 司[1,2], 大吉 崇文[3], 黒川 理樹[4], 小林 直宏[5], 永田 崇[1,2], 片平 正人[1,2]（[1]京都大学・エネルギー理工学研究所, [2]京都大学・エネルギー科学研究科, [3]静岡大学・理学部, [4]埼玉医科大学・ゲノム医学研究センター, [5]大阪大学・蛋白質研究所）
Keiko Kondo[1], Tsukasa Mashima[1,2], Takanori Oyoshi[3], Riki Kurokawa[4], Naohiro Kobayashi[5], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Institute of Advanced Energy, Kyoto University*, [2]*Graduate School of Energy Science, Kyoto University*, [3]*Department of Chemistry, Shizuoka University*, [4]*Research Center for Genomic Medicine, Saitama Medical University*, [5]*Institute for Protein Research, Osaka University*)

1G1544 The mechanism of R42me2a promoting the transcription
Zhenhai Li, Hidetoshi Kono (*QST*)

1G1556 Modeling Sequence-Specific Protein-DNA Interaction from High-Throughput Experiments
Cheng Tan, Shoji Takada (*Graduate School of Science, Kyoto University*)

1G1608 Proteomic analysis of the lncRNA-protein complexes in colon cancer cells
Lumi Negishi, Kenzui Taniue, Yoshihiro Kawasaki, Kosuke Matsumura, Akiko Takahashi, Tetsu Akiyama (*IMCB., Univ. Tokyo*)

13:20〜16:20　H 会場（全学教育棟 3 階 E303）／Room H (Room E303, General Education Bldg. 3F)
1H　細胞生物学的課題Ⅰ / Cell biology I

1H1320 Actin polymerization signal emitted at the raft nanodomains of the clusters of the anthrax-toxin-receptor complex: a single-molecule study

An-An Liu[1], Yukihiko Kudo[2], Shihui Liu[3], Kenichi Suzuki[4], Takahiro Fujiwara[2], Dai-Wen Pang[5], Stephen Leppla[3], Akihiro Kusumi[1,2] ([1]*Membrane Cooperativity Unit, Okinawa Institute of Science and Technology Graduate University (OIST)*, [2]*Institute for Integrated Cell-Material Sciences, Kyoto University Institute for Advanced Study*, [3]*Division of Intramural Research, NIAID, NIH*, [4]*Center for Highly Advanced Integration of Nano and Life Sciences (G-CHAIN), Gifu University*, [5]*College of Chemistry and Molecular Sciences, Wuhan University*)

1H1332 Functional signaling-fluorescent fusion protein for the dynamics of signaling pathway in E.coli

Ryota Shiono, Akihiko Ishijima, Hajime Hukuoka (*Grad. Sch. Frontier Biosci., Osaka Univ*)

1H1344 高速 AFM によるダイナミン 1ーアンフィファイジン複合体の動態観察

High-Speed AFM imaging of dynamics of Dynamin1-Amphiphysin1 complexes

○石黒 大輝[1], 竹田 哲也[3], 小財 稔矢[1], 背山 佳穂[3], 楊 恵然[3], 山田 浩司[3], 内橋 貴之[4], 安藤 敏夫[2], 竹居 孝二[3]（[1]金沢大・院・物理, [2]金沢大・bio-AFM, [3]岡山大・医歯薬, [4]名大理学）

Daiki Ishikuro[1], Tetsuya Takeda[3], Toshiya Kozai[1], Kaho Seyama[3], Huiran Yang[3], Hiroshi Yamada[3], Takayuki Uchihashi[4], Toshio Ando[2], Kohji Takei[3] ([1]*Grad. Sch. Phys., Kanazawa Univ*, [2]*Bio-AFM. FRC., Kanazawa Univ*, [3]*Graduate School of Medicine, Dentistry and Pharmaceutical Sciences, Okayama Univ*, [4]*Dept. Phys., Nagoya Univ*)

1H1356 高速 AFM による生細胞表面の分子イメージング

Molecular imaging on living bacterial cell surface by high speed AFM

○山下 隼人[1,2], 田岡 東[3,4], 福森 義宏[3], 阿部 真之[1]（[1]阪大・院基礎工, [2]JSTさきがけ, [3]金沢大・理工, [4]金沢大・バイオAFMセンター）

Hayato Yamashita[1,2], Azuma Taoka[3,4], Yoshihiro Fukumori[3], Masayuki Abe[1] ([1]*Grad. Sch. of Eng. Sci. Osaka Univ.*, [2]*PRESTO, JST*, [3]*Inst. Sci. and Eng., Kanazawa Univ.*, [4]*Bio-AFM Frontier Research Center, Kanazawa Univ.*)

1H1408 First evaluation of permeabilities across the actin-based compartment barriers in the plasma membrane

Alexey Yudin[1], Takahiro Fujiwara[2], Takaaki Tsunoyama[1], Akihiro Kusumi[1,2] ([1]*Membrane Cooperativity Unit, Okinawa Institute of Science and Technology Graduate University (OIST)*, [2]*Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto University*)

休憩（Coffee Break）　14:20–14:26

1H1426* メカノストレスによる歯周組織リモデリング機構の解明

Effects of Mechanical Stress on Remodeling of Periodontal Ligament

○藤田 彩乃[1,2], 森松 賢順[2], 西山 雅祥[3], 高柴 正悟[1], 成瀬 恵治[2]（[1]岡山大学大学院医歯薬学総合研究科歯周病態学分野, [2]岡山大学大学院医歯薬学総合研究科システム生理学, [3]京都大学大学院医学研究科人間健康科学系専攻）

Ayano Fujita[1,2], Masatoshi Morimatsu[2], Masayoshi Nishiyama[3], Shogo Takashiba[1], Keiji Naruse[2] ([1]*Department of Pathophysiology-Periodontal Science, Okayama University Graduate School of Medicine, Dentistry and Pharmaceutical Sciences*, [2]*Department of Pathophysiology-Periodontal Science, Okayama University Graduate School of Medicine, Dentistry and Pharmaceutical Sciences*, [3]*Human Health Sciences, Graduate School of Medicine, Kyoto University*)

1H1438 加圧・脱圧による芽胞ジピコリン酸の流出：高圧 NMR によるリアルタイム観測

How can pressure release DPA from bacterial spores? A study by high pressure NMR

○赤坂 一之[1], 前野 覚大[2], 金折 賢二[3], 山崎 彬[4]（[1]京都府立医大, [2]関西医大, [3]京都工繊大, [4]越後製菓）

Kazuyuki Akasaka[1], Akihiro Maeno[2], Kenji Kanaori[3], Akira Yamazaki[4] ([1]*Kyoto Prefectural University of Medicine*, [2]*Kansai Medical University*, [3]*Kyoto Institute of Technology*, [4]*Echigoseika Co.*)

1H1450 光照射によるインアクティブな珪藻細胞の刺激

Stimulation of inactive diatom cells by light irradiation

○梅村 和夫[1], 近藤 駿佑[1], 熊代 善一[2], 真山 茂樹[3]（[1]東理大・理, [2]東女医大, [3]東学大）

Umemura Kazuo[1], Shunsuke Kondo[1], Yoshikazu Kumashiro[2], Shigeki Mayama[3] ([1]*Tokyo Univ Sci*, [2]*Tokyo Women's Medical University*, [3]*Tokyo Gakugei University*)

1H1502* 滑走するヒト肺炎原因菌 *Mycoplasma pneumoniae* の“あし”P1 adhesin

P1 adhesin, the leg for gliding of *Mycoplasma pneumoniae*

○松本 優[1], 川本 晃大[2], 加藤 貴之[2], 川北 祥人[1], 見理 剛[3], 森 茂太郎[3], 難波 啓一[2,4], 宮田 真人[1,5]（[1]大市大・院理, [2]阪大・院生命機能, [3]感染研・武蔵村山, [4]理研・吹田, [5]大市大・複合先端）

U Matsumoto[1], Akihiro Kawamoto[2], Takayuki Kato[2], Yoshito Kawakita[1], Tsuyoshi Kenri[3], Shigetaro Mori[3], Keiichi Namba[2,4], Makoto Miyata[1,5] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Grad. Sch. Front. Biosci., Univ. Osaka*, [3]*Dept. Bacteriology II, NIID*, [4]*QBiC, RIKEN*, [5]*OCARINA, Osaka City Univ.*)

1H1514* 非熱的に駆動された細胞内部の混み合いガラス状態

Molecular crowding glass driven by metabolic activity in cells

○西澤 賢治, 水野 大介（九大物理）

Kenji Nishizawa, Daisuke Mizino (*Dept. of Phys., Kyushu Univ.*)

休憩（Coffee Break） 15:26–15:32

1H1532* NF-κB 転写因子の細胞質 - 核内移行の一細胞動態はその発現量によって自己制御される
Single-cell cytoplasmic-nuclear shuttling of transcription factor NF-κB is auto-regulated by the expression level
○宮本 佑[1], 有吉 哲郎[2], 稲葉 岳彦[3], 岩本 一成[4], 長谷 耕二[1], 佐甲 靖志[3], 岡田 康志[2], 岡田 眞里子[4]（[1]慶應大 院薬, [2]理研 QBiC, [3]理研 和光, [4]大阪大 蛋白研）
Yu Miyamoto[1], Tetsuro Ariyoshi[2], Takehiko Inaba[3], Kazunari Iwamoto[4], Koji Hase[1], Yasushi Sako[3], Yasushi Okada[2], Mariko Okada[4] ([1]*Keio Univ. Parmacy*, [2]*RIKEN QBiC*, [3]*RIKEN Wako*, [4]*Osaka Univ. Protein Research*)

1H1544* 誘引場への追従性能と細胞の前後極性から理解する好中球様 HL60 細胞の走化性運動
Chemotactic analysis of neutrophil-like HL60 cells based on cells' persistent polarity and immediate responsiveness to chemoattractant
○石田 元彦[1], 中島 昭彦[2], 澤井 哲[1,2]（[1]東京大学大学院総合文化研究科広域科学専攻, [2]複雑系生命システム研究センター）
Motohiko Ishida[1], Akihiko Nakajima[2], Satoshi Sawai[1,2] ([1]*Dept. Basic Sci., Grad. Sch. of Arts & Sci., Univ. of Tokyo*, [2]*Research Center for Complex Systems Biology, Grad. Sch. of Arts & Sci., Univ. of Tokyo*)

1H1556* 植物細胞内でシロイヌナズナアクチンアイソフォーム（ACT2, ACT7）は異なった局在を示す
Arabidopsis vegetative actin isoforms, ACT2 and ACT7, show distinct localization in a living plant cell
○貴嶋 紗久[1,2], Staiger Christopher J.[3], 加藤 薫[1], 光田 展隆[4], 上田 太郎[1,5]（[1]産総研 バイオメディカル, [2]筑波大学 生命環境科学, [3]Purdue大学 生物科学, [4]産総研 生物プロセス, [5]早稲田大学 先進理工）
Saku T. Kijima[1,2], Christopher J. Staiger[3], Kaoru Katoh[1], Nobutaka Mitsuda[4], Taro Q.P. Uyeda[1,5] ([1]*Biomedical Res. Inst., AIAT*, [2]*Grad. Sch. Sci., Univ. Tsukuba*, [3]*Dep. Biol. Sci., Purdue Univ.*, [4]*Bioproduction Res. Inst., AIST*, [5]*Dep. of Physics, Fac. Sci. Engin., Waseda Univ.*)

1H1608* 大腸菌走化性受容体クラスターにおける状態発振モデルの作成
Computational simulation of spontaneous transition between active and inactive in whole chemoreceptor array in *E. coli*
○濱元 樹[1], 佐川 貴志[2], 小口 伸[3], 福岡 創[1,3], 石島 秋彦[1,3]（[1]阪大・基礎工, [2]情報通信研究機構, [3]阪大・生命機能）
Tatsuki Hamamoto[1], Takashi Sagawa[2], Shin Koguchi[3], Hajime Fukuoka[1,3], Akihiko Ishijima[1,3] ([1]*Sch. Eng. Sci., Osaka Univ*, [2]*NICT*, [3]*Grad. Sch. Frontier Biosci., Osaka Univ*)

13:20〜16:20 I 会場（全学教育棟 3 階 E305）／Room I (Room E305, General Education Bldg. 3F)
1I 光生物： 視覚・光受容 I， 光合成 I， 光遺伝学・光制御 I /
Photobiology: Vision & Photoreception I, Photosynthesis I, Optogenetics & Optical Control I

1I1320* 新たに発見された光駆動型外向きプロトンポンプ DTS ロドプシンの機能解析と分光研究
Functional analysis and spectroscopic study of newly discovered light-driven outward proton pump DTS rhodopsins
○片岡 千尋[1], 井上 圭一[1,2], 神取 秀樹[1]（[1]名工大院工, [2]JSTさきがけ）
Chihiro Kataoka[1], Keiichi Inoue[1,2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*PRESTO, JST*)

1I1332* FTIR study of the T94I rhodopsin mutant in night blindness
Akiko Enomoto[1], Kota Katayama[1], Hiroo Imai[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Primate Res. Inst., Kyoto Univ.*)

1I1344* 海洋性真核藻類がもつ光駆動カチオンチャネル *Gt*CCR4 の分光解析
Spectroscopic analysis of a light-gated cation channel *Gt*CCR4 from marine algae
○山内 夢叶[1], 今野 雅恵[1,2], 伊藤 奨太[1], 角田 聡[1,2,3], 井上 圭一[1,2,3,4], 神取 秀樹[1,2]（[1]名工大・院・工, [2]名工大・オプトバイオ, [3]JST・さきがけ, [4]名工大・フロンティア）
Yumeka Yamauchi[1], Masae Konno[1,2], Shota Ito[1], Satoshi Tsunoda[1,2,3], Keiichi Inoue[1,2,3,4], Hideki Kandori[1,2] ([1]*Life Sci. Appl. Chem., Grad. Sch. Eng., NIT*, [2]*OBTRC, NIT*, [3]*PREST, JST*, [4]*FRIMS, NIT*)

1I1356 KR2 の Na^+輸送経路に位置する水分子の構造変化
Structural Changes of Water Molecules in the Na^+ Transport Pathway of KR2
○富田 紗穂子[1], 伊藤 奨太[1], 井上 圭一[1,2], 神取 秀樹[1]（[1]名古屋工業大学 神取研, [2]JSTさきがけ）
Sahoko Tomida[1], Shota Ito[1], Keiichi Inoue[1,2], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*PRESTO, JST*)

1I1408 低温赤外分光法を用いた(6-4)光産物の修復中間体の測定
Low-temperature FTIR study of the repair processes by Xenopus (6-4) photolyase
○山田 大智[1], 山元 淳平[2], 岩田 達也[3], 神取 秀樹[1]（[1]名工大院工, [2]阪大基礎工, [3]東邦大薬）
Daichi Yamada[1], Junpei Yamamoto[2], Tatsuya Iwata[3], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*Grad. Sch. Eng. Sci., Osaka Univ.*, [3]*Fac. Pharm. Sci., Toho Univ.*)

休憩（Coffee Break） 14:20–14:26

1I1426* 過渡回折格子法を用いた光センサータンパク質 EL222 の DNA 結合反応測定
Transient grating method revealed a DNA binding process of a light sensor protein EL222
○高門 輝, 中曽根 祐介, 寺嶋 正秀（京大院理）
Akira Takakado, Yusuke Nakasone, Masahide Terazima (*Grad. Sch. Sci. Kyoto Univ.*)

1I1438 光回復酵素/クリプトクロムファミリーにおける FAD 酸化還元制御メカニズム研究
The redox control mechanism of FAD in Photolyase/Cryptochrome family
○酒井 結衣[1], 山田 大智[1], 岩田 達也[2], 神取 秀樹[1]（[1]名古屋工業大学, [2]東邦大学薬学部）
Yui Sakai[1], Daichi Yamada[1], Tatsuya Iwata[2], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*Fac. Pharm. Sci. Toho Univ.*)

1I1450 分光法と QM/MM 計算を用いた Photoactive Yellow Protein 活性部位の構造解析
Active Site Structures of Photoactive Yellow Protein Revealed by Spectroscopy and QM/MM Calculations
○原口 翔次郎[1], Ren Jie[2], 藤澤 知績[1], Hoff Wouter D.[2], 海野 雅司[1]（[1]佐賀大院・工学系, [2]オクラホマ州立大）
Shojiro Haraguchi[1], Jie Ren[2], Tomotsumi Fujisawa[1], Wouter D. Hoff[2], Masashi Unno[1] ([1]*Grad. Sch. Sci. Eng., Saga Univ.*, [2]*Dept. Genet. Mol. Biol., Oklahoma State Univ.*)

1I1502* Acquirement of the water splitting ability and uni-directionality of the electron transfer pathway in O_2-evolving photosystem II
Keisuke Kawashima[1], Hiroshi Ishikita[1,2] ([1]*Grad. Sch. Eng., Univ. of Tokyo*, [2]*RCAST, Univ. of Tokyo*)

1I1514* フェムト秒過渡吸収分光による光化学系 II dimer のサブユニット間エネルギー移動ダイナミクスの解明
Intersubunit Energy Transfer Dynamics of Photosystem II Dimer Revealed by Femtosecond Transient Absorption Spectroscopy
○米田 勇祐[1], 片山 哲郎[1], 長澤 裕[2,3], 宮坂 博[1], 梅名 泰史[4]（[1]阪大・院基礎工, [2]立命館大・生命科学, [3]JSTさきがけ, [4]岡大・異分野）
Yusuke Yoneda[1], Tetsuro Katayama[1], Yutaka Nagasawa[2,3], Hiroshi Miyasaka[1], Yasufumi Umena[4] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Coll. Life. Sci., Ritsumeikan Univ.*, [3]*JST PREST*, [4]*Research Inst. Interdisciplinary Sci., Okayama Univ.*)

休憩（Coffee Break） 15:26–15:32

1I1532* The pH-Dependent Optical Property of Chlorophyll c bound to the Light-Harvesting Complex from a Diatom, Chaetoceros calcitrans
Nami Yamano[1], Tadashi Mizoguchi[2], Ritsuko Fujii[1,3] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [3]*OCARINA, Osaka City Univ.*)

1I1544* 光依存的に環状ヌクレオチド分解活性を示す新規酵素型ロドプシン
A novel enzyme rhodopsin with light- dependent cyclic nucleotide phosphodiesterase activity
○吉田 一帆[1], 角田 聡[1,2], Leonid Brown S.[3], 神取 秀樹[1]（[1]名工大・院工, [2]JST さきがけ, [3]ゲルフ大学）
Kazuho Yoshida[1], Satoshi Tsunoda[1,2], Brown S. Leonid[3], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*JST PRESTO*, [3]*Univ. Guelph*)

1I1556* タンパク質間 NO 転移反応を用いた SNO タンパク質の合成及びその機能の光制御
Photocontrol of SNO protein modified by protein-to-protein transnitrosylation
○黒田 剛[1], 佐藤 一平[1], 黒井 邦巧[1], 平松 弘嗣[2], 中林 孝和[1]（[1]東北大・院薬学, [2]交通大・応化学）
Takeshi Kurota[1], Ippei Sato[1], Kunisato Kuroi[1], Hirotsugu Hiramatsu[2], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [2]*Dept. Appl. Chem., NCTU*)

1I1608 光制御型 bZIP モジュール Photozipper の構造変化の分子機構
Molecular mechanisms for the conformational switching of a light-regulated bZIP module, Photozipper
○久冨 修（阪大・院理）
Osamu Hisatomi (*Grad. Sch. Sci., Osaka Univ.*)

13:20〜16:08 J 会場（全学教育棟 4 階 C401）／Room J (Room C401, General Education Bldg. 4F)
1J 非平衡・生体リズム，数理生物学Ⅰ，化学受容，神経・感覚 /
Nonequilibrium state & Biological rhythm, Mathematical biology I, Chemoreception, Neuroscience & Sensory systems

1J1320 時計タンパク質概日リズムを表現する素過程ベースの反応モデル
An elementary-process-based reaction model of the circadian rhythm of clock proteins
○甲田 信一[1,2], 斉藤 真司[1,2]（[1]分子研, [2]総研大）
Shin-ichi Koda[1,2], Shinji Saito[1,2] ([1]*IMS*, [2]*SOKENDAI*)

1J1332* Kai タンパク質間相互作用のリン酸化状態依存性による概日周期の安定性への影響
The influence of phosphorylation states dependence of Interaction between Kai proteins on stability of the circadian cycle
○杉山 翔吾[1], 盛 徹也[2], Byrne Mark[3], 内橋 貴之[4], Johnson Carl H.[2], 安藤 敏夫[1,5]（[1]金大自, [2]Dept. of Biol. Sci., Vanderbilt Univ., [3]Dept. Chem. Phys. and Eng., Spring Hill Col., [4]名大理, [5]金大バイオAFM FRC）
Shogo Sugiyama[1], Tetsuya Mori[2], Mark Byrne[3], Takayuki Uchihashi[4], Carl H. Johnson[2], Toshio Ando[1,5] ([1]*Dept. of Phys., Kanazawa Univ.*, [2]*Dept. of Biol. Sci., Vanderbilt Univ.*, [3]*Dept. Chem. Phys. and Eng., Spring Hill Col.*, [4]*Dept. of Phys., Nagoya Univ.*, [5]*Bio-AFM FRC., Kanazawa Univ.*)

1J1344 空間形状による Min たんぱく質の非線形波のコントロール
Geometric control of wave instability in Min oscillations
○義永 那津人[1,2]（[1]東北大学 材料科学高等研究所, [2]産総研 数理先端材料モデリング オープンイノベーションラボラトリ）
Yoshinaga Natsuhiko[1,2] ([1]*WPI-AIMR Tohoku University*, [2]*MathAM-OIL AIST*)

1J1356* ナノスケールでの化学的非平衡性を利用し、規則運動するｃｍサイズの液滴：生物が動く仕組みの実空間モデル
How to generated regular motion from nano-scaled fluctuating chemical machinery: Real-world modeling of motors in living organisms
○佐藤 志帆, 作田 浩輝, 吉川 研一（同志社大・生命医科）
Shiho Sato, Hiroki Sakuta, Kenichi Yoshikawa (*Grad. Sch. Life and Medical Sciences, Doshisha Univ.*)

1J1408* 力学-化学ハイブリッドモデルによる細胞集団形成ダイナミクス解析
Dynamic analysis of collective cell migration by mechanochemical hybrid model
○丸本 萌[1], 萩原 将也[2]（[1]大阪府大・院理学・生物, [2]大阪府大・Nanosquare拠点研究所）
Moegi Marumoto[1], Masaya Hagiwara[2] ([1]*Grad. Sch. Sci., Osaka Pref. Univ.*, [2]*N2RI, Osaka Pref. Univ.*)

休憩（Coffee Break） 14:20–14:26

1J1426 Numerical simulations of one dimensional cell crawling and traction force analysis
Hsuan-Yi Chen[1,2] ([1]*Natl. Cent. Univ., Taiwan*, [2]*Academia Sinica, Taiwan*)

1J1438 ネットワークのデザイン原理と構成要素の応答性
Network Designing and Response Sensitivity of Components
○井上 雅世[1], 金子 邦彦[2]（[1]明治大 総合数理, [2]東大 総合文化）
Masayo Inoue[1], Kunihiko Kaneko[2] ([1]*IMS, Meiji*, [2]*Univ. of Tokyo*)

1J1450 Lag Phase, Stationary Phase の理論モデル
Transitions among Log, Dormant, and Death Phases: Proposition of a simple model and quantitative characterization of dormancy and lag time
○姫岡 優介, 金子 邦彦（東大総文）
Yusuke Himeoka, Kunihiko Kaneko (*Tokyo Univ. Department of Arts and Sciences*)

1J1502 Generalized-Ensemble Simulations of Membrane Proteins
Te-Lun Mai[1], Chi-Ming Chen[2] ([1]*Genomic Research Center, Academia Sinica, Taiwan*, [2]*Department of Physics, National Taiwan Normal University*)

1J1514* コレラ菌走化性受容体 Mlp24, Mlp37 のリガンド認識機構の差異
Distinct mechanisms of ligand recognition between Mlp24 and Mlp37, chemoreceptor proteins of *Vibrio cholerae*
○高橋 洋平[1], 住田 一真[1], 西山 宗一郎[2], 川岸 郁朗[2], 今田 勝巳[1]（[1]阪大 院理, [2]法大 生命科学）
Yohei Takahashi[1], Kazumasa Sumita[1], So-ichiro Nishiyama[2], Ikuro Kawagishi[2], Katsumi Imada[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Dept. Front. Biosci. Sci., Hosei Univ.*)

休憩（Coffee Break） 15:26–15:32

1J1532* ATR-FTIR 分光測定によるヒト苦味受容体 TAS2R16 のリガンド結合機構の構造解析
Structural analysis of ligand binding in human bitter taste receptor by ATR-FTIR spectroscopy
○日置 茉優[1], 片山 耕大[1], 大橋 知明[1], 岩城 雅代[1], 吉住 怜[1], 今井 啓雄[2], 神取 秀樹[1]（[1]名工大・院工, [2]京大・霊長研）
Mayu Hioki[1], Kota Katayama[1], Tomoaki Ohashi[1], Masayo Iwaki[1], Rei Abe-Yoshizumi[1], Hiroo Imai[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Primate Res. Inst, Kyoto Univ.*)

1J1544 グルタミン酸受容体を介した植物の長距離 Ca^{2+} シグナル
Glutamate receptor channels essential for a long-distance Ca^{2+} waves in plants
○豊田 正嗣[1,2]（[1]埼玉大学・院・理, [2]University of Wisconsin-Madison）
Masatsugu Toyota[1,2] ([1]*Saitama University*, [2]*University of Wisconsin-Madison*)

1J1556 神経グロビンによる知覚変化の情報処理機構
Information processing mechanism underlying a perceptual change by a neuroglobin
○小田 茂和[1], 豊島 有[2], デゥボノ マリオ[3]（[1]岡崎統合バイオサイエンスセンター 定量生物学研究部門（基礎生物学研究所）, [2]東京大学大学院理学系研究科生物科学専攻, [3]MRC分子生物学研究所）
Shigekazu Oda[1], Yu Toyoshima[2], Mario De Bono[3] ([1]*Okazaki Institute for Integrative Science, Division of Quantitative Biology (National Institute for Basic Biology)*, [2]*Department of Biological Sciences, Graduate School of Science, University of Tokyo*, [3]*MRC Laboratory of Molecular Biology*)

第 2 日目（9 月 20 日（水））／Day 2（Sep. 20 Wed.）

13:55〜16:25　B 会場（全学教育棟 2 階 B201）／Room B (Room B201, General Education Bldg. 2F)
2B　分子モーターⅡ / Molecular motor II

2B1355 骨格筋ミオシン分子動態の直接可視化に基づく協同的な力発生の解明
Understanding of cooperative force generation among skeletal myosins based on direct observation of individual myosin dynamics
○茅 元司, 樋口 秀男（東京大学 大学院理学系研究科物理学専攻 樋口秀男研究室）
Motoshi Kaya, Hideo Higuchi (*Dept Physics, Univ of Tokyo*)

2B1407 ダイニン - ダイナクチン相互作用について
Interaction of dynactin complex with dynein
○斎藤 慧[1], 小林 琢也[1], 村山 尚[2], 豊島 陽子[1]（[1]東大・総合文化, [2]順天堂・医・薬理）
Kei Saito[1], Takuya Kobayashi[1], Takashi Murayama[2], Yoko Y Toyoshima[1] ([1]*Grad. Sch. Arts Sci., Univ. Tokyo*, [2]*Dept. of Pharmacology, Juntendo Univ. Sch. of Med.*)

2B1419 Yeast cytoplasmic dynein's small group takes a biased random walk toward the left-right

Mitsuhiro Sugawa[1], Shin Yamaguchi[1], Hiroaki Takagi[2], Mitsuhiro Iwaki[3], Keitaro Shibata[1], Yoko Y. Toyoshima[1], Junichiro Yajima[1] ([1]*Graduate School of Arts and Sciences, The Univ. of Tokyo*, [2]*Department of Physics, Nara Medical University*, [3]*QBiC, RIKEN*)

2B1431 単頭ダイニンのステップサイズと微小管結合時間の測定

The step size and microtubule-binding time of single-headed dynein

○木下 慶美[1], 神原 丈敏[1,2], 西川 香里[1], 茅 元司[1], 樋口 秀男[1]（[1]東京大学大学院, [2]理化学研究所QBiC）

Yoshimi Kinoshita[1], Taketoshi Kambara[1,2], Kaori Nishikawa[1], Motoshi Kaya[1], Hideo Higuchi[1] ([1]*The University of Tokyo*, [2]*RIKEN, QBiC*)

2B1443 Plus-end directionality present in kinesin conserved catalytic motor core

Masahiko Yamagishi, Junichiro Yajima (*Grad. Sch. Arts and Sci., The Univ. of Tokyo*)

2B1455 キネシンのエネルギー論

Nonequilibrium energetics of kinesin

○有賀 隆行[1], 富重 道雄[2], 水野 大介[1]（[1]九大・院理・物理, [2]青山学院大・理工・物理数理）

Takayuki Ariga[1], Michio Tomishige[2], Daisuke Mizuno[1] ([1]*Dept. Phys., Kyushu Univ.*, [2]*Dept. Phys. Math., Aoyama Gakuin Univ.*)

休憩（Coffee Break） 15:07–15:13

2B1513 高圧力で誘起される磁性細菌の遊泳運動能

Pressure-induced activation of the swimming motility of magnetotactic bacterium

○西山 雅祥[1], 阮 娟芳[2,3], 下權谷 祐児[3], 加藤 貴之[2], 南野 徹[2], 難波 啓一[2], 石川 拓司[3], 精山 明敏[1], Wu Long-Fei[4], 原田 慶恵[1,2]（[1]京都大学, [2]大阪大学, [3]東北大学, [4]Aix-Marseille University）

Masayoshi Nishiyama[1], Ruan Juanfang[2,3], Yuji Shimogonya[3], Takayuki Kato[2], Toru Minamino[2], Keiichi Namba[2], Takuji Ishikawa[3], Akitoshi Seiyama[1], Long-Fei Wu[4], Yoshie Harada[1,2] ([1]*Kyoto University*, [2]*Osaka University*, [3]*Tohoku University*, [4]*Aix-Marseille University*)

2B1525 金ナノプローブで明らかになった霊菌 Serratia marcescens 由来キチナーゼ A の 1 nm ステップ運動と運動律速段階

One nanometer steps and the rate-limiting step of Serratia marcescens chitinase A resolved by gold nanoprobe

○中村 彰彦[1,2], 飯野 亮太[1,2,3]（[1]自然科学研究機構 岡崎統合バイオサイエンスセンター, [2]総合研究大学院大学, [3]分子科学研究所）

Akihiko Nakamura[1,2], Ryota Iino[1,2,3] ([1]*Okazaki Inst. for Integr. Biosci.*, [2]*SOKENDAI*, [3]*Institute for Molecular Science*)

2B1537 腸球菌 V-ATPase 膜内在ローターリングの阻害剤結合型の X 線結晶構造解析

Crystal structure of inhibitor bound membrane rotor ring of Enterococcus hirae V-ATPase

○魏 川華[1], 薬師寺 ファビアナ リカ[1], 森山 克彦[1], 鈴木 花野[1], 水谷 健二[2], 村田 武士[1,3]（[1]千葉大・院理学, [2]横浜市立大・院生命医科学, [3]JST さきがけ）

Senka Gi[1], Fabiana Lica Yakushiji[1], Katsuhiko Moriyama[1], Kano Suzuki[1], Kenji Mizutani[2], Takeshi Murata[1,3] ([1]*Grad. Sch. Sci., Univ. Chiba*, [2]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [3]*PRESTO, JST*)

2B1549 How fast can bacteria grow their flagella?

Chien-Jung Lo (*Department of Physics, National Central University*)

2B1601 角度分割・時分割 X 線結晶構造解析による、哺乳類 F1-ATPase のリン酸解離駆動の回転力発生機構の分析

Molecular mechanism of Phosphate-driven rotation of mammalian F1 by the angle-divided and time-resolved X-ray crystallographic studies

○鈴木 俊治[1,2,3], 平田 邦生[4], 山下 栄樹[5], 飯田 直也[6], 遠藤 斗志也[2], 久堀 徹[3], 吉田 賢右[2], 野地 博行[1]（[1]東大院・工・応化, [2]京産大・総合生命, [3]東工大・化学生命研, [4]理研・SPring8センター, [5]阪大・蛋白研, [6]早大・物理）

Toshiharu Suzuki[1,2,3], Kunio Hirata[4], Eiki Yamashita[5], Naoya Iida[6], Toshiya Endo[2], Toru Hisabori[3], Masasuke Yoshida[2], Hiroyuki Noji[1] ([1]*Shool of Eng. Univ of Tokyo*, [2]*Dept of Mol Biosci, Kyoto-Sangyo Univ*, [3]*CLS, Tokyo Inst of Tech*, [4]*SPring8 Center, RIKEN*, [5]*Inst for Protein Res*, [6]*Dept of Physics, Waseda Univ*)

2B1613 Biophysical Characterization of the Chemomechanical Coupling of F_1 ATPase of *Paracoccus denitrificans*

Mariel Zarco Zavala[1], Duncan G.G. Mcmillan[2], Toshiharu Suzuki[1], Hiroshi Ueno[1], Rikiya Watanabe[1], Francisco Mendoza Hoffmann[3], José J. García Trejo[3], Hiroyuki Noji[3] ([1]*Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo*, [2]*Department of Biotechnology, Delft University of Technology*, [3]*Department of Biology, Chemistry Faculty, National Autonomous University of Mexico*)

13:55〜16:13 C 会場（全学教育棟 2 階 B202）／Room C (Room B202, General Education Bldg. 2F)
2C 生体膜・人工膜Ⅱ，生命の起源・進化，生態／環境 /
Biological & Artificial membrane II, Origin of life & Evolution/Ecology & Environment

2C1355 Characterization of prokaryotic voltage-gated calcium channel

Katsumasa Irie[1,2], Takushi Shimomura[3], Yoshiki Yonekawa[2], Yoshinori Fujiyoshi[1,4] ([1]*CeSPI, Nagoya Univ.*, [2]*Grad. Sch. Pharm., Nagoya Univ.*, [3]*Div. Biophys. and Neurobiol., NIPS*, [4]*CeSPIA Co., Ltd.*)

2C1407 電位依存性プロトンチャネルの亜鉛阻害におけるヒスチジンとカルボン酸の役割
The role of histidine and carboxylate residues for zinc inhibition in the voltage-gated proton channel Hv1/VSOP
○岩城 雅代[1], 竹下 浩平[2,3,4], 有馬 大貴[5], 岡村 康司[5], 中川 敦史[2], 神取 秀樹[1]（[1]名工大, [2]阪大・蛋白研, [3]阪大・未来戦略機構, [4]JST-さきがけ, [5]阪大院・医）
Masayo Iwaki[1], Kohei Takeshita[2,3,4], Hiroki Arima[5], Yasushi Okamura[5], Atsushi Nakagawa[2], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*Inst. Protein Res., Osaka Univ.*, [3]*Inst. Acad. Initiat., Osaka Univ.*, [4]*JST-PRESTO*, [5]*Grad. Sch. Med., Osaka Univ.*)

2C1419 光駆動型ナトリウムポンプロドプシンは異なる２つのイオン輸送モードを持つ
Two distinct ion transporting modes of sodium pumping rhodopsin, NaR
○小﨑 裕子[1], 細島 頌子[1], 角田 聡[1,2], 神取 秀樹[1]（[1]名工大 院工, [2]JST さきがけ）
Yuko Kozaki[1], Shoko Hososhima[1], Satoshi Tsunoda[1,2], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*PRESTO, JST*)

2C1431 高速 AFM による K+チャネル KcsA とポア結合性サソリ毒ペプチド Agtx2 の一分子結合動態解析
HS-AFM revealed single-molecule blocking dynamics of a scorpion toxin on the KcsA potassium channel
○角野 歩[1,2], 内橋 貴之[3], 炭竈 享司[4], 老木 成稔[4]（[1]金沢大・新学術創成, [2]金沢大・バイオAFM, [3]名大・院理, [4]福井大・医）
Ayumi Sumino[1,2], Takayuki Uchihashi[3], Takashi Sumikama[4], Shigetoshi Oiki[4] ([1]*InFiniti, Kanazawa Univ.*, [2]*Bio-AFM FRC, Kanazawa Univ.*, [3]*Dept. Phys., Nagoya Univ.*, [4]*Facult. Med. Sci., Univ. Fukui*)

2C1443 アルギニンペプチド修飾型エクソソームのマクロピノサイトーシス誘導と効率的な細胞内移行
Exosomal membrane modification with arginine-rich peptides for enhanced macropinocytotic uptake of exosomes
○中瀬 生彦[1], 野口 公輔[1,2], 青木 絢子[1,2], 中瀬 朋夏[3], 藤井 郁雄[2], 二木 史朗[4]（[1]阪府大 N2RI, [2]阪府大院理, [3]武庫女大薬, [4]京大化研）
Ikuhiko Nakase[1], Kosuke Noguchi[1,2], Ayako Aoki[1,2], Tomoka Takatani-Nakase[3], Ikuo Fujii[2], Shiroh Futaki[4] ([1]*N2RI, Osaka Prefecture Univ.*, [2]*Graduate School of Sci., Osaka Prefecture Univ.*, [3]*School of Pharm. Pharm. Sci., Mukogawa Women's Univ.*, [4]*ICR, Kyoto Univ.*)

2C1455 微細加工基板上の自立脂質二分子膜における浸透圧変化と相分離
Phase separation of freestanding planar bilayer lipid membrane on Si microwell under osmotic pressure change
○大嶋 梓[1], 住友 弘二[2], 中島 寛[1]（[1]NTT物性基礎研, [2]兵県大・院工）
Azusa Oshima[1], Koji Sumitomo[2], Hiroshi Nakashima[1] ([1]*NTT Basic Res. Labs.*, [2]*Grad. Sch. Eng., Univ. Hyogo*)

休憩（Coffee Break） 15:07–15:13

2C1513 Negative chemotaxis molecular robots migrated by osmotic pressure difference
Kan Shoji, Ryuji Kawano (*Dept. Biotech. and Life Sci., TUAT*)

2C1525 アクチン線維封入巨大リポソームの光刺激による可逆的な形態制御
Light-induced and reversible morphological control of F-actin-encapsulating giant liposomes
○林 真人[1], 田中 駿介[2], 滝口 金吾[2]（[1]理研・脳科学総合研究センター, [2]名大・理）
Masahito Hayashi[1], Shunsuke Tanaka[2], Kingo Takiguchi[2] ([1]*RIKEN BSI*, [2]*Grad. Sch. Sci., Nagoya Univ.*)

2C1537 人工 RNA 複製系を用いて試験管内で宿主・寄生体の進化的軍拡競争を観察する
Evolutionary arms races between artificial host-parasite RNA replicators in vitro
○古林 太郎[1], 番所 洋輔[1], 市橋 伯一[2]（[1]阪大・生命機能, [2]阪大・情報科学）
Taro Furubayashi[1], Yohsuke Bansho[1], Norikazu Ichihashi[2] ([1]*Grad. Sch. of Frontbio, Osaka Univ*, [2]*Grad. Sch. of InfoTech, Osaka Univ*)

2C1549 マイクロデバイスと大腸菌の融合を利用した新規人工細胞系の開発
Development of a new artificial cell system based on the fusion of micron-scaled device and *E. coli*
○森泉 芳樹[1,2], 田端 和仁[1,2,3], 渡邉 力也[1,3,4], 堂浦 智裕[5], 神谷 真子[3,5], 浦野 泰照[5,6,7], 野地 博行[1,2]（[1]東京大・院工学・応用化, [2]内閣府・ImPACT, [3]JST・さきがけ, [4]AMED・PRIME, [5]東京大・院医学, [6]東京大・院薬学, [7]AMED・CREST）
Yoshiki Moriizumi[1,2], Kazuhito Tabata[1,2,3], Rikiya Watanabe[1,3,4], Tomohiro Doura[5], Mako Kamiya[3,5], Yasuteru Urano[5,6,7], Hiroyuki Noji[1,2] ([1]*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*ImPACT, Cab. Office*, [3]*PRESTO, JST*, [4]*PRIME, AMED*, [5]*Grad. Sch. Med., Univ. Tokyo*, [6]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [7]*CREST, AMED*)

2C1601 バクテリアの長期定常期における密度依存的なリサイクリング活動
Density-dependent recycling in the long-term stationary phase of bacterial populations
高野 壮太朗[2], Pawlowska Bogna J.[3], Gudelj Ivana[3], 四方 哲也[4], ○津留 三良[1]（[1]東大・生物普遍性研究機構, [2]筑波大・生命環境系, [3]Biosci., Univ. of Exeter, [4]Inst. of Biol. and Inf. Sci., East China Normal Univ.）
Sotaro Takano[2], Bogna J. Pawlowska[3], Ivana Gudelj[3], Tetsuya Yomo[4], **Saburo Tsuru**[1] ([1]*Univ. Biol. Inst., The Univ. of Tokyo*, [2]*Life and Env. Sci., Univ. of Tsukuba*, [3]*Biosci., Univ. of Exeter*, [4]*Inst. of Biol. and Inf. Sci., East China Normal Univ.*)

13:55～16:25　D 会場（全学教育棟 2 階 E201）／Room D (Room E201, General Education Bldg. 2F)
2D　バイオイメージングⅡ / Bioimaging II

2D1355 スマートフォン顕微鏡イノベーション
Smartphone Microscope Innovation
○永山 國昭[1,2], 白根 純人[2]（[1]LisCo 永山顕微鏡研, [2]Life Is Small. Co）
Kuniaki Nagayama[1,2], Sumito Shirane[2] ([1]*Nagayama Microsc. Lab., LisCo*, [2]*Life Is Small. Co*)

2D1407 高速 AFM による抗体 IgG のリアルタイム観察と挙動解析
High-Speed AFM revealed dynamic behavior of antibody
○小谷 則遠, 川元-尾崎 洋子, Ramanujam Kumaresan, 中塚 涼, 森居 隆史, 岡田 孝夫（株式会社生体分子計測研究所）
Norito Kotani, Yoko Kawamoto-Ozaki, Kumaresan Ramanujam, Ryo Nakatsuka, Takashi Morii, Takao Okada (*Research Institute of Biomolecule Metrology*)

2D1419 High-speed atomic force microscopy (HS-AFM) revealed dynamic structural changes of Bacteriophage T4 sheath
Hiroki Watanabe[1], Shuji Kanamaru[2], Takayuki Uchihashi[3] ([1]*RIBM*, [2]*Dept. of Life Sci. and Tech., Tokyo Institute of Technology*, [3]*Dept. of Phys., Nagoya Univ.*)

2D1431 高速 AFM による天然変性タンパク質 CAMP の構造動態観察
Structural dynamics of the intrinsically disordered protein CAMP revealed by high-speed AFM
○成田 知恕[1], 池田 真教[2], 田中 耕三[2], 古寺 哲幸[3]（[1]金沢大・院数物, [2]東北大・加齢研・分子腫瘍, [3]金沢大・バイオAFM）
Tomoyuki Narita[1], Masanori Ikeda[2], Kozo Tanaka[2], Noriyuki Kodera[3] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*Dept. Mol. Oncol., Inst. Dev. Aging Center, Tohoku Univ.*, [3]*Bio-AFM FRC, Kanazawa Univ.*)

2D1443 高速 AFM による立体パターン基板を用いたタンパク質の動態観察
HS-AFM Observations of Protein Dynamics on 3D-patterned Substrate
○後藤 朱音[1], 柴田 幹大[2,3], 角野 歩[2,3], 古寺 哲幸[3]（[1]金沢大・院数物, [2]金沢大・新学術創成, [3]金沢大・バイオAFM）
Akane Goto[1], Mikihiro Shibata[2,3], Ayumi Sumino[2,3], Noriyuki Kodera[3] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ*, [2]*InFiniti., Kanazawa Univ*, [3]*Bio-AFM. FRC., Kanazawa Univ*)

2D1455 高速 AFM による脂質膜の曲率に依存したタンパク質-脂質膜の相互作用の直接観察
Direct observation of proteins-lipid membrane interactions depending on the physical shape of lipid membrane by high-speed AFM
○豊田 貴大[1], 後藤 朱音[1], 角野 歩[2,3], 柴田 幹大[2,3], 古寺 哲幸[3]（[1]金沢大・院数物, [2]金沢大・新学術創成, [3]金沢大・バイオAFM）
Takahiro Toyoda[1], Akane Goto[1], Ayumi Sumino[2,3], Mikihiro Shibata[2,3], Noriyuki Kodera[3] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*InFiniti., Kanazawa Univ*, [3]*Bio-AFM FRC, Kanazawa Univ.*)

休憩（Coffee Break） 15:07–15:13

2D1513 生細胞のクロマチン構造の超解像イメージング
Dynamic organization of chromatin domains revealed by super-resolution live-cell imaging
野崎 慎, ○前島 一博（国立遺伝学研究所構造遺伝学研究センター）
Tadasu Nozaki, **Kazuhiro Maeshima** (*NIG*)

2D1525 G タンパク質共役型受容体（GPCR）と G タンパク質の二色一分子観察をもとにした GPCR の活性化状態評価
Evaluation of G-protein coupled receptor (GPCR) signaling activity based on dual color single molecule imaging of GPCR and G-protein
○西口 知輝, 吉村 英哲, 小澤 岳昌（東大・院理）
Tomoki Nishiguchi, Hideaki Yoshimura, Takeaki Ozawa (*Grad. Sch. Sci., The Univ. Tokyo*)

2D1537 高光度化学発光タンパク質ナノ-ランタンを用いた走化性タンパク質の新規観察法
Novel imaging method for chemotaxis protein using a super-duper chemiluminescent protein, Nano-lantern
○麻生 慎太郎[1], 中野 雅裕[2], 福岡 創[1], 永井 健治[2], 石島 秋彦[1]（[1]大阪大学生命機能研究科, [2]大阪大学産業科学研究所）
Shintaro Aso[1], Masahiro Nakano[2], Hajime Fukuoka[1], Takeharu Nagai[2], Akihiko Ishijima[1] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [2]*ISIR, Osaka Univ.*)

2D1549 Trafficking of endocytic vesicles in live cancer cells
Seohyun Lee[1], Kohsuke Gonda[2], Motoshi Kaya[1], Hideo Higuchi[1] ([1]*Dept. of Physics, Graduate School of Science, The University of Tokyo*, [2]*Dept. of Medical Physics, Graduate School of Medicine, Tohoku University*)

2D1601 Linking Raman spectroscopy and gene expression profiles for genotype-phenotype prediction
Arno Germond[1], Takaaki Horinouchi[1], Chikara Furusawa[1,2], Toshio Yanagida[1], Taro Ichimura[1], Tomonobu M. Watanabe[1,3] ([1]*RIKEN, Quantitative Biology Center (QBiC)*, [2]*Universal Biology Institute, The University of Tokyo*, [3]*Graduate School of Frontier Bioscience, Osaka University*)

2D1613 遺伝子コードされた超音波エコーイメージング造影剤の開発
Development of genetically-encoded contrast agent for ultrasonography
○水島 良太[1], 井上 加奈子[2], 岩根 敦子[1], 渡邊 朋信[1]（[1]理研-QBiC, [2]阪大超高圧電顕センター）
Ryota Mizushima[1], Kanako Inoue[2], Atsuko Iwane[1], Tomonobu Watanabe[1] ([1]*RIKEN-QBiC*, [2]*Uhvem, Osaka Univ*)

13:55～16:01　E 会場（全学教育棟 2 階 E203）／Room E (Room E203, General Education Bldg. 2F)
2E　計測Ⅱ，数理生物学Ⅱ，化学受容，行動，その他 / Measurements II, Mathematical biology II, Chemoreception, Behavior, Miscellaneous topics

2E1355 実時間選択的回収による免疫細胞の網羅的遺伝子発現解析
Single-cell transcriptome analysis of stimulated immune cells with real-time collection
○田中 優実子[1], 白崎 善隆[1,2], 山岸 舞[1,2], 宮田 楓[1], 鈴木 信勇[1,2], 小原 收[2], 茂呂 和世[2], 上村 想太郎[1]（[1]東大・院・理, [2]理研・IMS）
Yumiko Tanaka[1], Yoshitaka Shirasaki[1,2], Mai Yamagishi[1,2], Kaede Miyata[1], Nobutake Suzuki[1,2], Osamu Ohara[2], Kazuyo Moro[2], Sotaro Uemura[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*IMS., RIKEN*)

2E1407 走査型イオンコンダクタンス顕微鏡による一次繊毛のナノスケール形状測定
Measuring nanoscale morphology of primary cilia using scanning ion-conductance microscopy
○周 緑殊[1], 斎藤 将樹[2], 宮本 貴史[1], 福間 剛士[1], 高橋 康史[1,3]（[1]金沢大・理工・電情, [2]東北大院・医・分子薬理, [3]JST・さきがけ）
Yuanshu Zhou[1], Masaki Saito[2], Takafumi Miyamoto[1], Takeshi Fukuma[1], Yasufumi Takahashi[1,3] ([1]*Fac. of Ele. & Com., Inst. of Sci. & Eng., Univ. Kanazawa*, [2]*Dept. of Mol. Pharmacol., Grad. Sch. of Med., Univ. Tohoku*, [3]*JST-PRESTO*)

2E1419 夾雑物存在下でマイクロ RNA を電気測定により検知する技術の開発
Detection of target microRNA in a crude sample by electrical measurement
○藤井 聡志[1], 三澤 宣雄[1], 神谷 厚輝[1], 大崎 寿久[1,2], 竹内 昌治[1,2]（[1]神奈川県立産業技術総合研究所, [2]東京大学生産技術研究所）
Satoshi Fujii[1], Nobuo Misawa[1], Koki Kamiya[1], Toshihisa Osaki[1,2], Shoji Takeuchi[1,2] ([1]*Kanagawa Institute of Industrial Science and Technology (KISTEC)*, [2]*Institute of Industrial Science (IIS), The University of Tokyo*)

2E1431 in vitro 三次元培養における計測制御プラットフォームの構築
In vitro 3D culture platform for environmental control and imaging
○萩原 将也[1], 野畑 李奈[2], 川原 知洋[3]（[1]大阪府大NanoSquare拠点研究所, [2]大阪府大院・生物, [3]九工大院生命体工学）
Masaya Hagiwara[1], Rina Nobata[2], Tomohiro Kawahara[3] ([1]*N2RI, Osaka Pref. Univ.*, [2]*Osaka Pref. Univ.*, [3]*Kyushu Inst. of Tech.*)

2E1443 バイオメディカルアプリケーションのための 8 タップ電荷変調画素に関する研究
An 8-tap Time Resolved CMOS Lock-In Pixel Imager for Biomedical Applications
○白川 雄也[1], 徐 珉雄[2], 安富 啓太[2], 香川 景一郎[2], 寺西 信一[2], 川人 祥二[2]（[1]静岡大・院工学, [2]静岡大・電子工学研）
Yuya Shirakawa[1], Min-Woong Seo[2], Keita Yasutomi[2], Keiichiro Kagawa[2], Nobukazu Teranishi[2], Shoji Kawahito[2] ([1]*Grad. Sch. Engi., Univ. Shizuoka*, [2]*Res. Ins. Elec, Univ. Shizuoka*)

2E1455 A mechanical model for diversified insect wing margin shapes
Yukitaka Ishimoto[1], Kaoru Sugimura[2] ([1]*Akita Pref. U.*, [2]*iCeMS, Kyoto U.*)

休憩（Coffee Break） 15:07–15:13

2E1513 アレルゲン免疫療法の理論的解析
Mathematical study of allergen immunotherapy
○原 朱音[1], 巌佐 庸[2]（[1]九大・院・システム生命, [2]九大・院・理学・生物科学）
Akane Hara[1], Yoh Iwasa[2] ([1]*Grad. Sch. Sys. Life Sci. Kyushu Univ.*, [2]*Dept. Biol., Fac. Sci., Kyushu Univ.*)

2E1525 機械学習を用いた大腸菌走化性受容体に作用する誘引物質の予測
Prediction of attractants for the chemoreceptors of *Escherichia coli* using machine learning
○佐川 貴志[1], 猿子 良太[2], 横田 悠右[1], 成瀬 康[1], 曽和 義幸[3], 川岸 郁朗[3], 岡田 真人[1,4], 大岩 和弘[1], 小嶋 寛明[1]（[1]情報通信研究機構, [2]長岡技科大・生物, [3]法政大・生命科学, [4]東大・複雑理工学）
Takashi Sagawa[1], Ryota Mashiko[2], Yusuke Yokota[1], Yasushi Naruse[1], Yoshiyuki Sowa[3], Ikuro Kawagishi[3], Masato Okada[1,4], Kazuhiro Oiwa[1], Hiroaki Kojima[1] ([1]*NICT*, [2]*Dept. Bioeng., Nagaoka Univ. Tech.*, [3]*Dept. Frontier Biosci., Hosei Univ.*, [4]*Dept. Complexity Sci. Eng., Univ. Tokyo*)

2E1537 二者の同調歩行における歩行パターン分析：受動と能動の中間的状況における身体性の拡張
Analysis for the changes in the gait patterns in paired walking: Expanded bodily self by the ambiguity of passive/active leadership
○箕浦 舞[1], 郡司 幸夫[1], 白川 智弘[2]（[1]早稲田大学 基幹理工学部 表現工学科 郡司研究室, [2]防衛大学校電気情報学群情報工学科）
Mai Minoura[1], Yukio-Pegio Gunji[1], Tomohiro Shirakawa[2] ([1]*School of Fundamental Science and Engineering, Waseda University*, [2]*Department of Computer Science, School of Electrical and Computer Engineering, National Defense*)

2E1549 Surfactant role on microbead manipulation by saw-tooth shaped electrode
Marcos Masukawa, Masahiro Takinoue (*Tokyo Institute of Technology, Takinoue Lab*)

13:55〜16:25　F 会場（全学教育棟 2 階 E205）／Room F (Room E205, General Education Bldg. 2F)
2F　蛋白質： 構造・構造機能相関Ⅱ / Proteins: Structure, Structure-function relationship II

2F1355 Structural analysis of Chrimson, a red-light activated channelrhodopsin
Kazumasa Oda, Satomi Oishi, Reiya Taniguchi, Tomohiro Nishizawa, Ryuichiro Ishitani, Osamu Nureki (*Grad. Sch. Sci., Univ. Tokyo*)

2F1407 A novel enzyme which folds into active form only with its counterpart
Kohei Sawada[1], Atsushi Minami[2], Taro Ozaki[2], Hiroyuki Kumeta[3], Tomohide Saio[2], Koichiro Ishimori[2], Min Yao[3], Hideaki Oikawa[2], Katsumi Maenaka[1], Toyoyuki Ose[1,3] ([1]*Faculty of Pharm. Sci, Hokkaido Univ.*, [2]*Faculty of Sci, Hokkaido Univ.*, [3]*Faculty of Adv. Life Sci., Hokkaido Univ.*)

2F1419 NMR characterization of the substrate-binding domains of protein disulfide isomerase using paramagnetic effects
Methanee Hiranyakorn[1,2], Saeko Yanaka[1,2], Maho Yagi-Utsumi[1,2], Koichi Kato[1,2] ([1]*Inst. Mol. Sci, Natl. Inst. Nat. Sci.*, [2]*SOKENDAI*)

2F1431 X 線自由電子レーザー回折像を用いた巨大生体分子三次元構造の復元
Three-dimensional structure reconstruction of large biological molecule from diffraction images obtained by XFEL using computer simulation
○中野 美紀[1], 宮下 治[1], Jonic Slavica[2], 徳久 淳師[1], Tama Florence[1,3,4]（[1]理研 計算科学研究機構, [2]IMPMC, Sorbonne Univ. CNRS, UPMC Univ Paris 6, MNHN, IRD, [3]名古屋大院理学研究科, [4]名古屋大トランスフォーマティブ生命分子研究所）
Miki Nakano[1], Osamu Miyashita[1], Slavica Jonic[2], Astushi Tokuhisa[1], Florence Tama[1,3,4] ([1]*RIKEN AICS*, [2]*IMPMC, Sorbonne Univ. CNRS, UPMC Univ Paris 6, MNHN, IRD*, [3]*Grad. Sch. Science, Nagoya Univ.*, [4]*ITbM, Nagoya Univ.*)

2F1443 Efficient strategy to retrieve potential 3D models directly from a small amount of single particle projection data
Sandhya Tiwari[1], Florence Tama[1,2,3], Osamu Miyashita[1] ([1]*RIKEN AICS*, [2]*ITbM, Nagoya University*, [3]*Dept. of Physics Nagoya University*)

2F1455 光回復酵素と DASH 型クリプトクロムにおける紫外線損傷二本鎖 DNA の結合に寄与する因子の特定
Identification of the factors that contribute to binding UV-damaged duplex DNA for Photolyase and Cryptochrome-DASH
○佐藤 竜馬, 重田 育照（筑波大学 計算科学研究センター）
Ryuma Sato, Yasuteru Shigeta (*Center for Computational Sciences, University of Tsukuba*)

休憩（Coffee Break） 15:07–15:13

2F1513 荷電性アミノ酸の粗視化モデルの開発
Development of a coarse-grained model for charged amino acid residues
○川口 一朋, 中川 聖, 長尾 秀実（金沢大学理工研究域数物科学系）
Kazutomo Kawaguchi, Satoshi Nakagawa, Hidemi Nagao (*Inst. Sci. Eng., Kanazawa Univ.*)

2F1525 Dimerization of full-length Aβ peptides by the Hamiltonian replica-permutation method
Satoru Itoh[1,2], Hisashi Okumura[1,2] ([1]*IMS*, [2]*SOKENDAI*)

2F1537 クライオ電子顕微鏡像フィッティングのための新規 MD 法の開発と応用
Development of a new method for efficient cryo-EM fitting simulation
○森 貴治[1,2], 宮下 治[3], Kulik Marta[1], Tama Florence[3,4], 杉田 有治[1,2,3,5]（[1]理研 杉田理論分子科学, [2]理研 iTHES, [3]理研 AICS, [4]名大院・理, [5]理研 QBiC）
Takaharu Mori[1,2], Osamu Miyashita[3], Marta Kulik[1], Florence Tama[3,4], Yuji Sugita[1,2,3,5] ([1]*RIKEN Theor. Mol. Sci. Lab.*, [2]*RIKEN iTHES*, [3]*RIKEN AICS*, [4]*Nagoya University*, [5]*RIKEN QBiC*)

2F1549 MD シミュレーションを用いた構造サンプリングによるドッキングタンパク質ータンパク質複合体結合自由エネルギー評価の精密化
Refining binding free energies of docked protein-protein complexes by sampling conformations during molecular dynamics simulations
○信夫 愛, 竹村 和浩, 北尾 彰朗（東大・分子研）
Ai Shinobu, Kazuhiro Takemura, Akio Kitao (*Inst. Mol. Cell. Bio., Univ. Tokyo*)

2F1601 Improvement of PaCS-MD based Flexible Docking Methods
Phuoc Duy Tran[1], Akio Kitao[1,2] ([1]*Graduate School of Frontier Sciences, The University of Tokyo*, [2]*Institute of Molecular and Cellular Biosciences, The University of Tokyo*)

2F1613 アミロイド核前駆体として機能する前駆中間凝集体のキャラクタリゼーション
A specific form of prefibrillar aggregates that functions as a precursor of amyloid nucleation
○山本 直樹, 津原 祥子, 田村 厚夫, 茶谷 絵理（神戸大学大学院理学研究科）
Naoki Yamamoto, Shoko Tsuhara, Atsuo Tamura, Eri Chatani (*Grad. Sch. Sci.*)

13:55〜16:25　H 会場（全学教育棟 3 階 E303）／Room H (Room E303, General Education Bldg. 3F)
2H　光生物： 光合成Ⅱ，電子状態，ヘム蛋白質Ⅱ，細胞生物学的課題Ⅱ，筋肉Ⅱ / Photobiology: Photosynthesis II, Electronic state, Heme proteins II, Cell biology II, Muscle II

2H1355 光化学系 I の低温単一分子分光: ブリンキングの起源
Single-Molecule Spectroscopy of Photosystem I at Low Temperature: the Origin of the Blinking
ジャナ サンカー[1], 小林 誉宗[1], 杜 婷[1], 長尾 遼[2], 野口 巧[3], ○柴田 穣[1]（[1]東北大学理学研究科化学専攻, [2]岡山大学異分野基礎科学研究所, [3]名古屋大学大学院理学研究科物質理学専攻）
Sankar Jana[1], Takanori Kobayashi[1], Ting Du[1], Ryo Nagao[2], Takumi Noguchi[3], **Yutaka Shibata**[1] ([1]*Grad. School of Sci. Tohoku Univ.*, [2]*Research Institute for Interdisciplinary Science, Okayama University*, [3]*Graduate School of Science, Nagoya University*)

2H1407 光化学系 II 酸素発生中心における酸素分子放出過程についての QM/MM 解析
QM/MM study on the O2 release mechanism of the oxygen-evolving complex in photosystem II
○庄司 光男[1], 磯部 寛[2], 重田 育照[1], 中嶋 隆人[3], 山口 兆[4]（[1]筑波大CCS, [2]岡山大, [3]理研AICS, [4]阪大）
Mitsuo Shoji[1], Hiroshi Isobe[2], Yasuteru Shigeta[1], Takahito Nakajima[3], Kizashi Yamaguchi[4] ([1]*Univ. Tsukuba*, [2]*Okayama Univ.*, [3]*RIKEN AICS*, [4]*Osaka Univ.*)

2H1419 単一分子分光で明らかになった光合成光保護機構
Photosynthetic photoprotection mechanism revealed by single-molecule spectroscopy
○近藤 徹[1,2], ピノーラ アルベルタ[3], チェン ウェイジア[1], ダロスト ルカ[3], バッシ ロベルト[3], シュラウコーエン ガブリエラ[1,2]（[1]マサチューセッツ工科大学, [2]Mit-Harvard エキシトン工学センター, [3]ヴェローナ大学）
Toru Kondo[1,2], Alberta Pinnola[3], Wei Jia Chen[1], Luca Dall'Osto[3], Roberto Bassi[3], Gabriela Schlau-Cohen[1,2] ([1]*Mit*, [2]*Mit-Harvard Center for Excitonics*, [3]*Univ. Verona*)

2H1431 Monitoring of quinone reduction in the thermophilic purple bacterium Thermochromatium tedium by means of isotope-edited FTIR spectroscopy
Michie Imanishi[1], Rikako Kishi[1], Masayuki Kobayashi[2], Seiu Otomo[3], **Yukihiro Kimura**[1] ([1]*Grad. Sch. Agro., Kobe Univ.*, [2]*Ariake Nat. Col. Tech*, [3]*Fac. Sci., Ibaraki Univ.*)

2H1443 時間分解 EPR でとらえる光合成反応中心初期電荷分離の制御機構
Regulation of Initial Charge Separation in Photosynthetic Reaction Center detected by Transient EPR
○三野 広幸[1], 佃野 弘幸[1], 武藤 理沙[2,3], 長嶋 宏樹[1,4], 小堀 康博[4], 栗栖 源嗣[2], 大岡 宏造[5]（[1]名大院理, [2]阪大蛋白研, [3]福岡大理, [4]神戸大フォト, [5]阪大院理）
Hiroyuki Mino[1], Hiroyuki Tsukuno[1], Risa Mutoh[2,3], Hiroki Nagashima[1,4], Yasuhiro Kobori[4], Genji Kurisu[2], Hirozo Oh-oka[5] ([1]*Grad. School of Sci., Nagoya Univ.*, [2]*Inst. for Protein Res., Osaka Univ.*, [3]*Fac. of Sci., Fukuoka Univ.*, [4]*Mol. Photosci. Res., Kobe Univ*, [5]*Grad. School of Sci., Osaka Univ.*)

2H1455 溶液中のクロロフィル a とフィオフィチン a の励起状態に関する理論的研究
Theoretical Study on Excited States of Chlorophyll a and Pheophytin a in Solutions
○水谷 亮, 東 雅大（琉球大・院理工）
Ryo Mizutani, Masahiro Higashi (*Grad. Sch. Univ. The Ryukyus*)

休憩（Coffee Break） 15:07–15:13

2H1513 Crystal structure of biliverdin reductase shows unexpected substrate binding manner; two substrates bind to the one catalytic cleft
Masakazu Sugishima[1], Haruna Takao[2,3], Yoshinori Hagiwara[4], Ken Yamamoto[1], Keiichi Fukuyama[5], Kei Wada[2] ([1]*Kurume Univ. Sch. Med.*, [2]*Fac. Med., Univ. Miyazaki*, [3]*Grad. Sch. Med. and Vet. Med., Univ. Miyazaki*, [4]*Dept. Biochem. and Appl. Chem., Nat. Inst. Tech., Kurume College*, [5]*Grad. Sch. Eng., Osaka Univ.*)

2H1525 カンチレバーを用いた高感度多周波 EPR 測定法の開発とヘミンへの応用
Development of cantilever-detected high-sensitive multi-frequency EPR method and its application to hemin
○岡本 翔[1], 高橋 英幸[2], 大道 英二[1], 太田 仁[3]（[1]神戸大・院理, [2]神戸大・先端, [3]神戸大・分子フォトセ）
Tsubasa Okamoto[1], Hideyuki Takahashi[2], Eiji Ohmichi[1], Hitoshi Ohta[3] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Arg. Adv. Integ. Res., Kobe Univ.*, [3]*Mol. Photosci. Res. Ctr., Kobe Univ.*)

2H1537 高分解能二次イオン質量分析法による電気細菌代謝の一細胞レベル追跡
NanoSIMS Analysis of Single Electrogenic Cell Reveals Feedback from Extracellular Electron Transport to Upstream Reactions
○岡本 章玄[1], 斎藤 淳貴[2], 橋本 和仁[1]（[1]物材機構 エネルギー・環境材料, [2]東京大学院応用化学）
Akihiro Okamoto[1], Junki Saito[2], Kazuhito Hashimoto[1] ([1]*National Institute for Material Sciences*, [2]*Dept. Appl. Chem., Univ. of Tokyo*)

2H1549 海洋性ビブリオ菌極べん毛の側における形成を抑制する新規因子 SflB の解析
Characterization of SflB, a novel factor that prevents peritrichous flagellar formation in marine *Vibrio*
錦野 達郎, 三野 平, ○小嶋 誠司, 本間 道夫（名大・院理・生命理学）
Tatsuro Nishikino, Taira Mino, **Seiji Kojima**, Michio Homma (*Div. of Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

2H1601 クライオ電子顕微鏡法で明らかになった、3.8 A 分解能のアクチン-コフィリン複合体構造
Actin-cofilin complex structure at 3.8 A resolution revealed by cryo-EM
田中 康太郎[1], 武田 修一[1], 光岡 薫[3], 小田 俊郎[2], 前田 雄一郎[1], ○成田 哲博[1]（[1]名大、理、構造生物学研究センター, [2]東海学院大, [3]阪大、超高圧電子顕微鏡センター）
Kotaro Tanaka[1], Shuichi Takeda[1], Kaoru Mitsuka[3], Toshiro Oda[2], Yuichiro Maeda[1], **Akihiro Narita**[1] ([1]*Struct. Biol. Res. Center, Nagoya Univ.*, [2]*Tokai Gakuin Univ.*, [3]*Res. Center for UHV EM, Osaka Univ.*)

2H1613 細胞性粘菌のアクチンのカルボキシ末端領域の二型性と Pro109 に導入した変異の関係
The relationship between the dimorphism of the carboxyl-terminal region and the mutagenesis introduced to Pro109 of *Dictyostelium* actin
○五味渕 由貴[1], 上田 太郎[2], 若林 健之[1]（[1]帝京大・理工, [2]早稲田・先進理工）
Yuki Gomibuchi[1], Taro Q.P. Uyeda[2], Takeyuki Wakabayashi[1] ([1]*Teikyo Univ.*, [2]*Waseda Univ.*)

13:55〜16:25 I 会場（全学教育棟 3 階 E305）／Room I (Room E305, General Education Bldg. 3F)
2I 光生物： 視覚・光受容Ⅱ, 光遺伝学・光制御Ⅱ / Photobiology: Vision & Photoreception II, Optogenetics & Optical Control II

2I1355 光駆動型ナトリウムイオンポンプロドプシンで見られる弁別的な機能・光化学特性
Distinctive functional and photochemical properties among light-driven sodium ion pumping rhodopsins
○栗原 眞理恵[1], 橋本 美沙[2], 吉澤 晋[3], 小島 慧一[1], 塚本 卓[1,2], 菊川 峰志[4,5], 須藤 雄気[1,2]（[1]岡大・院・医歯薬（薬）, [2]岡大・薬（薬）, [3]東大・大気海洋研, [4]北大・院・先端生命, [5]北大・国際連携研究教育局）
Marie Kurihara[1], Misa Hashimoto[2], Susumu Yoshizawa[3], Keiichi Kozima[1], Takashi Tsukamoto[1,2], Takashi Kikukawa[4,5], Yuki Sudo[1,2] ([1]*Grad. Sch. of Med. Dent. & Pharm. Sci., Univ. Okayama*, [2]*Fac. of Pharm. Sci., Univ. Okayama*, [3]*AORI, The Univ. of Tokyo*, [4]*Fac. Adv. Life Sci., Univ. Hokkaido*, [5]*GSS, GI-CoRE, Univ. Hokkaido*)

2I1407 ナトリウムポンプ型ロドプシン中間体の過渡共鳴ラマン分光法による研究
Transient Resonance Raman Spectroscopy of a Light-Driven Sodium-Ion-Pump Rhodopsin from Indibacter alkaliphilus
○梶本 航介[1]（[1]佐賀大 院工学系, [2]北大 先端生命科学研究院, [3]北海道大 国際連携研究教育局ソフトマターグローバルステーション）
Kosuke Kajimoto[1] ([1]*Grad. Sch. Sci. Eng. Saga-Univ*, [2]*Fac. Adv. Life Sci., Hokkaido Uni*, [3]*GSS, GI-CoRE, Hokkaido Univ.*)

2I1419 海洋性細菌 *Rubricoccus marinus* SG-29^T 株由来の内向き H^+ポンプ型ロドプシン *Rm*XeR の分光学的解析
Spectroscopic analysis of *Rm*XeR, an inward H^+ pump rhodopsin from the marine bacterium *Rubricoccus marinus* SG-29^T
○井上 紗希[1], 吉澤 晋[2], 小島 慧一[1], 塚本 卓[1], 菊川 峰志[3,4], 須藤 雄気[1]（[1]岡大・院・医歯薬（薬）, [2]東大・大気海洋研, [3]北大・院・先端生命, [4]北大・ 国際連携教育研究局）
Saki Inoue[1], Susumu Yoshizawa[2], Keiichi Kojima[1], Takashi Tsukamoto[1], Takashi Kikukawa[3,4], Yuki Sudo[1] ([1]*Grad. Sch. of Med. Dent. & Pharm. Sci., Okayama Univ.*, [2]*AORI, The Univ. of Tokyo*, [3]*Fac. Adv. Life Sci., Hokkaido Univ.*, [4]*GSS, GI-CoRE, Hokkaido Univ.*)

2I1431 ラマン光学活性分光を用いた微生物型ロドプシンにおけるレチナール発色団のコンフォメーション解析
Raman optical activity probes the conformation of the retinal chromophore in microbial rhodopsins
○松尾 淳平[1], 菊川 峰志[2,3], 海野 雅司[4], 藤澤 知績[5]（[1]佐賀大学大学院工学系研究科循環物質化学専攻, [2]北海道大学 先端生命科学研究院, [3]北海道大学国際連携研究教育局ソフトマターグローバルステーション, [4]佐賀大学 工学系研究科, [5]佐賀大学 工学系研究科）
Junpei Matsuo[1], Takashi Kikukawa[2,3], Masashi Unno[4], Tomotsumi Fujisawa[5] ([1]*Grad. Sch. Eng. Saga Univ*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*, [3]*GSS, GI-CoRE, Hokkaido Univ.*, [4]*Grad. Sch. Eng. Saga Univ*, [5]*Grad. Sch. Eng. Saga Univ*)

2I1443 Towards the structural study of the photocycle of bistable rhodopsin
Midori Murakami (*Dept. Physics, Nagoya Univ.*)

2I1455 In situ 光照射固体ＮＭＲによるバクテリオロドプシンとその変異体に生成する光反応中間体の定常捕捉
Stationary trapping of photo-intermediates during the photo cycles of bR and its mutants by in situ photoirradiation solid-state NMR
○内藤 晶[1], 大島 恭介[1], 大谷 優人[1], 重田 安里寿[1], 槙野 義輝[1], 川村 出[1], 沖津 貴志[2], 和田 昭盛[2], 辻 暁[3], 岩佐 達郎[4]（[1]横浜国立大学 大学院工学研究院, [2]神戸薬科大学, [3]兵庫県立大学, [4]室蘭工業大学）
Akira Naito[1], Kyosuke Oshima[1], Yuto Otani[1], Arisu Shigeta[1], Yoshiteru Makino[1], Izuru Kawamura[1], Takashi Okitsu[2], Akimori Wada[2], Satoru Tuzi[3], Tatsuo Iwasa[4] ([1]*Yokohama National University*, [2]*Kobe Phamacutical University*, [3]*University of Hyogo*, [4]*Muroran Institute of Technology*)

休憩（Coffee Break） 15:07–15:13

2I1513 メラノプシンの 3 平衡状態光反応による光量感知
Melanopsin tristability: a new model of photoresponse for irradiance detection
○松山オジョス 武[1], 高橋 政代[1], 七田 芳則[2]（[1]理化学研究所CDB, [2]京都大学理学研究科）
Takesi Matsuyama Hoyos[1], Masayo Takahashi[1], Yoshinori Shichida[2] ([1]*RIKEN CDB*, [2]*Kyoto University Graduate School of Science*)

2I1525 松果体オプシンパラピノプシンの分子特性の細胞応答への寄与
Contribution of a molecular property of a pineal opsin parapinopsin to cellular responses
和田 清二[1], 沈 宝国[1], 山下（川野） 絵美[1], 永田 崇[1], 保 智己[2], 小柳 光正[1], ○寺北 明久[1]（[1]大阪市大・院理, [2]奈良女子大・理）
Seiji Wada[1], Baoguo Shen[1], Emi Kawano-Yamashita[1], Takashi Nagata[1], Satoshi Tamotsu[2], Mitsumasa Koyanagi[1], **Akihisa Terakita**[1] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Fac. Sci., Nara Women's Univ.*)

2I1537 暗所視を司る錐体視物質の低い熱雑音の進化的獲得
Evolutionary acquisition of low thermal noise of cone pigments for scotopic vision
○小島 慧一[1,2], 松谷 優樹[2], 柳川 正隆[3], 山下 高廣[2], 今元 泰[2], 久冨 修[4], 山野 由美子[5], 和田 昭盛[5], 七田 芳則[2,6]（[1]岡山大学大学院医歯薬学総合研究科, [2]京都大学大学院理学研究科, [3]理研・細胞情報, [4]大阪大学大学院理学研究科, [5]神戸薬科大学, [6]立命館大学・総研機構）
Keiichi Kojima[1,2], Yuki Matsutani[2], Masataka Yanagawa[3], Takahiro Yamashita[2], Yasushi Imamoto[2], Osamu Hisatomi[4], Yumiko Yamano[5], Akimori Wada[5], Yoshinori Shichida[2,6] ([1]*Grad. Sch. of Med. Dent. Pharm. Sci., Okayama Univ*, [2]*Grad. Sch. Sci., Kyoto Univ.*, [3]*Cell. Info. Lab., RIKEN*, [4]*Grad. Sch. Sci., Osaka Univ.*, [5]*Kobe Pharm. Univ.*, [6]*Ritsumeikan Univ.*)

2I1549 光遺伝学に向けた長波長シフト型ナトリウムポンプロドプシンの作製
Red-shifted sodium pump rhodopsin variants for optogenetic application
○井上 圭一[1,2], 中村 良子[1], 神取 秀樹[1]（[1]名古屋工業大学, [2]JST･さきがけ）
Keiichi Inoue[1,2], Ryoko Nakamura[1], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*JST PRESTO*)

2I1601 光依存型グアニル酸シクラーゼである微生物型ロドプシン(BeGC1)の機能解析
Functional characterization of rhodopsin-guanylate cyclase, BeGC1
○角田 聡[1,2,3], 吉田 一帆[2], 神取 秀樹[2,3]（[1]JST さきがけ, [2]名工大 院 工, [3]オプトバイオ）
Satoshi Tsunoda[1,2,3], Kazuho Yoshida[2], Hideki Kandori[2,3] ([1]*JST, PRESTO*, [2]*NIT*, [3]*OBTR*)

2I1613 ハロロドプシンはヒドロキシイオンを輸送できるか？
Can halorhodopsin pump hydroxyl ions ?
○神山 勉, 鈴木 健太, 成瀬 圭汰, Chan Siu Kit（名古屋大学大学院理学研究科）
Tsutomu Kouyama, Kenta Suzuki, Keita Naruse, Siu Kit Chan (*Graduate School of Science, Nagoya University*)

13:55〜16:01　J 会場（全学教育棟 4 階 C401）／Room J (Room C401, General Education Bldg. 4F)
2J　発生・分化，核酸Ⅱ，ゲノム生物学 / Development & Differentiation, Nucleic acid II, Genome biology

2J1355 細胞の異方的なメカノレスポンスが発生過程の精巣上体細管の径を維持する
Anisotropic Cellular Mechanoresponse Maintains the Radial Size of Developing Epididymal Tubules
○平島 剛志[1], 安達 泰治[2]（[1]京都大学大学院医学研究科 基礎病態学講座 病態生物医学分野, [2]京都大学 ウイルス・再生医科学研究所）
Tsuyoshi Hirashima[1], Taiji Adachi[2] ([1]*Grad Sch Med, Kyoto Univ*, [2]*Inst Front Life Med Sci, Kyoto Univ*)

2J1407 3 次元的な形態の多様性を説明する細胞の力学の理論的な推定
Theoretical inference of cell mechanics for explaining 3-dimensional morphological diversity
○小山 宏史[1,2], 藤森 俊彦[1,2]（[1]基生研 初期発生, [2]総研大）
Hiroshi Koyama[1,2], Toshihiko Fujimori[1,2] ([1]*Div. Embryology, NIBB*, [2]*SOKENDAI*)

2J1419 マウス ES 細胞は、フラッシュラチェット様式をとりながら、集団で分化する
Flashing ratchet-driven collective cell-state transition in mouse embryonic stem cells
○岡本 和子[1], ジェルモン アルノ[1], 藤田 英明[1,2], 古澤 力[1,3], 岡田 康志[1,3,4], 渡邉 朋信[1,4]（[1]理研 QBiC, [2]阪大 免フロ, [3]東大 院理, [4]阪大 生命機能）
Kazuko Okamoto[1], Arno Germond[1], Hideaki Fujita[1,2], Chikara Furusawa[1,3], Yasushi Okada[1,3,4], Tomonobu Watanabe[1,4] ([1]*RIKEN QBiC*, [2]*WPI, IFReC, Osaka Univ.*, [3]*Sch. of Sci, Univ. of Tokyo*, [4]*FBS, Osaka Univ.*)

2J1431 植物組織では異方的な細胞成長が滑らかな境界形成を促進する。
Anisotropic cell growth promotes smooth boundary formation of stem cell tissue in plant roots
○藤原 基洋, 藤本 仰一（大阪大・理）
Motohiro Fujiwara, Koichi Fujimoto (*Science Dept. Osaka Univ.*)

2J1443 Bicistronic 2A-peptide-based co-expression reporter revealed the gene expression profiles in developing human photoreceptors
Kohei Homma (*Keio Univ. Sch. of Med. Dpt. of Ophthalmol.*)

2J1455 Two-dimensional fluorescence lifetime correlation spectroscopy reveals μs-dynamics and distinct folding mechanisms of $preQ_1$ riboswitch
Bidyut Sarkar[1], Kunihiko Ishii[1,2], Tahei Tahara[1,2] ([1]*Molecular Spectroscopy Laboratory, RIKEN*, [2]*RIKEN Center for Advanced Photonics, RIKEN*)

休憩（Coffee Break） 15:07–15:13

2J1513 The reaction mechanism of pH-dependent RecA-mediated DNA strand exchange
Hsiu-Fang Fan (*National Yang-Ming University*)

2J1525 DNA ナノデバイスの温度応答性能の設計
Engineering thermal response of a DNA nanodevice
○小宮 健[1], 小林 聡[2], ローズ ジョン[3]（[1]東工大 情報理工, [2]電通大 院情報理工, [3]立命館APU APS）
Ken Komiya[1], Satoshi Kobayashi[2], John A. Rose[3] ([1]*Sch. Comp., Tokyo Tech.*, [2]*Dept. Comp. Sci., The Univ. Electro-Commun.*, [3]*College APS, Ritsumeikan APU*)

2J1537 Nucleosome Repositioning Investigated by Coarse-Grained MD Simulations and Markov State Modeling
Giovanni Brandani, Toru Niina, Cheng Tan, Shoji Takada (*Dept Biophysics, Div Biology, Grad School Science, Kyoto University*)

2J1549 Osmotic mechanism of loop extrusion process
Tetsuya Yamamoto[1], Helmut Schiessel[2] ([1]*Nagoya Univ., Dep. of Mat. Phys.*, [2]*Leiden U., Inst. Lorentz for Theo. Phys.*)

口頭発表 座長一覧

建物名	フロア	会場名	部屋名	9月19日(火)	9月20日(水)
				13:20–16:20	13:55–16:25
全学教育棟	2F	B会場	B201	1B 筋肉Ⅰ, 分子モーターⅠ	2B 分子モーターⅡ
				成田 哲博(名大)、村田 武士(千葉大)	豊島 陽子(東大)、昆 隆英(阪大)
		C会場	B202	13:20–16:20	13:55–16:13
				1C 生体膜・人工膜Ⅰ, バイオエンジニアリング, 計測Ⅰ	2C 生体膜・人工膜Ⅱ, 生命の起源・進化, 生態／環境
				瀧ノ上 正浩(東工大)、瀧口 金吾(名大)	古谷 祐詞(分子研)、中野 実(富山大)
		D会場	E201	13:20–16:20	13:55–16:25
				1D バイオイメージングⅠ	2D バイオイメージングⅡ
				永井 健治(阪大)、金城 正孝(北大)	永山 國昭(LisCo 永山顕微鏡研)、松田 知己(阪大)
		E会場	E203	13:20–16:20	13:55–16:01
				1E 水・水和／電解質, 蛋白質: 物性, 蛋白質工学, 生命情報科学, 核酸Ⅰ	2E 計測Ⅱ, 数理生物学Ⅱ, 化学受容, 行動, その他
				高橋 聡(東北大)、富井 健太郎(産総研)	安永 卓生(九工大)、佐甲 靖志(理研)
		F会場	E205	13:20–16:08	13:55–16:25
				1F 蛋白質: 構造, 構造機能相関Ⅰ, 計測・解析の方法論	2F 蛋白質: 構造・構造機能相関Ⅱ
				濡木 理(東大)、櫻井 実(東工大)	杉原 崇憲(バイオ産業情報化コンソ)、海野 昌喜(茨城大)
	3F	G会場	C301	13:20–16:20	—
				1G 蛋白質: 機能, ヘム蛋白質Ⅰ, 核酸結合蛋白質	—
				河野 秀俊(量研)、新井 宗仁(東大)	—
		H会場	E303	13:20–16:20	13:55–16:25
				1H 細胞生物学的課題Ⅰ	2H 光生物: 光合成Ⅱ, 電子状態, ヘム蛋白質Ⅱ, 細胞生物学的課題Ⅱ, 筋肉Ⅱ
				難波 啓一(阪大)、岡田 眞理子(阪大)	柴田 穣(東北大)、城 宜嗣(兵県大)
		I会場	E305	13:20–16:20	13:55–16:25
				1I 光生物: 視覚・光受容Ⅰ, 光合成Ⅰ, 光遺伝学・光制御Ⅰ	2I 光生物: 視覚・光受容Ⅱ, 光遺伝学・光制御Ⅱ
				寺嶋 正秀(京大)、海野 雅司(佐賀大)	七田 芳則(京大)、藤澤 知積(佐賀大)
	4F	J会場	C401	13:20–16:08	13:55–16:01
				1J 非平衡・生体リズム, 数理生物学Ⅰ, 化学受容, 神経・感覚	2J 発生・分化, 核酸Ⅱ, ゲノム生物学
				安藤 敏夫(金沢大)、細川 千絵(産総研)	中村 春木(阪大)、片平 正人(京大)

ポスター　Poster

第1日目（9月19日（火））／Day 1（Sep. 19 Tue.）全学教育棟2階 C201, C202, D201, D202, D203; 全学教育棟3階 D301, D302, D303 ／ Room C201, C202, D201, D202, D203, General Education Bldg. 2F; D301, D302, D303, General Education Bldg. 3F

蛋白質：構造 / Protein: Structure

1Pos001 **X線結晶解析スクリーニングによるBRD4阻害剤の探索とBRD4－阻害剤複合体の中性子結晶構造解析**
Discovery of BRD4 inhibitors by X-ray crystallographic screening and neutron crystallographic analysis of BRD4-inhibitor complex
Takeshi Yokoyama, Kazunori Matsumoto, Yuko Nabeshima, Mineyuki Mizuguchi (*Fac. of Pharm. Sci., Univ. of Toyama*)

1Pos002 **P-loopを用いたATP結合タンパク質のゼロからの設計**
Toward design of ATP-binding proteins from scratch using P-loop
Kengo Nakamura[1,2], Takahiro Kosugi[1,2], Nobuyasu Koga[1,2,3] ([1]*SOKENDAI*, [2]*IMS CIMoS*, [3]*JST PRESTO*)

1Pos003 **gREST法によるTrpcageのフォールディングと自由エネルギー地形**
Folding simulation and free energy landscape analysis of Trpcage by gREST
Motoshi Kamiya[1], Yuji Sugita[1,2,3] ([1]*RIKEN AICS*, [2]*RIKEN TMS*, [3]*RIKEN QBiC*)

1Pos004 **AMED創薬等ライフサイエンス研究支援基盤事業が提供する最先端クライオ電子顕微鏡システム**
State-of-the Art Cryo-EM system provided by AMED Platform Project for Supporting Drug Discovery and Life Science Research
Kenji Iwasaki, Kiyo Tsunezumi, Mika Hirose, Naoyuki Miyazaki (*IPR, Osaka Univ.*)

1Pos005 **リガンド結合シミュレーションへのタンパク質構造揺らぎの取り込み**
Incorporation of protein flexibility into ligand binding simulation
Suyong Re[1], Hiraku Oshima[1], Motoshi Kamiya[2], Yuji Sugita[1,2,3] ([1]*RIKEN QBiC*, [2]*RIKEN AICS*, [3]*RIKEN TMS*)

1Pos006 **Cryo-cooling effect on crystalline DHFR studied by replica-exchange molecular dynamics**
Tetsuro Nagai[1], Osamu Miyashita[2], Florence Tama[1,2,3] ([1]*Nagoya Univ., Grad. School of Science*, [2]*RIKEN AICS*, [3]*Nagoya Univ., ITbM*)

1Pos007 **GPUを用いた加重アンサンブルシミュレーションによるタンパク質の機能性ダイナミクスの探索**
Investigation of protein functional dynamics by GPU-accelerated weighted ensemble simulation
Hironori Kokubo, Atsutoshi Okabe, Etsurou Watanabe (*Research, Takeda Pharmaceutical*)

1Pos008 **The head structure of the Staphylococcus aureus phage S13' at near atomic resolution by cryo-electron microscopy single particle analysis**
Naoyuki Miyazaki[1], Jumpei Uchiyama[2], Shigenobu Matsuzaki[3], Kazuyoshi Murata[4], Kenji Iwasaki[1] ([1]*Institute for Protein Research, Osaka University*, [2]*Azabu University*, [3]*Kochi University*, [4]*National Institute for Physiological Sciences*)

1Pos009 **自由エネルギー変分原理に基づくPim-1キナーゼ阻害剤系の相対的結合自由エネルギーの予測.リガンド構造の分類**
Relative binding free energy predictions for ligands with Pim-1 kinase based on the free energy variational principle: classify of ligands
Anna Hirai, Takeshi Ashida, Takeshi Kikuchi (*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*)

1Pos010 **The amino acid sequences analysis of Titin by methods based on the inter-residue average distance statistics**
Panyavut Aumpuchin, Takeshi Kikuchi (*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*)

1Pos011 **分子動力学法を用いたHras-GTP/GDP複合体の構造と溶媒水との水素結合との関連性の研究**
Molecular dynamics study of relationship between the structures of the Hras-GTP/GDP complexes and hydrogen bonds to the solvent water
Takeshi Miyakawa[1], Ryota Morikawa[1], Masako Takasu[1], Kimikazu Sugimori[2], Kazutomo Kawaguchi[2], Hidemi Nagao[2] ([1]*Tokyo University of Pharmacy and Life Sciences*, [2]*Kanazawa University*)

1Pos012 **親水性/疎水性界面におけるアミロイドβフラグメントの凝集の分子動力学シミュレーション**
All-atom molecular dynamics simulations of amyloid-β fragment aggregation at hydrophilic/hydrophobic interface
Hisashi Okumura[1,2], Satoru G. Itoh[1,2] ([1]*IMS*, [2]*SOKENDAI*)

1Pos013 **単一ミオシン結合状態アクトミオシンの高分解能化**
F-actin structural changes induced by a single myosin head
Takahiro Namise, Takuo Yasunaga, Kazuaki Yoshida (*Kyushu Institute of Technology*)

1Pos014 **XFELテンプレートマッチング法と粗視化法を用いたクロマチン多重立体配座解析の実現可能性に関する研究**
Feasibility study for the multiple conformation analysis of the chromatin structure by using the XFEL template matching and CG simulation
Atsushi Tokuhisa[1,5], Ryo Kanada[1], Yuta Isaka[3,4], Biao Ma[3,4], Shuntaro Chiba[1], Yasushi Okuno[1,2,4,5] ([1]*RIKEN, RC*, [2]*Kyoto University, Graduate School of Medicine*, [3]*FBRI, Pro-Cluster Kobe*, [4]*FBRI, IBRI Laboratory*, [5]*RIKEN, AICS*)

1Pos015 **タンパク質構造の安定化における糖の役割**
Role of sugars on the stabilization of protein structure
Satoshi Ajito, Mitsuhiro Hirai (*Grad. Sch. Sci. and Tec., Univ. Gunma*)

1Pos016 **ポリエチレングリコールの存在下でのタンパク質構造安定性の研究**
Study of protein structure stability in the presence of polyethylene glycol
Yugo Maezawa, Mitsuhiro Hirai (*Grad. Sch. Sci & Tec., Univ. Gunma*)

1Pos017 **分子動力学シミュレーションの緩和モード解析**
Relaxation mode analysis of molecular dynamics simulations
Ayori Mitsutake, Hiroshi Takano (*Dept. Phys, Keio Univ.*)

1Pos018 **NMR-based structural analysis of the locally disordered conformation of outer surface protein A**
Takuro Wakamoto[1], Ryo Kitahara[2] ([1]*Graduate School of Life Sciences, Ritsumeikan University*, [2]*College of Pharmaceutical Sciences, Ritsumeikan University*)

1Pos019 **Free energy analysis of cosolvent-induced denaturation through molecular dynamics simulation and energy-representation method**
Yu Yamamori, Nobuyuki Matubayasi (*Osaka Univ. Grad. Sch. Eng. Sci.*)

1Pos020 **Structure and Dynamics of α-crystellin under crowding condition**
Yusuke Sakamaki[1], Rintaro Inoue[2], Nobuhiro Sato[2], Masaaki Sugiyama[2] ([1]*Grad. Sch. Sci., Kyoto Univ.*, [2]*KURRI*)

蛋白質：構造機能相関 / Protein: Structure & Function

1Pos021 **Quantum-chemical analysis of pKa and structural change of amino acid residues in catalytic center of Ser286-mutant firefly luciferases**
Naohisa Wada[1], Kazuya Kato[1], Hironori Sakai[2] ([1]*Food and Nutritional Sciences, Toyo University*, [2]*Institute of Fluid Science, Tohoku University*)

1Pos022 **結晶中の小さな構造変化からタンパク質のアロステリック機構を読み解く**
Deciphering protein allosteric mechanisms from small structural changes in crystals
Naoya Shibayama[1], Ayana Sato[1], Mio Ohki[2], Sam-Yong Park[2] ([1]*Jichi Med. Univ., Div. of Biophys.*, [2]*Yokohama City Univ., Drug Design Lab.*)

1Pos023 **3D−RISM 理論を応用した溶液中におけるアスパラギン、 Met−enkephalin の構造揺らぎの解析**
Analysis of structural fluctuations of ASN and Met-encephalin in the solution phase by means of 3D-RISM theory
Masatake Sugita[1], Fumio Hirata[2] ([1]*Dept. of Bioinfo., Col. of Life Sci., Ritsumeikan Univ.*, [2]*Toyota Phys. & Chem. Res. Inst.*)

1Pos024 **アルカン合成関連酵素の機能発現に重要なアミノ酸残基の変異解析**
Mutational analysis of amino acid residues important for the function of an enzyme for alkane biosynthesis
Masashi Nomura, Hisashi Kudo, Yuuki Hayashi, Munehito Arai (*Dept. Life Sci., Univ. Tokyo*)

1Pos025 **Regression method for comparison of multiple protein conformations**
Takashi Amisaki, Shin-ichi Fujiwara (*Fac of Med, Tottori Univ*)

1Pos026 **親水性タンパク質ータンパク質間会合の駆動力に関する MD 及び 3D-RISM 計算**
Driving force of hydrophilic protein-protein associations as studied by MD and 3D-RISM calculations
Honami Sakaizawa, Tadaomi Furuta, **Minoru Sakurai** (*Cent. Biores. Bioinf., Tokyo Tech*)

1Pos027 **粗視化モデルと全原子モデルを用いた蛋白質複合体シミュレーション**
Simulations of Protein Dimers using a Coarse-Grained Model and All-Atom Models
Takao Yoda, Takuya Yamada, Toshiyuki Tsuji, Tsuyoshi Shirai (*Computer Bioscience, Nagahama Institute of Bio-Science and Technology*)

1Pos028 **hERG イオンチャネルと薬剤分子の相互作用予測手法の開発**
Prediction of interactions between the hERG potassium ion channel and drug molecules
Tatsuki Negami, Tohru Terada (*Grad. Sch. Agri. and Life Sci., The Univ. of Tokyo*)

1Pos029 **ヘモグロビンの酸素親和性制御に関係する大振幅ヘリックス揺らぎの実験的検証：テラヘルツ（THz）分光による研究**
Experimental Investigation of Large Amplitude Fluctuations of Helices Related with Oxygen Affinity of Hemoglobin using THz Spectroscopy
Shigenori Nagatomo[1], Kohji Yamamoto[2], Masako Nagai[3], Teizo Kitagawa[4] ([1]*Dept. Chem., Univ. Tsukuba*, [2]*Res. Center Develop. Far-IR Region, Univ. Fukui*, [3]*Res. Center Micro-Nano Tech., Hosei Univ.*, [4]*Grad. Sch. Life Sci., Univ. Hyogo*)

1Pos030 **Study on the pH-dependent changes in the structure and ligand-binding properties of the perireceptor proteins**
Durige Wen[1], Mituhiro Hirai[2], Mamiko Ozaki[3], Tatsuo Iwasa[4] ([1]*Department of Applied Science and Engineering, Muroran Institute of Technology*, [2]*Graduate School of Science and Technology, Gunma University*, [3]*Department of Biology, Graduate School of Science, Kobe University*, [4]*Center of Environmental Science and Disaster Mitigation for Advanced Research, Muroran Institute of Technology*)

1Pos031 **pH 一定の分子動力学シミュレーションによって発生させたアミノ酸の様々なプロトン化状態に基づく結合自由エネルギー計算**
Binding free energy calculation using various protonation states of amino acids generated by constant pH molecular dynamics simulations
Shin-ichi Fujiwara, Takashi Amisaki (*Fac. Med., Tottori Univ.*)

1Pos032 **MD シミュレーションを用いた CD44 のヒアルロン酸との結合に関する理論的研究**
Theoretical Study on Hyaluronan-Binding to CD44 Using Molecular Dynamics Simulation
Yota Horioka[1], Saki Hongo[1], Yuki Inazuka[1], Yoshifumi Fukunishi[2], Juha M. Lintuluoto[3], Masami Lintuluoto[1] ([1]*Grad. Sch. of Life and Environ. Sci., Kyoto Pref. Univ.*, [2]*Nati. Instit. of Adv. Indust. Sci. and Technol.*, [3]*Grad. Sch. of Eng., Kyoto Univ.*)

1Pos033 **XOR の結合ポケットの中における基質の運動についてー分子動力学による研究ー**
The motion of the substrate in the binding pocket of XOR: molecular dynamics study
Hiroto Kikuchi[1], Hiroshi Fujisaki[1], Tadaomi Furuta[2], Ken Okamoto[3], Takeshi Nishino[4] ([1]*Dept. of Phys., Nippon Med. Sch.*, [2]*Sch. of Life Sci. & Tech., Tokyo Tech.*, [3]*Dept. of Biochem., Nippon Med. Sch.*, [4]*Grad. Sch. of Agri. & Life Sci., Univ. Tokyo*)

1Pos034 **基質結合蛋白質の天然変性領域の網羅的探索および機構解析**
Comprehensive search and mechanism analysis of intrinsically disordered region of ligand binding proteins
Satoshi Omori, Hafumi Nishi, Kengo Kinoshita (*Grad. Sch. of Info. Sci., Tohoku Univ.*)

蛋白質：物性 / Protein: Property

1Pos035 **Relating slow-down in diffusion and transient oligomer formation in concentrated villin solutions**
Po-Hung Wang[1], Nawrocki Grzegorz[2], Isseki Yu[1], Takanori Kigawa[3], Michael Feig[2], Yuji Sugita[1,4,5,6] ([1]*RIKEN TMSL (Wako)*, [2]*MSU, USA*, [3]*RIKEN QBiC (Yokohama)*, [4]*RIKEN AICS (Kobe)*, [5]*RIKEN QBiC (Kobe)*, [6]*RIKEN iTHES (Wako)*)

1Pos036 **LEA モデルペプチド及びトレハロースによるリゾチームの熱変性防止**
Protective effect of LEA peptides and trehalose on the thermal denaturation of lysozyme
Takao Furuki, Minoru Saukrai (*Tokyo Institute of Technology*)

1Pos037 **カーボンナノチューブによるシステイン残基の酸化**
Oxidation of cysteine residues of proteins on carbon nanotubes
Atsushi Hirano[1], Tomoshi Kameda[2], Shun Sakuraba[3], Momoyo Wada[1], Takeshi Tanaka[1], Hiromichi Kataura[1] ([1]*NMRI, AIST*, [2]*AIRC, AIST*, [3]*Grad. Sch. Front. Sci., Univ. Tokyo*)

1Pos038 **Structural and thermodynamic analysis for metal-induced three helix-bundle formation**
Satomi Inaba[1], Daiki Usui[2], Hiroshi Sekiguchi[1], Toshiki Tanaka[3], Masayuki Oda[2] ([1]*JASRI/SPring-8*, [2]*Grad. Sch. Life Environ. Sci., Kyoto Pref. Univ.*, [3]*Grad. Sch. Eng., Nagoya Inst. Technol.*)

1Pos039 **考慮する因子を段階的に増やすモデル解析に基づく蛋白質の折り畳み機構の理論的解明**
Unraveling protein folding mechanism by analyzing the hierarchy of models with increasing level of detail
Tomohiko Hayashi[1], Satoshi Yasuda[1,2,3], Skrbic Tatjana[4], Giacometti Achille[4], Masahiro Kinoshita[1] ([1]*Inst. Adv. Energ., Kyoto Univ.*, [2]*Grad. Sch. Sci., Chiba Univ.*, [3]*MCRC, Chiba Univ.*, [4]*Dept. of Molecular Sciences and Nanosystems, Venezia Univ.*)

1Pos040 **アルコール中のメリチンとマストパランのヘリックス構造熱安定性**
Thermal stability of helical conformation of melittin and mastoparan in alcohol
Yoshinori Miura (*Center for Advanced Instrumental Analysis, Kyushu University*)

1Pos041 **NtrC の構造転移の経路とその遷移状態のカメレオンモデルによる研究**
Characterization of the pathways and transition states of conformational transition of NtrC by the chameleon model
Shinya Abe[1], Masaki Sasai[2], Tomoki P. Terada[2] ([1]*Dept. Comput. Sci. Eng., Grad. Sch. Eng., Nagoya Univ.*, [2]*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

1Pos042 **定温定圧レプリカ置換分子動力学シミュレーションによって明らかになったシニョリンの準安定状態の温度・圧力依存性**
Temperature and pressure dependence of metastable state of a chignolin revealed by an isothermal-isobaric replica-permutation method
Masataka Yamauchi[1,2], Hisashi Okumura[1,2] ([1]*SOKENDAI*, [2]*IMS*)

1Pos043 **Structural stability of halorhodopsin from Natronomonas pharaonis under acidic condition**
Shinichiro Hayashi, Takanori Sasaki (*Grad. Sch. Adv. Math. Sci., Meiji Univ*)

1Pos044 **分子回転拡散係数のビリアル展開によるタンパク質間相互作用の解析**
Protein-protein interaction on crystallization revealed by the virial expansion of molecular rotational diffusion coefficient
Akane Kato[1], Yudai Katsuki[1], Etsuko Nishimoto[2] ([1]*Grad. Sch. Bioresour. Bioenviron. Sci., Kyushu Univ.* , [2]*Fac. Agr., Kyushu Univ.*)

1Pos045 **タンパク質構造変化における経路の多様性：マルコフ状態モデルによる解析**
A variety of pathways for a conformational change of a protein analyzed using a Markov state model
Sotaro Fuchigami (*Grad. Sch. of Medical Life Science, Yokohama City Univ.*)

1Pos046 **何故 4 つのイントロン位置は、タンパク質立体構造上で、平面を形成するか?**
Why four intron positions form a plane in the tertiary structure of protein?
Michiko Nosaka (*Naional Institute of Technology, Sasebo College*)

膜蛋白質 / Membrane proteins

1Pos047 **1 分子イメージングによる GPCR の活性推定**
Single-molecule imaging-based estimation of GPCR activity
Masataka Yanagawa[1], Michio Hiroshima[1,2,3], Yuichi Togashi[4], Takahiro Yamashita[5], Yoshinori Shichida[5,6], Masayuki Murata[7], Masahiro Ueda[2,8], Yasushi Sako[1] ([1]*RIKEN*, [2]*QBiC, RIKEN*, [3]*JST, CREST*, [4]*Grad. Sch. Sci., Hiroshima Univ.*, [5]*Grad. Sch. Sci., Kyoto Univ.*, [6]*Research Org. Sci. & Tech., Ritsumeikan Univ.*, [7]*Grad. Arts & Sci., Univ. Tokyo*, [8]*Grad. Frontier Biosci., Osaka Univ.*)

1Pos048 **脂質ータンパク協同性による上皮成長因子受容体の膜近傍ドメイン二量体形成機構**
Lipid-protein cooperativity in the regulation of juxtamembrane domain dimer formation in epidermal growth factor receptor
Ryo Maeda[1], Takeshi Sato[2], Kenji Okamoto[1], Yasushi Sako[1] ([1]*Cellular Informatics Lab., RIKEN*, [2]*Kyoto Pharmaceutical Univ.*)

1Pos049 **レプリカ交換 MD シミュレーションによる FGFR3 膜貫通領域の構造サンプリング**
Conformation Sampling of FGFR3 TM dimer using replica exchange MD simulation
Daisuke Matsuoka, Motoshi Kamiya, Yuji Sugita (*RIKEN*)

1Pos050 **活性型 G タンパク質共役受容体の熱安定化置換の同定**
Identification of PtThermostabilizing mMutations for a G-protein coupled receptor in the active state
Simon Hikiri[1,2], Ryosuke Nakano[1], Nanao Suzuki[1], Satoshi Yasuda[1,2,3], Yuta Kajiwara[4], Masahiro Kinoshita[2], Takeshi Murata[1,3,5] ([1]*Graduate School of Science, Chiba University*, [2]*Institute of Advanced Energy, Kyoto University*, [3]*Molecular Chirality Research Center, Chiba University*, [4]*Graduate School of Energy Science, Kyoto University*, [5]*JST, PRESTO*)

1Pos051 **置換により多くの Class A の G タンパク質共役型受容体を安定化するアミノ酸残基の理論的決定**
Theoretical Identification of Hot-Spot Residues to be Mutated Common in G Protein-Coupled Receptors of Class A
Satoshi Yasuda[1,2,3], Yuta Kajiwara[4], Yosuke Toyoda[5], Kazushi Morimoto[5], Ryoji Suno[5], So Iwata[5], Yakuya Kobayashi[5], Takeshi Murata[1,2,6], Masahiro Kinoshita[3] ([1]*Grad. Sch. Sci., Chiba Univ.*, [2]*MCRC, Chiba Univ.*, [3]*IAE, Kyoto Univ.*, [4]*Grad. Sch. Ener. Sci., Kyoto Univ.*, [5]*Grad. Sch. Med., Kyoto Univ.*, [6]*JST, PRESTO*)

1Pos052 活性型アデノシン A2a 受容体の 4 重置換がもたらす安定化の物理起源
Physical origin of stabilization by a quadruple mutation for the adenosine A2a receptor in the active state
Yuta Kajiwara[1], Satoshi Yasuda[2,3,4], Mitsunori Ikeguchi[5], Takeshi Murata[2,3,6], Masahiro Kinoshita[4] ([1]*Graduate School of Energy Science, Kyoto University*, [2]*Graduate School of Science, Chiba University*, [3]*Molecular Chirality Research Center, Chiba University*, [4]*Institute of Advanced Energy, Kyoto University*, [5]*Graduate School of Medical Life Science, Yokohama City University*, [6]*JST, PRESTO*)

1Pos053 コレステロールを介した上皮成長因子受容体のクラスター形成は EGF シグナル伝達に不可欠である
Cholesterol Mediated Cluster Formation Is Indispensable for the Downstream Signaling of Epidermal Growth Factor Receptor
Michio Hiroshima[1,2], Nario Tomishige[2], Masahiro Ueda[1], Yasushi Sako[2] ([1]*RIKEN QBiC*, [2]*RIKEN*)

1Pos054 赤外分光法による GLIC の pH 依存性チャンネル開閉機構の研究
ATR-FTIR / SEIRAS study on the pH induced gating mechanisms of Gloeobacter violaceus pentameric ligand-gated ion channel (GLIC)
Kenichi Ataka[1], Haidai Hu[2], Marc Delarue[2], Joachim Heberle[1] ([1]*Freie Universitaet Berlin, Fachbereich Physik, Experimental Molecular Biophysics*, [2]*Institut Pasteur, Unit of Structural Dynamics of Macromolecules, CNRS URA*)

1Pos055 バクテリオロドプシンの DC-DFTB-MD シミュレーション： 光反応サイクル上でのプロトンダイナミクス
DC-DFTB-MD simulations of bacteriorhodopsin: Proton dynamics along the photocycle
Minori Imai[1], Junichi Ono[1], Yoshifumi Nishimura[2], Hiromi Nakai[1,2,3,4] ([1]*Grad. Sch. of Adv. Sci. & Eng., Waseda Univ.*, [2]*RISE, Waseda Univ.*, [3]*JST-CREST*, [4]*ESICB, Kyoto Univ.*)

1Pos056 生細胞での膜タンパク質の拡散運動の網羅的解析
Comprehensive Diffusion Analysis of Membrane Proteins in Living Cells
Kazutoshi Takebayashi[1,2], Yukihiro Miyanaga[3], Masahiro Ueda[1,3] ([1]*QBiC, RIKEN*, [2]*Grad. Sch. Sci., Univ. Osaka*, [3]*Grad. Sch. FBS., Univ. Osaka*)

1Pos057 膜貫通タンパク質の細胞内局在要因の同定
Identification of the subcellular localization factors of transmembrane proteins
Tatsuki Kikegawa, Yuri Mukai (*Dept. Electronics, Grad. Sch. Sci. Tech., Meiji Univ.*)

1Pos058 **Membrane binding structure of Bombinin H2 and H4 peptides in leishmania mimetic membrane as studied by solid-state NMR and MD simulation**
Mijiddorj Batsaikhan[1,2], Shiho Kaneda[1], Namsrai Javkhlantugs[2], Kazuyoshi Ueda[1], Hisako Sato[3], Akira Naito[1], **Izuru Kawamura**[1] ([1]*Yokohama Natl. Univ.*, [2]*National University of Mongolia*, [3]*Ehime University*)

1Pos059 **Novel microsystem for high throughput production of small liposome with size uniformity**
Naoki Soga[1], Rikiya Watanabe[1,2], Hiroyuki Noji[1] ([1]*Dept. of App. Chem., The Univ. of Tokyo*, [2]*AMED-PRIME*)

1Pos060 バクテリオロドプシンの DC-DFTB-MD シミュレーション： プロトン放出基における余剰プロトンの非局在化ダイナミクス
DC-DFTB-MD simulations of bacteriorhodopsin: Delocalization dynamics of an excess proton in proton releasing group
Junichi Ono[1], Minori Imai[1], Yoshifumi Nishimura[2], Hiromi Nakai[1,2,3,4] ([1]*Grad. Sch. of Adv. Sci. & Eng., Waseda Univ.*, [2]*RISE, Waseda Univ.*, [3]*JST-CREST*, [4]*ESICB, Kyoto Univ.*)

1Pos061 ナノポアと DNA を用いたナノ空間内におけるホフマイスター効果の検証
Investigation of Hofmeister effect in nanospace using nanopore and DNA as a probe
Masaki Matsushita, Ryuji Kawano (*Grad. Sch. Biotech. and Life Sci., TUAT*)

電子状態 / Electronic state

1Pos062 ホタルルシフェリン酸化反応経路の pH 依存性
pH dependence of oxidation reaction pathway of firefly luciferin
Miyabi Hiyama[1], Hidefumi Akiyama[1,2], Nobuaki Koga[3] ([1]*ISSP, Univ. Tokyo*, [2]*OPERANDO-OIL*, [3]*Grad. Sch. Info. Sci., Nagoya Univ.*)

1Pos063 光電子放出を用いたサーモフィリックロドプシン膜の電子構造の観測
Electronic structure of a thermophilic rhodopsin film observed by techniques using photoelectron emission
Daisuke Sano[1], Astushi Matsuzaki[1], Yuki Takeda[1], Takuya Miyauchi[1], Takeshi Murata[2,3], Yuki Sudo[4], Hisao Ishii[1,3,5] ([1]*Graduate School Science and Engineering Chiba University*, [2]*Graduate School of Science Chiba University*, [3]*Molecular Chirality Research Center Chiba University*, [4]*Graduate School of Medicine Dentistry and Pharmaceutical Science Okayama University*, [5]*Center for Frontier Science*)

1Pos064 アミロイドβ凝集における亜鉛イオンの役割の計算解析
Computational analysis of the role of a zinc ion in the amyloid-β aggregation
Hiroaki Nishizawa[1], Hisashi Okumura[1,2] ([1]*IMS*, [2]*SOKENDAI*)

水・水和・電解質 / Water & Hydration & Electrolyte

1Pos065 部分波展開法と 3D-RISM 法の結合による新たな溶媒和自由エネルギー計算式の提案
New solvation free energy expression for the 3D-RISM combined with the distributed partial wave expansion
Shoichi Tanimoto, Norio Yoshida, Haruyuki Nakano (*Grad. Sch. Sci., Kyushu Univ.*)

1Pos066 **Size-consistent multipartitioning QM/MM 法により量子化学効果を取り込んだ陽イオンの溶媒和**
Cation solvation with quantum chemical effect incorporated by size-consistent multi-partitioning QM/MM method
Hiroshi Watanabe[1,2], Maximilian Kubillus[3], Tomas Kubar[3], Robert Stach[4], Boris Mizaikoff[4], Hiroshi Ishikita[1] ([1]*UTokyo, RCAST*, [2]*UTokyo, ACHEM*, [3]*Karlsruhe Institute of Technology*, [4]*University of Ulm*)

1Pos067　蛋白質構造の安定性と熱変性に関する相互作用成分解析
Interaction-component analysis of protein stability with regard to heat denaturation
Yoshihiko Tokunaga, Yu Yamamori, Ryosuke Ishizuka, Nobuyuki Matubayasi (*Grad. Eng. Sci., Univ. Osaka*)

1Pos068　機械学習による水和水の研究
Machine-learning approach for behavior of hydration water
Taku Mizukami[1], Viet Cuong Nguyen[3], Tien Lam Pham[2], Heiu Chi Dam[2] ([1]*JAIST, Materials Science*, [2]*JAIST, Knowledge Science*, [3]*HPC Systems*)

1Pos069　筋原線維懸濁液の ATP 分解素過程中のプロトン NMR 緩和経過
Spin-spin relaxation of 1H NMR signals from myofibril suspension during cross-bridge cycling
Tetsuo Ohno (*Dept. Physiol., The Jikei Univ. Sch. Med.*)

1Pos070　水溶液からアルキルアミン含有有機溶媒へのリン酸化合物分配の熱力学的解析
Thermodynamic analysis for partitioning of phosphoric compounds between water and organic solvent containig alkyl amine
Hideyuki Komatsu (*Biosci. & Bioinfo. Kyushu Inst. Tech.*)

1Pos071　蛋白質の二次構造と水和ダイナミクスの相関に関する分子動力学的研究
Molecular dynamics study on the relationship between the protein secondary structure and its hydration dynamics
Takafumi Fujiyoshi[1], Kota Kasahara[2], Takuya Takahashi[2] ([1]*Graduate School of Life Science, Ritsumeikan University*, [2]*College of Life Science, Ritsumeikan University*)

1Pos072　イオン周囲の水分子の運動性を再現する新規 Lennard-Jones パラメータの検討
Reproduction of the water mobility around an ion by introducing a new Lennard-Jones parameter
Yuki Takimoto[1], Kota Kasahara[2], Takuya Takahashi[2] ([1]*Grad. Life. Sci., Ritsumeikan Univ.*, [2]*Col. Life. Sci., Ritsumeikan Univ.*)

1Pos073　疎水表面による静電相互作用の強化
Enhancement of electrostatic interaction by hydrophobic surface
Takato Sato[1], Tohru Sasaki[1], Jun Ohnuki[1], Koji Umezawa[2,3], Mitsunori Takano[1] ([1]*Dept. of Pure & Appl. Phys., Waseda Univ.*, [2]*Grad. Sch. of Sci. & Tech., Shinshu Univ.*, [3]*IBS, Shinshu Univ.*)

1Pos074　小角散乱、中性子準弾性散乱、及び中性子結晶学による蛋白質水和水の統一的解析
Coordinated analysis of protein hydration water by small-angle scattering, quasielastic neutron scattering, and neutron crystallography
Satoru Fujiwara[1], Tatsuhito Matsuo[1], Fumiaki Kono[1], Shin-ichi Takata[2], Yasunobu Sugimoto[3], Tatsuya Kikuchi[2], Kenji Nakajima[2], Toshiyuki Chatake[4] ([1]*QuBS, QST*, [2]*J-PARC Center*, [3]*Nagoya Univ.*, [4]*RRI, Kyoto Univ.*)

1Pos075　リゾチームの動的ストークスシフト測定と分子動力学計算によるその解釈
Measurement of dynamic Stokes shift of lysozyme and its interpretation by molecular dynamics simulation
Asahi Fukuda[1,2], **Tomotaka Oroguchi**[1,2], Masayoshi Nakasako[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*)

分子モーター / Molecular motor

1Pos076　演題取り消し

1Pos077　細胞質ダイニンの歩行運動の異方性に関する理論的研究
Theoretical study on the anisotropy of Cytoplasmic dynein locomotion
Shintaoh Kubo, Shoji Takada (*Grad. Sci., Univ. Kyoto*)

1Pos078　確率的モデリングによるミオシン V の化学ー力学ネットワーク
Chemomechanical network modeling of myosin V
Tomonari Sumi (*Res. Inst. Interdisciplinary Sci., Okayama Univ.*)

1Pos079　Two antagonistic regulatory domains of DCTN1 modulate the microtubule-binding affinities of both dynein and dynactin
Takuya Kobayashi[1], Kei Saito[1], Takuya Miyashita[1], Takashi Murayama[2], Yoko Y Toyoshima[1] ([1]*Department of Life Sciences, Graduate School of Arts and Sciences, The University of Tokyo*, [2]*Department of Pharmacology, Juntendo University School of Medicine*)

1Pos080　Development of a nano-patterning of kinesins to control the number and arrangement of motors by combining Au nano-pillars and SAM
Taikopaul Kaneko[1], Shotaro Ohba[1], Ken'ya Furuta[2], Kazuhiro Oiwa[2], Hirofumi Shintaku[1], Hidetoshi Kotera[1], Ryuji Yokokawa[1] ([1]*Kyoto Univ. Eng. Micro.*, [2]*NICT*)

1Pos081　微小管結合タンパク質アルファシヌクレインの微小管および微小管依存細胞内輸送における機能解析
Alpha-synuclein binds unconventional microtubules that have a unique function
Shiori Toba[1], Mingyue Jin[1], Masami Yamada[1], Sakiko Matsumoto[1], Takuo Yasunaga[2,3,4], Yuko Fukunaga[5,6], Atsuo Miyazawa[5,6], Hiroaki Kojima[7], Yoshiyuki Arai[8], Takeharu Nagai[8], Shinji Hirotsune[1] ([1]*Osaka City Univ. Grad. Sch. of Medicine*, [2]*Faculty of Computer Science and Systems Engineering, Kyushu Inst. of Technology*, [3]*JST-SENTAN*, [4]*JST-CREST*, [5]*Grad. Sch. of Life Science, Univ. of Hyogo*, [6]*RIKEN SPring-8 Center*, [7]*Advanced ICT Research Inst., National Inst. of Information and Communications Technology*, [8]*Inst. of Scientific and Industrial Research, Osaka Univ.*)

1Pos082　アーキアべん毛の回転を駆動するモーターは速度一定型である
The Archaellar Motor Produces Variable Torques to Maintain Constant Rotation Speed
Seiji Iwata, Yoshiaki Kinosita, Daisuke Nakane, Takayuki Nishizaka (*Dept. of Phys., Gakushuin Univ., Japan*)

1Pos083　真核生物鞭毛軸糸の Ca^{2+}濃度による構造変化の X 線繊維回折による解析
Structural responses of *Chlamydomonas* flagellar axonemes to Ca^{2+} studied with X-ray fiber diffraction
Kazuhiro Oiwa[1,2,3], Junya Kirima[2], Misaki Shiraga[2], Hiroyuki Iwamoto[4] ([1]*Adv. ICT Res. Inst. NICT*, [2]*Grad. Sch. Life Sci. Univ. Hyogo*, [3]*CREST Biodynamics*, [4]*Japan Sync. Rad. Res. Inst. SPring-8*)

1Pos084 **Cell-like locomotion of self-organized motor-filament complex**
Takayuki Torisawa[1,2], Masahiro Sawada[2,3], Daisuke Taniguchi[4], Shuji Ishihara[2,3], Kazuhiro Oiwa[1,2] ([1]*Advanced ICT Inst., NICT*, [2]*CREST, JST*, [3]*Grad. Sch. Arts and Sciences, Univ. Tokyo*, [4]*Dept. of Pharm., Grad. Sch. Med, Kyoto Univ.*)

1Pos085 ***de novo* 設計した人工コイルドコイルは回転子として機能する。**
The *de novo* designed artificial coiled-coil functions as a rotor of rotary motor
Jun-ichi Kishikawa, Mihori Baba, Atsuko Nakanishi, Ken Yokoyama (*Dept. Mol. Biosci., Kyoto Sangyo Univ.*)

1Pos086 **Structural and mechanistic insights into the ε subunit from bacterial ATP synthases**
Alexander Krah[1,2], Shoji Takada[2], Changbong Hyeon[1] ([1]*School of Computational Sciences, Korea Institute for Advanced Study (KIAS)*, [2]*Department of Biophysics, Graduate School of Science, Kyoto University*)

1Pos087 **DNA ペイント法を用いた RNA ポリメラーゼの超解像イメージングと細胞個性の分子メカニズムの解明**
Super-resolution imaging of RNA polymerases with DNA-PAINT for understanding the molecular mechanism of cell individuality
Keisuke Fujita[1,2], Toshio Yanagida[1,2], Mitsuhiro Iwaki[1,2] ([1]*QBiC, RIKEN*, [2]*Grad. Sch. of Front. Bioscience., Osaka Univ.*)

1Pos088 **F_1-ATPase のシリンダー部分の 1 分子立体構造変化観察**
Single-molecule observation of conformational dynamics in the cylinder part of F_1-ATPase
Ryuichi Yokota[1], Mitsuhiro Sugawa[2], Yuta Nomura[1], Junichiro Yajima[2], Tomoko Masaike[1,3] ([1]*Dept. Appl. Biol., Sch. Sci. and Tech., Tokyo Univ. of Sci.*, [2]*Grad. Sch. Arts and Sci., Univ. of Tokyo*, [3]*Imaging Frontier Center, Tokyo Univ. of Sci.*)

1Pos089 **キネシン-微小管の運動性を利用したデフォーカス角度イメージングの単一蛍光色素のテンプレートの獲得**
Acquisition of raw sequential templates of a single fluorophore under defocused orientation imaging using kinesin-MT motility assay
Shoko Fujimura[1], Kazuki Goto[2], Kengo Adachi[3], Takayuki Nishizaka[2] ([1]*Sch. of Med, Keio Univ.*, [2]*Dept. Phys., Gakushuin Univ.*, [3]*Engin., Waseda Univ.*)

1Pos090 **Novel photochromic inhibitor of kinesin composed of dronpa tandem dimer**
Kohei Uchida, Shinsaku Maruta (*Grad. Sch. Eng., Univ. Soka*)

細胞生物学 / Cell biology

1Pos091 **細胞内シグナル伝達における膜電位の役割**
Role of membrane potential in intracellular signal transduction
Yusuke V. Morimoto[1,2,3], Masahiro Ueda[2,3] ([1]*Dept. of Biosci. Bioinfo., Kyushu Inst. Tech.*, [2]*RIKEN, QBiC*, [3]*Grad. Sch. Frontier Biosci., Osaka Univ.*)

1Pos092 **原始真核生物の細胞分裂過程を細胞内小器官の 3D 構造モデルから読み解く**
Reading out the cell division process of primitive eukaryotes from 3D structural model of intracellular organelles
Takako M. Ichinose[1,2], Rina Nagai[1,2], Hikari Mori[1], **Atsuko H. Iwane**[1,2] ([1]*RIKEN, QBiC, Cell Struct.*, [2]*Osaka Univ., Grad. Front. Biosci.*)

1Pos093 **角化細胞においてアクトミオシン活性が増殖の接触阻害に必須である**
Actomyosin activity is required for contact inhibition of keratinocyte proliferation
Hiroaki Hirata[1,2], Mikhail Samsonov[3], Masahiro Sokabe[1] ([1]*Nagoya Univ Grad Sch Med*, [2]*R-Pharm Japan*, [3]*R-Pharm*)

1Pos094 **エンドセリン B 受容体のシグナル伝達における GRP78 の役割**
Roles of GRP78 in endothelin B receptor signaling
Yuichi Mazaki[1], Tsunehito Higashi[1], Takahiro Horinouchi[1], Jin-Min Nam[2], Yasuhito Onodera[3] ([1]*Dept. Cell. Pharm., Grad. Sch. Med., Hokkaido Univ*, [2]*GSQ, GI-CoRE, Hokkaido Univ.*, [3]*Dept. Mol. Biol., Grad. Sch. Med., Hokkaido Univ.*)

1Pos095 **細胞形状が誘発するアメーバ細胞の集団運動**
Cell shape driving collective migration of amoeba cells
Katsuyoshi Matsushita (*Osaka University, School of Science, Depertment of Biological Science*)

1Pos096 **γ-tubulin は中心子のトリプレット微小管形成に関与する**
Evidence for involvement of γ-tubulin in assembly of centriolar triplet microtubules
Yuki Nakazawa[1,2], Mao Horii[3], Saki Watanabe[1], Moeko Otsuki[1], Akira Noga[3], Ken-ichi Wakabayashi[4], Masafumi Hirono[1] ([1]*Dept. Frontier Biosci., Fac. Biosci. Appl. Chem., Hosei Univ.*, [2]*JSPS*, [3]*Dept. Biosci., Grad. Sch. Sci., Univ. Tokyo*, [4]*Inst. Innov. Res., Tokyo Inst. Tech.*)

1Pos097 **単一心筋細胞に対する赤外レーザ照射の影響**
Influence of focused infrared laser irradiation on beating rate in single cardiomyocytes
Kento Nozawa, Yukino Motohashi, Maki Ishii, **Tomoyuki Kaneko** (*LaRC, FB, Hosei Univ.*)

1Pos098 **Protein with tau-like repeats (PTL-1)と細胞骨格線維の相互作用**
Interaction between cytoskeletal filaments and a protein with tau-like repeats, PTL-1
Kazufumi Matsui[1], Miki Tamura[1], Miyuki Shiga[1], Yurika Hashi[2], Susumu Kotani[3], Kiyotaka Tokuraku[1] ([1]*Div. Sust. Env. Eng., Muroran Inst. Tech.*, [2]*Gen. Dept. of Aesthetics, Yamano Col.*, [3]*Fac. Sci., Kanagawa Univ.*)

1Pos099 **ゾウリムシ繊毛メタクロナールウェーブの発振源**
Sources of Metachronal Wave in *Paramecium* Cilia
Naohiko Himata, Chika Okimura, Manabu Hori, **Yoshiaki Iwadate** (*Fac. Sci., Yamaguchi Univ.*)

1Pos100 **魚類表皮ケラトサイトの遊走のための車輪**
A Wheel for Migration in Fish Keratocyte
Chika Okimura[1], Atsushi Taniguchi[2], Shigenori Nonaka[2], Yoshiaki Iwadate[1] ([1]*Fac. Sci., Yamaguchi Univ.*, [2]*NIBB*)

1Pos101 マイコプラズマの滑走速度を示す分子速度計

Molecular speedometer indicating gliding speed in *Mycoplasma pneumoniae*

Kohki Murata[1], Tsuyoshi Kenri[2], Daisuke Nakane[1], Keigo Shibayama[2], Takayuki Nishizaka[1] ([1]*Dept. of Phys., Gakushuin Univ.*, [2]*Dept. of Bact II., NIID*)

1Pos102 単一細胞内グルココルチコイド受容体のホモ二量体形成と転写活性の関連解析

Quantitative analysis of glucocorticoid receptor dimerization and transcriptional activity in single cell using advanced imaging technique

Sho Oasa, Manisha Tiwari,, Johtaro Yamamoto,, Daisuke Yamashita,, Shintaro Mikuni,, **Masataka Kinjo** (*Adv. Life Sci., Hokkaido U.*)

1Pos103 **Actin-like MamK cytoskeleton tethers bacterial magnetosome organelles in a static chain**

Azuma Taoka[1,2], Ayako Kiyokawa[1], Yousuke Kikuchi[1], Yoshihiro Fukumori[3] ([1]*Fac. of Nat. Sys., Inst. Sci. and Eng., Kanazawa Univ.*, [2]*Bio-AFM FSC., Inst. Sci. and Eng., Kanazawa Univ.*, [3]*Vice President, Kanazawa Univ.*)

1Pos104 ロクロクビムシのプロボーシスの伸縮機構

Extension and Contraction Mechanism of the Proboscis of a Ciliate, *Lacrymaria olor*

Ryuji Yanase[1], Yukinori Nishigami[2], Masatoshi Ichikawa[2], Atsushi Taniguchi[3], Shigenori Nonaka[3], Tohru Yoshihisa[1], Seiji Sonobe[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Dept. Phys. Grad. Sch. Sci., Kyoto Univ.*, [3]*Spatiotemp. Reg., NIBB*)

1Pos105 バクテリアべん毛輸送ゲート複合体構成蛋白質間の相互作用

Interactions between flagellar type III export gate proteins

Miki Kinoshita[1], Akihiro Kawamoto[1], Keiichi Namba[1,2], Tohru Minamino[1] ([1]*Graduate School of Frontier Biosciences, Osaka Univ.*, [2]*QBiC, RIKEN*)

1Pos106 べん毛蛋白質輸送装置の基質認識モード切り替えにおける FlhA リンカー領域の役割

The role of a flexible linker of FlhA in substrate specificity switching of the bacterial flagellar type III export apparatus

Yumi Inoue[1], Mamoru Kida[2], Miki Kinoshita[1], Katsumi Imada[2], Keiichi Namba[1,3], **Tohru Minamino**[1] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [2]*Grad. Sch. Sci., Osaka Univ.*, [3]*QBiC, RIKEN*)

1Pos107 細菌べん毛モーター固定子付随蛋白質 FliL のペリプラズム領域の構造

Structure of a periplasmic fragment of FliL, a bacterial flagellar stator associated protein from *Vibrio alginolyticus*

Norihiro Takekawa[1], Miyu Isumi[1], Mayuko Sakuma[2,3], Seiji Kojima[2], Michio Homma[2], Katsumi Imada[1] ([1]*Dept. of Macromol. Sci., Grad. Sch. of Sci., Osaka Univ.*, [2]*Div. of Biol. Sci., Grad. Sch. of Sci., Nagoya Univ.*, [3]*Radioisotope Res. Cent., Nagoya Univ.*)

1Pos108 多電極電位計測システムを用いたライン状心筋細胞の伝導速度測定

Measuring Conduction Velocity of Line-Networked Cardiomyocyte

Tetsuro Yoshida, Yui Okabe, Tomoyuki Kaneko (*LaRC, FB, Hosei Uni.*)

1Pos109 1 細胞レベルで再構成した心筋細胞ネットワークによる外部電気刺激への応答解析

Analysis of response to external electric stimulations by cardiomyocytes-network arranged at single-cell-level

Koki Fujii[1], Fumimasa Nomura[2], Tomoyuki Kaneko[1] ([1]*Laboratory for Reconstructive Cell Biology, Frontier Bioscience, Hosei University*, [2]*Department of Biomedical Information, Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University*)

1Pos110 新規マイクロ流体システムで解明する赤血球の非線形非平衡変形能

Non-linear and non-equilibrium deformability of a red blood cell unraveled with a novel microfluidic platform

Hiroaki Ito[1], Ryo Murakami[1], C.-H. Dylan Tsai[1], Motomu Tanaka[2,3], Makoto Kaneko[1] ([1]*Grad. Sch. Eng., Osaka Univ.*, [2]*iCeMS, Kyoto Univ.*, [3]*Phys. Chem. Inst., Univ. Heidelberg*)

1Pos111 **Dynamics of Actin Cytoskeleton Remodeling Induced by Femtosecond Laser Ablation**

Kwokhoi Ng[1], Takuya Takeshige[1], Ryuzo Kawamura[1], Seiichiro Nakabayashi[1], Yosuke Yoneyama[2], Fumihiko Hakuno[2], Shin-ichiro Takahashi[2], Hiroshi Yoshikawa[1] ([1]*Dept. Chem., Saitama Univ.*, [2]*GSALS., The Univ. of Tokyo*)

生体膜・人口膜：構造・物性 / Biological & Artificial membrane: Structure & Property

1Pos112 ベシクル可溶化法によるリン脂質ーリン脂質間相互作用熱力学量の測定

Phospholipid-Phospholipid Interactions in Bilayers Determined by Vesicle Solubilization

Keisuke Ikeda, Minoru Nakano (*Grad. Sch. Med. Pharm. Sci., Univ. Toyama*)

1Pos113 コレステロール含有ホスファチジルエタノールアミン膜とシトクロム P450 基質薬剤クロルゾキサゾンの相互作用

Interaction between cholesterol-containing phosphatidylethanolamine bilayers and cytochrome P450 substrate drug chlorzoxazone

Hiroshi Takahashi (*Grad. Sch. Sci. & Tech., Gunma Univ.*)

1Pos114 ガラス基板に固定した細胞膜中の脂質と膜タンパク質の電気泳動

Electrophoresis of lipids and membrane proteins in the cell membrane fixed on a glass substrate

Miki Okazaki[1], Takashi Okuno[2] ([1]*Grad. Sch. Eng., Yamagata Univ.*, [2]*Fac. Sci, Yamagata Univ.*)

1Pos115 分子動力学シミュレーションを用いたメリチンによる膜細孔形成の自由エネルギー解析

Free energy analysis of membrane pore formation by melittin using molecular dynamics simulations

Yusuke Miyazaki, Wataru Shinoda, Susumu Okazaki (*Grad. Sch. Eng., Univ. Nagoya*)

1Pos116 界面通過法 GUV-膜タンパク質発現バキュロウイルス間膜融合の可視化解析

Analysis of membrane fusion between membrane protein-expressing baculovirus virions and GUVs prepared with a droplet transfer method

Misako Nishigami[1], Masahiro Tomita[1], Kingo Takiguchi[2], Kanta Tsumoto[1] ([1]*Grad. Sch. Eng., Mie Univ.*, [2]*Grad. Sch. Sci., Nagoya Univ.*)

1Pos117 **Change of binding ability of halorhodopsin for bacterioruberin accompanied by retinal binding / dissociation on archaeal membrane**
Shun Yano, Takanori Sasaki (*Graduate School of Advanced Mathematical Sciences, Meiji University*)

1Pos118 **Role of cholesterol in membrane phase separation observed via coarse-grained simulations of ternary mixtures**
George A. Pantelopulos, John E. Straub (*Chem. Dept., Boston U., USA*)

1Pos119 **Reconstitution amount of membrane proteins was controlled by components of asymmetric lipid vesicles**
Koki Kamiya[1], Toshihisa Osaki[1,2], Ryuji Kawano[1], Shoji Takeuchi[1,2] ([1]*Kanagawa Institute of Industrial Science and Technology*, [2]*IIS, University of Tokyo*)

1Pos120 **リガンド添加による脂質二分子膜相転移温度変化の熱力学的解釈**
Thermodynamic interpretation for variation in phase-transition temperatures of lipid bilayer membranes by adding a ligand
Masaki Goto[1], Hirotsugu Okamoto[2], Toshiki Nakao[2], Nobutake Tamai[1], Hitoshi Matsuki[1] ([1]*Grad. Sch. Tech., Indus. & Soc. Sci., Tokushima Univ.*, [2]*Grad. Sch. Adv. Tech. & Sci., Tokushima Univ.*)

1Pos121 **ポア形成ベータシートペプチドのデザイン**
Design of pore-forming β-sheet peptides in lipid bilayer
Keisuke Shimizu[1], Naoki Saigo[1], Yusuke Sekiya[1], Kenji Usui[2], Ryuji Kawano[1] ([1]*Kawano Lab. Tokyo University of Agriculture and Technology*, [2]*Usui Lab. Konan University*)

1Pos122 **コレステロールによるジアルキルホスファチジルコリンの指組構造化の抑制**
Suppression of bilayer interdigitation of dialkyl-phosphatidylcholine by cholesterol
Nobutake Tamai[1], Takuya Izumikawa[2], Maiko Uemura[2], Masaki Goto[1], Hitoshi Matsuki[1] ([1]*Grad. Sch. Technol. Indus. Soc. Sci., Tokushima Univ.*, [2]*Grad. Sch. Adv. Technol. Sci., Tokushima Univ.*)

1Pos123 **Quantitative analysis of water permeation into model lipid membranes for the stratum corneum intercellular lipids by FTIR-ATR**
Kohei Oka, Hiromitsu Nakazawa, Satoru Kato (*Grad. Sch. Sci & Tech., Univ. Kwansei Gakuin*)

1Pos124 **マイクロ流路デバイスを用いた細胞サイズ液滴の充填パターン**
Hexagonal packing of cell-sized lipid droplets using microfluidic device
Shougo Fujiwara, Kan Shouji, Ryuji Kawano, **Miho Yanagisawa** (*Tokyo Univ. Agri. Technol.*)

1Pos125 **粗視化モデルによる混合脂質ベシクルの構造安定性に関する理論的研究**
Theoretical study on the structural stability of vesicle consisting of mixed lipids by coarse-grained model
Tetsu Matsuura, Shohei Takagi, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Sch. Nat. Sci. Tech., Kanazawa. Univ*)

生体膜・人口膜：ダイナミクス / Biological & Artificial membrane: Dynamics

1Pos126 **親水性アミノ酸残基の位置に依存した膜貫通ペプチドのリン脂質 flip-flop 促進能の評価**
Effect of hydrophilic amino acid residues and their relative position in transmembrane peptides on phospholipid flip-flop promotion
Yuta Sugimoto[1], Hiroyuki Nakao[2], Keisuke Ikeda[2], Minoru Nakano[2] ([1]*Fac. of Pharm. and Pharm. Sci., Univ. of Toyama*, [2]*Grad. Sch. of Med. and Pharm. Sci., Univ. of Toyama*)

1Pos127 **脂質膜の熱的揺らぎは細胞透過ペプチド・トランスポータン 10(TP10)の単一ベシクルへの侵入に影響を与える**
Thermal Fluctuation of Lipid Bilayers Affect the Entry of Cell-Penetrating Peptide Transportan 10 (TP10) into Single Vesicles
Md. Zahidul Islam[1], **Sabrina Sharmin**[1], Victor Levadnyy[1,2], Sayed Ul Alam Shibly[1], Masahito Yamazaki[1,3,4] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Rus. Acad. Sci.*, [3]*Res. Inst. Ele., Shizuoka Univ.*, [4]*Grad. Sch. Sci., Shizuoka Univ.*)

1Pos128 **混合脂質二重膜中における孔側壁の線張力係数の孔径依存性：分子動力学シミュレーション**
Pore Radius Dependence of Nano-Pore Edge Tension in Mixed Lipid Bilayers: Molecular Dynamics Simulation
Taiki Shigematsu[1], Kenichiro Koshiyama[2], Shigeo Wada[2] ([1]*Global Center for Medical Engineering and Informatics, Osaka University*, [2]*Graduate School of Engineering Science, Osaka University*)

1Pos129 **A New Coarse-Grained Lipid Model for the Study of Lipid-Membrane Protein Systems**
Diego Ugarte, Shoji Takada (*Dept. Biophysics, Div. Biology, Grad. Sch. Sci., Kyoto University*)

1Pos130 **脂質膜の張力は水の膜透過係数を増加させる**
Lateral Tension increases membrane permeability of water in lipid membranes
Rajib Ahmed[1], Sayed Ul Alam Shibly[1], Md. Zahidul Islam[1], Masahito Yamazaki[1,2,3] ([1]*Grad. Sch. Sci., Shizuoka Univ.*, [2]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [3]*Res. Inst. Ele., Shizuoka Univ*)

1Pos131 **細胞透過ペプチド・トランスポータン 10 の脂質膜透過に与える膜電位の効果**
Effect of Membrane Potential on the Translocation of Cell-Penetrating Peptide Transportan 10 (TP10) across Lipid Bilayers
Md Mizanur Moghal[1], Md. Zahidul Islam[1], Sharmin Sabrina[1], Masahito Yamazaki[1,2,3] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Res. Inst. Ele., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

生体膜・人口膜：興奮・チャネル / Biological & Artificial membrane: Excitation & Channels

1Pos132 **コリネ型バクテリアの機械受容チャネル MscCG の C 末端構造による開閉機構の制御**
Modulation of gating MscCG, the mechanosensitive channel of Corynebacterium glutamicum, by the C-terminal domain
Yoshitaka Nakayama[1], Michael Becker[2], Haleh Ebrahimian[3], Tomoyuki Konishi[4], Hisashi Kawasaki[4], Reinhard Kramer[2], Boris Martinac[1,5] ([1]*Victor Chang Cardiac Research Institute*, [2]*University of Cologne*, [3]*Wollongong University*, [4]*Tokyo Denki University*, [5]*University of New South Wales*)

1Pos133 **N 末端変異リアノジン受容体における分子動力学計算法とカルシウムシグナルの相関解析**

Correlation of molecular dynamics analysis and Calcium dynamics in mutant type 1 ryanodine receptors

Toshiko Yamazawa[1], Takashi Murayama[2], Maki Yamaguchi[1], Hideto Oyamada[3], Nagomi Kurebayashi[2], Junji Suzuki[4], Kazunori Kanemaru[4], Takashi Sakurai[2], Masamitsu Iino[4,5] ([1]*Dept Mol. Physiol., Jikei Univ. Sch. Med.*, [2]*Dept. Pharmacol., Juntendo Univ. Sch. Med.*, [3]*Dept. Pharmacol., Sch. Med., Showa Univ.*, [4]*Dept. Pharmacol., Grad. Sch. Med., The Univ. Tokyo*, [5]*Dept. Cell. Mol. Pharmacol., Nihon Univ. Sch. Med.*)

1Pos134 **哺乳類 2 ポアドメインカリウムチャネル TWIK-1 の機能特性と機能制御メカニズムの解析**

Functional properties and the regulating mechanisms of a mammalian two-pore domain potassium channel TWIK-1

Hisao Tsukamoto[1], Koichi Nakajo[2,3], Yoshihiro Kubo[3], Yuji Furutani[1] ([1]*Institute for Molecular Science*, [2]*Osaka Medical College*, [3]*National Institute for Physiological Sciences*)

1Pos135 **イオンチャネル電流測定の自動化**

Automated system for channel current measuremen

Minako Hirano[1], Nobuyuki Kawashima[2], Masahisa Tomita[2], Toru Ide[3] ([1]*GPI*, [2]*SYSTEC Corporation*, [3]*Grad. Schl Sci. Tech. Okayama Univ.*)

1Pos136 **電位依存性ホスファターゼ VSP の疎水的な膜相互作用部位の重要性**

The critical role of the hydrophobic membrane interacting region in voltage-sensing phosphatase (VSP)

Akira Kawanabe[1], Masaki Hashimoto[1], Tomoko Yonezawa[1], Yuka Jinno[1], Souhei Sakata[2], Yasushi Okamura[1] ([1]*Grad. Sch. Med., Osaka Univ.*, [2]*Fac. Med., Osaka Med. Col.*)

1Pos137 **KcsA チャネルからのイオンの自発的流出**

Spontaneous exits of ions from the KcsA channel

Takashi Sumikama, Shigetoshi Oiki (*Univ of Fukui*)

1Pos138 **Single channel recordings of ion channels immobilized on a solid substrate**

Toru Ide[1,2], Masahiro Yamakami[1], Minako Hirano[2], Hiroaki Yokota[2], Junya Ichinose[1] ([1]*Grad Schl Nat Sci Tech, Okayama Univ*, [2]*GPI*)

1Pos139 **A simple method for promoting liposome-bilayer fusion**

Kohei Miyatani[1], Minako Hirano[2], Toru Ide[1] ([1]*Okayama Univ*, [2]*GPI*)

1Pos140 **Characterization of the channel pore formed by Cry46Ab toxin from soil bacterium Bacillus thuringiensis**

Akira Sakakibara[1], Tohru Hayakawa[1], So Takebe[2], Toru Ide[1] ([1]*Univ. Okayama*, [2]*Kindai Univ.*)

生体膜・人口膜：輸送 / Biological & Artificial membrane: Transport

1Pos141 **ミトコンドリア凝集に伴う表面 p H の変化の計算**

Calculation of surface pH change of mitochondria due to aggregation

Takuya Takahashi[1], Kota Kasahara[1], Yoshihiro Ohta[2] ([1]*Dept. of Biosci. and Bioinformatics, Ritsumeikan Univ.*, [2]*Div. of Biotech. and Life Sci., Inst. of Eng., Tokyo Univ. of Agr. and Tech.*)

1Pos142 **反転膜を用いたべん毛 III 型蛋白質輸送の定量測定**

Quantitative analysis of the flagellar type III protein export using the inverted membrane vesicles

Tsuyoshi Tono[1], Hiroyuki Terashima[1,2], Kazuhito Tabata[3], Hiroshi Ueno[3], Hiroyuki Noji[3], Katsumi Imada[1] ([1]*Grad. Sch. of Sci., Osaka Univ.*, [2]*Grad. Sch. of Sci., Nagoya Univ.*, [3]*Sch of Eng., Univ. of Tokyo*)

1Pos143 **シグナルペプチド配列のバリエーションと細胞内局在に関する考察**

Sequence variation of signal-peptides and protein subcellular localization

Tomonao Iibuchi, Tatsuki Kikegawa, Keiya Inoue, Naoyuki Takachio, Kenji Etchuya, Yuri Mukai (*Dept. Electronics, Grad. Sch. Sci. & Tech., Meiji Univ.*)

1Pos144 **浸透圧がミトコンドリアの活性に及ぼす影響**

Effects of osmolality on mitochondrial activities

Sawako Kimura, Yoshihiro Ohta (*Tokyo University of Agriculture and Technology*)

1Pos145 **基質存在下・非存在下での多剤排出輸送体 AcrAB-TolC の細胞内動態解析**

Analysis of the in cell dynamics of a multi-drug exporter AcrB in the absenc e and presence of substrates

Tomoki Matsuda, Seiji Yamasaki, Kunihiko Nishino, Takeharu Nagai, Akihito Yamaguchi (*ISIR, Osaka Univ*)

1Pos146 **ERK 情報処理過程の共焦点局所画像を用いた定量解析**

Quantitative measurement for information processing of ERK using localized confocal image analyses

Kazunari Mouri[1], Yasushi Okada[1,2] ([1]*RIKEN, QBiC*, [2]*Univ. Tokyo, Grad. Sch. Sci., Dept. Phys*)

生体膜・人口膜：情報伝達 / Biological & Artificial membrane: Signal transduction

1Pos147 **In vitro 1 分子イメージングによる PTEN-PI(4,5)P2 相互作用の解析**

In vitro single molecule-imaging analysis of interactions between PTEN and phosphatidylinositol 4, 5-bisphosphate

Daisuke Yoshioka[1,3], Seiya Fukushima[1,3], Daichi Okuno[3], Satomi Matsuoka[3], Toru Ide[4], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. of Sci., Osaka Univ.*, [2]*Grad. Sch. of Front. Biosci., Osaka Univ.*, [3]*RIKEN QBiC*, [4]*Grad. Sch. of Nat. Sci. and Tech., Okayama Univ.*)

1Pos148 **MCF7 細胞内における p52shc の細胞膜移行ダイナミクス計測**

p52SHC translocation to the plasma membrane of MCF7 cells

Ryo Yoshizawa[1,2], Nobuhisa Umeki[2], Masataka Yanagawa[2], Masayuki Murata[1], Yasushi Sako[2] ([1]*Grad. Sch. Arts and Shi., Univ. Tokyo*, [2]*Wako Inst., RIKEN*)

1Pos149 **A single EGF molecule is sufficient to activate a preformed EGFR dimer**
Ei-ichiro Saita, Dingze Mang, Ichiro N. Maruyama (*OIST*)

1Pos150 **コレラ菌タウリン走性受容体 Mlp37 遺伝子の温度による発現制御**
Temperature-regulated expression of the gene encoding the taurine chemoreceptor Mlp37 of *Vibrio cholerae*
Shiori Onogi[1], Noriaki Sagoshi[1], So-ichiro Nishiyama[1,2], Yoshiyuki Sowa[1,2], **Ikuro Kawagishi**[1,2] ([1]*Dept. Frontier Biosci., Hosei Univ.*, [2]*Res. Cen. Micro-Nano. Tech., Hosei Univ.*)

1Pos151 **サルモネラ属細菌クエン酸走性受容体 Tcp のリガンド認識における 2 価金属イオンの役割**
Role of divalent metal cations in ligand recognition by the citrate chemoreceptor Tcp of *Salmonella enterica*
Mariko Matsuda[1], Tetsuya Shiroi[1], Katsumi Imada[2], So-ichiro Nishiyama[3,4], Mayuko Sakuma[5], Michio Homma[5], Ikuro Kawagishi[1,3,4] ([1]*Grad. Sch. Sci. Eng., Hosei Univ.*, [2]*Grad. Sch. Sci., Osaka Univ.*, [3]*Dept. Frontier Biosci., Hosei Univ.*, [4]*Res. Cen. Micro-Nano Tech., Hosei Univ.*, [5]*Grad. Sch. Sci., Nagoya Univ.*)

発生・分化 / Development & Differentiation

1Pos152 **ヒト人工多能性幹細胞由来の内胚葉及び中胚葉細胞により模倣されるヒト原腸形成期の細胞運動**
Cell Migration in the Human Gastrulation Stage Mimicked by Endoderm and Mesoderm Derived from Human Induced Pluripotent Stem Cells
Kenshiro Maruyama, Shota Miyazaki, Kiyoshi Ohnuma (*Grad. Sch. Eng., Univ. Nagaoka Tech.*)

1Pos153 **形態形成における集団運動を制御する細胞間シグナル伝達の動態の変遷**
Transition of the dynamics of cell-cell communication controlling collective cell migration during morphogenesis of Dictyostelium cells
Hidenori Hashimura[1,2], Masato Yasui[1], Yusuke Morimoto[1,3], Masahiro Ueda[1,2,4] ([1]*RIKEN QBiC*, [2]*Dep. Biol. Sci., Grad. Sch. of Sci., Osaka Univ.*, [3]*Dept. of Biosci. Bioinfo., Kyushu Inst. Tech.*, [4]*Grad. Sch. of Front. Biosci., Osaka Univ.*)

1Pos154 **Mechanics of the Nucleus and Cell Body during Early Mouse Development with Implications for Reproductive Medicine**
Fransisca As Van Esterik[1], Masahiro Ikenaga[1], Hitoshi Niwa[2], Daisuke Mizuno[1] ([1]*Dept. of Physics, Kyushu University*, [2]*Dept. of Pluripotent Stem Cell Biology, IMEG, Kumamoto University*)

1Pos155 **高時間分解・長時間撮影による、線虫 *C.elegans* の原腸貫入運動の解析**
Particle tracking analysis of gastrulation in C. elegans embryos
Yukinobu Arata[1], Yuki Shindo[1], Hiroaki Takagi[2], Yashushi Sako[1] ([1]*Cell. Info., RIKEN*, [2]*Dept. of Phys. Nara Med. Univ.*)

1Pos156 **高速三次元光シート顕微鏡によるマウス胚ノード流の三次元解析**
Three-dimensional analysis of the nodal flow in the mouse embryo by the rapid 3-D light-sheet microscopy
Atsushi Taniguchi, Shigenori Nonaka (*Spatiotemp. Reg., Natl. Inst. Basic Biol.*)

1Pos157 **上皮組織変形の連続体モデル**
Continuum model of epithelial mechanics
Shuji Ishihara[1], Marcq Philippe[2], Kaoru Sugimura[3] ([1]*Grad. Sch. Arts. Sci., Univ. Tokyo*, [2]*Inst. Curie, Univesite Paris 6*, [3]*iCeMS, Kyoto Univ.*)

1Pos158 **in vitro でのヒト原腸形成期における細胞運動に対する細胞間相互作用の影響**
The effects of cell-cell interaction on the cell dynamics during human gastrulation in vitro
Shota Miyazaki, Kenshiro Maruyama, Gen Kato, Tohru Sasaki, Kiyoshi Ohnuma (*Grad. Sch. Eng., Univ. Nagaoka Tech.*)

神経科学・感覚 / Neuroscience & Sensory systems

1Pos159 **カエルの神経筋伝達の短期間シナプス可塑性におけるドッキングタンパク質の新たな役割**
Novel Distinctive Roles of Docking Proteins in Short-term Synaptic Plasticity of Frog Neuromuscular Transmission
Yasuhiro Imafuku[1], Koh-ichi Enomoto[2], Hiroko Kataoka[2], Isao Ito[1], Takashi Maeno[3] ([1]*Dept Biol., Kyushu Univ.*, [2]*Shimane Univ.*, [3]*Prof. Emeritus, Shimane Med. Univ.*)

1Pos160 **海馬神経シナプスを制御する神経ステロイドの non-genomic 信号系**
Non-genomic signaling of neurosreroids, regulating synapses in the hippocampus
Suguru Kawato[1,2] ([1]*Dep. Cognitive Neuroscience, Pharma-Science, Teikyo Univ.*, [2]*Dep. Urology, Grad Sch Medicine, Juntendo Univ.*)

1Pos161 **微小管の物理的特性に与える MAPs の影響**
Influence of microtubule-associated proteins on the physical properties of microtubules
Miki Tamura[1], Kazufumi Matsui[1], Miyuki Siga[1], Kabir Arif Md. Rashedul[2], Akira Kakugo[2], Susumu Kotani[3], Kiyotaka Tokuraku[1] ([1]*Div. Sust. Env. Eng., Muroran Inst. Tech.*, [2]*Fac. Sci., Hokkaido Univ.*, [3]*Fac. Sci, Kanagawa Univ.*)

1Pos162 **神経細胞における細胞骨格アクチンの修復の分子メカニズム**
Molecular Mechanism of Cytoskeletal Actin Repairing in Nerve Cells
Tomoya Higo[1], Takuo Yasunaga[2], Shinji Aramaki[3] ([1]*Kyushu Institute of Technology*, [2]*Kyushu Institute of Technology*, [3]*Tvips GmbH*)

1Pos163 **演題取り消し**

1Pos164 **チャコウラナメクジの匂い味覚条件付け学習における記憶形成に対するエピカテキンの影響**
Epicatechin enhances the long-term memory of odor aversive learning in the land slug
Yoshimasa Komatsuzaki[1,2], Taiyou Nakamura[1], Ken Lukowiak[2], Minoru Saito[3] ([1]*Dept. of Phys., CST, Nihon Univ.*, [2]*Hotchkiss Brain Inst, Cumming Sch of Med, Univ of Calgary, Canada*, [3]*Dept. of Biosci., CHS, Nihon Univ.*)

神経回路・情報処理 / Neuronal circuit & Information processing

1Pos165 **Structure of the Neuron-to-Neuron Network of Drosophila Connectome**
Chi-Tin Shih (*Tunghai University*)

1Pos166 **神経細胞ネットワークの 1 細胞レベル自発発火を解析する拡張型コンパクトオンチップ細胞外電位計測技術の開発**
Extracellular electrophysiological measurement of spontaneous firing of single neurons in neuronal circuit using expandable on-chip assay
Shota Aoki[1], Takahito Kikuchi[2], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Masao Odaka[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., WASEDA Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*)

1Pos167 **オンチップ 1 細胞培養系を用いた神経細胞から伸長する神経突起の特性の解析**
Neurite elongation characteristics in the width-controlled channels using an in situ on-chip photothermal microfabrication assay
Takahito Kikuchi[1], Shota Aoki[2], Hideyuki Terazono[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Masao Odaka[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*Waseda Biosci. Res. Ins. in Singapore (WABIOS)*)

1Pos168 **カエル神経筋接合部シナプスにおける促通 2 成分間の数学的関係性の解明：加算的なのか積算的なのか和のベキ的関係なのか**
What mathematical relationship of two components of facilitation at the frog NMJ: Additive, multiplicative, or power of summation ?
Naoya Suzuki, Junpei Yamaguchi (*Dept. Phys., Grad. Sch. Sci., Nagoya Univ.*)

1Pos169 **線虫の whole-brain イメージングデータに関する因果性解析**
Causality analysis on whole-brain imaging data of C. elegans
Yuishi Iwasaki[1,7], Takayuki Teramoto[2,7], Suzu Oe[2,7], Terumasa Tokunaga[3,7], Osamu Hirose[4,7], Stephen Wu[5,7], Yu Toyoshima[6,7], Moon Sun Jang[6,7], Ryo Yoshida[5,7], Yuichi Iino[6,7], Takeshi Ishihara[2,7] ([1]*Fac. Eng., Ibaraki Univ.*, [2]*Grad. Sch. Sci., Kyushu Univ.*, [3]*Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Institute Tech.*, [4]*Institute. Sci. and Eng., Kanazawa Univ.*, [5]*Institute Stat. Math.*, [6]*Grad. Sch. Sci., Univ. Tokyo*, [7]*JST, CREST*)

1Pos170 **ニワトリ胚由来の神経細胞から伸長する軸索の制御**
Control of axon elongation of neuron derived from chicken embryos
Hayato Toriumi, Tomoyuki Kaneko (*LaRC, FB, Hosei Univ.*)

1Pos171 **集光フェムト秒レーザーによる単一神経細胞の光刺激メカニズム**
Stimulation Mechanisms in Living Neuronal Cells with a Focused Femtosecond Laser
Yuji Fujioka[1,2], Suguru N. Kudoh[2], Takahisa Taguchi[3], Chie Hosokawa[1,2,4] ([1]*Biomed. Res. Inst., AIST*, [2]*Grad. Sci. &Tech., Kwansei Gakuin Univ.*, [3]*CiNet, NICT*, [4]*PhotoBIO-OIL, AIST*)

1Pos172 **脳における発火頻度依存性シナプス可塑性の数理的解析**
Numerical simulations and mathematical analysis of synaptic plasticity based on the rates of presynaptic firing
Katsuhiko Hata[1,2,6], Osamu Araki[3], Osamu Yokoi[2,4], Toshiaki Kaminaka[2,4], Izumi Kuboyama[1], Susumu Ito[5] ([1]*Sch. Emerg. Med. Sys. Kokushikan Univ.*, [2]*Res Cent for Math Med*, [3]*Dept of Ap Phys TUS*, [4]*DPEMS, Kokushikan Univ*, [5]*High-Tech Res. Cent., Kokushikan Univ.*, [6]*Sakurai Hosp.*)

1Pos173 **経頭蓋磁気刺激法における細胞外媒質まで考慮したケーブル理論**
Cable theory considering extracellular medium in transcranial magnetic stimulation method
Toshiaki Kaminaka[1,2], Osamu Yokoi[1,2], Katsuhiko Hata[2,3,4] ([1]*DPEMS, Kokushikan Univ*, [2]*Res Cent for Math Med*, [3]*Sch. Emerg. Med. Sys. Kokushikan Univ*, [4]*Sakurai Hosp*)

1Pos174 **反復リップルノイズを使った聴性脳幹反応の聴覚レベル判定**
Auditory level determination of auditory brainstem response using iterated ripple noise
Osamu Yokoi[1,2], Toshiaki Kaminaka[1,2], Katuhiko Hata[1,2,3] ([1]*DPEMS Kokushikan Univ*, [2]*Res Cent for Math Med*, [3]*Dept of Emerg. Med. Sys., Kokushikan Univ*)

1Pos175 **人工ニューラルネットワークによる運動想起脳波信号の多クラス特徴抽出**
Artificial neural network for multiclass feature extraction from motor imagery EEG
Ippei Yabe[1], Takuya Inoue[1], Hideo Mukai[1,2] ([1]*Dept. Comp. Sci., Grad. Sch. Sci. & Tech., Meiji Univ.*, [2]*Dept. Comp. Sci., Sch. Sci. & Tech., Meiji Univ.*)

バイオインフォマティクス：構造ゲノミクス / Bioinformatics: Structural genomics

1Pos176 **Specific Nucleotide Distributions and Nucleosome Positioning around Simple Sequence Repeats in the Human Genome**
Takeru Kameda, Atsushi Ikegaya, Naoaki Sakamoto, Akinori Awazu (*Dept. of Mathematical and Life Sciences, Hiroshima University*)

1Pos177 **MNase, as a probe to study the sequence-dependent site exposure in the +1 nucleosomes of yeast**
D. Luo[1], D. Kato[2], J. Nogami[3], Y. Ohkawa[3], H. Kurumizaka[2], H. Kono[1] ([1]*National Institutes for Quantum and Radiological Science and Technology*, [2]*Waseda University*, [3]*Kyushu University*)

1Pos178 **相互作用プロファイルによる細菌走化性タンパク質間相互作用ネットワーク解析**
Protein interaction surfaces of protein-protein interaction networks in bacterial chemotaxis networks using profile methods
Nobuyuki Uchikoga[1], Yuri Matsuzaki[1], Masahito Ohue[2], Yutaka Akiyama[1,2] ([1]*Tokyo Tech. ACLS*, [2]*Tokyo Tech, Sch. of Computing, Dept. of Computer Sci.*)

1Pos179 **生体内低分子化合物三次元構造データベースのアップデートと構造精度向上のための取り組み**
Recent development of 3DMET database: New release and efforts to improve data accuracy
Miki Maeda, Tomomi Komaba, Tomoki Yonezawa (*NARO AAC*)

1Pos180 **Revisiting a classical threading method with novel scoring function of sequence-structure compatibility**
Kyosuke Tomoda, Yota Masuyama, George Chikenji (*Grad. Sch. Eng., Nagoya Univ.*)

1Pos181 **ホモダイマー構造変化の網羅的解析**
Structural changes of homodimers in PDB
Ryotaro Koike, Takayuki Amemiya, Tatsuya Horii, Motonori Ota (*Grad. Sch. Info., Nagoya U.*)

1Pos182 **SLC 輸送体の構造および変異特性の統合解析のための情報基盤構築**
Platform for integrated computational analyses of structural property and mutation effect on SLC transporters
Akiko Higuchi[1], Kei Yura[2,3] ([1]*Grad. Sch. Fornt. Sci. , Univ. Tokyo*, [2]*Cent. Info. Bio., Ochanomizu Univ.*, [3]*Sch. Adv. Sci. Engr., Waseda Univ.*)

1Pos183 **Towards predicting functional consequences of genetic variants in humans through supramolecular complex structures**
Atsushi Hijikata[1], Toshiyuki Tsuji[1,2], Masafumi Shionyu[1], Tsuyoshi Shirai[1] ([1]*Nagahama Inst. Bio-Sci. Tech.*, [2]*Mita Intl. Sch.*)

1Pos184 **マルチカノニカル分子動力学法を用いた転写因子天然変性領域による DNA 結合制御メカニズムの検討**
Multicanonical molecular dynamics study of transcription factor-DNA binding regulation via the intrinsically disordered region
Kota Kasahara[1], Masaaki Shiina[2], Junichi Higo[3], Kazuhiro Ogata[2], Takuya Takahashi[1], Haruki Nakamura[3] ([1]*Col. Life Sci., Ritsumeikan Univ.*, [2]*Grad. Sch. Med., Yokohama City Univ.*, [3]*IPR, Osaka Univ.*)

非平衡・生体リズム / Nonequilibrium state & Biological rhythm

1Pos185 **生物表面に見られる曲面の機能：曲面による進行波の分裂**
Functions of living matter surfaces: Curvature-driven splitting of a traveling wave
Kazuya Horibe[1], Ken-ichi Hironaka[2], Katsuyoshi Matsushita[2], Koichi Fujimoto[2] ([1]*Grad. Sch. of Info Sci and Tech., Osaka U.*, [2]*Grad. Sch. of Sci., Osaka U.*)

1Pos186 **細胞外領域への伝導不均一性の導入による致死性不整脈の抑制**
Suppression of life-threatening cardiac arrhythmia by introducing inhomogeneity of electric conductivity in extracellular region
Kojiro Inoue (*Future Univ Hakodate*)

1Pos187 **多様な環境で生育するシアノバクテリア由来 KaiC ATPase の生化学的解析**
Biochemical characterization of KaiC ATPases from cyanobcateria living in various habitants
Atsushi Mukaiyama[1,2], Yoshihiko Furuike[1,2], Shuji Akiyama[1,2] ([1]*IMS*, [2]*SOKENDAI*)

1Pos188 **人工自走粒子から見る、集団運動の普遍性**
Universality of Collective Motion investigated in Artificial Systems
Junichiro Iwasawa[1], Daiki Nishiguchi[1,2], Masaki Sano[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*CEA, Saclay*)

1Pos189 **温度補償能を欠損した時計タンパク質 KaiC 変異体の同定**
Identification of Clock Protein KaiC Mutants Losing Temperature Compensation Ability
Yoshihiko Furuike[1,2], Atsushi Mukaiyama[1,2], Eiki Yamashita[3], Takao Kondo[4], Shuji Akiyama[1,2] ([1]*Research Center of Integrative Molecular Systems (CIMoS), Institute for Molecular Science (IMS)*, [2]*Department of Functional Molecular Science, SOKENDAI (The Graduate University for Advanced Studies)*, [3]*Institute for Protein Research, Osaka University*, [4]*Graduate School of Science, Nagoya University*)

1Pos190 **概日反応における時計蛋白質 KaiA のプロトマーの役割**
Functional roles of each protomer of homodimeric clock protein KaiA in circadian rhythm
Risa Imada[1], Shun Terauchi[1], Takahiro Iida[2], Hiroyuki Noji[3], Masahiro Ishiura[4], Kosuke Maki[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Faculty Sci., Fukuoka Univ.*, [3]*Grad. Sch. Eng., Univ of Tokyo*, [4]*Nagoya Univ*)

1Pos191 **C. elegans 集団が形作る動的ネットワーク構造**
Dynamical network structure in C. elegans group
Ken Nagai[1], Hiroshi Ito[2], Takuma Sugi[3] ([1]*JAIST*, [2]*Kyushu Univ.*, [3]*Shiga Univ. Med. Sci.*)

バイオイメージング / Bioimaging

1Pos192 **走査型イオンコンダクタンス顕微鏡を用いた神経細胞のナノスケールイメージング**
Nanoscale Neuron Topography Imaging using Scanning Ion Conductance Microscopy
Yasufumi Takahashi[1,2], Takafumi Miyamoto[1], Yuanshu Zhou[1], Takeshi Fukuma[1] ([1]*Kanazawa Univ.*, [2]*JST PREST*)

1Pos193 **アルギン酸細胞封入技術を使った細胞塊分取技術の検討**
A simple method for encapsulating single cells in alginate microspheres
Masao Odaka[1,2], Akihiro Hattori[1,2], Kenji Matsuura[1,2], Moe Iwamura[3], Yuki Yamanaka[3], Kento Iida[4], W.Davis Ronald[5], D.Crosby Laurel[5], Kenji Yasuda[1,2,3,4] ([1]*Org. Univ. Res. Initiatives, Waseda Univ.*, [2]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*, [3]*Dept. Pure & Appl. Phys., Grad. Schl. Adv. Sci. & Eng., Waseda Univ.*, [4]*Dept. Pure & Appl. Phys., Schl. Adv. Sci. & Eng., Waseda Univ.*, [5]*Stanford Genome Tech. Ctr., Stanford Univ.*)

1Pos194 **集束光による局所直接加熱技術を用いたゼラチン微細加工技術の開発**
Development of real time microfabrication technology of gelatin with focused photo-thermal etching
Kento Iida[1], Yuki Yamanaka[2], Moe Iwamura[2], Masao Odaka[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[3,4] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*WASEDA Biosci. Res. Ins. in Singapore(WABIOS)*)

1Pos195　集束光による局所直接加熱技術を用いたナノ粒子埋包アガロース微細加工技術の開発

Development of real time microfabrication technology of nano-particle suspended agarose microstructures with focused photo-thermal etching

Yuki Yamanaka[1], Kento Iida[2], Moe Iwamura[1], Masao Odaka[3,4], Kenji Matuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*)

1Pos196　軟 X 線ライブセルイメージングによるシアノバクテリアの細胞内元素濃度の可視化

Visualization of Intracellular Element Concentration in cyanobacteria with soft x-ray live cell imaging

Takahiro Teramoto[1], Chihiro Azai[2], Masashi Yoshimura[3], Kazuki Terauchi[2], Toshiaki Ohta[3] ([1]*Col. Sci & Eng, Ritsumeikan Univ.*, [2]*Col. Life Sci, Ritsumeikan Univ.*, [3]*SR Center, Ritsumeikan Univ.*)

1Pos197　Visualization of microvilli dynamics on living cell surface using high speed scanning ion-conductance microscopy

Hiroki Ida[1], Yasufumi Takahashi[2,3], Akichika Kumatani[1], Hitoshi Shiku[4], Tomokazu Matsue[1] ([1]*Grad. Sch. Env., Univ. Tohoku*, [2]*Div. Elec. Eng. and Com. Sci., Univ. Kanazawa*, [3]*PRESTO, JST*, [4]*Div. Eng., Univ. Tohoku*)

1Pos198　線虫 *C. elegans* 胚発生における細胞形状の自動抽出

An automated cell shape extraction in *C. elegans* embryogenesis

Yusuke Azuma, Shuichi Onami (*QBiC, RIKEN*)

1Pos199　新規誘電率顕微鏡(SE-ADM)による生きた培養細胞と CD44 膜タンパク質結合ビーズのナノスケール観察

Nanoscale imaging of living cells bound by nanobeads-connected anti-CD44 antibody in medium using newly developed dielectric microscopy

Tomoko Okada, **Toshihiko Ogura** (*National Institute of Advanced Industrial Science and Technology, Biomedical Research Institute*)

1Pos200　Two-dimensional crystals of tamavidin 2 for a quick and easy method of immobilization of biotinylated biomolecules

Daisuke Noshiro[1], Noriyuki Kodera[1], Toshio Ando[1,2] ([1]*Bio-AFM FRC, Inst. of Sci. & Eng., Kanazawa Univ.*, [2]*CREST, JST*)

1Pos201　高速 AFM 及び光ピンセット複合システム開発による一分子操作された分子の直接観察

Developing a Combined System of High-Speed AFM and Optical Tweezers for Direct Visualization of Single-Molecules under Manipulation

Motonori Imamura[1], Shin'nosuke Yamanaka[2], Toshio Ando[1] ([1]*Bio-AFM FRC, Kanazawa Univ.*, [2]*Grad. Sch. Sci., Kanazawa Univ.*)

1Pos202　ソフトウェア「閻魔」を用いた XFEL-CXDI 実験データの分類

Classification of XFEL-CXDI Imaging Experimental Data using the Software "EMMA"

Takashi Yoshidome[1], Yuki Sekiguchi[2,3], Yamamoto Takahiro[2,3], Oroguchi2 Tomotaka[2,3], Nakasako Masayoshi[2,3], Ikeguchi Mitsunori[4] ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*Fac. of Sci. and Tech., Keio Univ.*, [3]*RIKEN SPring-8 Center*, [4]*Grad. Sch. of Med. Life Sci. Yokohama City Univ.*)

1Pos203　低温コヒーレント X 線回折イメージング・トモグラフィー実験による分裂期原始紅藻シゾンの三次元構造解析

Three-dimensional structure of Cyanidioschyzon merolae by using coherent X-ray diffraction imaging tomography at cryogenic temperature

Amane Kobayashi[1,2], Yuki Takayama[3], Yuki Sekiguchi[1,2], Mao Oide[1,2], Asahi Fukuda[1,2], Takahiro Yamamoto[1,2], Koji Okajima[1,2], Tomotaka Oroguchi[1,2], Sachihiro Matsunaga[4], Yoshiki Kohmura[2], Masaki Yamamoto[2], **Masayoshi Nakasako**[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*, [3]*Schl. Sci. Univ. Hyogo*, [4]*Faclt. Sci. Tech. Tokyo Univ. Sci.*)

バイオエンジニアリング / Bioengineering

1Pos204　サイズ分画機能を備えた画像認識型セルソーターによる血中循環腫瘍細胞の測定

Monitoring of circulating tumor cell clusters in blood using size classifying imaging cell sorter

Moe Iwamura[1], Masao Odaka[3,4], Yuki Yamanaka[1], Kento Iida[2], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ*, [4]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*)

1Pos205　Direct observation and analysis of bacteria within giant liposomes

Masamune Morita, Naohiro Noda (*Biomed. Res. Inst., Natl. Inst. Adv. Ind. Sci. Tech. (AIST)*)

1Pos206　人工細胞での DNA 論理回路を用いた最小限の意識を生み出すオートマトン

Automata that generates minimum consciousness using DNA logic circuits in artificial cells

Hiroki Watanabe[1], Ryuji Kawano[2], Masahiro Takinoue[1] ([1]*Dept. Compt. Sci., Tokyo Tech*, [2]*Dept. Bio. Life Sci., Tokyo Univ. Agri. Tech.*)

1Pos207　カップ形状 AFM チップを用いた様々な基板に対する細胞接着強度の評価

Adhesion strengths of living cells for various substrates measured by using cup-shaped AFM chip

Hyonchol Kim[1,2], Kenta Ishibashi[2], Kosuke Matsuo[3], Atsushi Kira[3], Yui Onomura[1], Tomoko Okada[1], Chikashi Nakamura[1,2] ([1]*Biomed. Res. Inst., AIST*, [2]*Grad. Sch. Eng., Tokyo Univ. Agric. Technol.*, [3]*Japan Aviation Electronics Ind., Ltd.*)

1Pos208　Photo-regulation of Small GTPase Ras Using Photochromic Peptide

Masahiro Kuboyama[1], Nobuyuki Nishibe[1], Kazuo Fujiwara[1], Kazunori Kondo[1], Mitsuo Ikebe[2], Shinsaku Maruta[1] ([1]*Grad. Sch. Bioinfo., Soka Univ.*, [2]*The University of Texas Health Science Center at Tyler*)

1Pos209　DNA 分子ロボットのためのマイクロドロップレットの機械的安定性評価

Evaluation of mechanical stability of microdroplet-based DNA molecular robots

Misato Tsuchiya[1], Daisuke Ishikawa[1], Yuki Suzuki[2], Masayuki Endo[3], Masahiro Takinoue[1] ([1]*Dept. Comput. Sci., Tokyo Tech.*, [2]*Fronti. Res. Inst. Interdiscip. Sci., Tohoku Univ.*, [3]*WPI-iCeMS., Kyoto Univ.*)

1Pos210 バーコード様 DNA と生体ナノポアによる胆管癌特異的マイクロ RNA 発現パターンの認識
MicroRNA pattern recognition for cholangiocarcinoma using barcode-like DNA and biological nanopore
Moe Hiratani, Ryuji Kawano (*The Dep. of Biotech. and Life Sci., Tokyo Univ. of Agr. and Tech.*)

1Pos211 **Construction of steric cardiac tissue by three dimensional printer using gelatin-agarose mixed scaffold**
Naoki Tadokro, Ami Takasaki, Tomoyuki Kaneko (*Hosei Univ. FB LaRK*)

1Pos212 バクテリア走化性応答の解析に基づく水溶液識別法の構築
Construction of aqueous solution discrimination method based on analysis of bacterial chemotactic response
Hiroto Tanaka[1], Yasuaki Kazuta[1], Ikuro Kawagishi[2], Yoshiyuki Sowa[2], Yasushi Naruse[3], Yukihiro Tominari[1], Masato Okada[4], Kazuhiro Oiwa[1], Hiroaki Kojima[1] ([1]*Adv ICT Res Inst, NICT*, [2]*Housei Univ*, [3]*CiNet, NICT*, [4]*Tokyo Univ*)

1Pos213 固体試料における紫膜の積層ならびにバクテリオロドプシンの機能に対する固体化媒体の影響
Comparative study on purple membrane stacking and bacteriorhodopsin functionality in immobilized samples with various hydrogels
Shunsuke Yano[1], Hiakru Tanaka[1], Yasunori Yokoyama[1], Hiroshi Takahashi[2], Masashi Sonoyama[2], Takashi Kikukawa[3,4], Koshi Takenaka[1] ([1]*Grad. Sch. Eng., Nagoya Univ.*, [2]*Grad. Sch. Sci. & Tech., Gunma Univ.*, [3]*Grad. Sch. Life Sci., Hokkaido Univ.*, [4]*Gl-CoRE, Hokkaido Univ.*)

1Pos214 演題取り消し

その他 / Miscellaneous topics

1Pos215 シッフ塩基形成反応を利用したゴシポール配糖体の合成とその分子特性
Synthesis and properties of gossypol schiff-bases having two-glycoside appendages
Masaki Nakamura[1], Yoshitsugu Amano[1], Teruaki Hasegawa[2] ([1]*Grad. Sch. of Life Sci., Toyo Univ.*, [2]*Dept. of Life Sci., Toyo Univ.*, [3]*Bio-Nano Electronics Research Centre, Toyo Univ.*)

1Pos216 **Self-assembly of two-dimensional DNA origami lattices with designed geometries on lipid membranes**
Yuki Suzuki[1,2], Ibuki Kawamata[2], Satoshi Murata[2] ([1]*Fronti. Res. Inst. Interdiscrip. Sci., Tohoku Univ.*, [2]*Grad. Sch. Eng., Tohoku Univ.*)

1Pos217 **Development of a cell-sized molecular robot controlled by an external molecular signal**
Yusuke Sato[1], Yuki Suzuki[2], Ibuki Kawamata[1], Satoshi Murata[1], Yuichi Hiratsuka[3], Ken Komiya[4], Masayuki Endo[5], Shin-ichiro M. Nomura[1] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*FRIS, Tohoku Univ.*, [3]*Sch. Mat. Sci., JAIST*, [4]*Sch. Comp., Tokyo Tech.*, [5]*iCeMS*)

1Pos218 フォトクロミック分子の光刺激による二酸化硫黄発生の反応機構
Reaction mechanism on sulfur dioxide generation by photoexcitation of a photochromic molecule
Satoshi Yokojima[1], Ryuhei Kodama[2], Kimio Sumaru[3], Shinichiro Nakamura[4], Kingo Uchida[2] ([1]*Tokyo University of Pharmacy and Life Sciences*, [2]*Ryukoku University*, [3]*AIST*, [4]*RIKEN*)

第2 日目（9 月20 日（水））／Day 2（Sep. 20 Wed.）全学教育棟 2 階 C201, C202, D201, D202, D203; 全学教育棟 3 階 D301, D302, D303 ／ Room C201, C202, D201, D202, D203, General Education Bldg. 2F; D301, D302, D303, General Education Bldg. 3F

蛋白質：構造 / Protein: Structure

2Pos001 自由エネルギー変分原理に基づく check point kinase1 阻害剤系における相対的結合自由エネルギー予測
Prediction of relative binding free energy based on a free energy variational principal for the Check point kinase1-inhibitor system
Daichi Kondo, Takeshi Ashida, Takeshi Kikuchi (*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*)

2Pos002 **Property of sequences analysis of beta-Trefoil protins with irregular structures on their folding**
Risako Kimura, Takeshi Kikuchi (*Depat. of Bioinf Col. Life Sci Ritsumeikan Univ*)

2Pos003 **Estimation of relative binding free energy for the CDK2 protein-ligand system**
Takayuki Kawano, Takeshi Ashida, Takeshi Kikuchi (*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*)

2Pos004 P53 タンパク質四量体化ドメインへの残基間平均距離統計に基づくコンタクトマップによる天然変性領域の予測法の応用
Application of the prediction technique of IDRs to tetramerization domain of p53 protein
Takumi Shimomura, Takeshi Kikuchi (*Dept. of Bioinf., Col. of Life Sci., Ritsumeikan Univ.*)

2Pos005 紅色光合成細菌由来の電子伝達複合体の共結晶化
Co-crystallization of a bacterial photosynthetic electron-transfer complex
T. Kawakami[1], T. Liang[1], K. Okazaki[1], Y. Kimura[2], S. Otomo[1] ([1]*Ibaraki Univ.*, [2]*Grad. Sch. Agri. Sci., Kobe Univ.*)

2Pos006 新規抗体断片 Fv-clasp を用いたラミニン受容体インテグリン α6β1 の結晶化と構造決定
Crystallization and structure determination of laminin-binding integrin α6β1 aided by the use of Fv-clasp technology
Takao Arimori, Junichi Takagi (*IPR, Osaka Univ.*)

2Pos007 MM/3D ー RISM 法を用いた水・エタノール混合溶液中での HP-β-シクロデキストリンによるフルアステロン包摂反応の結合自由エネルギー予測
Binding free energy calculation of fluasterone and HPβCD in cosolvent by MM / 3D-RISM method
Kazuma Kondo[1], Masatake Sugita[1], Takeshi Kikuchi[1], Humio Hirata[2] ([1]*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*, [2]*Toyota Phys. & Chem. Res. Inst.*)

2Pos008 **Barrier-to-autointegration factor の変異による構造変化解析**
Structural change analysis by mutation of Barrier-to-autointegration factor
Chiaki Yamaguchi[1], Masatake Sugita[1], Toshiya Hayano[2], Takeshi Kikuchi[1] ([1]*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*, [2]*Dept. of Biomed., Col. Life Sci., Ritsumeikan Univ.*)

2Pos009 **自由エネルギー変分原理を用いたタンパク - リガンド間相対的結合自由エネルギー計算の DHFR-TMP 系への応用**
Calculation of relative binding free energy between DHFR-TMP system on the basis of free energy variational principle
Naoto Nishimura, Takeshi Kikuchi (*Dept. of Bioinf. Col. of Life Sci. , Ritsumeikan Univ*)

2Pos010 **ビタミンＤ受容体リガンド結合ドメインのアポ体及びアンタゴニスト複合体の溶液構造解析**
Apo- and antagonist-binding structures of vitamin D receptor ligand-binding domain elucidated by SAXS experiments and MD simulations
Yasuaki Anami[1], Nobutaka Shimizu[2], **Toru Ekimoto**[3], Daichi Egawa[1], Toshimasa Itoh[1], Mitsunori Ikeguchi[3], Keiko Yamamoto[1] ([1]*Showa Pharmaceutical Univ.*, [2]*KEK PF*, [3]*Yokohama City Univ.*)

2Pos011 **Crystallization of Hepatitis B virus Core Protein in genotype C**
Katsumi Omagari, Yasuhito Tanaka (*Dept. of Virology, Medical School, Nagoya City University*)

2Pos012 **MM/3D-RISM 法を用いた HP-b-CD と HP-g-CD によるコレステロールの結合様式と結合自由エネルギーの予測**
Estimation of the binding free energy for inclusion processes of cholesterol by HP-b-CD and HP-g-CD using MM/3D-RISM method
Yuji Hayashino[1], Masatake Sugita[1], Tetsumi Irie[2], Fumio Hirata[3], Takeshi Kikuchi[1] ([1]*Dept. of Bioinfo., Col. Life Sci., Ritsumeikan Univ*, [2]*Dept. of Clin. Chem. Inf., Kumamoto Univ*, [3]*Toyota Phys. Chem. Res. Inst.*)

2Pos013 **バクテリオロドプシンの高分解能Ｘ線結晶構造解析**
Crystallographic analysis of bacteriorhodopsin at high resolution
Nagayuki Hasegawa, Hideyuki Jonotsuka, Kazuki Takeda, Kunio Miki (*Grad. Sch. Sci., Kyoto Univ.*)

2Pos014 **常磁性効果を用いた溶液 NMR 法による蛋白質の立体構造解析**
Protein structural refinement using paramagnetic effects in solution NMR
Mayu Okada[1], Teppei Ikeya[1], Rajesh Sundaresan[1], Eri Nojiri[1], Tsutomu Mikawa[2], Yutaka Ito[1] ([1]*Grad. Sch. of Sci. & Eng., Tokyo Met. Univ.*, [2]*RIKEN, QBiC*)

2Pos015 **小さな膜タンパク質 KcsA のクライオ電子顕微鏡法による構造解析の取り組み**
An Approach to Structural Analysis of a Small Membrane Protein KcsA by Cryo-electron Microscopy
Hiroko Takazaki[1,2], Hirofumi Shimizu[3], Naoko Kajimura[4], Kaoru Mitsuoka[2,4], Takuo Yasunaga[1,2] ([1]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*, [2]*Abis*, [3]*Fac. Med. Sci., Univ. Fukui*, [4]*Research Center for Uhvem, Univ. Osaka*)

2Pos016 **X 線結晶構造解析を目指した精製二量体 VSOP の特性に関する研究**
Studies of characteristics the purified dimeric VSOP for X-ray crystallography
Satoko Mochida[1], Yusuke Goto[1], Akima Yamamoto[1], Satomi Shibumura[1], Yasushi Okamura[4,5], Atsushi Nakagawa[1,5], Kohei Takeshita[1,2,3] ([1]*IPR, Osaka Univ.*, [2]*JST, PRESTO*, [3]*IAI, Osaka Univ.*, [4]*Grad. Sch. of Med., Osaka Univ.*, [5]*JST, CREST*)

2Pos017 **β-シート中の隣接した strand 上の Cys-Cys ペアは好まれる**
Cys-Cys pairs on the strands arranged adjacently are preferred in β-sheets
Hiromi Suzuki (*Sch. Agri., Meiji Univ.*)

2Pos018 **クライオ電子顕微鏡によるグルタミン酸脱水素酵素ドメイン運動の研究**
Cryo-electron microscopy study toward detecting domain motion of glutamate dehydrogenase
Mao Oide[1,2], Takayuki Kato[3], Tomotaka Oroguchi[1,2], Keiichi Namba[3,4], Masayoshi Nakasako[1,2] ([1]*Grad. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*, [3]*Grad. Sch. of Front. Biosci., Osaka Univ.*, [4]*RIKEN, QBiC*)

2Pos019 **Implementation of Fragment Molecular Orbital Replica-Exchange method (FMO-REM) in GAMESS-US simulation package**
Shingo Ito[1], Stephan Irle[2], Yuko Okamoto[1] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*Oak Ridge National Laboratory*)

2Pos020 **分子動力学シミュレーションによる抗 HIV 中和抗体 PG16 の CDR-H3 の変異における中和能への影響の解析**
Molecular dynamics study of mutation effects on the neutralizing ability in CDR-H3 of an anti-HIV antibody PG16
Ryo Kiribayashi[1], Hiroko X. Kondo[1], Daisuke Kuroda[2,3], Toru Saito[1], Jiro Kohda[1], Akimitsu Kugimiya[1], Yasuhisa Nakano[1], Kouhei Tsumoto[2,3], Yu Takano[1] ([1]*Grad. Sch. Info. Sci., Hiroshima City Univ.*, [2]*Grad. Sch. Eng., Univ. Tokyo*, [3]*Ins. Med., Univ. Tokyo*)

2Pos021 **The Free Energy Profile for Dissociation of Ligand from Zn2+ Ion of CA I Activesite**
Arwansyah Muhammad Saleh, Isman Kurniawan, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Sch. of Nat. Sci. and Tech. Kanazawa University*)

蛋白質：構造機能相関 / Protein: Structure & Function

2Pos022 **タンパク質の基準振動モードのネットワーク解析：中心性指標 betweenness とアロステリック機構**
Network analysis of normal modes of proteins: betweenness centrality and allosteric behavior
Hiroshi Wako[1], Shigeru Endo[2] ([1]*Sch. of Soc. Sci., Waseda Univ.*, [2]*Sch. of Sci., Kitasato Univ.*)

2Pos023 **ガス圧 NMR 法を用いた酸素結合部位の解析：Outer Surface protein A**
Analysis of O2-binding sites in proteins using gas-pressure NMR spectroscopy: outer surface protein A
Takahiro Kawamura[2], Takuro Wakamoto[2], Soichiro Kitazawa[1], Shun Sakuraba[3], Tomoshi Kameda[4], **Ryo Kitahara**[1] ([1]*Coll. Pharm. Sci., Ritsumeikan Univ.*, [2]*Grad. Sch. Life. Sci.*, [3]*Grad. Sch. Frontier Sci., Univ. Tokyo*, [4]*AIST*)

2Pos024 **Conformational dynamics of Human Protein Kinase CK2α and its effect on function and inhibition**
Ashutosh Srivastava[1], Tsuyoshi Hirota[1,2], Stephan Irle[1], Florence Tama[1,3,4] ([1]*Inst. of Transformative Bio-Molecules, Nagoya University*, [2]*PRESTO, JST, Nagoya Univ., Nagoya*, [3]*Dept. Phys., Sch. Sci., Nagoya Univ., Nagoya*, [4]*Adv. Inst. Comp. Sci, RIKEN*)

2Pos025 **生体系の結合標準自由エネルギー計算の新しい手続き**
A new calculation workflow for the standard free energy of binding in biomolecular system
Yoshiaki Tanida, Azuma Matsuura (*Fujitsu Laboratories Ltd.*)

2Pos026 **差分距離行列によるタンパク質構造変化の研究**
Difference Distance Matrix enhanced molecular dynamics study on protein
Yasushige Yonezawa (*IAT, Kindai*)

2Pos027 **B 細胞抑制性因子 CD72 の分子表面電荷分布によるリガンド結合制御機構**
Charge distribution regulates the ligand-binding affinity of B cell inhibitory receptor CD72
Nobutaka Numoto[1], Chizuru Akatsu[2], Kenro Shinagawa[1], Takeshi Tsubata[2], Nobutoshi Ito[1] ([1]*Dept. Struct. Biol., Med. Res. Inst., Tokyo Med. & Dent. Univ.*, [2]*Dept. Immunol., Med. Res. Inst., Tokyo Med. Dent. Univ.*)

2Pos028 **EGF 受容体 C-末端天然変性ドメインの１分子 FRET 計測**
Single-molecule FRET measurement of the intrinsically disordered C-tail domain of the epidermal growth factor receptor
Kenji Okamoto, Yasushi Sako (*RIKEN*)

2Pos029 **ヘテロ３量体 G 蛋白質相互作用因子 Gip1 の網羅的アラニンスキャン変異解析**
Comprehensive alanine scanning analysis of heterotrimeric G protein interacting partner Gip1
Hiroyasu Koteishi[1], Takero Miyagawa[2], Yoichiro Kamimura[1], Yukihiro Miyanaga[2], Masahiro Ueda[1,2] ([1]*RIKEN, QBiC*, [2]*Fron. Biosci., Osaka Univ.*)

2Pos030 **クモ糸タンパク質ナノファイバーの自己集合**
Self-assembly of nanofibers from spider silk fibroin
Yugo Hayashi[1], Tomoaki Murakami[1], Mai Arakawa[1], Keito Yoshida[1], Yoichi Yamazaki[1], Takehiro K. Sato[2], Hironari Kamikubo[1] ([1]*Grad. Sch. Mat. Sci. Nara Inst. Sci. Tech.*, [2]*Spiber Inc.*)

2Pos031 **抗体 G2 は異なる 3 つの配列を強く特異的に認識する**
A three-in-one monoclonal antibody G2 recognizes completely different epitope sequences with high affinity
Md. Nuruddin Mahmud[1], Masayuki Oda[2], Daiki Usui[2], Yasuo Inoshima[1,3], Naotaka Ishiguro[1,3], **Yuji O. Kamatari**[4] ([1]*United Grad. Sch. of Vet. Sci., Gifu Univ.*, [2]*Grad. Sch. of Life and Environ. Sci., Kyoto Pref. Univ.*, [3]*Fac. of Appl. Bio. Sci., Gifu Univ.*, [4]*Life Sci. Res. Ctr., Gifu Univ.*)

2Pos032 **二次構造に基づいた蛋白・蛋白相互作用面の階層的分類**
Hierarchical classification of protein-protein interfaces based on their secondary structures
Takashi Fujii, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. of Bioinformatics. Soka Univ.*)

2Pos033 **Gip1 は Gγ の脂質修飾部位を疎水性空隙で覆うことで三量体 G 蛋白質を細胞基質に隔離する**
Gip1 sequesters heterotrimeric G proteins in the cytosol by masking their lipid-modification site with the hydrophobic cavity
Takero Miyagawa[1], Yoichiro Kamimura[2], Hiroyasu Koteishi[2], Kohei Takeshita[3], Atsushi Nakagawa[3], Masahiro Ueda[1,2] ([1]*Grad. Sch. Front. Biosci., Osaka Univ.*, [2]*QBiC, RIKEN*, [3]*IPR, Osaka Univ.*)

2Pos034 **Framework for computational protein science written in functional language Scala**
Itaru Onishi, **Masayuki Irisa** (*Comp. Sci. and Sys. Eng., Kyushu Inst. of Tech.*)

2Pos035 **ファミリー 4 ウラシル DNA グリコシラーゼ–DNA 複合体の結晶構造解析**
Crystal structure of family 4 uracil-DNA glycosylase in complex with DNA
Akito Kawai[1], Teruya Nakamura[2], Kazumi Shimono[1], Yuriko Yamagata[3], Shuichi Miyamoto[1] ([1]*Fac. of Pharmaceut. Sci., Sojo Univ.*, [2]*Priority Organization for Innovation and Excellence, Kumamoto Univ.*, [3]*Grad. Sch. of Pharm. Sci., Kumamoto Univ.*)

2Pos036 **細胞内アクチンの分子構造に対するミオシン阻害剤の効果**
Effect of myosin inhibitor on the atomic structure of actin in cells
Shiori Nishinaka[1], Q.P. Taro Uyeda[2], Q.P. Taro Noguchi[1] ([1]*National Institute of Technology, Miyakonojo College*, [2]*Waseda University*)

蛋白質：物性 / Protein: Property

2Pos037 **ヒトフェリチン L 鎖の解離と変性に関する研究**
A study on dissociation and unfolding of recombinant human ferritin L chain
Tomoki Yamamoto[1], Daisuke Sato[2], Kazuo Fujiwara[2], Masamichi Ikeguchi[1,2] ([1]*Grad. Sch. Bioinfo., Univ. Soka*, [2]*Fac. Sci. and Eng., Univ. Soka*)

2Pos038 **新規 NMR 法を用いた ALS 関連タンパク質 SOD1 の線維形成メカニズムの解明**
Elucidation of fibrillization mechanism of ALS-related protein SOD1 using novel NMR spectroscopy
Naoto Iwakawa[1], Daichi Morimoto[1], Erik Walinda[2], Kenji Sugase[1], Masahiro Shirakawa[1] ([1]*Grad. Sch. Eng., Kyoto Univ.*, [2]*Grad. Sch. Med., Kyoto Univ.*)

2Pos039 **Measurement of microtubule persistence length with sub-pixel resolution revealed its dependency on the growth rate**
Naoto Isozaki[1], Kazuki Ukita[1], Hirofumi Shintaku[1], Hidetoshi Kotera[1], Taviare L. Hawkins[2], Jennifer L. Ross[3], Ryuji Yokokawa[1] ([1]*Dept. Micro Eng., Grad. Sch. Eng., Kyoto Univ.*, [2]*Dept. Phys., UW-La Crosse*, [3]*Dept. Phys., UMass Amherst*)

2Pos040 **アルカリ条件下におけるカロテノイドと古細菌脂質の結合に伴うハロロドプシンの熱安定化**
Thermal stabilization of Halorhodopsin by binding carotenoid and archaeal lipids under alkaline condition
Kenichi Takeda[1], Takashi Kikukawa[2], Makoto Demura[2], Takanori Sasaki[1] ([1]*Grad. Sch. Adv. Math. Sci., Meiji Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

2Pos041 **酵素処理が LDL の物性に与える影響**
Effect of enzymes treatment on physical properties of low-density lipoprotein
Seiji Takeda[1], Agus Subagyo[2], Shu-Ping Hui[1], Hirotoshi Fuda[1], Kazuhisa Sueoka[2], Hitoshi Chiba[1] ([1]*Faculty of Health Sci, Hokkaido Univ.*, [2]*Grad Sch of Inf Sci and Tech, Hokkaido Univ.*)

2Pos042 **一価陽イオン溶液におけるリゾチームの回転及び並進拡散運動に基づくビリアル係数**
The virial coefficients based on the rotational and translational diffusions of lysozyme in the monovalent cation solutions
Yudai Katsuki[1], Akane Kato[1], Etsuko Nishimoto[2] ([1]*Grad. Sch. Bioresour. Bioenviron. Sci., Kyushu Univ.* , [2]*Fac. Agr., Kyushu Univ.*)

2Pos043 **時間分割スペクトルによるヒト血清アルブミンの Trp214 残基周辺の水和状態に対する 1 価陽イオンの影響の解析**
Effect of monovalent cation on the hydration state near Trp214 of human serum albumin revealed by the time-resolved fluorescence spectrum
Shoutaro Kubo[1], Etsuko Nishimoto[2] ([1]*Grad. Sch. Bioresour. Bioenviron. Sci., Kyushu Univ.* , [2]*Fac. Agr., Kyushu Univ.*)

2Pos044 ***Archaeoglobus fulgidus* ferritin assembly studied by time-resolved small-angle X-ray scattering**
Daisuke Sato[1], Yuta Okada[2], Boyce Hong Ping Law[3], Ambrish Kumar[3], Sierin Lim[3], Masamichi Ikeguchi[1,2] ([1]*Fac. Sci. and Eng., Soka Univ.*, [2]*Dept. Bioinfo., Gra. Sch. Eng., Soka Univ.*, [3]*Sch. Chem. and Biomed. Eng., Nanyang Tech. Univ., Singapore*)

2Pos045 **キチン結合タンパク質(CBP21)の構造安定性に対する銅イオンの効果**
Effects of copper ions on the structural stability of chitin-binding protein 21
Hayuki Sugimoto[1], Erina Katagiri[1], Akiyoshi Tanaka[2], Takeshi Watanabe[1], Kazushi Suzuki[1] ([1]*Fac. Agri., Niigata Univ.*, [2]*Grad. Sch. Bioresources, Mie Univ.*)

2Pos046 **競争的凝集形成機構に基づいた蛋白質異常凝集の理解**
Understanding of aberrant protein aggregation based on the competitive aggregation mechanism
Masayuki Adachi, Masatomo So, Yuji Goto (*Inst. Protein Res., Osaka Univ.*)

2Pos047 **時間分割蛍光測定による生体防御タンパク質 momorcharin のアンフォールディング/リフォールディング中間体に関する研究**
The time-resolved fluorescence studies on the unfolding and refolding intermediate state of defense-related protein, momorcharins
Chie Matsunaga[1], Etsuko Nishimoto[2] ([1]*Grad. Sch. Bioresour. Bioenviron. Sci., Kyushu Univ.* , [2]*Fac. Agr., Kyushu Univ.*)

2Pos048 **ストップトフロー過渡回折格子法のタンパク質変性反応への適用**
Application of stopped-flow TG method to denaturation dynamics of a photosensory protein
Shunki Takaramoto, Yusuke Nakasone, Masahide Terazima (*Dep. Chem., Sch. Sci., Kyoto Univ.*)

蛋白質：機能 / Protein: Function

2Pos049 **テトラヒメナ外腕ダイニンにおける変異導入システムの確立と α 重鎖 P ループの機能**
Establishment of a mutation system in *Tetrahymena* outer arm dynein and P-loop functions of the alpha heavy chain (Dyh3p)
Masaki Edamatsu (*Dept. Life Sci., Grad. Sch. Arts Sci., Univ. Tokyo*)

2Pos050 **Identification of residues in SecM that are responsible for stabilizing the translation arrest**
Mikihisa Muta, Ryo Iizuka, Takashi Funatu (*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*)

2Pos051 **TnaC 翻訳アレスト中のリボソームにおける解離因子の作用**
Action of release factors on the stalled ribosome during translation of TnaC
Tomoki Shinozawa, Ryo Iizuka, Zhuohao Yang, Takashi Funatsu (*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*)

2Pos052 **A single-molecule kinetic analysis of ATP hydrolysis and substrate degradation by the 26S proteasome**
Akira Sato, Takahiro Saito, Takashi Okuno (*Grad. Sch. Sci., Univ. Yamagata*)

2Pos053 **大腸菌で生産される *Pyrovaculum islandicum* 由来グルタミン酸脱水素酵素の活性に対する FK506 結合タンパク質の影響**
Effect of FK506 binding protein in the activity of glutamate dehydrogenase from *Pyrovaculum islandicum* produced in *Escherichia coli*
Shuichiro Goda, Junpei Yagi, Hideaki Unno, Tomomitsu Hatakeyama (*Grad. Sch. of Eng., Nagasaki Univ.*)

2Pos054 **[NiFe]ヒドロゲナーゼの活性準備状態 Ni-SI$_r$ と活性状態 Ni-SI$_a$ 間の酸塩基平衡機構の解明**
Elucidation of the acid-base equilibrium mechanism between the ready Ni-SI$_r$ and active Ni-SI$_a$ states of [NiFe] hydrogenase
Hulin Tai[1,2], Liyang Xu[1], Koji Nishikawa[3], Yoshiki Higuchi[2,3], Shun Hirota[1,2] ([1]*Grad. Sch. Mater. Sci., NAIST*, [2]*CREST, JST*, [3]*Grad. Sch. Life Sci., Univ. Hyogo*)

2Pos055 **Zymoseptoria tritici 真菌チューブリンは異常な特性を有する**
***Zymoseptoria tritici* fungal tubulin has unusual properties**
Douglas Drummond[1], Naomi Sheppard[2], Robert Cross[2] ([1]*Kyushu Univ.*, [2]*Univ. of Warwick, UK*)

2Pos056 **Spectroscopic studies of hydrogen sensing [FeFe] hydrogenase from *Thermotoga maritima***
Nipa Chongdar[1], Krzysztof Pawlak[1], James A. Birrell[1], Wolfgang Lubitz[1], **Hideaki Ogata**[1,2] ([1]*MPI CEC*, [2]*ILTS Hokkaido Univ.*)

2Pos057 **線虫 Cytochrome b_{561} ホモログ・Cecytb-2 の分子機能解明**
Elucidation of the molecular function of *Caenorhabditis elegans* Cecytb-2, a cytochrome b_{561} homologue
Mika Fujimura, Masahiro Miura, Tetsunari Kimura, Motonari Tsubaki (*Dept. of Chem., Grad. Sch. Sci., Kobe Univ.*)

2Pos058 **Theoretical study on light-activation mechanism of LOV photoreceptor protein**
Masahiko Taguchi, Cheng Cheng, Chika Higashimura, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

2Pos059 **複数のアミロイド性ペプチドの混在する複雑な系におけるアミロイド線維形成機構**
Amyloid Fibrillation in Promiscuous Systems Containing Various Amyloidgenic Peptides
Hiroya Muta[1], Masatomo So[1], Kazumasa Sakurai[2], Yuji Goto[1] ([1]*IPR, Osaka Univ.*, [2]*Inst. of Advan. Tech., Kindai Univ.*)

蛋白質：計測・解析 / Protein: Measurement & Analysis

2Pos060 **機械学習を用いたシミュレーションと実験の統合によるタンパク質ダイナミクス解析**
Linking single-molecule experiment and simulation of protein dynamics by machine learning
Yasuhiro Matsunaga[1,2], Yuji Sugita[1,3,4] ([1]*RIKEN AICS*, [2]*JST PRESTO*, [3]*RIKEN TMS*, [4]*RIKEN QBiC*)

2Pos061 **ヒドロゲナーゼ/シトクローム c_3 間電子移動における静電相互作用の役割**
Role of the electrostatic interactions in the electron transfer from [NiFe] hydrogenase to cytochrome c_3
Yu Sugimoto[1], Yoshitaka Moriwaki[1], Thoru Terada[1], Kenji Kano[2], Kentaro Shimizu[1] ([1]*Grad. Sch. of Agri. and Life Sci. Univ. of Tokyo*, [2]*Grad. Sch. of Agri. Kyoto Univ*)

2Pos062 **X 線 1 分子追跡法による TRPV1 チャネルの分子運動解析**
3D MOTION MAPS OF TRPV1 CATION CHANNEL DEPICTED BY DIFFRACTED X-RAY TRACKING METHOD
Kazuhiro Mio[1], Keigo Ikezaki[2], Masahiro Kuramochi[2], Hiroshi Sekiguchi[3], Tai Kubo[1], Yuji C. Sasaki[2] ([1]*OPERANDO-OIL, AIST*, [2]*Frontier Science, Univ. of Tokyo*, [3]*JASRI*)

2Pos063 **高次構造に特異的な人工タンパク質を用いた抗体医薬品の品質評価モニタリング**
Quality control monitoring of therapeutic antibodies based on an artificial protein specific for higher order structures of IgG
Hideki Watanabe[1], Seiki Yageta[1,2], Hiroshi Imamura[1], Shinya Honda[1,2] ([1]*BMRI, AIST*, [2]*Grad. Sch. of Frontier Sci., The Univ. of Tokyo*)

2Pos064 **チオフラビン T とアミロイドβ凝集体の結合：蛍光寿命測定による解析**
Thioflavin T binding to amyloid-beta peptide aggregates: Analyses with fluorescence lifetime measurements
Akinori Oda, Hiroshi Satozono, Tomomi Shinke (*Hamamatsu Photonics K. K.*)

2Pos065 **タンパク質間相互作用観測を目指した蛍光相関分光装置の開発**
Development of Fluorescence Correlation Spectrometer for the Elucidation of Protein Interactions
Asami Izaki[1,2], Hiroyuki Oikawa[1,2], Takeshi Tomita[3], Satoshi Takahashi[1,2] ([1]*IMRAM, Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*, [3]*Dept. Pharmacol., Tokyo Women's Medical Univ.*)

2Pos066 **Influence of the PYP domain on Photoreaction of the phytochrome domain in Ppr**
Jia Siang Sum, Yoichi Yamazaki, Yugo Hayashi, Hironari Kamikubo (*Grad. Sch. of Mater. Sci., NAIST*)

2Pos067 **分子動力学シミュレーションによるβシート凝集の自由エネルギー解析**
Free energy analysis of β-sheet aggregation by molecular dynamics simulation
Keiichi Masutani, Kang Kim, Nobuyuki Matubayasi (*Graduate School of Engineering Science, Osaka University*)

2Pos068 **赤色蛍光タンパク質, Akane families (*Scleronephthya gracillima*) の緑と赤の蛍光は海域によらない共通特性**
Common properties of red fluorescent protein Akane families having green and red emissions irrespective of ocean areas
Yuko Kato[1,2], Ikki Fujimoto[2], Yukimitsu Imahara[3], Mitsuru Jimbo[4], Kei Amada[2], Toshio Yamaguchi[1], Shu Nakachi[3] ([1]*Univ. Fukuoka*, [2]*Fukuoka Inst. Tech.*, [3]*Kuroshio Bio Research*, [4]*Univ. Kitasato*)

2Pos069 **PF-AR NW12A における顕微分光装置の開発**
The development of spectroscopic system for UV-visible absorption at PF-AR NW12A
Masahide Hikita[1], Yusuke Yamada[1], Masahiko Hiraki[2], Naohiro Matsugaki[1], Toshiya Senda[1] ([1]*PF/SBRC, IMSS, KEK*, [2]*Mechanical Engineering Center, Applied Research Laboratory, KEK*)

蛋白質工学 / Protein: Engineering

2Pos070 **理想タンパク質の安定性のオリジンを探る**
Stability for de novo designed ideal proteins revisited
Mami Yamamoto[1,2], Rie Koga[1], Takahiro Kosugi[1,2], Nobuyasu Koga[1,2,3] ([1]*IMS, CIMoS*, [2]*SOKENDAI*, [3]*JST, PRESTO*)

2Pos071 **エングレイルドホメオドメインを用いた新たな転写因子の設計**
Designing a new artificial transcription factor based on engrailed homeodomain
Tomoko Sunami, Hidetoshi Kono (*QST*)

2Pos072 **タンパク質へのワンポット飽和変異導入におけるヌクレオチドとアミノ酸のバイアス**
Bias in nucleotides and amino acids in one-pot saturation mutagenesis of protein
Akasit Visootsat[1], Fumihiro Kawai[2], Akihiko Nakamura[2,3], **Ryota Iino**[1,2,3] ([1]*IMS, NINS*, [2]*OIIB, NINS*, [3]*SOKENDAI*)

2Pos073 **天然に存在しないフォールドを持つタンパク質の合理的デザイン**
Rational design of new fold proteins yet-unexploited in nature
Shintaro Minami[1], Rie Koga[1], George Chikenji[2], Nobuyasu Koga[1,3] ([1]*CIMoS, IMS*, [2]*Grad. Sch. of Eng., Nagoya Univ.*, [3]*PRESTO, JST*)

2Pos074 **多様な all-α タンパク質のデザイン**
Design of diverse all-α proteins
Koya Sakuma[1,2], Rie Koga[2], Takahiro Kosugi[1,2], Nobuyasu Koga[1,2,3] ([1]*SOKENDAI*, [2]*CIMoS, IMS*, [3]*JST, PRESTO*)

2Pos075 **水酸化酵素 PHBH の没食子酸産生変異体の構築とその理論的考察**
Modification of *p*-Hydroxybenzoate to produce gallic acid and its theoretical insight
Yoshitaka Moriwaki[1], Tohru Terada[2], Kentaro Shimizu[1] ([1]*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [2]*Agri. Bioinfo. Res. Unit, Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

2Pos076 **可逆的光架橋プローブを用いた翻訳の制御**
Photo-control of the ribosome movement along mRNA using a reversible photo-crosslinking probe
Shunsuke Yamashiro[1], Ryo Iizuka[2], Takashi Funatsu[2] ([1]*Dept. of Pharm., Fac. of Pharm. Sci., The Univ. of Tokyo*, [2]*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*)

2Pos077 **カルモジュリン融合・共発現系を用いた抗菌ペプチド fowlicidin 大量生産法**
Mass production of fowlicidin, a cathelicidin antimicrobial peptide by a calmodulin-peptide fusion and coexpression system
Koki Onuma[1], Hiroaki Ishida[2], Takasumi Kato[1], Takashi Tsukamoto[1,3], Takashi Kikukawa[1,3], Makoto Demura[1,3], Hans J. Vogel[2], Tomoyasu Aizawa[1,3] ([1]*Grad. Sci. Life Sci, Hokkaido Univ.*, [2]*Biochem. Res. Grp., Dep. of Biol. Sci., Univ. of Calgary*, [3]*GI-CoRE, Hokkaido Univ.*)

2Pos078 **Some factors that make a structure of a beta-sheet protein more designable**
Hayao Imakawa[1], Nobuyasu Koga[2], George Chikenji[1] ([1]*Dept. of App. Phys., Nagoya Univ.*, [2]*CIMoS, IMS*)

核酸結合蛋白質 / Nucleic acid binding proteins

2Pos079 **転写因子 NF-kB の核内クラスター形成の観察**
Analysis of NF-kB clusters formation in the cell nucleus
Takhiko Inaba[1], Yu Miyamoto[2], Kazunari Iwamoto[2], Hisaaki Shinohara[3], Mariko Okada[2], Yasushi Sako[1] ([1]*RIKEN, Cellular Informatics Laboratory*, [2]*Inst. Protein Research, Osaka U.*, [3]*RIKEN, Yokohama*)

2Pos080 **ヌクレオソーム動態解析を指向した化学合成ヒストンタンパク質**
Chemically synthesized histone proteins for analysis of nucleosome dynamics
Gosuke Hayashi[1], Takuma Sueoka[1], Akimitsu Okamoto[1,2] ([1]*Dept. Chem. and Biotech., Univ. of Tokyo*, [2]*RCAST, Univ. of Tokyo*)

2Pos081 **大腸菌非六量体型 DNA ヘリカーゼ UvrD 変異体の多量体形成の 1 分子イメージング**
Single-molecule imaging of the oligomeric form of the non-hexameric *Escherichia coli* helicase UvrD mutants
Hiroaki Yokota (*Grad. Sch. Creation Photon Indust.*)

2Pos082 **Structural change of ALS-liked mutant of TDP-43**
Akira Kitamura, Sachiko Yuno, Ai Shibasaki, Fusako Gan, Makoto Oura, Johtaro Yamamoto, Masataka Kinjo (*Laboratory of Molecular Cell Dynamics, Faculty of Advanced Life Science, Hokkaido University*)

2Pos083 **Sequence Dependent Spontaneous Nucleosome Slidings Revealed by Molecular Dynamics Simulation**
Toru Niina, Giovanni Brandani, Cheng Tan, Shoji Takada (*Grad. Sch. Sci., Kyoto Univ.*)

2Pos084 **Real-time observation of flexible domain movements in Cas9**
Saki Osuka, **Kazushi Isomura**, Shohei Kajimoto, Tomotaka Komori, Hiroshi Nishimasu, Tomohiro Shima, Osamu Nureki, Sotaro Uemura (*Grad. Sch. Sci, Univ. Tokyo*)

核酸：構造・物性 / Nucleic acid: Structure & Property

2Pos085 **2 つのヌクレオソームの配向多様性は H4 tail により生成しうる。**
The diversity in the orientation of two nucleosomes is potentially produced by H4 tails
Hisashi Ishida, Hidetoshi Kono (*QST, Molecular Modeling and Simulation*)

2Pos086 **Model building of overlapping dinucleosome from SAXS and SANS data**
Atsushi Matsumoto[1], Hidetoshi Kono[1], Rintaro Inoue[2], Masaaki Sugiyama[2], Daiki Kato[3], Yasuhiro Arimura[3], Hitoshi Kurumizaka[3] ([1]*QST*, [2]*Kyoto Univ.*, [3]*Waseda Univ.*)

2Pos087 **マイクロ液滴界面上での相分離による人工細胞核の形成の DNA ユニット依存性の解析**
Analyses of DNA unit dependence of artificial cell nuclei formed by phase separation on microdroplet interface
Yu Kasahara, Risa Watanabe, Masahiro Takinoue (*Tokyo Institute of Technology/School of Computing/Computer Science*)

2Pos088 **マイクロ液滴界面を利用した RNA 転写可能な人工細胞核の構築**
Construction of artificial cell nuclei with RNA transcription capability using a microdroplet interface
Risa Watanabe[1], Masamune Morita[1,2], Miho Yanagisawa[3], Masahiro Takinoue[1] ([1]*Dept. Comput. Sci., Tokyo Tech.*, [2]*Biomedical Res. Inst., AIST*, [3]*Dept. Appl. Phys., Tokyo Univ. Agri. Tech.*)

2Pos089 **TIRF 顕微鏡を用いた良溶媒中の直鎖／環状 DNA の形状揺らぎの長時間観察と相関時間の計測**
Long-time observations of linear/circular DNA in a good solvent by TIRF to measure a correlation time of configuration fluctuations
Takafumi Iwaki, Masato Tanigawa (*Fac. Med., Oita Univ.*)

2Pos090 **クラスター凝集モデルに基づく球面上の DNA マイクロ構造体形成の数値シミュレーション**
Numerical simulations of DNA fractal microstructure formation on spherical surface based on cluster-cluster aggregation
Tetsuro Sakamoto, Risa Watanabe, Masamune Morita, Takinoue Masahiro (*Department of Computer Science, Tokyo Institute of Technology*)

2Pos091 **二次構造予測から三次構造予測へ：検証と分子動力学シミュレーションを用いた応用**
From secondary structure prediction to three dimensional structure prediction: the validation and application using MD simulation
Tomoshi Kameda (*AIRC, AIST*)

核酸：相互作用・複合体形成 / Nucleic acid: Interaction & Complex formation

2Pos092 **シスプラチンとトランスプラチンによる DNA の高次構造と機能への影響の比較研究**
The effect of cisplatin and transplatin on the higher order structure and function of DNA
Toshifumi Kishimoto[1], Yuko Yoshikawa[2], Kenichi Yoshikawa[1] ([1]*Fac. Life Med. Sci., Univ. Doshisha*, [2]*Nano. Bio., Univ. Doshisha*)

2Pos093 **Structure and function of DNA in the presence of linear-chain polyamines with a valency from 2+ to 5+**
Hiroko Tanaka[1], Ai Kanemura[1], Yuko Yoshikawa[2], Naoki Umezawa[3], Takahiro Kenmotsu[1], Kenichi Yoshikawa[1] ([1]*Fac. Life Med. Sci., Univ. Doshisha.*, [2]*Nano. Bio., Univ. Doshisha.*, [3]*Grad. Sch. Phar Sci., Univ. Nagoya City.*)

2Pos094 **金属イオンがグロビュール状 DNA-ヒストン凝集体の大きさに与える影響**
Effects of metal ions on the size of globular DNA-histone aggregates
Kyoji Natsume, Yoshifumi Amamoto, Yuichi Masubuchi, Tetsuya Yamamoto (*Grad. Sch. Eng., Univ. Nagoya*)

2Pos095 **直鎖・分岐ポリアミン存在下での DNA 高次構造の特異性と温度依存的な変化**
Temperature-dependent structural changes of large DNA in the presence of linear- and blanched-chain polyamines
Takashi Nishio[1], Kenichi Yoshikawa[1], Yuko Yoshikawa[1], Naoki Umezawa[2] ([1]*Lab. Biol. Phys., Facul. Life Med. Sci., Doshisha Univ.*, [2]*Pharmaceutical. Sci., Nagoya City Univ.*)

2Pos096 **How a small change in ligand functional groups affects the dynamics of an aminoglycoside riboswitch?**
Marta Kulik[1,2], Takaharu Mori[1], Yuji Sugita[1], Joanna Trylska[2] ([1]*RIKEN*, [2]*Univ. of Warsaw, Poland*)

2Pos097 **トリヌクレオソーム構造のリンカー DNA の長さ依存性**
Tri-nucleosome folding dependent on the linker DNA length
Hiroo Kenzaki[1], Shoji Takada[2] ([1]*ACCC, RIKEN*, [2]*Grad. Sch. Sci., Univ. Kyoto*)

2Pos098 **Protective effect of PEG against DNA double-strand breaks caused by photo irradiation**
Moe Usui, Yuko Yoshikawa, Kenichi Yoshikawa (*Grad. Sch. Life and Medical Sciences, Doshisha Univ*)

2Pos099 **塩基配列非特異的に誘起された長鎖 DNA の折り畳みにおよぼす共存イオンの効果**
The Effects of Ions on the Folding of Giant ds DNA Chains Induced by Nonspecific Interaction with Poly-cations and Proteins
Tatsuo Akitaya[1], Toshio Kanbe[2], Anatoly Zinchenko[3], Shizuaki Murata[3], Makoto Demura[4], Kenichi Yoshikawa[5] ([1]*Asahikawa Medical Univ.*, [2]*Nagoya Univ.*, [3]*Nagoya Univ.*, [4]*Hokkaido Univ.*, [5]*Doshisha Univ.*)

2Pos100 **Pt(II)化合物の DNA 高次構造に対する影響のその場計測：レーザー・マニピュレーション**
Evaluation of the effect of dinuclear Pt(II) complexes on DNA conformation through laser manipulation
Yusuke Kashiwagi[1], Masatoshi Ichikawa[2], Seiji Komeda[3], Koichiro Sadakane[1], Yuko Yoshikawa[1], Kenichi Yoshikawa[1] ([1]*Grad. Sch. Life and Medical Sciences, Doshisha Univ.*, [2]*Grad. Sch. Physics, Kyoto Univ.*, [3]*Fac. Pharm. Sch. Suzuka Univ Med Sci*)

2Pos101 **Reverse mapping to reconstruct atomistic structures from coarse-grained models for DNA-protein complexes**
Masahiro Shimizu, Shoji Takada (*Grad. Sch. Sci., Kyoto Univ.*)

2Pos102 **Reconstitution system of Siwi- and Vasa-coupled piRNA biogenesis**
Tomotaka Komori, Ryo Murakami, Tomohiro Shima, Mikiko Siomi, Sotaro Uemura (*Univ. of Tokyo*)

分子遺伝学・遺伝子発現 / Molecular genetics & Gene expression

2Pos103 **人工細胞デバイスを用いた T7 プロモーター配列の進化分子工学手法の開発**
Directed evolution of T7 promoter sequence with artificial cell reactor device
Tomoya Nishimura[1], Yi Zhang[1,2], Hiroshi Ueno[1], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*JAMSTEC*)

2Pos104 **人工細胞デバイス内における無細胞タンパク質発現ノイズの解析**
Gene expression noise of cell-free system in artificial cell reactors
Shiori Fujimoto[1], Yi Zhang[1,2], Hiroshi Ueno[1], Kazuhito Tabata[1], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*JAMSTEC*)

分子モーター / Molecular motor

2Pos105 **Protein-peptide dissociation at high pressure studied by parallel cascade selection molecular dynamics simulations**
Hiroaki Hata[1], Yasutaka Nishihara[1], Masayoshi Nishiyama[2], Ikuro Kawagishi[3], Akio Kitao[1] ([1]*IMCB, UTokyo*, [2]*The Hakubi Center, Kyoto Univ.*, [3]*Dept. of Frontier Biosci., Hosei Univ.*)

2Pos106 **Rng2 がアクチンフィラメントとミオシン間の協同的結合に与える影響の解析**
Analysis of influence of Rng2 on cooperative binding between myosin and F-actin
Taiga Imai[1], Masak Takaine[2], Kentaro Nakano[2], Osamu Numata[2], Taro Uyeda[3], Kiyotaka Tokuraku[1] ([1]*Muroran Institute of Technology*, [2]*University of Tsukuba*, [3]*Waseda University*)

2Pos107 **Minicell tethered assay that enables simultaneous observation of a flagellar motor rotation and the incorporation of stators to the motor**
Takao Nakajima, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Biosci., Osaka Univ.*)

2Pos108 **Repetitive buckling of microtubules driven by dynein arms reconstituted on singlet microtubules**
Misaki Shiraga[2], Jyunya Kirima[2], Kazuhiro Ooiwa[1,2] ([1]*NICT*, [2]*Grad. Sch. Sci., Univ. Hyogo*)

2Pos109 **係留されたキネシン頭部の微小管への結合解離の直接観察**
Direct observation of the binding and unbinding motions of the tethered kinesin head to microtubule
Kohei Matsuzaki[1], Michio Tomishige[2] ([1]*Dept. Appl. Phys., Grad. Sch. Eng., Univ. Tokyo*, [2]*Dept. Math. Phys., Col. Sci. Eng., Aoyama Univ.*)

2Pos110 **温度適性に着目した、糸状菌由来のキネシンの特性**

Properties of kinesins from filamentous fungi focused on the thermal aptitude

Youske Shimizu, Toru Togawa, Shigeru Chaen (*Col. Humanities and Sciences, Nihon Univ.*)

2Pos111 **Conformational change in azimuth and tilting angles of F_1-ATPase revealed with defocused orientation imaging**

Kazuki Gotoh[1], Shoko Fujimura[2], Takayuki Nishizaka[1] ([1]*Dept. Phys., Gakushuin Univ.*, [2]*Sch. of Med, Keio Univ.*)

2Pos112 **Morelloflavone による有糸分裂キネシン Eg5 の阻害効果の生化学的解析**

Biochemical analysis on the effect of morelloflavone as a novel inhibitor of mitotic kinesin Eg5

Kenichi Taii[1], Tomisin Happy Ogunwa[3], Shuya Yano[1], Kei Sadakane[2], Shinsaku Maruta[2,4], Takayuki Miyanishi[3] ([1]*Soka University, Faculty of Science and Engineering, Department of Bioinformatics Engineering*, [2]*Soka University Graduate School, School of Engineering, Major of Bioinformatics Engineering*, [3]*Nagasaki University, School of Fisheries and Environmental Sciences*, [4]*Soka University, Faculty of Science and Engineering, Department of Symbiotic Creation Science and Engineering*)

2Pos113 **Modification of V_1 rotary molecular motor of *Thermus thermophilus***

Aiko Endo[1], Naho Mitani[2], Jun-ichi Kishikawa[2], Ken Yokoyama[2] ([1]*Grad. Sch. Biochem., Kyoto Sangyo Univ.*, [2]*Dept. Mol. Biosci., Kyoto Sangyo Univ.*)

2Pos114 **DNA オリガミ-ミオシン II モーター混合システムの高速原子間力顕微鏡観察**

High-speed AFM imaging of DNA origami-myosin II motor hybrid system

Masashi Ohmachi[1], Hiroki Fukunaga[2], Keisuke Fujita[1], Keigo Ikezaki[3], Toshio Yanagida[1,2], Mitsuhiro Iwaki[1,2] ([1]*QBiC, RIKEN*, [2]*Grad. Sch. Front. Biosci., Osaka Univ.*, [3]*Grad. Sch. Sci., Univ. Tokyo*)

2Pos115 **新規フォトクロミック阻害剤であるスピロピラン誘導体を利用した有糸分裂キネシン Eg5 の光制御**

Photoregulation of mitotic kinesin Eg5 using a novel photochromic inhibitor composed of spiropyran

Kei Sadakane[1], Kenichi Taii[2], **Shinsaku Maruta**[1] ([1]*Dept. of Bioinfo. Grad. Sch. Engin. Soka Univ.*, [2]*Dept. of Sci. & Engin. Soka Univ.*)

2Pos116 **High speed AFM imaging of structural changes in actin filaments bound tropomyosin-troponin in presence of myosin S1 and ATP**

Kien Xuan Ngo[1,2], Taro QP Uyeda[1], Noriyuki Kodera[3] ([1]*Department of Physics, Faculty of Science and Engineering, Waseda University, Tokyo, Japan*, [2]*Brain Science Institute, RIKEN, Wako, Japan*, [3]*Department of Physics and Bio-AFM Frontier Research Center, Kanazawa University, Kanazawa, Japan*)

2Pos117 **Development of simultaneous observation system for flagellar components and motor rotation with external load by electrorotation**

Kenta Morishima, Akihiko Ishijima, **Hajime Fukuoka** (*Grad. Sch. Frontier Biosci., Osaka Univ.*)

2Pos118 **Can we make KIF5 faster?**

Taketoshi Kambara[1], Yasushi Okada[1,2] ([1]*RIKEN, QBiC*, [2]*Univ. of Tokyo, Grad. Sch. of Sci.*)

2Pos119 **生体分子モーターと光応答性 DNA を用いた分子輸送技術の構築**

Construction of a nano-transportation system by using a biomolecular motor and photoresponsive DNA

Kentaro Kayano[1], Ryuhei Suzuki[1], Arif Md. Rashedul Kabir[2], Kazuki Sada[1,2], Akinori Kuzuya[3], Hiroyuki Asanuma[4], Akira Kakugo[1,2] ([1]*Graduate School of Chemical Sciences and Engineering, Hokkaido University*, [2]*Faculty of Science, Hokkaido University*, [3]*Faculty of Science, Kansai University*, [4]*Graduate School of Science, Nagoya University*)

細胞生物学 / Cell biology

2Pos120 **細菌べん毛 III 型分泌装置の精製と再構成**

Purification and reconstitution of the flagellar type III protein export apparatus

Hiroyuki Terashima[1,2], Katsumi Imada[2] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Grad. Sch. Sci., Osaka Univ.*)

2Pos121 **LAT 小胞はマスト細胞の中で自己完結型信号伝達場として働く：1 分子観察による解明**

The LAT vesicle works as a self-contained signaling platform in mast cells; discovery by single molecule tracking

Koichiro M. Hirosawa[1,2], Nao Hiramoto-Yamaki[2], Kenta J. Yoshida[2], Shohei Nozaki[3], Taka A. Tsunoyama[4], Bo Tang[5], Kenichi G.N. Suzuki[1], Kazuhisa Nakayama[3], Takahiro Fujiwara[2], Akihiro Kusumi[4] ([1]*G-CHAIN, Gifu Univ.*, [2]*iCeMS, Kyoto Univ.*, [3]*Grad. Sch. Pharma., Kyoto Univ.*, [4]*OIST*, [5]*Wuhan Univ.*)

2Pos122 **Detection of the activity in receptor cluster by single cell FRET and motor rotation in Escherichia coli cell**

Yu Mitoro (*Grad. Sch. Biosci., Univ. Osaka*)

2Pos123 **β-arrestin independent mechanism is involved in the temporal trapping of diffusing GPCR on cell surface**

Rinshi Kasai[1], Asuka Inoue[2], Takahiro Fujiwara[3], Akihiro Kusumi[4] ([1]*Inst. Front. Life Med. Sci., Kyoto Univ.*, [2]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [3]*KUIAS-iCeMS, Kyoto Univ.*, [4]*OIST*)

2Pos124 **Rotation assay of the proton-driven bacterial flagellar motor under near zero load**

Yuta Hanaizumi[1], Shuichi Nakamura[1,2], Yusuke V. Morimoto[2,3], Tohru Minamino[2], Keiichi Namba[2,4] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [3]*Kyushu Institute of Technology*, [4]*QBiC, RIKEN*)

2Pos125 **原子間力顕微鏡によるマウス顎下腺上皮組織のレオロジー測定**

Rheological properties of epithelium in mouse submandibular gland measured by atomic force microscopy

Kenta Sugimoto[1], Hiroaki Taketa[2], Takuya Matsumoto[2], Takaharu Okajima[1] ([1]*Grad. Schl. Inform. Sci. and Technol., Hokkaido Univ.*, [2]*Dept. of Biomat Okayama Univ.*)

2Pos126 **Flagella-associated protein in Chlamydomonas flagella, FAP85 is one of the microtubule inner proteins (MIPs)**

Junya Kirima[1], Hiroaki Kojima[2], Kazuhiro Oiwa[1,2] ([1]*Grad. Sch. of Life Sci., Univ. of Hyogo*, [2]*Adv. ICT Res. Inst., NICT*)

2Pos127 **細菌べん毛モーターの固定子組み込みとトルク発生におけるプロトン透過の関わり**
Implication of proton translocation for stator assembly and torque generation in the bacterial flagellar motor
Yuya Suzuki[1], Kodai Oono[1], Fumio Hayashi[2], Yusuke V. Morimoto[3], Seishi Kudo[1], Kenji Oosawa[4], Shuichi Nakamura[1] ([1]*Grad. Sch. Eng.*, [2]*Center for Inst. Anal., Gunma Univ.*, [3]*Grad. Sch. Computer Sci. & System Eng. Kyushu Inst. of Tech*, [4]*Div. Mol. Sci., Fac. Sci. and Tech.*)

2Pos128 **アクチン繊維の集団運動により形成される構造は繊維の物理的性質によって決まる**
The characterization of size and filament distances of band patterns of moving actin filaments
Hirotaka Taomori[1], Yuuji Setoguchi[1], Kentaro Ozawa[1], Itsuki Kunita[2], Shigeru Sakurazawa[3], Hajime Honda[1] ([1]*Dept. Bioeng., Nagaoka Univ. Tech.*, [2]*Univ. Ryukyus*, [3]*Future Univ. Hakodate*)

2Pos129 ***Bacillus alcalophilus* 由来べん毛固定子蛋白質の MotS のペリプラズムフラグメントの構造**
Structural of a periplasmic fragment of MotS, a flagellar stator protein of *Bacillus alcalophilus*
Koki Nishiuchi[1], Mami Yamamoto[2], Masahiro Ito[2], Katsumi Imada[1] ([1]*Grad. Sch of Sci., Osaka Univ*, [2]*Faculty of Life Sciences, Toyo Univ*)

2Pos130 **細胞内温度への微小管の寄与の検討**
Investigating the contribution of microtubules on intracellular temperature variation
Takashi Yanagi[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Phemac. Sci., Univ. Tokyo*, [2]*JST, PRESTO*)

2Pos131 **Polarized ArfA activation directs PTEN to posterior plasma membrane for eukaryotic cell migration**
Takuma Degawa[1], Satomi Matsuoka[2], Masahiro Ueda[1,2,3] ([1]*Dep. Biol. Grad. Sch. of Sci. Osaka Univ.*, [2]*RIKEN QBiC*, [3]*Grad. Sch. of Front. Bio Sci. Osaka Univ.*)

2Pos132 **ネスチンと緑茶カテキン(-)エピガロカテキンガレートの細胞弾性への効果**
Effect of nestin and (-)-epigallocatechin gallate on cell elasticity
Moe Susaki[2], Ayana Yamagishi[1,2], Keisuke Iida[3], Hyonchol Kim[1,2], **Chikashi Nakamura**[1,2] ([1]*AIST*, [2]*TUAT*, [3]*Chiba Univ.*)

2Pos133 **ビブリオ菌極べん毛数と位置へ影響する FlhF の精製とその GTPase 活性検出**
Purification of FlhF to detect the GTPase activity effecting on the number and location of the polar flagellum of *Vibrio alginolyticus*
Shota Kondo, Michio Homma, Seiji Kojima (*Grad. Sch. of Sci., Nagoya Univ.*)

2Pos134 **ERK, Akt の多重可視化よる細胞周期制御機構の定量的な解析**
Quantitative analysis of cell-cycle control mechanisms by multiplexed imaging of ERK and Akt activity
Gembu Maryu[1,3], Michiyuki Matsuda[1,2], Kazuhiro Aoki[3] ([1]*Lab. Bioimaging Cell Signal., Grad. Sch. Biostudies, Kyoto Univ.*, [2]*Dept. Pathol. Biol. Dis, Grad. Sch. Med., Kyoto Univ.*, [3]*Div. Qant. Biol., Nat. Inst. Basic Biol.*)

2Pos135 **運動性シアノバクテリアの双方向性運動の解析**
Analysis of bidirectional motion of motile cyanobacteria
Takashi Kosaki, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

2Pos136 **繊維状インフルエンザウイルスの運動様式**
Motility of filamentous influenza virus
Tatsuya Sakai, Mineki Saito (*Department of Microbiology, Kawasaki Medical School*)

2Pos137 **外腕ダイニン中間鎖の点突然変異によるクラミドモナス鞭毛運動性の低下**
A novel *Chlamydomonas* mutant harboring a point mutation in an intermediate chain gene of outer-arm dynein displays lowered motility
Tomoka Ogawa[1], Emiri Kanno[2], Yusuke Kondo[1], Masafumi Hirono[3], Takako Kato-Minoura[2], Ritsu Kamiya[2], **Toshiki Yagi**[1] ([1]*Dept. Life Sci., Pref. Univ. Hiroshima*, [2]*Dept. Biol. Sci., Fac. Sci. & Eng., Chuo Univ.*, [3]*Dept. of Biosci., Hosei Univ.*)

2Pos138 **システイン変異導入によるべん毛モーター固定子タンパク質 PomA のペリプラズムループ領域の解析**
Characterization of periplasmic loop regions of PomA, a stator protein of flagellar motor, using cysteine mutagenesis
Hiroto Iwatsuki, Hiroyuki Terashima, Seiji Kojima, Michio Homma (*Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

2Pos139 **分散培養心筋細胞と心臓組織片の拍動同期**
Synchronization of beating between dispersed culture of cardiomyocytes and cardiac tissue slice
Chiho Nihei, Tomoyuki Kaneko (*LaRC, Grad. Sch. Sci. & Eng., Hosei Univ.*)

2Pos140 **シュードモナス属細菌の運動性およびべん毛回転測定**
Measurements of motility and flagellar rotation in Pseudomonas species
Taro Hariu[1], Takuto Tensaka[1], Naoya Terahara[2], Seishi Kudo[1], Shuichi Nakamura[1,2] ([1]*Grad. Sch. Applied Phys., Tohoku Univ.*, [2]*Grad. Sch. of Frontier Biosc., Osaka Univ.*)

化学受容 / Chemoreception

2Pos141 **Guanylate Cyclase mediates chemotaxis by transducing high-frequency signals for pseudopod formation**
Yuki Tanabe[1,3,4], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. Sci., Univ. Osaka*, [2]*Grad. Sch. Frontier Biosci., Univ. Osaka*, [3]*QBiC, RIKEN*, [4]*JSPS*)

2Pos142 **受容体の細胞膜上空間分布解析**
Spatial distribution analysis of membrane receptors
Hiroaki Takagi[1], Yukihiro Miyanaga[2], Michio Hiroshima[3], Yasushi Sako[4], Masahiro Ueda[2,3] ([1]*Sch. Med., Nara Med. Univ.*, [2]*Grad. Sch. Front. Biosci., Osaka Univ.*, [3]*QBiC, RIKEN*, [4]*RIKEN*)

2Pos143 **大腸菌温度感覚レセプター Tar-Tap キメラ体の温度受容能**
Thermosensing abilities of Tar-Tap chimeric receptors of *Escherichia coli*
So-ichiro Nishiyama[1,2], Takashi Sagawa[3], Hana Sato[4], Hiroaki Kojima[3], Kazuhiro Oiwa[3,4], Ikuro Kawagishi[1,2] ([1]*Dept. Frontier Biosci., Hosei Univ.*, [2]*Res. Cen. Micro-Nano Tech., Hosei Univ.*, [3]*Adv. ICT Res. Inst., NICT*, [4]*Grad. Sch. Life Sci., Univ. Hyogo*)

光生物：視覚・光受容 / Photobiology: Vision & Photoreception

2Pos144 **脊椎動物の光受容タンパク質 Opn5 の分子特性の多様化とその変換**
Comparison and conversion of diversified molecular properties in vertebrates Opn5 group
Yukimi Nishio[1], Takahiro Yamashita[1], Keita Sato[2], Yasushi Imamoto[1], Hideyo Ohuchi[2], Yoshinori Shichida[1] ([1]*Grad. Scl. of Sci., Kyoto Univ.*, [2]*Okayama Univ. Grad. Sch. of Med.*)

2Pos145 **Rc-PYP の光依存的複合体種の形成機構**
Light dependent multiple complex formation of Rc-PYP
Yoichi Yamazaki[1], Yohei Shibata[1], Yugo Hayashi[1], Nathumi Endo[1], Kentaro Ishii[2], Susumu Uchiyama[2,3], Takayuki Uchihashi[4], Hironari Kamikubo[1] ([1]*Grad. Sch. Ms, NAIST*, [2]*Okazaki Inst. Integrative Bioscience, NINS*, [3]*Grad. Sch. Eng., Osaka Univ.*, [4]*Grad. Sch. Sci., Nagoya Univ.*)

2Pos146 **Light-Driven Cl^- Transport Mechanism of *Nonlabens marinus* Rhodopsin-3 Studied by Static and Time-Resolved Spectroscopy**
Takashi Tsukamoto[1,2], Susumu Yoshizawa[3], Takashi Kikukawa[1,2], Makoto Demura[1,2] ([1]*Fac. Adv. Life Sci., Hokkaido Univ.*, [2]*Glob. Sta. for Soft Matt., GI-CoRE, Hokkaido Univ.*, [3]*AORI, The Univ. of Tokyo*)

2Pos147 **The photochemical properties of archaerhodopsin and its mutants found in *Halorubrum* sp. ejinoor**
Xiong Geng[1], Luomeng Chao[2], Gang Dai[3], Takashi Kikukawa[4], Tatsuo Iwasa[5] ([1]*Adv. Production Syst. Eng., Muroran Ins. Technol., Japan*, [2]*Anim. Sci. Technol., Inner Mongolia Nationalities Univ., China*, [3]*Coll. Chem. Environ. Sci., Inner Mongolia Normal Univ., China*, [4]*Grad. Sch. Life. Sci., Hokkaido Univ., Japan*, [5]*Div. Eng. Composite Funct., Muroran Ins. Technol., Japan*)

2Pos148 **桿体・錐体外節膜における脂質組成の解析**
Analysis on lipid compositions in outer segment membranes of rod and cone photoreceptor cells
Kyoko Kadomatsu[1], Keiji Seno[2], Yuki Ito[3], Satoru Kawamura[3], Shuji Tachibanaki[3] ([1]*Faculty of Science, Osaka University*, [2]*Department of Biology, Faculty of Medicine, Hamamatsu University School of Medicine*, [3]*Grad. Sch. of Frontier Biosci., Osaka University*)

2Pos149 **脊椎動物の視物質とピノプシンの熱活性化効率の比較解析**
Comparison of thermal activation rates between vertebrate visual pigments and pinopsin
Takahiro Yamashita[1], Keita Sato[2], Keiichi Kojima[1], Kazumi Sakai[1], Yuki Matsutani[1], Masataka Yanagawa[3], Yumiko Yamano[4], Akimori Wada[4], Naoyuki Iwabe[1], Hideyo Ohuchi[2], Yoshinori Shichida[1] ([1]*Grad. Sch. Sci., Kyoto Univ.*, [2]*Okayama Univ. Grad. Sch. Med. Dent. & Pharmaceut. Sci.*, [3]*RIKEN*, [4]*Kobe Pharmaceut. Univ.*)

2Pos150 **光駆動ナトリウムポンプ KR2 の多量体形成に重要なアミノ酸残基**
Aromatic amino acids of a light-driven sodium pump KR2 are important to form an oligomer
Rei Abe-Yoshizumi[1], Shota Ito[1], Kento Ikeda[2], Mikihiro Shibata[3,4], Keiichi Inoue[1,5], Takayuki Uchihashi[6], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*Grad. Sch. Phys., Kanazawa Univ.*, [3]*InFiniti., Kanazawa Univ.*, [4]*Bio-AFM FRC*, [5]*JST PRESTO*, [6]*Dept. Phys., Nagoya Univ.*)

2Pos151 **紫外共鳴ラマン分光法によるオレンジカロテノイドタンパク質の光活性化機構**
Evidence for close-to-open photoactivation of orange carotenoid protein from ultraviolet resonance Raman spectroscopy
Yushi Nakamizo[1], Momoka Nagamine[2], Tomotsumi Fuzisawa[1], Cheryl Kerfeld[3], Masashi Unno[4] ([1]*Advanced Technology Fusion, Saga University*, [2]*Faculty of Science and Engineering, Department of Chemistry and Applied Chemistry, Saga University*, [3]*Michigan Sate University*, [4]*Department of Chemistry and Applied Chemistry, Saga University*)

2Pos152 **霊長類青感受性視物質の極大吸収波長における内部結合水の役割**
The role of internal water molecules in λ_{max} of primate blue-sensitive visual pigment
Kota Katayama[1], Yuki Nonaka[1], Kei Tsutsui[2], Hiroo Imai[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Primate Res. Inst., Kyoto Univ.*)

2Pos153 **Na^+ポンプ型ロドプシンの Na^+輸送過程の解析**
Analysis of Na^+ transfer reactions of Na^+-pumping rhodopsin
Keisuke Murabe[1], Takashi Kikukawa[1,2], Takashi Tsukamoto[1,2], Tomoyasu Aizawa[1,2], Naoki Kamo[1], Makoto Demura[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ*, [2]*GSS, GI-CoRE, Hokkaido Univ*)

2Pos154 ***Gloeobacter* rhodopsin の多量体構造における機能的役割の解明**
Functional importance of trimer formation of light-driven H^+pump*Gloeobacter* rhodopsin
Azusa Iizuka[1], Takashi Kikukawa[1,2], Kousuke Kajimoto[3], Tomoki Fujisawa[3], Takashi Tsukamoto[1,2], Tmoyasu Aizawa[1,2], Naoki Kamo[1], Masashi Unno[3], Makoto Demura[1,2] ([1]*Glad. Sch. Life Sci., Hokkaido Univ*, [2]*GSS, GI-CoRE, Hokkaido Univ.*, [3]*Grad. Sch. Sci. Eng., Saga Univ.*)

生態／環境 / Ecology & Environment

2Pos155 **Challenge for direct observation of bacterial growth and death in long-term starvation**
Sotaro Takano[1,2], Ryo Miyazaki[2] ([1]*Life and Env. Sci., Univ. of Tsukuba*, [2]*AIST, Bioprod. Inst.*)

2Pos156 **運動性シアノバクテリアのコロニー形成による増殖活性の解析**
Analysis of proliferation rate depending on colonial morphologies in motile cyanobacteria, Pseudanabaena sp
Keita Mizoe, Atsuko Takamatsu, Taku Kimura (*Waseda University*)

2Pos157 **微生物生態系における種の共存と代謝ネットワーク**
Metabolic network enables to live together in microbial ecosystems
Kenshi Suzuki[1], Masahiro Honjyo[2], Tomoka Nishimura[3], Yosuke Tashiro[2], Hiroyuki Futamata[1,2,4] ([1]*Grad. Sch. Sci. and Technol., Shizuoka Univ.*, [2]*Grad. Sch. Integ. Sci. and Technol., Sizuoka Univ.*, [3]*Dept. Appl. Chem. and Biochem. Eng., Shizuoka Univ.*, [4]*Res. Ins. Green Sci. and Technol., Shizuoka Univ.*)

数理生物学 / Mathematical biology

2Pos158 フグ種別鑑別システムのためのフグ模様再現モデルの構築
Skin patterns replicate model of puffer fish for the crossbreed puffer fish identification system
Takeshi Ishida, Daiki Tadokoro (*National Fisheries University*)

2Pos159 NMDA 受容体を介した Ca2+上昇による情報伝達の小体積効果
Small-Volume Effect of Information Transmission by NMDA receptor-mediated Ca2+ increase
Takehiro Tottori[1], Masashi Fujii[2], Shinya Kuroda[2] ([1]*Fac. Sci., Univ. Tokyo*, [2]*Grad. Sch. Sci., Univ. Tokyo*)

2Pos160 **A Modified Sequence-Dependent Coarse-Grained Elastic-Network Model for DNA**
Yan Zhao, Akinori Awazu, Hiraku Nishimori (*Grad. Sch. Sci., Univ. Hiroshima*)

2Pos161 **A stochastic simulation study on the mechanism of correlation between circadian oscillation and ATPase activity of KaiC hexamer**
Sumita Das[1], Shota Hashimoto[1], Tomoki P. Terada[1,2], Masaki Sasai[1,2] ([1]*Department of Computational Science and Engineering, Nagoya University*, [2]*Department of Applied Physics, Nagoya University*)

2Pos162 **Extraction of statistical dynamics of a stochastic neuronal model**
Takanobu Yamanobe (*Sch. Med., Hokkaido Univ.*)

2Pos163 DNA 損傷認識タンパク質による核内哨戒効率の理論的考察
Theoretical study of nuclear patrol efficiency by DNA damage recognition protein
Takamasa Yamamoto, Hiraku Nishimori, Akinori Awazu (*Dept. Math and Life Sci. Hiroshima Univ.*)

2Pos164 核膜変形と核内流体を考慮した分裂酵母減数分裂期染色体のモデル
Model of fission yeast meiotic chromosome considering nuclear envelope deformation and intranuclear hydrodynamics
Kazutaka Takao, Hiraku Nishimori, Akinori Awazu (*Dept. Math and Life Sci., Hiroshima Univ.*)

2Pos165 **Understanding the Selection Effect through Lineage-Removal Operations**
Shunpei Yamauchi, Yuichi Wakamoto (*Graduate School of Arts and Sciences, The University of Tokyo*)

2Pos166 ヌクレオソーム排他的 DNA 配列のインスレーター機能の解析
Analysis of insulator function of nucleosome exclusive DNA sequence
Yuki Matsushima, Hiraku Nishimori, Akinori Awazu (*Dept. Math and Life Sciences, Grad. Sch. of Sci., Hiroshima Univ.*)

2Pos167 **Theoretical study of YAP-dependent actomyosin network contribution to morphogenesis under gravity**
Kazunori Takamiya, Seirin Ri, Hiraku Nishimori, Akinori Awazu (*Hiroshima University Graduate Graduate School of Science Department of Mathematical and Life Sciences*)

計測 / Measurements

2Pos168 緑色光が及ぼす水素化アモルファスシリコン薄膜上のアミノ酸含有ゲルの電圧電流特性への効果
Green light effect on voltage current property of amino acid containing hydrogel on hydrogenated amorphous silicon film
Makoto Horigane[1], **Kouki Kagawa**[1], Mahoko Sano[1], Honoka Endo[1], Hiroshi Masumoto[2], Takashi Goto[3], Yutaka Tsujiuchi[1] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary*, [3]*Institute for Materials Research, Tohoku University*)

2Pos169 オンチップ 1 細胞計測系によるマクロファージの貪食試料の最適化
Optimization of antigen of macrophage phagocytosis using on-chip single cell measurement assay
Yuya Furumoto[1], Yoshiki Nakata[2], Masao Odaka[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*Waseda Biosci. Res. Ins. in Singapore (WABIOS)*)

2Pos170 強制拍動刺激周期の変化に応答した心筋細胞集団の細胞外電位変化
Adaptation of field potential duration in cardiomyocyte clusters under forced electrical stimulation intervals
Natsuki Seki[1], Naoki Takahashi[2], Masao Odaka[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*Waseda Biosci. Res. Ins. in Singapore (WABIOS)*)

2Pos171 オンチップ 1 細胞計測系によるマクロファージの同一点連続貪食の応答解析
Analysis of sequential single point phagocytosises in macrophages using on-chip single cell measurement assay
Yoshiki Nakata[1], Yuya Furumoto[2], Masao Odaka[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Hideyuki Terazono[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*Waseda Biosci. Res. Ins. in Singapore (WABIOS)*)

2Pos172 心筋細胞クラスターの拍動周期の起源：心筋細胞ネットワークの拍動周期の選択ルールの解明
Origin of cardiomyocyte cluster beating intervals: Elucidation of selection rule of interbeat intervals of cardiomyocyte network
Naoki Takahashi[1], Natuki Seki[2], Masao Odaka[3,4], Hideyuki Terazono[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*Waseda Biosci. Res. Ins. in Singapore (WABIOS)*)

2Pos173 **Study of the Structure change in protein using Polarization-dependent Fluorescence Correlation Spectroscopy (Pol-FCS)**
Fusako Gan[1], Johtaro Yamamoto[2], Masataka Kinjo[2] ([1]*Grad. Sch. Life Sci., Univ. Hokkaido*, [2]*Fac. Adv. Life Sci., Univ. Hokkaido*)

2Pos174　角度ダイナミックレンジ広範化に向けたサンプル傾斜角度走査型 X 線 1 分子追跡法の開発

Development of Sample Angular Scanning Diffracted X-ray Tracking for Enhancing Angular Dynamic Range

Hiroshi Sekiguchi[1], Yuji Sasaki[1,2] ([1]*JASRI/SPring-8*, [2]*Dept. of Adv. Mater. Sci., Univ. of Tokyo*)

2Pos175　SQUID とネオジウム磁石片を用いて，繊毛運動を測定する

Measurement of ciliary movement using SQUID gradiometer and a small neodymium magnet piece

Ryota Makibatake[1], Daisuke Oyama[2], Jun Kawai[2], Hitoshi Tatsumi[1] ([1]*Department of Applied Bioscience, Kanazawa Inst. of Technol., Ishikawa, Japan*, [2]*Applied Electronics Laboratory, Kanazawa Inst. of Technol., Ishikawa, Japan*)

2Pos176　冷却 HPD による広視野 1 分子蛍光寿命測定

Wide-field single-molecule fluorescence lifetime measurement by a cooled hybrid photo-detector (HPD)

Atsuhito Fukasawa[1], Gaku Nakano[1], Takayasu Nagasawa[1], Shigeru Ichikawa[1], Minako Hirano[2], Toru Ide[3], Yasuharu Negi[1], Tomohiro Ishizu[1], Hiroaki Yokota[2] ([1]*Hamamatsu Photonics K. K.*, [2]*Grad. Sch. Creation Photon. Indust.*, [3]*Grad. Sch. Nat. Sci. Tecnol., Okayama Univ.*)

バイオイメージング / Bioimaging

2Pos177　PC12 細胞の神経分化における細胞内温度イメージング

Imaging of intracellular temperature in PC12 cell nerve differentiation

Taishu Akiyama[1,4], Masaki Kinoshita[1], Kohki Okabe[2,3], Hisashi Tadakuma[4], Yoshie Harada[4] ([1]*Grad. Sch. Life Sci., Univ. Kyoto*, [2]*Grad. Sch. Pharm., Univ. Tokyo*, [3]*PRESTO, JST*, [4]*Inst. Protein Res., Univ. Osaka*)

2Pos178　蛍光イメージング定量解析で明らかになった ATP に依存した INO80 クロマチン再構成複合体の核内動態

ATP dependent dynamics of INO80 chromatin remodeling complex revealed by quantitative fluorescence imaging

Yuma Ito[1], Masahiko Harata[2], Kumiko Sakata-Sogawa[2], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

2Pos179　Screening of chemical compounds to find new inhibitors against ATP synthesis in mitochondria by MASC assay

Yuki Hayashida[1], Jun-ichi Kishikawa[2], Makoto Fujikawa[3], Hiromi Imamura[4], Ken Yokoyama[2] ([1]*Grad. Sch. Biochem., Kyoto Sangyo Univ.*, [2]*Dept. Mol. Biosci., Kyoto Sangyo Univ.*, [3]*Dept. Pharmacol Neurobiol, Grad. School of Med., Tokyo Medical and Dental.*, [4]*Lab. Funct. Biol., Grad. School of Biostudies, Kyoto Univ.*)

2Pos180　線形ゼロモード導波路を用いたアクチン重合の 1 分子観察

Single-molecule analysis of actin polymerization mechanism using linear zero-mode waveguides

Soichiro Fujii[1], Ryo Iizuka[1], Masamichi Yamamoto[1], Makoto Tsunoda[1], Takashi Tanii[2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [2]*Fac. Sci. Eng., Waseda Univ.*)

2Pos181　ストレス顆粒内内在性 mRNA のナノスケール構成

Nanoscale Organization of Endogenous mRNAs in Stress Granules

Ko Sugawara[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [2]*JST, PRESTO*)

2Pos182　酸化ストレス応答における Nrf2 動態の生細胞 1 分子イメージング

Dynamics changes of transcriptional factor Nrf2 in living cells upon exposure to oxidative stress using single-molecule imaging

Takahiro Maeda[1], Yuma Ito[1], Shunei Doi[1], Masaaki Shiina[2], Kumiko Sakata-Sogawa[3], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*, [3]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

2Pos183　金，銀ナノ粒子を用いたマルチカラー 1 分子イメージング法の開発

Development of multi-color single-molecule imaging method using gold and silver nanoparticles

Jun Ando[1,2,3], Akihiko Nakamura[2,3], Tatsuya Iida[1,2,3], Akasit Visootsat[1], Ryota Iino[1,2,3] ([1]*Institute for Molecular Science*, [2]*Okazaki Inst. for Integrative Bioscience*, [3]*The Graduate University for Advanced Studies (SOKENDAI)*)

2Pos184　RNA 顆粒形成過程の細胞内温度測定

Intracellular temperature measurement during RNA granule formation

Beini Shi[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [2]*PRESTO, JST*)

2Pos185　金ナノ粒子を利用した単一細胞内局所加熱法の開発

Development of a method of local heating a single cell using gold nanoparticles

Takaaki Honda[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharma. Sci., Univ. Tokyo*, [2]*JST, PRESTO*)

2Pos186　相平衡状態にある核小体内領域における核小体構成タンパク質の 1 分子動態解析

Single-molecule dynamics of nucleolar proteins in different compartments of nucleolus

Daiki Matsumoto[1], Yuma Ito[1], Noriko Saitoh[2], Kumiko Sakata-Sogawa[3], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Dept. of Cancer Biol., The Cancer Inst. JFCR.*, [3]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

2Pos187　蛍光イメージングによる転写伸長メディエーター MED26 のダイナミクス解析

Molecular dynamics analysis of Mediator subunit MED26 controlling transcription elongation by fluorescence imaging in the nucleus

Shinnosuke Kunimi[1], Yuma Ito[1], Hidehisa Takahashi[2], Kumiko Sakata-Sogawa[3], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Fac. of Med., Hokkaido Univ.*, [3]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

2Pos188　X 線自由電子レーザーを用いたコヒーレント X 線回折イメージングによる異なる細胞周期にある酵母細胞核の三次元構造解析

3D structural analyses of yeast nuclei in different cell phases by coherent X-ray diffraction imaging using X-ray free electron laser

Takahiro Yamamoto[1,2], Yuki Sekiguchi[1,2], Amane Kobayashi[1,2], Mao Oide[1,2], Asahi Fukuda[1,2], Koji Okajima[1,2], Tomotaka Oroguchi[1,2], Masaki Yamamoto[2], Masayoshi Nakasako[1,2] ([1]*Grad. Sci. Tech., Keio Univ.*, [2]*RSC, RIKEN*)

バイオエンジニアリング / Bioengineering

2Pos189 **Photoregulation of Calmodulin using bifunctional Photochromic compound**
Takayuki Ogiwara[1], Hideki Shishido[2], Shinsaku Maruta[1] ([1]*Grad. Sch. Bioinfo., Univ. Soka*, [2]*Cystic Fibrosis Foundation Thrapeutics, Inc.*)

2Pos190 **Introducing mitochondria to heterologous cells by electrofusion of giant unilamellar vesicles into cells**
Yui Kawagishi[1,2], Atsushi Kubo[2,3], Ken Matsumoto[2,3], Atsushi Tanaka[4], Toshihiko Ogura[2,3], Shin-ichiro M Nomura[1,2] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*AMED-CREST*, [3]*Inst. of Dev., Aging and Canc, Tohoku Univ.*, [4]*Inst. for Prom. of Med. Sci. Res., Facul. of Med., Yamagata Univ.*)

2Pos191 **Photocontrol of interaction between small G protein Ras and its regulatory factor SOS using water soluble azobenezene**
Nobuyuki Nishibe[1], Kenichi Taii[2], Masahiro Kuboyama[1], Toshio Nagashima[3], Toshio Yamazaki[3], Shinsaku Maruta[1] ([1]*Grad. Sch. Bioinfo., Univ. Soka*, [2]*Dep. Sci. Eng., Univ. Soka*, [3]*Yokohama Inst., RIKEN*)

2Pos192 **Development of an automated microarray system for rapid microRNA profiling**
Ryo Iizuka[1,2], Shoichi Tsuchiya[2], Taro Ueno[3], Takanori Ichiki[2,4], Takashi Funatsu[1] ([1]*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*, [2]*iCONM*, [3]*Nikon Corp.*, [4]*Grad. Sch. of Eng., The Univ. of Tokyo*)

2Pos193 **Function control of vitamin D_3 hydroxilase toward efficient bio-sensing and bio-production**
Hikari Sasaki, **Yasuhiro Mie**, Yoshiaki Yasutake, Tomohiro Tamura (*Bioproduction Res. Inst., AIST*)

2Pos194 **一分子検出のための生体ナノポアと固体ナノポアの特性比較**
CHARACTERISTICS COMPARISON OF BIOLOGICAL AND SOLID-STATE NANOPORES FOR A SINGLE MOLECULE DETECTION
Natsumi Takai[1], Masaki Matsushita[1], Kan Shoji[1], Tei Maki[2,3], Ryuji Kawano[1] ([1]*Dept. Biotech. Life Sci., TUAT*, [2]*Res. Ctr. for Sci. Tech., TUAT*, [3]*EM Biz. Unit, JEOL. Ltd*)

2Pos195 **人体システムにおける線形性と非線形性**
Linearity and Non-linearity in Human Body System
Susumu Ito[1], Izumi Kuboyama[2], Katsuhiko Hata[2] ([1]*High-Tech Res. Cent., Kokushikan Univ.*, [2]*Sch. Emerg. Med. Sys. Kokushikan Univ.*)

2Pos196 **Automated cell manipulation system by using high-speed two fingered micro-hand**
Masaru Kojima[1], Eunhye Kim[1], Yasushi Mae[1], Tatsuo Arai[2,3] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Glob. Alliance Lab., The Univ. of Electro-Communications*, [3]*Beijing Inst. of Tech.*)

2Pos197 **ヘリックス相互作用認識を利用したエクソソームの細胞受容体標的**
Receptor clustering and activation using artificial coiled-coil peptide-modified exosomes
Natsumi Ueno[1,2], Miku Katayama[1,2], Kosuke Noguchi[1,2], Tomoka Takatani-Nakase[3], Nahoko Bailey Kobayashi[4,5], Tetsuhiko Yoshida[4,5], Ikuo Fujii[2], Shiroh Futaki[6], Ikuhiko Nakase[1] ([1]*N2RI, Osaka Prefecture Univ.*, [2]*Grad. Sch. Sci., Osaka Prefecture Univ.*, [3]*Sch. of Pham. Pham. Sci., Mukogawa Women's Univ.*, [4]*KARC, Keio Univ.*, [5]*Toagosei Co., Ltd.*, [6]*ICR, Kyoto Univ.*)

2Pos198 **希釈がもたらす生命システムの非線形濃度応答とその人工細胞技術への応用**
Nonlinear concentration dependence of biosystems on dilution and its application on artificial cell technology
Kei Fujiwara (*Department of Biosciences and Informatics, Keio University*)

2Pos199 **Interaction of HVR domain of small GTPase Ras with catalytic domain**
Takashi Hashimoto[1], Nobuhisa Umeki[2], Yasunobu Sugimoto[3], Shinsaku Maruta[1] ([1]*Grad. Sci. Bioinfo., Univ. Soka*, [2]*Wako Inst., RIKEN*, [3]*NUSR*)

2Pos200 **撹拌操作が引き起こすゲノム DNA の二本鎖切断：新規実験手法の提案**
How to keep genome-sized DNA safe against stirring stress: Quantitative analysis through single DNA observation
Hayato Kikuchi, Yuko Yoshikawa, Rinko Kubota, Kenichi Yoshikawa (*Lab. Biol. Phys., Facul. Life Med. Sci., Doshisha Univ.*)

結晶成長・結晶化技術 / Crystal growth & Crystallization technique

2Pos201 **Protocol to optically measure pH in nanopores of protein crystals**
Kazuo Mori, Bernd Kuhn (*OIST*)

その他 / Miscellaneous topics

2Pos202 **高周波磁場によるナノ粒子の加熱効果の検証**
Heat production of bio-synthesized nano-particles in altering magnetic field
Daisuke Katayama[1], Naoki Takashima[1], Hideyuki Yoshimura[2] ([1]*Biophysics Third Lab., Physics Major, Grad. Sch. Science and Technology, Univ. Grad. Sch. Meiji*, [2]*Univ. Meiji*)

2Pos203 **生命構造の維持・形成に関わる力場についての一考察**
A concept for understanding biological dynamics, which would maintain and reproduce biological structure
Ryutaro Izumi (*Nihon University*)

2Pos204 **ゼロモード導波路(ZMW)の量産化と生体分子観察への応用**
High-throughput fabrication of Zero-Mode Waveguide (ZMW) and its application to observation of bio-molecules
Kimiko Nakao[1], Hisashi Tadakuma[1], Yong-Woon Han[2], Kodai Fukumoto[1], Yoshie Harada[1] ([1]*Inst. for Protein Res. Osaka Univ.*, [2]*School of Life Science and Technology, Tokyo Tech.*)

2Pos205 **Combining a docking software with a ligand-based virtual screening method, VS-APPLE**
Daisuke Kobayashi, George Chikenji (*Nagoya University*)

蛋白質：構造 / Protein: Structure

3Pos001 **L グルタミン酸酸化酵素の基質特異性変換の構造基盤**
Structural basis of the conversion of substrate specificity of L-glutamate oxidase
Nanako Ito[1], **Masaki Kitagawa**[1], Shinnsaku Matsuo[2], Michiko Nemoto[2], Takashi Tamura[2], Hitoshi Kusakabe[3], Kennji Inagaki[2], Katsumi Imada[1] ([1]*Dept. MacroMol., Grad. Sch. Sci., Osaka Univ*, [2]*Grad. Sch. Env. & Life Sci., Okayama Univ*, [3]*Enzyme Sensor Co. Ltd*)

3Pos002 **Development of the software with an intelligent strategy for serial data analysis measured by SEC-SAXS/UV-Vis. Spectroscopy**
Kento Yonezawa, Masatsuyo Takahashi, Keiko Yatabe, Shinya Saijo, Nobutaka Shimizu (*Photon Factory, IMSS, KEK*)

3Pos003 **二重スピンラベルたんぱくの cwEPR 距離測定に対するウエーブレット変換の応用**
An application of wavelet transform to distance measurement by continuous wave EPR of doubly spin labeled protein
Yasunori Ohba[1], Shoji Ueki[2], Toshiaki Arata[3] ([1]*IMRAM, Tohoku Univ.*, [2]*Fac. Pharm. Sci., Tokushima Bunri Univ.*, [3]*Grad. School of Sci., Osaka City Univ.*)

3Pos004 ***Porphyromonas gingivitis* の線毛蛋白質 FimA の構造**
Structure of FimA, a major component protein of fimbriae of *Porphyromonas gingivitis*
Kodai Okada[1], Koji Nakayama[2], Mikio Shoji[2], Katsumi Imada[1] ([1]*Grad. Sch. Sci. Osaka Univ.*, [2]*Grad. Sch. Biomedical Sci. Nagasaki Univ.*)

3Pos005 **タンパク質の構造コンプライアンス適合運動の解析**
Analysis of SC (Structural Compliance) Consistent Motion in Proteins
Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)

3Pos006 **GPI アンカー型タンパク質におけるシグナル配列の二次構造解析**
Secondary structural analysis of signal sequence in GPI-anchored protein
Keiya Inoue, Tomonao Iibuchi, Daiki Takahashi, Tatsuki Kikegawa, Kenji Etchuya, Yuri Mukai (*Dept. Electronics, Grad. Sch. Sci. & Tech., Meiji Univ.*)

3Pos007 **蛍光異方性解消法を用いたタンパク質の構造変性時における回転拡散係数および局所構造動きに関する研究**
Rotational diffusion coefficients and the fluctuation of local structure of proteins along denaturation curve
Tomoyuki Yoshitake, Masahide Terazima (*Kyoto University*)

3Pos008 **レプリカ交換分子動力学シミュレーションによる酸性条件下でのポリグルタミン酸の最安定構造**
The dominant structure of polyglutamic acids under an acidic conditions analyzed by replica-exchange molecular dynamics simulations
Ryosuke Iwai[1], Tetsuro Nagai[2], Kota Kasahara[3], Takuya Takahashi[3] ([1]*Grad. Sci. Life Sci., Ritsumeikan Univ*, [2]*Dept. Of Phys., Nagoya Univ*, [3]*Coll. Life. Sci., Ritsumeikan Univ*)

3Pos009 **Nontargeted parallel cascade selection molecular dynamics using convex hull for structure selection**
Kenichiro Takaba[1,2] ([1]*Asahi Kasei Pharma Co., Ltd.*, [2]*Grad. Sch. Sci., Univ. Tokyo*)

3Pos010 **位相板を用いたクライオ電子顕微鏡法での腸内連鎖球菌 V-ATPase 単粒子構造解析**
Single Particle Analysis of *Eh*V-ATPase by Phase-Plate electron cryo-microscopy
Jun Tsunoda[1,2], Chihong Song[2], Takeshi Murata[3], Hiroshi Ueno[4], Naoyuki Miyazaki[5], Kenji Iwasaki[5], Ryota Iino[6], Kazuyoshi Murata[1,2] ([1]*SOKENDAI*, [2]*NIPS*, [3]*Dept. Chem., Chiba Univ.*, [4]*Dept. Appl. Chem., Sch. Eng., Univ. Tokyo*, [5]*IPR*, [6]*OIIB/IMS*)

3Pos011 **HIV-1 プロテアーゼにおける触媒的加水分解反応に関する理論化学的研究**
Theoretical study on catalysis of HIV-1 protease
Masahiro Kaneso, Masahiko Taguchi, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

3Pos012 **Improved method for soluble expression and rapid purification of yeast TFIIA**
Naruhiko Adachi[1,2,3], Kyohei Aizawa[2], Shinya Saijo[1], Nobutaka Shimizu[1,2], Toshiya Senda[1,2] ([1]*SBRC, IMSS, KEK*, [2]*Soken Univ.*, [3]*PRESTO, JST*)

3Pos013 **クライオ電顕を用いた好熱菌プロトン回転型 ATPase の単粒子解析**
Cryo EM structure of intact rotary H+-ATPase/synthase from Thermus thermophilus
Atsuko Nakanishi[1], Jun-ichi Kishikawa[1], Kaoru Mistuoka[2], **Ken Yokoyama**[1] ([1]*Department of Molecular Biosciences, Kyoto Sangyo University*, [2]*Research Center for Ultra-High Voltage Electron Microscopy*)

3Pos014 **分子動力学法による緑色蛍光タンパク質のフォールディングとアグリゲーション**
Folding and Aggregation of Green Fluorescent Protein Studied by Molecular Dynamics Simulation
Mashiho Ito[1], Shoji Takada[2] ([1]*Nagoya Univ.*, [2]*Kyoto Univ.*)

3Pos015 **Flexible docking and affinity calculation between CDK2 and its inhibitor CS3 using multicanonical MD and thermodynamic integration**
Gert-Jan Bekker[1], Narutoshi Kamiya[2], Mitsugu Araki[3], Ikuo Fukuda[1], Yasushi Okuno[3], Haruki Nakamura[1] ([1]*IPR, Osaka Univ.*, [2]*Grd. Sch., Univ. Hyogo*, [3]*Grd. Sch. Med., Kyoto Univ.*)

3Pos016 **A structural study of the novel chemokine receptor-binding protein, R1-15**
Hiroko Takasaki[1], Sosuke Yoshinaga[1], Soichiro Ezaki[1], Mitsuhiro Takeda[1], Yuya Terashima[2], Etsuko Toda[2], Kouji Matsushima[2], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*Grad. Sch. Med., Univ. Tokyo*)

3Pos017 **ユニークな Coiled-coil 構造を有する VSOP の電気生理学的および構造学的研究**
Electrophysiological and structural studies of a unique coiled-coil region of VSOP
Akima Yamamoto[1], Takashi Tanibayashi[1], Satomi Shibumura[1], Yuichirou Fujiwara[4], Yasushi Okamura[4,5], Atsushi Nakagawa[1,5], Kohei Takeshita[1,2,3] ([1]*IPR, Osaka Univ.*, [2]*JST, PRESTO*, [3]*IAI, Osaka Univ.*, [4]*Grad. Sch. of Med., Osaka Univ.*, [5]*JST, CREST*)

3Pos018 **小角散乱によるヒト α-シヌクレインのアミロイド線維の構造解析**
Structural characterization of amyloid fibrils of human α-synuclein by small-angle scattering
Fumiaki Kono[1], Tatsuhito Matsuo[1], Shin-ichi Takata[2], Yasunobu Sugimoto[3], Satoru Fujiwara[1] ([1]*QuBS, QST*, [2]*J-PARC Center*, [3]*SR Center, Nagoya Univ.*)

3Pos019 **A SAXS study of thermal denaturation and coagulation of a major soybean storage protein β-conglycinin**
Nobuhiro Sato[1], Yuki Higashino[2], Rintaro Inoue[1], Masaaki Sugiyama[1], Reiko Urade[2] ([1]*Res. React. Inst., Kyoto Univ.*, [2]*Grad. Sch. Agric., Kyoto Univ.*)

3Pos020 **ガウス関数入力型混合正規分布モデルによる３次元密度マップの近似表現**
Gaussian-input Gaussian mixture model for approximate representation of 3D density map
Takeshi Kawabata, Haruki Nakamura (*Inst. Prot. Res., Osaka U.*)

3Pos021 **バックグラウンドイメージより抽出した CTF を使ったネガティブ染色電子顕微鏡像の CTF 補正**
The CTF correction of negative-staining electron micrographs by using the CTF extracted from the background image
Hitoshi Sakakibara (*Nat. Inst. Inf. Com. Tech. Bio-Function Sec.*)

蛋白質：構造機能相関 / Protein: Structure & Function

3Pos022 **細胞内のアクチン構造は細胞への機械刺激により変化する。**
Atomic structure of actin within cells is changed by external mechanical stimulus
Urara Tokuishi[1], Q.P. Taro Uyeda[2], Q.P. Taro Noguchi[1] ([1]*National Institute of Technology, Miyakonojo College*, [2]*Waseda University*)

3Pos023 **Shootin1 の複数のリン酸化体とその構造**
Multiple phosphorylated species of shootin1 and their solution structure
Shoki Nakata[1], Kentarou Baba[2], Yugo Hayashi[1], Yoichi Yamazaki[1], Naoyuki Inagaki[2], Hironari Kamikubo[1] ([1]*Grad. Sch. of Mater. Sci., NAIST.*, [2]*Grad. Sch. of Biol. Sci., NAIST.*)

3Pos024 **アシル CoA の分子力学力場パラメータの改良**
Refinement of molecular mechanics force field of acyl-CoA
Kyosuke Sato (*Dept. Mol. Physiol., Fac. Life Sci., Kumamoto Univ.*)

3Pos025 **ラン藻でのアルカン合成に必要な 2 つの酵素間の相互作用**
Interaction between two enzymes essential for cyanobacterial alkane biosynthesis
Mari Chang[1], Keigo Shimba[2], Hisashi Kudo[2], Hidenobu Kawai[2], Yoshiki Oka[2], Manami Wada[2], Yuuki Hayashi[2], Munehito Arai[1,2] ([1]*Dept. Phys., Univ. Tokyo*, [2]*Dept. Life Sci., Univ. Tokyo*)

3Pos026 **クライオ EM マップ及び多階層構造を対象とした状類構造検索サービス「Omokage 検索」の改良**
Improvement in Omokage search, shape similarity search for cryo-EM maps and multi-scale structure data
Hirofumi Suzuki[1,2], Takeshi Kawabata[1], Genji Kurisu[1,2], Haruki Nakamura[1,2] ([1]*IPR, Osaka-Univ*, [2]*PDBJ*)

3Pos027 **単分子動態計測によって明らかになる KcsA チャネル開閉構造変化の遷移過程における立体構造安定性**
Structural Stabilities during Gating Transitions in the KcsA Potassium Channel Revealed by Single-Molecule Dynamics Recordings
Hirofumi Shimizu, Masayuki Iwamoto (*Univ. Fukui. Fac. Med. Sci.*)

3Pos028 **NMR と MRS による α-シヌクレインの生体内オリゴマー化の解析**
NMR and MRS analyses of α-Synuclein oligomerization *in vivo*
Keika Saito, Mitsuhiro Takeda, Sosuke Yoshinaga, Hiroaki Terasawa (*Fac. Life Sci., Kumamoto Univ.*)

3Pos029 **リン酸化タンパク質におけるリン酸基周辺の水和水動態解析**
Analysis of water dynamics around phosphorylated protein
Hiroya Yamazaki, Shige H. Yoshimura (*Grad. Sch. Biostudies., Univ. Kyoto*)

3Pos030 **アデニル酸キナーゼの反応機構に関する計算化学的研究**
Computational Study on the Reaction Mechanism of Adenylate Kinase
Kenshu Kamiya (*Dept. Phys., Sch. Sci., Kitasato Univ.*)

3Pos031 **T 細胞受容体による特異的および交差反応的な抗原認識機構の解明**
Analyses of the structural mechanisms of specific and crossreactive recognitions of antigen peptide-MHC by TCRs
Yuko Tsuchiya[1], Yoshiki Namiuchi[2], Hiroshi Wako[3], Hiromichi Tsurui[4] ([1]*IPR, Osaka Univ.*, [2]*QBiC, RIKEN*, [3]*Sch. of Social Sci., Waseda Univ.*, [4]*Sch. of Med., Juntendo Univ.*)

3Pos032 **Virtual system coupled canonical molecular dynamics simulation to enhance sampling along a reaction coordinate**
Bhaskar Dasgupta[1,2], Kota Kasahara[3], Haruki Nakamura[1], Junichi Higo[1] ([1]*IPR, Osaka University*, [2]*Technology Research Association for Next Generation Natural Products Chemistry*, [3]*College of Life Sciences, Ritsumeikan University*)

3Pos033 **シトクロム P450 還元酵素における荷電状態変化に応じた物理状態変化**
Physical state change in NADPH-cytochrome P450 oxidoreductase in response to the charged state change
Mikuru Iijima, Takato Sato, Ryota Moritake, Tohru Sasaki, Mitsunori Takano (*Dept. of Pure. & Appl. Phys., Waseda Univ.*)

3Pos034 **タンパク質の協同的な折れたたみとループのつながり方の関係: 4α-2β タンパク質トポロジーに関する網羅的解析**
Relation between cooperative protein folding and loop connections: comprehensive analysis over 2α-4β protein topologies
Nobu C. Shirai[1], Shintaro Minami[2] ([1]*Center for Information Technologies and Networks, Mie University*, [2]*Graduate School of Information Science, Nagoya University*)

3Pos035 **MD シミュレーションを用いた ATP 作動性イオンチャネル P2X における競合的阻害剤 TNP-ATP の作用機序の解明**
MD simulation of ATP-gated P2X receptors reveals the inhibitory mechanism of a competitive antagonist TNP-ATP
Ryoki Nakamura[1], Go Kasuya[1], Mizuki Takemoto[1], Motoyuki Hattori[2], Ryuichiro Ishitani[1], Osamu Nureki[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Sci., Fudan Univ.*)

3Pos036 **Real-time imaging of Na^+-induced structural transitions of MotPS stator complex of flagellar motor by HS-AFM**
Naoya Terahara[1], Noriyuki Kodera[2], Takayuki Uchihashi[3], Toshio Ando[2], Keiichi Namba[1], Tohru Minamino[1] ([1]*Grad. Sch. Frontier Bioscience, Osaka Univ.*, [2]*Bio-AFM Frontier Research Center, Kanazawa Univ.*, [3]*Grad. Sch. Sci, Nagoya Univ.*)

蛋白質：物性 / Protein: Property

3Pos037 **Comparison of amyloid fibrillation between wild type and I2E mutant of VL domains of antibody light chain**
Takafumi Naito[1], Masahiro Noji[1], Masatomo So[1], Kenji Sasahara[1], Johannes Buchner[2], Goto Yuji[1] ([1]*IPR*, [2]*Technical University Munich*)

3Pos038 **味覚受容体細胞外領域ヘテロ二量体の発現・精製および性状解析**
Expression, purification, and characterization of the entire heterodimeric extracellular regions of fish taste receptor
Hiroki Maruhashi[1], Daisuke Noshiro[2], Norihisa Yasui[1], Toshio Ando[2], Atsuko Yamashita[1] ([1]*Grad. Sch. Med. Dent. Pharm. Sci., Okayama Univ.*, [2]*Bio-AFM FRC, Inst. of Sci. & Eng., Kanazawa Univ.*)

3Pos039 **ポリリン酸による α-synuclein のアミロイド線維形成誘導のメカニズム**
The mechanisms of polyphosphate-induced amyloid fibrillation of α-synuclein
Tatsuya Fujikawa, Masatomo Sou, Yuji Goto (*Osaka Univ. IPR*)

3Pos040 **Structure elements are closely related to intramolecular residue-residue contacts**
Yasumichi Takase, Yugo Hayashi, Yoichi Yamazaki, Hironari Kamikubo (*NAIST MS*)

3Pos041 **弱酸性条件における $A\beta_{1-40}$ のアミロイド線維化**
Amyloid fibrillation of $A\beta_{1-40}$ under weak acidic conditions
Kaori Mageshi, Naoki Yamamoto, Takato Hiramatsu, Eri Chatani (*Grad. Sch. of Sci., Kobe Univ.*)

3Pos042 **示差走査熱量測定によるマルチドメイン蛋白質の不可逆熱転移の速度論的解析**
Kinetic analysis of the irreversible thermal transition of multi-domain proteins by Differential Scanning Calorimetry
Shigeyoshi Nakamura[1,2], Hiroka Suzuki[3], Pitchanan Nimpiboon[4], Priya Kaewpathomsri[4], Piamsook Pngsawasdi[4], Wataru Nunomura[4], Shun-ichi Kidokoro[4] ([1]*NIT, Ube College*, [2]*Nagaoka Univ. of Tech.*, [3]*Akita Univ.*, [4]*Chulalongkorn Univ.*)

3Pos043 **Conformational fluctuation of phosphorylated-ubiquitin studied by high-pressure NMR spectroscopy**
Soichiro Kitazawa, Yu Aoshima, Junki Iga, Takuro Wakamoto, Ryo Kitahara (*Ritsumeikan Univ.*)

3Pos044 **Solubilization and structural analysis of heat-aggregated keratin protein**
Atsushi Baba[1], Momoko Furuta[1], Kentaro Shiraki[2], Len Ito[1] ([1]*MILBON Co., Ltd.*, [2]*Fac. Pure and App. Sci., Univ. Tsukuba*)

3Pos045 **マイクロ波照射環境での酵素反応のエントロピー低下**
Entropy reduction of enzymatic reaction in microwave irradiated environment
Fujiko Aoki, Takeo Yoshimura, **Shokichi Ohuchi** (*Dept Biosci Bioinform, Kyushu Inst Tech*)

3Pos046 **統計力学モデルによるマルチドメインタンパク質のフォールディング経路の解析**
Folding pathways of multi-domain proteins predicted by a statistical mechanical model
Koji Ooka[1], Munehito Arai[1,2] ([1]*Dept. Phys., Univ. Tokyo*, [2]*Dept. Life Sci., Univ. Tokyo*)

3Pos047 **張力によって誘起されたアクチンの静電的変化：アクチンフィラメントの圧電性**
Tension-induced electrostatic change in actin: piezoelectricity of an actin filament
Jun Ohnuki, Hideyo Okamura, Akira Yodogawa, Takato Sato, Taro Q.P. Uyeda, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

3Pos048 **トリガーファクターが補助するタンパク質フォールディングの 高速原子間力顕微鏡を用いたリアルタイム観測**
Real time observation of Trigger Factor assisted protein folding using high-speed atomic force microscope
Taiji Namba[1], Tomohide Saio[1,2,3], Koichiro Ishimori[1,2], Noriyuki Kodera[4] ([1]*Grad. Sch. Sci. Eng., Univ. Hokkaido*, [2]*Grad. Sch. Sci., Univ. Hokkaido*, [3]*PRESTO. JST*, [4]*Sci. Tec., Univ. Kanazawa*)

3Pos049 **対イオンで誘起されるアクチンの静電的変化：リエントラント重合における大域斥力と局所引力のバランス**
Counter-ion-induced electrostatic change in actin: the balance between global repulsion and local attraction in reentrant polymerization
Akira Yodogawa, Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

蛋白質：機能 / Protein: Function

3Pos050 **単一アクチンフィラメントの両末端におけるモノマー間の変動の差異**
Differences of inter-monomer fluctuations of single actin filament at either ends
Ryota Mashiko[1], Hirotaka Ito[1], Hajime Honda[1], Kenji Kamimura[2] ([1]*Nagaoka University of Technology, Department of Bioengineering*, [2]*National Institute of Thechnology, Nagaoka College, Department of Electronic Control Engineering*)

3Pos051 セルロース合成の時分割 X 線小角散乱による計測
Time-resolved SAXS measurement of cellulose synthesized in vitro
Hirotaka Tajima[1], Paavo Penttilä[2], Tomoya Imai[1], Junji Sugiyama[1], Yoshiaki Yuguchi[3] ([1]*RISH, Kyoto Univ.*, [2]*ILL*, [3]*Fac. Engineer., OECU*)

3Pos052 タンパク質レベルでの発現が確認されていないスプライシングアイソフォームの機能性推定
Estimating functionality of expression-unconfirmed splicing isoforms at the protein level
Teerasetmanakul Pramote, **Masafumi Shionyu** (*Grad. Sch. of Bio-Sci., Nagahama Inst. Bio-Sci. Tech.*)

3Pos053 グラム陽性菌 ***Bacillus subtilis*** 由来 ferredoxin-NADP$^+$酸化還元酵素パラログ YcgT の酵素学的解析
Enzymatic characterization of ferredoxin-NADP$^+$ oxidoreductase paralogue YcgT from gram-positive bacterium *Bacillus subtilis*
Daisuke Seo[1], Masaharu Kitashima[2], Kazuhito Inoue[2], Hirofumi Komori[3] ([1]*Div. Mat. Sci., Grad. Sch. Nat. Sci. Tec., Kanazawa Univ*, [2]*Dep. Biol. Sci., Kanagawa Univ*, [3]*Fac. Educ., Kagawa Univ*)

3Pos054 タウタンパク質に対する Pin1 由来のプロテアーゼの活性の定量的評価
Quantitative evaluation of activity of a protease derived from Pin1 for tau protein
Teikichi Ikura, Nobutoshi Ito (*Med. Res. Inst., Tokyo Med. Dent. Univ.*)

3Pos055 拡張アンサンブル分子動力学シミュレーションを用いたヒストン脱メチル化酵素阻害剤のアイソザイム選択制に関する研究
Study for Isozyme Selectivity of Lysine Demethylase Inhibitor by Using Generalized Ensemble Molecular Dynamics Simulations
Shuichiro Tsukamoto[1,3], Yoshitake Sakae[2], Yukihiro Itoh[2,3], Takayoshi Suzuki[2,3], Yuko Okamoto[1,3,4,5,6] ([1]*Grad. Sch. Sci., Nagoya Univ*, [2]*Grad. Sch. Med. Sci., Kyoto Pref. Univ. Med.*, [3]*JST-CREST*, [4]*Struc. Bio. Res. Cen., Grad. Sch. Sci., Nagoya Univ.*, [5]*Cen. Comput. Sci., Grad. Sch. Eng., Nagoya Univ.*, [6]*Info. Tech. Cen., Nagoya Univ.*)

3Pos056 プラストシアニンとシトクロム *f* との反応過程に対する分子間静電相互作用の寄与に関する理論的研究
Theoretical study on contribution of electrostatic intermolecular interaction to reaction process of Plastocyanin with Cytochrome *f*
Satoshi Nakagawa, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Sch. Nat. Sci. Tech., Kanazawa Univ.*)

3Pos057 ADP/ATP 交換輸送体のミトコンドリアにおける活性調節の計測
Measurements of activity regulation of adenine nucleotide translocator in mitochondria
Mayu Yoneda, Saki Yamashita, Yoshihiro Ohta (*Ohta. Lab., Univ. Noko*)

3Pos058 **Single α-helix alone in a shaft of F_1-ATPase cannot fully transmit the torque but closely cooperate with the stator**
Shou Furuike, Yasushi Maki, Hideji Yoshida (*Phys., Osaka Med. Col.*)

3Pos059 OPA1 プロテオリポソームによるミトコンドリア内膜形態制御機構の解明
Elucidating the regulation of mitochondrial inner membrane morphology using OPA1 proteoliposome
Tadato Ban, Naotada Ishihara (*Dept. of Protein Biochem., Inst. of Life Science, Kurume Univ.*)

3Pos060 抗菌性ペプチドも進化するのか？：チャネル電流計測を用いたヒトとサルにおける抗菌ペプチドの膜障害活性評価からの推察
Do pore-forming activities of antimicrobial peptides change with evolution between Human and Gibbon?
Naoki Saigo, Yusuke Sekiya, Ryuji Kawano (*Dept. Biotech and Biosci*)

蛋白質工学 / Protein: Engineering

3Pos061 結晶性多糖を分解する双方向性リニア分子モーターの計算機合理設計と構造解析
Computational design and structural analysis of bi-directional linear molecular motor hydrolyzing crystalline polysaccharide
Fumihiro Kawai[1], Akihiko Nakamura[1,2], Mayuko Yamamoto[1], Yasuko Okuni[1], Ryota Iino[1,2,3] ([1]*Okazaki Institute for Integrative Bioscience*, [2]*The Graduate University for Advanced Studies (SOKENDAI)*, [3]*Institute for Molecular Science*)

3Pos062 モモ由来システインリッチアレルゲン peamaclein の大量発現
Over expression of recombinant peamaclein, a cysteine-rich plant allergenic peptide derived from peach pulp
Hiromu Suzuki[1], Takasumi Kato[1], Mihoko Yasumoto[1], Kento Iwama[1], Akiho Okamura[1], Tomoya Kato[1], Naoya Kitada[1], Md. Ruhul Kuddus[1], Farhana Rumi[1], Takashi Tsukamoto[1,2], Takashi Kikukawa[1,2], Makoto Demura[1,2], Tomoyasu Aizawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*GI-CoRE, Hokkaido Univ.*)

3Pos063 **V_1-ATPase 非活性界面を再設計することで分子モーターを理解する試み**
An Attempt to Understand Molecular Motor by Redesigning Non-Catalytic Interface of V_1-ATPase
Takahiro Kosugi[1,2], Tatsuya Iida[2,3], Fumihiro Kawai[3], Minako Kondo[1], Mikio Tanabe[5], Ryota Iino[1,2,3], Nobuyasu Koga[1,2,5] ([1]*CIMoS, IMS*, [2]*SOKENDAI*, [3]*Okazaki. Inst. Integ. Biosci.*, [4]*KEK*, [5]*JST, PRESTO*)

3Pos064 **Generation of a ruthenium-binding peptide motif containing genetically encoded bipyridylalanine as ligand**
Marziyeh Karimiavargani[1], Noriko Minagawa[2], Seiichi Tada[2], Takuji Hirose[1], Yoshihiro Ito[2], Takanori Uzawa[2] ([1]*Graduate School of Science and Engineering, Saitama University*, [2]*Nano Medical Engineering Laboratory, RIKEN*)

3Pos065 人工設計タンパク質間結合面の移植による新規タンパク質間相互作用の創出
Development of a novel protein complex by grafting an artificial protein-protein binding interface
Sota Yagi[1], Satoshi Akanuma[2], Tatsuya Uchida[1], Akihiko Yamagishi[1] ([1]*Dep. Appl. Life Sci., Tokyo Univ. Pharm. Life Sci.*, [2]*Facul. Hum. Sci., Waseda Univ.*)

3Pos066 リポソームディスプレイ法を用いた多剤排出トランスポーター EmrE の in vitro 機能進化
In vitro evolution of E. coli multidrug efflux transporter EmrE by using liposome display
Sae Uchida, Atsuko Uyeda, Hajime Watanabe, Tomoaki Matsuura (*Dep. Biotechnol, Grad. Sch. Eng., Osaka Univ*)

3Pos067 **アルカリフォスファターゼの変異導入率と酵素活性分布の関係**
The relationship between mutation rate and enzymatic activity distribution of alkaline phosphatase
Makoto Kato[1], Yi Zhang[1,2], Hiroshi Ueno[1], Kazuhito Tabata[1], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*JAMSTEC*)

3Pos068 **細胞内における脂肪酸アルデヒド生成量のリアルタイム検出とその応用**
***In vivo* real-time measurement of fatty aldehyde and its application**
Yuuki Hayashi, Munehito Arai (*Dept. Life Sci., Univ. Tokyo*)

ヘム蛋白質 / Heme proteins

3Pos069 **ATP 結合型外向きヘム輸送体の計算的モデリング**
Computational Modeling of the ATP-Bound Outward-Facing Form of a Heme Importer
Koichi Tamura[1], Hiroshi Sugimoto[2,3], Yoshitsugu Shiro[2], Yuji Sugita[1,4,5,6] ([1]*RIKEN AICS*, [2]*Grad. Sch. Life Sci., Univ. Hyogo*, [3]*RIKEN SPring-8*, [4]*RIKEN TMS*, [5]*RIKEN iTHES*, [6]*RIKEN QBiC*)

3Pos070 **呼吸鎖ヘム・銅酸素還元酵素 A タイプのプロトン移動経路の pKa 解析**
pKa analysis of the proton transfer pathway in respiratory A-type heme-copper oxygen reductase
Kazumasa Muramoto (*Dept. Life Sci., Univ. of Hyogo*)

3Pos071 **ヘムタンパク質中のヘムの歪みの統計および量子化学計算による解析**
Statistical and quantum-chemical analysis of heme distortion in hemoprotein
Yasuhiro Imada[1], Yusuke Kanematsu[2], Hiroko Kondo[2], **Yu Takano**[1,2] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sci. Info. Sci., Hiroshima City Univ.*)

3Pos072 **金属還元酵素ヒト Steap3 の分子機能解明**
Analyses on the molecular function of metalloreductase human Steap3
Akito Nakata[1], Mika Fujimura[1], Fusako Takeuchi[2], Motonari Tsubaki[1] ([1]*Dept. of Chem., Grad. Sch. Sci., Kobe Univ.*, [2]*IPHE., Kobe Univ.*)

3Pos073 **Computational design of heme-binding protein by remodeling NTF2-like structure**
Minako Kondo[1], Yoshitaka Moriwaki[2], Takahiro Kosugi[1], Norifumi Muraki[1,3], Shigetoshi Aono[1,3], Rie Koga[1], Nobuyasu Koga[1,4] ([1]*CIMoS, IMS*, [2]*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [3]*Okazaki. Inst. Integ. Biosci.*, [4]*JST, PRESTO*)

3Pos074 **コスモトロープ溶質による多量体アロステリック蛋白質の解体とその機能への影響**
Disassembly and Impact on Function of a Multimeric Allosteric Protein by Kosmotropes
Antonio Tsuneshige, Satoru Unzai (*Frontier Bioscience, Hosei University*)

3Pos075 **膜内在性一酸化窒素還元酵素 cNOR の保存されたバリン残基の役割**
Functional roles of a conserved valine residue in membrane-integrated nitric oxide reductase, cNOR
Raika Yamagiwa[1,2], Hitomi Sawai[1], Takehiko Tosha[2], Hiro Nakamura[3], Hiroyuki Arai[4], Yoshitsugu Shiro[1] ([1]*Grad. Sch. of Life Sci., Univ. of Hyogo*, [2]*RIKEN, SPring-8*, [3]*RIKEN, Yokohama*, [4]*GSALS, Univ. of Tokyo*)

3Pos076 **時間分解可視・赤外吸収分光法を用いた一酸化窒素還元酵素の NO 還元反応機構の解明**
Elucidation of the NO Reduction Mechanism of Nitric Oxide Reductase Using Time-resolved Vis / IR Spectroscopy
Hanae Takeda[1,2], Tetsunari Kimura[4], Takashi Nomura[3], Akiko Matsubayashi[1], Shoko Ishii[1], Takehiko Tosha[3], Yoshitsugu Shiro[1], Minoru Kubo[3,5] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*JRA, RIKEN*, [3]*SPring8-Center, RIKEN*, [4]*Grad. Sch. Sci., Kobe Univ.*, [5]*JST PREST*)

筋肉 / Muscle

3Pos077 **ミオシンによるポリ三リン酸の加水分解とアクトミオシン運動への影響**
Tripolyphosphate hydrolysis by myosin and its effect on the motility of actomyosin
Kuniyuki Hatori, Mitsuru Seino, Koji Ito (*Dept. Bio-Systems Eng., Yamagata Univ.*)

3Pos078 **溶液中のアクチンフィラメントは平面で運動するアクトミオシンに引き付けられる**
A motility induced concentration effects detected by QCM-microscopy
Shohta Takamori[1], Hirotaka Taomori[1], Kaho Yokomuro[1], Kazuya Soda[1], Takasi Ishiguro[2], Hajime Honda[1] ([1]*Dept . Of Bioeng., Nagaoka Univ. Tech.*, [2]*Taiyo Yuden CO., Ltd.*)

3Pos079 **Effects of E244D mutation of cardiac troponin T on the structure of thin filaments by small-angle x-ray scattering**
Tatsuhito Matsuo, Fumiaki Kono, Satoru Fujiwara (*QuBS, QST*)

3Pos080 **ヒト β-アクチン発現系の構築と変異体の解析**
System for Expressing and Purification of Human β-Actin and Analysis of Mutants
Mizuki Matsuzaki[1], Sae Kashima[1], Kayo Maeda[1], Tomoharu Matsumoto[1], Mahito Kikumoto[1], Motonori Ota[2], Akihiro Narita[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Grad. Sch. Info. Sci., Nagoya Univ.*)

3Pos081 **Structural analysis of human cardiac muscle thin filament by electron cryomicroscopy**
Yurika Yamada[1], Keiichi Namba[1,2], Takashi Fujii[2] ([1]*Grad. Sch. of Frontier Biosci., Osaka Univ.*, [2]*RIKEN QBiC*)

3Pos082 **心筋リン酸化調節に関与するトロポニン I と T の動的構造： 双極子 ESR を用いた距離測定法による研究**
Structural dynamics of cardiac troponin I and T regulated by phosphorylation, as studied by distance measurement using dipolar ESR
Toshiaki Arata[1,2,5], Kouichi Sakai[1], Chenchao Zhao[1], Hiroaki Yamashita[1], Takayasu Somiya[1], Shinji Takai[1], Masao Miki[3], Shoji Ueki[4] ([1]*Dept. Biol. Sci., Grad. Sch. Sci., Osaka Univ.*, [2]*Ctr. Adv. High Mag. Field Sci.*, [3]*Univ. Fukui*, [4]*Tokushima Bunri Univ.*, [5]*Dept. Biol., Grad. Sch. Sci., Osaka City Univ. (Present Address)*)

分子モーター / Molecular motor

3Pos083 **Rotation of the engineered F_1-ATPase with α-type P-loop on catalytic β subunit**

Hiroshi Ueno[1], Rie Koga[2], Tomoko Masaike[3], Nobuyasu Koga[2], Hiroyuki Noji[1,4] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*CIMoS, IMS*, [3]*Dept. Appl. Biol. Sci., Tokyo Univ. of Sci.*, [4]*ImPACT, JST*)

3Pos084 **光ピンセットで停止させたバクテリアべん毛モーターのトルク**

Stall torque of the bacterial flagellar motor measured by optical tweezers

Taishi Kasai[1], Yoshiyuki Sowa[1,2] ([1]*Reserch Center for Micro-Nano Tech., Hosei Univ.*, [2]*Dept. Frontier Biosci., Hosei Univ.*)

3Pos085 **人工筋肉の創成に向けたサルコメアユニットの設計**

Designing of sarcomere unit from microtubules and kinesins for construction of artificial muscles

Ai Saito[1], Kabir Arif Md. Rashedul[2], Yuichi Hiratsuka[3], Akinori Kuzuya[4], Akihiko Konagaya[5], Kazuki Sada[1,2], Akira Kakugo[1,2] ([1]*Grad. Sch. of Chem. Sci. and Eng., Hokkaido Univ.*, [2]*Fac. of Sci., Hokkaido Univ.*, [3]*Sch. Mat. Sci., JAIST*, [4]*Fac. Chem. Mater. Bioeng., Kansai Univ.*, [5]*DIS, TITECH.*)

3Pos086 **Na^+と K^+で駆動するバクテリアべん毛モーターの発生トルク**

Torque-IMF relationship of Na^+- and K^+-driven bacterial flagellar motor

Kenta Arai[1], Taishi Kasai[2], Yuka Takahashi[3], Masahiro Ito[3], **Yoshiyuki Sowa**[1,2] ([1]*Dept. Frontier Biosci, Hosei Univ.*, [2]*Reserch Center for Micro-Nano Tech., Hosei Univ.*, [3]*Fac. Life Sci., Toyo Univ.*)

3Pos087 **ハイブリッド F_1-ATPase の 1 分子回転観察**

Rotation of hybrid F_1-ATPase from bacterial rotor and mammalian stator ring

Ryo Watanabe, Hiroshi Ueno, Toshiharu Suzuki, Ryohei Kobayashi, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

3Pos088 **駆動力と集積力に依存するアクチン線維流の配向**

Alignment of actin-streams driven by myosin motors: Dependence on driving force and packing force

Takahiro Iwase[1], Yosiya Miyasaka[2], Kuniyuki Hatori[1] ([1]*Dept. Bio-Systems Eng., Yamagata Univ.*, [2]*Dept. Bio-Systems Eng., Yamagata Univ.*)

3Pos089 **Novel photochromic inhibitor of mitotic kinesin Eg5 composed of spiropyran and azobenzene**

Md Alrazi Islam[1], Ryouta Shimoyama[2], Shinsaku Maruta[1] ([1]*Soka University, Department of Bioinformatics, Graduate School of Engineering*, [2]*Dept. of Sci. and Eng. Faculty of Bioinfo.*)

3Pos090 **Structural basis of the mechanical properties of the flagellar distal rod and the hook**

Yumiko Saijo-Hamano[1], Hideyuki Matsunami[2], Keiichi Namba[1,3], Katsumi Imada[4] ([1]*FBS. Osaka Univ.*, [2]*OIST*, [3]*QBiC, RIKEN*, [4]*Dept. MacroMol. Sci., Grad. Sch. Sci., Osaka Univ.*)

3Pos091 **Structural analysis of the NATIVE state flagella hook by electron cryomicroscopy**

Takayuki Kato[1], Tomoko Miyata[1], Peter Horvath[1], Keiich Namba[1,2] ([1]*Grad. Front. Biosci, Osaka Univ*, [2]*QBiC, RIKEN*)

3Pos092 **細菌べん毛モーターの回転方向変換制御機構の解明**

Elucidation of the directional switching mechanism of the bacterial flagellar motor by electron cryomicroscopy

Tomoko Miyata[1], Takayuki Kato[1], Akihiro Kawamoto[1], Keiichi Namba[1,2] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [2]*QBiC, RIKEN*)

3Pos093 **High resolution structural analysis of the flagellar hook of Salmonella Typhimurium**

Peter Horvath[1], Takayuki Kato[1], Tomoko Miyata[1,2], Keiichi Namba[1] ([1]*FBS Osaka Uni.*, [2]*QBiC, RIKEN*)

3Pos094 **pH-indicator を用いた好熱菌 *Bacillus* PS3 由来 F_oF_1-ATP 合成酵素の ATP 加水分解と H^+輸送の共役機構**

Analyses of coupling mechanism between ATP-hydrolysis and H^+-translocation of *Bacillus* PS3 F_oF_1-ATP synthase using pH-indicator

Naoya Iida[1], Yuzo Kasuya[1], Naoki Soga[2], Taro Uyeda[1], Masasuke Yoshida[3], Kazuhiko Kinosita[1], Toshiharu Suzuki[2] ([1]*Dept. Physics, Waseda Univ.*, [2]*Dept. Eng, Univ. of Tokyo*, [3]*Dept. Mol Biochem, Kyoto Sangyo Univ*)

3Pos095 **Regulation of dynein motility by NDEL1**

Toshiaki Saito[1], Takuya Kobayashi[1], Takayuki Torisawa[2], Takashi Murayama[3], Yoko Y Toyoshima[1] ([1]*Grad. Sch. of Arts & Sci., Univ. Tokyo*, [2]*Bio ICT Lab, NICT*, [3]*Dept. Pharmacol., Juntendo Univ. Sch. of Med.*)

3Pos096 **F_O モーターの回転ブラウン運動の数値解析**

Computational Analysis of the Brownian rotation of F_O motor

Daiki Yamakoshi, Dan Parkin, Kota Tezuka, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

3Pos097 **微小管のグライディング運動における蛍光 ATP の Linear zero-mode waveguides を利用した 1 分子観察**

Single molecule observation of fluorescent ATP in microtubule gliding motility enabled by linear zero-mode waveguides

Kazuya Fujmoto[1], Ryota Iino[2], Michio Tomishige[3], Hirofumi Shintaku[1], Hidetoshi Kotera[1], Ryuji Yokokawa[1] ([1]*Kyoto Univ.*, [2]*Institute for Molecular Science*, [3]*Aoyama Gakuin Univ.*)

細胞生物学 / Cell biology

3Pos098 **Probing cell-wall synthetic dynamic using bacterial membrane protein-complex**

Yi-Ren Sun, Chien-Jung Lo (*Department of Physics and Graduate Institute of Biophysics, National Central University*)

3Pos099 **足場の形状によるアクチン波と細胞極性の制御**

Actin waves and cell polarity regulated by substrate geometry

Gen Honda[1], Akihiko Nakajima[2], Satoshi Sawai[1,2] ([1]*Department of Basic Science, Graduate School of Arts and Sciences, University of Tokyo*, [2]*Research Center for Complex Systems Biology, Graduate School of Arts and Sciences, University of Tokyo*)

3Pos100 **Manipulation and Detection of Ca^{2+} Concentration Change of Single Immotile Cilium in Mammalian Node**
Takanobu A Katoh[1], Katsutoshi Mizuno[2], Hiroshi Hamada[2], Takayuki Nishizaka[1] ([1]*Dept. Phys., Gakushuin Univ.*, [2]*CDB, RIKEN*)

3Pos101 **リニアモータータンパク質によるミトコンドリアの形態変化**
Mitochondrial Shape Changing by Linear Motor Proteins
Keitaro Shibata[1,2], Luca Scorrano[1,2] ([1]*Dept. of Biol., Univ. of Padua*, [2]*VIMM*)

3Pos102 **生体ゲル内ナノ粒子の移動量に基づく細胞浸潤時の力場計測**
Force map of collective cells invading into biological matrix gels
Yuto Sano, Seohyun Lee, Hideo Higuchi (*University of Tokyo, School of Science, Department Physics*)

3Pos103 **Universal glass-forming behavior of living cytoplasm**
Masahiro Ikenaga, Kenji Nishizawa, Daisuke Mizuno (*Dept. of Phys., Univ. Kyushu*)

3Pos104 **超解像顕微鏡で観察された、ラメリポーディア領域のファシンとアクチンメッシュ ワークの相互作用**
Interaction between fascin and actin meshwork in lamellipodial region revealed with superresolution microscopy
Minami Tanaka[1,2], Ryoki Ishikawa[3], Kaoru Katoh[2] ([1]*Grad. Sch. Life & Env. Sci., Univ. Tsukuba*, [2]*Bio Mes Res. Inst., AIST*, [3]*Gunma Pref. Coll. Health Sci*)

3Pos105 **Live-cell analysis of actin network by high-speed atomic force microscopy**
Yoshitsuna Itagaki, Yanshu Zhang, Aiko Yoshida, Masahiro Kumeta, Shige H. Yoshimura (*Grad. Sch. Biostudies, Kyoto Univ.*)

3Pos106 **原子間力顕微鏡による正常および肺高血圧症の肺動脈平滑筋細胞の弾性率測定**
Elastic modulus of pulmonary arterial smooth muscle cells in normal and pulmonary arterial hypertension patient by atomic force microscopy
Nao Tatsumi[1], Shinichi Katsuragi[2], Ryosuke Tanaka[1], Hidekazu Ishida[2], Shigetoyo Kogaki[2], Takaharu Okajima[1] ([1]*Grad. Schl. Inform. Sci. and Technol., Hokkaido Univ.*, [2]*Dept. Ped., Grad. Schl. Med., Osaka Univ.*)

3Pos107 **細胞競合現象における細胞内部環境のダイナミクス**
The dynamics of intracellular environments under cell competition
Katsuhiro Umeda[1], Wataru Nagao[1], Kenji Nishizawa[1], Shunsuke Kon[2], Yasuyuki Fujita[2], Daisuke Mizuno[1] ([1]*Grad. Sch. Sci., Univ. Kyushu*, [2]*Grad. Sch. Sci., Univ. Hokkaido*)

3Pos108 **光ゆらぎ法による酸化ストレスを受けた動物細胞の損傷度の計測**
Evaluation of oxidative stress in mammalian cell by intensity fluctuation method
Morito Sakuma, Yuichi Kondo, Hideo Higuchi (*Department of Physics, Graduate School of Science, The University of Tokyo*)

3Pos109 **On bending rigidity of microtubules measured from in vitro motility assay with external force**
Takahiro Nitta (*Applied Physics Course, Gifu Univ.*)

3Pos110 **GPI アンカー型受容体プリオンタンパク質と Thy1 の動的メゾスケール拡散停止：1 分子追跡による検出**
Dynamic mesoscale anchorage of GPI-anchored receptors prion protein and Thy1 in the cell membrane as revealed by single molecule tracking
Yuri L. Nemoto[1,2,4], Roger J. Morris[3], Hiroko Hijikata[1], Taka A. Tsunoyama[4], Akihiro C. E. Shibata[1,2], Rinshi S. Kasai[2], Akihiro Kusumi[1,2,4], Takahiro K. Fujiwara[1] ([1]*Center for Meso-Bio Single-Molecule Imaging (CeMI), Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto Univ.*, [2]*Institute for Frontier Life and Medical Sciences, Kyoto Univ.*, [3]*Department of Chemistry, King's College London*, [4]*OIST*)

3Pos111 **Stiffness measurement of bacterial cell using high-resolution imaging tracking**
Chih-Chao Liao, Chien-Jung Lo (*National Central University*)

3Pos112 **べん毛 III 型分泌装置のある構成因子は膜内部で Rhomboid プロテアーゼ GlpG による切断を受ける**
A component of the flagellar type III secretion system receives proteolytic cleavage by rhomboid protease GlpG inside the membrane
Yohei Hizukuri, Kosuke Terushima, Yoshinori Akiyama (*Inst. Front. Life Med. Sci., Kyoto Univ.*)

3Pos113 **単一細胞におけるミトコンドリアのダメージと活性酸素発生の同時観察**
Simultaneous measurements of mitochondrial damages and ROS generation in single cells
Emika Shida, Yoshihiro Ohta (*Ohta. Lab., Univ. Noko*)

3Pos114 **Molecular mechanism of T cell signaling termination**
Hiroaki Machiyama, Tadashi Yokosuka (*Dept. Immunol, Tokyo Med. Univ.*)

3Pos115 **Small GTPase, F-actin and cell morphology dynamics in migrating cells under well-defined noisy chemoattractant gradients**
Yoichi Irie[1], Taihei Fujimori[1], Akihiko Nakajima[2], Satoshi Sawai[1,2] ([1]*Grad. Sch. Arts Sci., Univ. Tokyo*, [2]*Res. Ctr. Complex Sys. Biol., Univ. Tokyo*)

3Pos116 **Investigating contribution of transcription to temperature in nucleus**
Shunsuke Takeda[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., The Univ. of Tokyo*, [2]*PRESTO, JST*)

3Pos117 **細胞性粘菌のアメーバ運動のブレブモードへの移行は、細胞外からの Ca^{2+}流入に依存しない**
Motility of *Dictyostelium* amoebae switches to the bleb mode without Ca^{2+} influx
Naoto Yoshinaga, Taro Uyeda (*Dept. Phys., Waseda Univ.*)

3Pos118 **前後運動する神経幹細胞における力測定**
Traction Force working on Reversive Motion of Neural Stem Cells
Masahito Uwamichi, Masaki Sano (*Dept. of Phys, Univ. of Tokyo*)

行動 / Behavior

3Pos119 **微速度撮影によるユーカリ苗の根生長速度における電界応答測定**
Electric response measurement of E. camaldulensis in seedling root growth by time lapse photography
Kazuki Sugawara[1], Yutaro Mukai[1], Hideki Suganuma[2], Shigeru Kato[1], Takuya Ito[1], Toshinori Kojima[1], **Seiichi Suzuki**[1] ([1]*Faculty of Science and Technology, Seikei University*, [2]*Kawasaki Environment Research Center*)

3Pos120 **繊毛虫テトラヒメナの空間の広がりに対する適応能**
Adaptive capacity in response to spatial expansion in the ciliate protozoan Tetrahymena
Itsuki Kunita[1], Tatsuya Yamaguchi[2], Atsushi Tero[2], Masakazu Akiyama[3], Shigeru Kuroda[3], Toshiyuki Nakagaki[3] ([1]*University of The Ryukyus*, [2]*Kyushu University*, [3]*Hokkaido University*)

3Pos121 **モジホコリ変形体における行動決定の揺らぎ**
Fluctuation in decision-making of Physarum plasmodium
Yuya Mitsutake, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

3Pos122 **モジホコリ変形体における周期刺激に対する輸送管ネットワークの適応**
Adaptation of transportation network against periodic stimuli in Physarum plasmodium
Akira Ishizaki, Satoshi Toyoda, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

光生物：視覚・光受容 / Photobiology: Vision & Photoreception

3Pos123 **Cloning of cryptochrome 2 gene from honey bee**
Yuhei Hosokawa, Shigenori Iwai, Junpei Yamamoto (*Grad. Sch. Eng. Sci., Univ. Osaka*)

3Pos124 **ナトリウムイオンポンプ型ロドプシンの細胞外側表面に位置する酸性残基の機能解析**
Functional analyses of Na^+-pumping rhodopsin focusing on acidic residues on the extracellular surface
Akiko Okamura[1], Takashi Kikukawa[1,2], Takashi Tsukamoto[1,2], Tomoyasu Aizawa[1,2], Naoki Kamo[1], Makoto Demura[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*GSS, GI-CoRE, Hokkaido Univ.*)

3Pos125 ***Natronomonas pharaonis* halorhodopsin T126E 変異体の機能解析**
Functional analysis of T126E mutant of *Natronomonas pharaonis* halorhodopsin
Shuhei Abe[1], Takashi Kikukawa[1,2], Takashi Tsukamoto[1,2], Tomoyasu Aizawa[1,2], Naoki Kamo[1], Makoto Demura[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*GSS, GI-CoRE, Hokkaido Univ.*)

3Pos126 **NTQ 型アニオンポンプの輸送機能と構造解析**
Functional and Structural Analysis of NTQ type Anion Pump Rhodopsins
Miwako Teranishi[1], Shota Ito[1], Manish Singn[1], Keiichi Inoue[1,2], Hideki Kamitori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*,, [2]*PRESTO, JST*)

3Pos127 **二量体化がロドプシンの光構造変化に与える影響**
Effect of dimerization on the light-induced helical rearrangement of visual rhodopsin
Yasushi Imamoto[1], Keiichi Kojima[2], Toshihiko Oka[3], Ryo Maeda[4], Yoshinori Shichida[5] ([1]*Kyoto Univ.*, [2]*Okayama Univ.*, [3]*Shizuoka Univ.*, [4]*RIKEN*, [5]*Ritsumeikan Univ.*)

3Pos128 **^{13}C NMR 化学シフト値計算によるセンサリーロドプシンの光中間体におけるレチナール構造の解析**
Quantum chemical calculation of ^{13}C NMR chemical shifts for retinal at photo-intermediates in the photocycle of sensory rhodopsin
Yoshiteru Makino[1], Izuru Kawamura[1], Takashi Okitsu[2], Akimori Wada[2], Yuki Sudo[3], Naoki Kamo[4], Akira Naito[1], Kazuyoshi Ueda[1] ([1]*Grad. Sch. Eng., Yokohama Natl. Univ.*, [2]*Kobe Pharm. Univ.*, [3]*Grad. Sch. Med. Dent. Pharm., Okayama Univ.*, [4]*Grad. Sch. Life Sci., Hokkaido Univ.*)

3Pos129 **ショウジョウバエ Rh7 の特徴的な幅広い吸収スペクトルの解析**
Drosophila melanogaster Rh7 is a UV-to-visible light sensor having extraordinarily broad absorption spectrum
Kazumi Sakai[1], Kei Tsutsui[1], Takahiro Yamashita[1], Naoyuki Iwabe[1], Keisuke Takahashi[1], Akimori Wada[2], Yoshinori Shichida[1] ([1]*Grad. Sch. Sci., Kyoto Univ.*, [2]*Organic Chemistry for Life Science, Kobe Pharm. Univ.*)

3Pos130 **青色光センサー PixD の光反応とその多様性**
Study on diversity of photoreactions among various homologous PixD proteins
Shunrou Tokonami, Yusuke Nakasone, Masahide Terazima (*Grad. Sch. Sci., Univ. Kyoto*)

3Pos131 **緑藻の光駆動プロトンポンプであるアセタブラリアロドプシン II のフォトサイクルにおける２つの O 中間体の存在**
Existence of two O intermediates in the photocycle of *Acetabularia* rhodopsin II, a light-driven algal proton pump
Jun Tamogami[1], Takashi Kikukawa[2,3], Toshifumi Nara[1], Makoto Demura[2,3], Tomomi Kimura-Someya[4,5], Mikako Shirouzu[4,5], Shigeyuki Yokoyama[4,6], Seiji Miyauchi[7], Kazumi Shimono[7,8], Naoki Kamo[2] ([1]*College Pharm. Sci., Matsuyama Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*, [3]*Glob. Sta. for Soft Mat., Glob. Ins. for Col. Res., Edu., Hokkaido Univ.*, [4]*RIKEN SSBC*, [5]*RIKEN CLST*, [6]*RIKEN Structural Biology Laboratory*, [7]*Grad. Sch. Pharm. Sci., Toho Univ.*, [8]*Fac. Pharm. Sci., Sojo Univ.*)

3Pos132 **Quantitative evaluation of UV-induced cell death and its resistance by drug in human epidermal keratinocytes**
Noritaka Masaki, Shigetoshi Okazaki (*Dept. Med. Spec., Hamamatsu Univ. Sch. Med.*)

3Pos133 **Comparison of chromophore environments between rhodopsin and cone visual pigment using Fourier transform infrared spectroscopy**
Naoto Noguchi[1], Takahiro Yamashita[1], Yoshinori Shichida[2], Yasushi Imamoto[1] ([1]*Kyoto University*, [2]*Ritsumeikan University*)

光生物：光合成 / Photobiology: Photosynthesis

3Pos134 **FTIR 分光電気化学法による光化学系 II 第一キノン Q_A の酸化還元電位計測：Mn 除去の影響**
Influence of Mn depletion on the redox potential of the primary quinone Q_A in photosystem II as revealed by FTIR spectroelectrochemistry
Ayaka Ohira, Ryo Nagao, Takumi Noguchi, Yuki Kato (*Grad. Sch. Sci., Nagoya Univ.*)

3Pos135 **ATR-FTIR 解析による光化学系 II における非ヘム鉄のヒスチジン配位子のプロトン化状態**
ATR-FTIR study on the protonation state of a histidine ligand to the non-heme iron in photosystem II
Masakazu Kimura, Shin Nakamura, Yuki Kato, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Univ.*)

3Pos136 **光化学系 II 結晶における水分解 S 状態遷移の ATR-FTIR 解析**
ATR-FTIR analysis of the S-state transitions during water oxidation in photosystem II crystals
Yuki Kato[1], Fusamichi Akita[2,3], Yoshiki Nakajima[2], Michihiro Suga[2], Yasufumi Umena[2], Jian-Ren Shen[2], Takumi Noguchi[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Res. Inst. Interdiscip. Sci., Okayama Univ.*, [3]*JST-PRESTO*)

3Pos137 **ヘリオバクテリア光合成反応中心のドナー側とアクセプター側における電子伝達反応の解析**
Analyses of electron transfer reactions on donor and acceptor sides in heliobacterial photosynthetic reaction center
Risa Kojima[1], Chihiro Azai[2], Shigeru Itoh[3], **Hirozo Oh-oka**[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*, [3]*Grad. Sch. Sci., Nagoya Univ.*)

3Pos138 **光化学系 II における Mn クラスターの光活性化過程の FTIR および量子化学計算による解析**
FTIR and quantum chemical calculation study of the photoactivation process of the Mn cluster in photosystem II
Shin Nakamura, Akihiko Sato, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Univ.*)

3Pos139 **北海道の河川から採取した紅色非硫黄細菌による水素生成に対する pH と基質濃度の影響**
Effect of pH and substrate concentration on hydrogen production by purple non-sulfur bacteria from rivers in Hokkaido
Mayoka Kanoh[1], Haruna Minakami[2], Seigo Kumakura[2], Yusuke Kato[2], Masahiro Hibino[1,2] ([1]*Div. Sustain. Environ. Eng., Muroran Inst. Tech.*, [2]*Dept. Appl. Sci., Muroran Inst. Tech.*)

3Pos140 **構造解明されている 2 種類の紅色光合成細菌の LH2 タンパク質からの B800 バクテリオクロロフィル a の脱離挙動解析**
Analysis of removal of B800 bacteriochlorophyll a from structure-determined LH2 proteins derived from two purple photosynthetic bacteria
Yoshitaka Saga[1,2], Keiya Hirota[1], Kokomi Doi[1] ([1]*Kindai Univ.*, [2]*PRESTO, JST*)

3Pos141 **新奇クロロフィルを持つシアノバクテリアにおけるクロロフィル *f* 蓄積過程のエネルギー移動の解析**
Spectral characterization of new chlorophyll containing cyanobacterium in the accumulation process of chlorophyll *f*
Toshiyuki Shinoda[1], Keishi Arai[2], Hiroki Tabushi[2], Seiji Akimoto[3], Tatsuya Tomo[1,2] ([1]*Grad. Sch. Sci., Tokyo Univ. Sci.*, [2]*Fac. Sci., Tokyo Univ. Sci.*, [3]*Fac. Sci., Kobe Univ.*)

3Pos142 **Spectral characterization of Photosystem II reaction center in a chlorophyll d-dominated cyanobacterium**
Reona Toyofuku[1], Kaichiro Endo[2], Toshiyuki Shinoda[1], Seiji Akimoto[3], Tatsuya Tomo[1] ([1]*Grad. Sch. Sci., Tokyo Univ. Sci.*, [2]*Grad. Sch. Sci., Tokyo Univ.*, [3]*Grad. Sch. Sci., Kobe Univ.*)

3Pos143 **ヘリオバクテリア反応中心の初期電荷分離スピン相関解析ラジカル対の捕捉**
Initial charge separated spin-polarized radical pair in reaction center of *Heliobacterium modesticaldum*
Hiroyuki Mino[1], Hiroyuki Tsukuno[1], Risa Mutoh[2,3], Hiroki Nagashima[1,4], Yasuhiro Kobori[4], Genji Kurisu[2], Hirozo Oh-oka[5] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*Inst. Protein. Res., Osaka Univ.*, [3]*Fac. Sci., Univ. Fukuoka*, [4]*Mol. Photosci. Res., Kobe Univ.*, [5]*Grad. Sch. Sci., Univ. Osaka*)

3Pos144 **光合成における電子伝達体のダイナミックスに関する理論的研究**
Theoretical studies on dynamics of electron carriers in photosynthesis
Hidemi Nagao, Satoshi Nakagawa, Isman Kurniawan, Koichi Kodama, Muhammad Arwansyah, Kazutomo Kawaguchi (*Kanazawa University*)

3Pos145 **光化学系複合体と炭素ナノ材料間の電子移動反応**
Linear electron transfer between photosystems and carbon nanomaterials
Shota Tanaka[1], Mariko Miyachi[2], Yoshinori Yamanoi[2], Akihide Iwase[1], Akihiko Kudo[1], Hiroshi Nishihara[2], Tatsuya Tomo[1] ([1]*Grad. Sch. Sci., Tokyo Univ. of Sci.*, [2]*Grad. Sch. Sci., Tokyo Univ.*)

3Pos146 **高等植物の光化学系 II における効率的な電荷分離反応のメカニズム**
The mechanism of efficient charge separation reaction in photosystem II of higher plants
Hiroki Nagashima[1,2], Masashi Hasegawa[3], Reina Minobe[3], Hiroyuki Mino[2], Yasuhiro Kobori[1,3] ([1]*Molecular Photoscience Research Center, Kobe Univ.*, [2]*Grad. Sch. Sci., Nagoya Univ.*, [3]*Grad. Sch. Sci. Kobe Univ.*)

3Pos147 **The dynamics of photosystem 2 and light-harvesting complex 2 in spinach grana membrane revealed by high-speed AFM**
Risa Mutoh, Takahiro Iida, **Daisuke Yamamoto** (*Faculty of Science, Fukuoka Univ.*)

3Pos148 **ステート遷移における光捕集系の膜内移動の検証**
Verification of Shuttling of Light-Harvesting Complexes upon State Transition
Yuki Fujita, Yutaka Shibata (*Tohoku University*)

光生物：光遺伝学・光制御 / Photobiology: Optogenetics & Optical Control

3Pos149 **水晶振動子微量天秤による光制御型 bZip モジュール photozipper 及び N131 変異体の DNA 結合の解析**
DNA-binding of a light-regulated bZIP module, photozipper and Asn131 mutants analyzed by quartz crystal microbalanc
Samu Tateyama, Osamu Hisatomi (*Grad. Sch. Sci., Univ. Osaka*)

3Pos150 フォトジッパーにおける Q317 の機能解明
Function of Q317 in Photozipper
Itsuki Kobayashi, Yuki Yabe, Yoichi Nakatani, Osamu Hisatomi (*Grad. Sci., Univ. Osaka*)

3Pos151 アニオンチャネルロドプシン 2(ACR2)の線虫における超高感度光神経抑制活性
Ultrasensitive neural silencing activity of Anion channelrhodopsin-2 (ACR2) in *Caenorhabditis elegans*
Misayo Maki[1], Satoko Doi[1], Keiichi Kojima[1], Srikanta Chowdhury[2], Takashi Tsukamoto[1], Akihiro Yamanaka[2], Shin Takagi[3], Yuki Sudo[1] ([1]*Grad. Sch. of Med. Dent. & Pharm. Sci., Univ. Okayama*, [2]*RIEM, Univ. Nagoya*, [3]*Grad. Sch. of Sci., Univ. Nagoya*)

3Pos152 光駆動ナトリウムポンプロドプシンの活性中心の水素結合構造
Hydrogen-bonding network in the active site of light-driven sodium pumping rhodopsins
Shota Ito, Sahoko Tomida, Hideki Kandori (*Nagoya Inst. Tech.*)

3Pos153 光捕集カロテノイドアンテナと相互作用する光駆動プロトンポンプ TR の創出
Production of a light-driven proton pump TR interacted with light-harvesting carotenoid antennae
Keigo Nishikawa[1], Keiichi Kojima[1], Shigeko Kawai-Noma[2], Sayaka Nemoto[3], Takeshi Murata[3], Daisuke Umeno[1,2], Yuki Sudo[1] ([1]*Grad. Med. Den. Pha., Univ. Okayama*, [2]*Dep. Applied Chemistry and Biotechnology., Univ. Chiba*, [3]*Grad. Sci., Univ. Chiba*)

3Pos154 光誘起チャネルロドプシンに関する理論研究
Theoretical study on molecular mechanism of photo-induced gate opening of channelrhodopsin
Cheng Cheng[1], Motoshi Kamiya[1], Norio Yoshida[2], Shigehiko Hayashi[1] ([1]*Grad. of Science, Kyoto Univ.*, [2]*Grad. of Science, Kyushu Univ.*)

3Pos155 光制御型 bHLH-ZIP 転写因子の開発
Development of a light-regulated bHLH-ZIP transcription factor
Yoichi Nakatani, Osamu Hisatomi (*Grad. Sch. of Sci., Osaka Univ.*)

3Pos156 光駆動イオントランスポーターハロロドプシンの理論的研究
Theoretical study on molecular mechanism of a light-driven ion transport of Halorhodopsin
Ryo Oyama, Taisuke Hasegawa, Shigehiko Hayashi (*Grad. Sch. Sci., Univ. Kyoto*)

放射線生物学・活性酸素 / Radiobiology & Active oxygen

3Pos157 **Effect of interaction between IP6 and NOX2 on monocytic differentiation**
Asuka Kato[1], Yuki Hirakawa[2], Wakako Hiraoka[2] ([1]*Department of Obstetrics and Gynecology, Fujita Health University School of Medicine*, [2]*Department of Physics, Graduate School of Science and Technology, Meiji University*)

3Pos158 放射線照射がミトコンドリア電子伝達系酸化還元関連分子に与える影響の電子スピン共鳴法を用いた評価。
Estimating physiological transition of electron transport chain with ESR in whole cell culture
Yukihaya Watanabe, Naoya Matsunaga, Wakako Hiraoka (*Dept. Phys., Grad. Sch. of Sci. & Tech., Meiji Univ.*)

3Pos159 **Cross talk between mitochondria and NOX2 in vitamin D_3-induced monocytic differentiation**
Naoya Matsunaga, Yukihaya Watanabe, Wakako Hiraoka (*Dept. Phys., Grad. Sch. Sci. & Tech., Meiji Univ.*)

生命の起源・進化 / Origin of life & Evolution

3Pos160 **Phenotypic Constraints Shaped by Evolution: Numerical and Experimental Approaches**
Chikara Furusawa[1,2], Kunihiko Kaneko[2,3] ([1]*QBiC, RIKEN*, [2]*UBI, Univ. Tokyo*, [3]*Grad. Sch. Art Sci., Univ. Tokyo*)

3Pos161 **Polymerization and information selection in template-directed ligation of information polymers**
Yasuhiro Magi, Shoichi Toyabe (*Appl. Phys., Tohoku Univ.*)

3Pos162 鋳型ライゲーションにおける拡散混合に対する情報保持の実験的証明
Experimental demonstration of information retention against diffusional mixing in templated ligation
Kazuki Hata, Yasuhiro Magi, Syoichi Toyabe (*Tohoku University, Applied Physics*)

3Pos163 アルカリ性熱水噴出孔における硫化鉄を触媒にした還元的炭素化合物生成過程の第一原理分子動力学シミュレーション
***Ab initio* molecular dynamics study of reducible carbon compounds production catalyzed by iron sulfides at an alkaline hydrothermal vent**
Kohei Shimamura[1], Fuyuki Shimojo[2], Aiichiro Nakano[3], Shigenori Tanaka[1] ([1]*Kobe Univ.*, [2]*Kumamoto Univ.*, [3]*Univ. of Southern California*)

3Pos164 凍結融解によるリポソーム融合を介した人工細胞への栄養供給法の確立
Sustainable biochemical reactions in liposoems by liposome fusion via the freeze-thaw
Gakushi Tsuji[1,2], Takeshi Sunami[1,2], Satoshi Fujii[1], Norikazu Ichihashi[1,3] ([1]*Grad. Sch. of IST, Osaka University*, [2]*IAI, Osaka University*, [3]*Grad. Sch. of FBS, Osaka University*)

ゲノム生物学：ゲノム構造 / Genome biology: Genome structure

3Pos165 出芽酵母の tRNA 遺伝子の転写量と核内における空間配置との相関解析
Analysis of Correlation Between tRNA Levels and Spatial Arrangement of tRNA Genes in the Budding Yeast Nucleus
Naoko Tokuda, Masaki Sasai (*Grad. Sch. Eng., Nagoya Univ.*)

3Pos166 **A quasi-harmonic approach to investigating chromatin domains**
S.S Ashwin[1], Tadasu Nozaki[2], Kazuhiro Maeshima[2], Masaki Sasai[1] ([1]*Department of Applied Physics, Nagoya University*, [2]*Structural Biology Center, National Institute of Genetics*)

3Pos167 **The phase-separation principle of human genome architecture**
Shin Fujishiro, Masaki Sasai (*Dept. Comp. Sci. & Eng., Nagoya Univ.*)

3Pos168 **Transient local contacts and meta-stable global organization of human interphase chromosomes**
Lei Liu, Changbong Hyeon (*Sch. Comp. Sci., KIAS*)

ゲノム生物学：ゲノム機能 / Genome biology: Genome function

3Pos169 **遺伝子発現におけるポリアミンの促進と阻害の二面性**
Dual effect of polyamines on gene expression: Acceleration and inhibition
Ai Kanemura[1], Yuko Yoshikawa[1], Takahiro Kenmotsu[1], Wakao Fukuda[2], Kenichi Yoshikawa[1] ([1]*Doshisha University*, [2]*Ritsumeikan University*)

3Pos170 **Microdroplet-based screening method for microbes producing polymer-degrading enzymes**
Kai Saito[1], Ryo Iizuka[1], Eiji Shigihara[1], Wataru Kawakubo[2], Dong Hyun Yoon[2], Tetsuji Sekiguchi[3], Shuichi Shoji[2], Yuji Hatada[4], Takashi Funatsu[1] ([1]*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*, [2]*Dept. of Nanosci. and Nanoeng., Waseda Univ.*, [3]*Res. Org. for Nano & Life Innov., Waseda Univ.*, [4]*Dept. of Life Sci. and Green Chem., Saitama Inst. of Technol.*)

バイオインフォマティクス：構造ゲノミクス / Bioinformatics: Structural genomics

3Pos171 **機械学習を用いたタンパク質と薬のドッキング予測**
A new prediction method for complex structures of protein and small molecule with machine learning
Fumiaki Sato, Kota Kasahara, Takuya Takahashi (*Col. Life Sci., Ritsumeikan Univ*)

3Pos172 **拡張アンサンブル分子動力学法のサンプリング効率向上のための最適条件の探索**
Investigation of appropriate conditions for enhancing sampling efficiency of multi-canonical molecular dynamics
Takuya Shimato[1], Kota Kasahara[1], Junichi Higo[2], Takuya Takahashi[1] ([1]*Col. Life Sci., Ritsumeikan Univ.*, [2]*IPR, Osaka Univ.*)

3Pos173 **Statistical analysis of correlation between amino acid sequence and protein function based on using Protein Data Bank**
Ryohei Kondo, Kota Kasahara, Takuya Takahashi (*Col. Life Sci., Ritsumeikan Univ.*)

3Pos174 **MEGADOCK-WEB: タンパク質間相互作用予測の統合データベース**
MEGADOCK-WEB: an integrated database of structure-based protein-protein interaction predictions
Masahito Ohue[1,2], Takanori Hayashi[1,3], Yuri Matsuzaki[3], Keisuke Yanagisawa[1,3], Yutaka Akiyama[1,2,3] ([1]*Dept CS, Sch Comput, Tokyo Tech*, [2]*ACDD, IIR, Tokyo Tech*, [3]*ACLS, Tokyo Tech*)

3Pos175 **生体膜系におけるヘリックス間の相互作用パターン解析**
Analysis of helix interaction pattern in each biological membrane environment
Masato Sakai[1], Masami Ikeda[2], Makiko Suwa[1,2] ([1]*Biol. Sci., Grad. Sci. Eng., Aoyama Gakuin Univ.*, [2]*Chem. Biol. Sci., Sci. Eng., Aoyama Gakuin Univ.*)

3Pos176 **ポリグルタミン酸のヘリックスコイル転移における末端の安定性に関する分子動力学法による検討**
Study on helix-coil transition stability of the termini of poly-glutamic acid using molecular dynamics method
Naoki Ogasawara[1], Ryosuke Iwai[1], Kota Kasahara[2], Takuya Takahashi[2] ([1]*Grad. Life. Sci., Ritsumeikan Univ.*, [2]*Col. Life. Sci., Ritsumeikan Univ.*)

3Pos177 **What are the structural features of superfolds? a case study of beta-sheet proteins**
George Chikenji[1], Hayao Imakawa[1], Shintaro Minami[2] ([1]*Dep. App. Phys., Nagoya Univ.*, [2]*CIMoS, IMS*)

3Pos178 **Annotation of missense genomic variations based on various protein 3D structures**
Matsuyuki Shirota[1,2,3] ([1]*Grad. Sch. Med., Tohoku Univ.*, [2]*ToMMo, Tohoku Univ.*, [3]*Grad. Sch. Inform. Sci. Tohoku Univ.*)

バイオインフォマティクス：分子進化 / Bioinformatics: Molecular evolution

3Pos179 **機能に関する選択圧による P-loop 蛋白質のフォールド多様性についてのシミュレーション**
Simulated diversification of the P-loop protein fold through functional selection
Kohei Inukai, Masaki Sasai, George Chikenji (*Department of Applied Physics, Nagoya University*)

数理生物学 / Mathematical biology

3Pos180 **Neo-logistic model precisely predicting a bacteria growth curve**
Tohru Tashiro[1], Fujiko Yoshimura[2] ([1]*Dept. Sci., Ochanomizu Univ.*, [2]*Sch. Comput., Tokyo Tech.*)

3Pos181 **細胞間および基質との接着を考慮した細胞集団の粒子モデル**
Individual cell-based model for cell population considering cell-cell and cell-matrix adhesion
Seiya Nishikawa, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

3Pos182 **ストレスを受けた概日時計における位相変動の数理モデル**
A mathematical model for stress induced phase shift in mammalian circadian systems
Yosuke Someya, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

3Pos183 **Mathematical model for motor-filament aster locomotion on motor-coated substrate**
Masahiro Sawada[1,2], Takayuki Torisawa[2,3], Kazuhiro Oiwa[2,3], Shuji Ishihara[1,2] ([1]*Grad. Sch. Arts and Sciences, Univ. Tokyo*, [2]*CREST, JST*, [3]*Advanced ICT Inst., NICT*)

3Pos184 **Probability eddy currents in a coupled genetic and epigenetic network**
Bhaswati Bhattacharyya, Masaki Sasai (*Nagoya University*)

3Pos185 **ヒト血糖値調節におけるホルモン・代謝物の血中動態の数理モデルを用いた解析**
Mathematical model analysis for blood glucose homeostasis regulated by blood hormones and metabolites in humans
Kaoru Ohashi[1], Masashi Fujii[1], Shinsuke Uda[2], Hiroyuki Kubota[2], Hisako Komada[3], Kazuhiko Sakaguchi[3], Wataru Ogawa[3], Shinya Kuroda[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Med. Ins. of Bioreg., Kyushu Univ.*, [3]*Grad. Sch. Med., Kobe Univ.*)

3Pos186 **ErbB シグナル転写ネットワークの新規統合数理モデルの構築と制御反応の同定**
A new integrated mathematical model of the ErbB signaling and transcriptional network reveals key reactions determining the ErbB response
Hiroaki Imoto, Mariko Okada, Kazunari Iwamoto (*IPR, Osaka Univ.*)

3Pos187 **真性粘菌変形体の細胞運動が有する Lévy-walk 的性質**
Levy-walk nature in the cell migration of Physarum plasmodium
Tomohiro Shirakawa[1], Takayuki Niiato[2], Hiroshi Sato[1], Ryota Ohno[1] ([1]*Department of Computer Science, School of Electrical and Computer Engineering, National Defense Academy of Japan*, [2]*Department of Intelligent Interaction Technologies, Graduate School of Systems and Information Engineering, University of Tsukuba*)

3Pos188 **細胞知覚の位相推定モデル**
Phase Detection Model of Cellular Sensing
Ryo Yokota, Tetsuya, J. Kobayashi (*Institute of Industrial Science, The University of Tokyo*)

3Pos189 **３次元フェイズフィールドモデルによるアメーバ細胞動態の解析**
Cellar 3D phase-field model for amoeboid movement
Nen Saito[1], Satoshi Sawai[2] ([1]*Graduate School of Science, University of Tokyo*, [2]*Department of Basic Science, Graduate School of Arts and Sciences, University of Tokyo*)

計測 / Measurements

3Pos190 **Imaging of cysteic acid produced in ultraviolet-irradiated hair using synchrotron radiation**
Kosuke Watanabe[1], Chinami Ariji[2], Daisuke Yoshida[2], Sho Kobayashi[1], Takaaki Maeda[1], Kazuyuki Suzuta[1], Len Ito[1] ([1]*MILBON CO., LTD.*, [2]*COSMOS TECHNICAL CENTER CO., LTD.*)

3Pos191 **光第二高調波顕微鏡によるタンパク質構造解析**
Optical second-harmonic generation microscope as a tool for protein structure analysis
Junichi Kaneshiro[1], Yasushi Okada[1,2], Tomohiro Shima[2], Mika Tsujii[3], Katsumi Imada[3], Taro Ichimura[1], Tomonobu M. Watanabe[1] ([1]*RIKEN QBiC*, [2]*Grad. Sch. Sci. Univ. Tokyo*, [3]*Grad. Sch. Sci. Osaka Univ.*)

3Pos192 **Continuous fluorescence observation without oxygen scavengers using a LED-based fluorescence microscope**
Shin Yamaguchi[1], Kazuki Nakajima[1], Junichiro Yajima[2], Yuichi Inoue[1] ([1]*SIGMAKOKI Co., LTD*, [2]*Dept. of Life Sciences, Graduate School of Arts and Sciences, The Univ. of Tokyo*)

3Pos193 **初期胚発生過程における細胞弾性率と細胞骨格構造の時空間変動**
Spatiotemporal change in elastic modulus and cytoskeletal structure of cells in early embryonic development
Yuki Fujii[1], Taichi Imai[2], Wataru Koizumi[2], Kohji Hotta[2], Kotaro Oka[2], Takaharu Okajima[1] ([1]*Grad. Schl. Inform. Sci and Tech. Hokkaido Univ.*, [2]*Grad. Schl. Biosci. and Bioinfo. Keio Univ.*)

3Pos194 **Analysis of the number density distribution of colloidal particles on a substrate before solidification: A study of biomineralization**
Amano Ken-ichi, Taira Ishihara, Nishi Naoya, Tetsuo Sakka (*Grad. Sch. Eng., Kyoto Univ.*)

3Pos195 **改良型蛍光 ATP センサーを用いた細胞内代謝変化の可視化**
Visualization of intracellular metabolic changes using an improved fluorescent ATP indicator in mammalian cells
Hideyuki Yaginuma, Yasushi Okada (*QBiC, RIKEN*)

3Pos196 **蛍光相互相関分析に及ぼすヘモグロビン光吸収の影響**
Effects of hemoglobin absorption on fluorescence cross correlation analysis
Atsushi Matsuo, Yasutomo Nomura (*Maebashi Institute of Technology*)

3Pos197 **単一細胞中でのミトコンドリア電子伝達の計測**
Measurements of mitochondrial electron transfer in a single cell
Hiroko Kashiwagi, Yoshihiro Ohta (*Ohta. Lab., Univ. Noko*)

3Pos198 **蛍光分子薄膜の紫外可視光変換システム解析**
Ultra violet visible light conversion system analysis of fluorescent molecular thin film
Shotaro Minato[1], Taiyo Tsurugai[1], Miku Kaneta[1], Honoka Endo[1], Hiroshi Masumoto[2], Takashi Goto[3], **Yutaka Tsujiuchi**[1] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary*, [3]*Institute for Materials Research, Tohoku University*)

バイオイメージング / Bioimaging

3Pos199 **Quantitative imaging analysis of microtubule-organizing center repositioning mediated by CLIP-170 phosphorylation during T cell activation**
Wei Ming Lim[1], Yuma Ito[1], Kumiko Sakata-Sogawa[2], Makio Tokunaga[1] ([1]*Sch. Lif. Sci. Tech., Tokyo Ins. Tech.*, [2]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

3Pos200 **Comparison of the analgesic effects of different types of therapeutic agents on allodynia-specific pain using fMRI**

Yuri Kitamoto[1], Sosuke Yoshinaga[1], Naoya Yuzuriha[1], Hiroshi Sato[2], Mitsuhiro Takeda[1], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Univ. Kumamoto*, [2]*Bruker Biospin*)

3Pos201 **１分子イメージングによる機能性 RNA TERRA の動態・局在解析**

Dynamics and localization of a non-coding RNA TERRA in living cells revealed by single molecule imaging

Hideaki Yoshimura, Toshimichi Yamada, Rintaro Shimada, Takeaki Ozawa (*Sch. Sci., Univ. Tokyo*)

3Pos202 **生物発光イメージング法を用いたグルカゴン分泌の可視化解析系の構築**

Video rate bioluminescence imaging of glucagon secretion from pancreatic alpha cells

Satoru Yokawa[1], Takahiro Suzuki[2], Satoshi Inouye[3], Yoshikazu Inoh[1], Ryo Suzuki[4], Naohide Hirashima[4], Tadahide Furuno[1] ([1]*Sch. Pharm., Aichi Gakuin Univ.*, [2]*Sch. Dent., Aichi Gakuin Univ.*, [3]*JNC Co., Yokohama*, [4]*Grad. Sch. Pharm. Sci., Nagoya City Univ.*)

3Pos203 **遊走細胞からの分泌を実時間で可視化する**

Real-time secretion tracking system for migrating single cells

Yoshitaka Shirasaki[1], Yosuke Yasuzawa[1], Yumiko Tanaka[1], Nobutake Suzuki[1], Sotaro Uemura[1], Kazuyo Moro[2] ([1]*Dep. Biol. Sci., Grad. Sch. of Sci., The Univ. of Tokyo*, [2]*IMS, RIKEN*)

3Pos204 **細胞・組織内生体分子の動態を可視化する逆ラマン顕微測定システムの開発**

Development of inverse Raman micro spectroscopic system toward visualizing the dynamics of biomolecule *in vivo* and *in cellulo*

Yuka Kawahara-Nakagawa, Satoru Nakashima, Takashi Ogura (*Grad. Sch. Sci., Univ. Hyogo*)

3Pos205 **細胞内温度変化による細胞機能制御の分子機構の解明**

Investigating molecular mechanism of intracellular temperature dependent cell functions

Yu Bi[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pha. Sci., Univ. Tokyo*, [2]*JST-PRESTO*)

3Pos206 **振動和周波検出赤外超解像顕微鏡法による爪・毛髪中のケラチンタンパク質の分布・配向観察**

Molecular distribution and orientation of keratins in human nails and human hairs observed by VSFG-detected IR super-resolution microscopy

Yuichiro Iwasaki, Maho Hata, Mitsuki Fujiwara, Ryo Morimoto, **Hirona Takahashi**, Makoto Sakai (*Okayama University of Science*)

3Pos207 **振動和周波検出赤外超解像顕微鏡法による羽毛 β-ケラチンの分子配向イメージング**

Orientation-sensitive molecular imaging of feather β-keratins by a VSFG-detected IR super-resolution microscopy

Kota Yamamoto, Kosuke Tatekabe, Tomoya Miyake, Yuya Kimura, Hirona Takahashi, **Makoto Sakai** (*Okayama University of Science*)

3Pos208 **Evaluation of anesthesia conditions for detecting odor responses in the mouse whole brain**

Fuyu Hayashi, Hirotsugu Funatsu, Sosuke Yoshinaga, Naoya Yuzuriha, Shunsuke Kusanagi, Mitsuhiro Takeda, Hiroaki Terasawa (*Fac. Life Sci., Kumamoto Univ.*)

3Pos209 **１分子軌跡追跡により時空間動態と結合解離を定量する解析法**

An analysis method for quantification of spatiotemporal dynamics and kinetics using single-molecule tracking

Yuma Ito[1], Kumiko Sakata-Sogawa[1,2], **Makio Tokunaga**[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

3Pos210 **マウスノロウイルス MNV-S7 のクライオ電顕単粒子構造解析**

Capsid Structure of Murine Norovirus S7 revealed by cryo-electron microscopy

Chihong Song[1], Naoyuki Miyazaki[2], Kenji Iwasaki[2], Motohiro Miki[3], Reiko Todaka[4], Kei Haga[4], Akira Fujimoto[4], Kazuhiko Katayama[4], Kazuyoshi Murata[1] ([1]*NIPS*, [2]*IPR*, [3]*Denka Co., Ltd.*, [4]*Kitasato Univ.*)

1SAA-1 Spatiotemporal dynamics of flow-related biological patterns: Overview

Takayuki Torisawa (*Advanced ICT Inst., NICT*)

"Everything flows": this statement by an ancient Greek philosopher now sheds light on a new direction of biophysical studies. In recent years, a wide variety of studies have emerged focusing on the diverse flow-related phenomena in biological systems, the components of which were cytoskeletal proteins, cilia, or cells. In this session, we would like to discuss the growing and interdisciplinary field of flow-related spatiotemporal dynamics ranging from a theory on a single element to an experiment on collective behavior of real cells with the promising young investigators with diverse backgrounds.

1SAA-2 Multiscale dynamics of red blood cells in flow

Stephanie Nix, Yukitaka Ishimoto (*Akita Pref. U.*)

Red blood cells must undergo large and complex deformations in order to fulfill their role to transport oxygen and carbon dioxide throughout the body. While the basic dynamics of red blood cells in simple flows has been clarified, much remains to be investigated in the relationships between red blood cell deformation, the applied flow, and their effects on related phenomena such as oxygen transport. In this presentation, we explore topics related to the microscale flow patterns of red blood cells, such as the effect of red blood cell deformation on mass transport and factors that may lead to the flow-induced rupture of red blood cells.

1SAA-3 細胞表層シートを用いた繊毛虫ゾウリムシ繊毛運動の解析
Analysis on the ciliary movements in *Paramecium* using the ciliated cortical sheet

Osamu Kutomi[1,2], Manabu Hori[3] ([1]*Grad. Sch. Sci. and Eng., Univ. Toyama*, [2]*Grad. Sch. Med., Univ. Yamanashi*, [3]*Fac. Sci., Yamaguchi Univ*)

In unicellular ciliates, *Paramecium*, there are several thousand cilia on the cell surface. The cilia beat with coordination, allowing the cell to swim freely. It is well known that the ciliary movement are regulated by second messengers, such as cAMP and Ca^{2+}, and generated by axonemal dynein-driven microtubule sliding. However, the molecular mechanisms of ciliary movement remain unclear. We have analyzed the ciliary movement in *Paramecium* using the ciliated cortical sheet, an experimental system enabling the visualization of ciliary movement *in vitro*, and the gene specific silencing by RNAi. In this symposium, we will present recent progress on the molecular function of axonemal dynein components in ciliary movement of *Paramecium*.

1SAA-4 Emergent collective motion of the unicellular green alga *Chlamydomonas*: 2-body swimming and beyond

Azusa Kage[1], Takayuki Torisawa[2], Ken H. Nagai[3] ([1]*Sch. Eng., Tohoku Univ.*, [2]*Advanced ICT Inst., NICT*, [3]*Sch. Materials Sci., JAIST*)

Chlamydomonas reinhardtii, a unicellular, biflagellated green alga, shows various types of collective motion such as bioconvection. Here we discuss these collective dynamics, particularly focusing on the novel "2-body swimming" of the *uni1-1* mutant. This mutant has only one flagellum and it shows "ciliary type" motion like the wild-type *Chlamydomonas* flagella. As a result, a *uni1-1* cell displays only local rotation rather than directed translational movement. We found that when two *uni1-1* cells attached through their flagella, there occurred the transition from the local rotation to the directed movement, suggesting a novel type of microswimmer. In addition to the 2-body swimming, the emergent, hydrodynamic "N-body problems" of *Chlamydomonas* will be discussed.

1SAA-5 遊泳バクテリアで捉える自己駆動粒子の集団運動における普遍性
Universality in collective motion of self-propelled elements captured through swimming bacteria

Daiki Nishiguchi[1,2,3], Ken H. Nagai[4], Hugues Chate[1,5], Masaki Sano[1] ([1]*CEA-Saclay*, [2]*Dept. of Phys., The Univ. of Tokyo*, [3]*Pasteur Institute*, [4]*JAIST*, [5]*Beijin CSRC*)

Collective motion of self-propelled elements, as seen in bird flocks, bacterial swarms, etc., is so ubiquitous. Evidence for universality in collective motion has been provided by many theoretical and numerical studies using simple flocking models such as agent-based models and hydrodynamic theories. However, no experiments had been fully convincing in demonstrating the existence of this universality until recently [1]. I will detail the theoretical predictions, e.g. long-range orientational order and giant density fluctuations, as well as past experimental endeavors to capture these properties using both living and non-living systems. Then how such universality emerges in bacterial systems will be discussed.

[1] Nishiguchi, et al., Phys. Rev. E 95, 020601(R) (2017).

1SAA-6 The impact of flow and environmental sensing on bacterial biofilm degradation

Knut Drescher[1, 2] ([1]*Max Planck Institute for Terrestrial Microbiology, 35043 Marburg, Germany*, [2]*Department of Physics, Philipps University Marburg, 35032 Marburg, Germany*)

Bacteria primarily live in multicellular communities, termed biofilms. The strategies used by bacteria to decide between remaining in a biofilm, or actively degrading the biofilm, are unclear, even though biofilm degradation is a central aspect of the biofilm life cycle and critical for infection transmission. We show that Vibrio cholerae integrates information about the flow and mass transport environment to control the biofilm degradation response: By combining information from individual-level and collective-level sensory inputs of diffusible molecules, biofilm-dwelling bacteria can make robust decisions to disperse from large biofilms under distress, while preventing premature dispersal when biofilm populations are small.

1SBA-1 ヘムタンパク質の電子論
Electronic Theory of Hemoprotein Chemistry

Yasuhiko Yamamoto (*Department of Chemistry, University of Tsukuba*)

Functional properties of myoglobin (Mb) is regulated through the intrinsic heme Fe reactivity, in addition to the heme environment furnished by nearby amino acid residues. We found that not only the oxygen (O2) affinity and autoxidation, i.e., a spontaneous oxidation process of the ferrous Fe state of the oxygenated protein, but also the discrimination between O2 vs. carbon monoxide (CO) of Mb is regulated through a change in the electron density of the heme Fe atom. These functional regulations of the protein could be interpreted in terms of the resonance between the two canonical structures of the Fe-O2 fragment, i.e., Fe(2+)-O2 and Fe(3+)-O2(-)-like species. Thus our study succeeded in resolving the electronic mechanism of the O2 vs CO discrimination of the protein.

1SBA-2 核共鳴非弾性散乱分光により解き明かす鉄蛋白質活性点の構造化学とダイナミックス
Nuclear resonance vibrational spectroscopic studies of the geometric structure and dynamics of iron-containing biomolecules

Takehiro Ohta (*Grad. Sch. Sci., Univ. Hyogo*)

Spectroscopic studies of the coordination geometries and electronic structures of the active sites of iron-containing biomolecules are important as biological iron sites are involved in chemical reactions essential to life. Nuclear resonance vibrational spectroscopy (NRVS) is a synchrotron based vibrational spectroscopy, which detects sidebands of the 14.4 keV iron-57 nuclear Mossbauer transition. NRVS band intensity is proportional to the displacement of iron-57 in normal mode, thus powerful for obtaining the structural information when the data is analyzed with density functional theory calculation. Recent studies of NRVS on iron-containing biomolecules, which provide a link between bioinorganic chemistry and biophysics, will be discussed.

1SBA-3 Mononuclear Nonheme Iron(IV)-Oxo Complexes with Tripodal Ligands in Oxidation Reactions

Mi Sook Seo, Wonwoo Nam (*Ewha Womans University*)

High-valent iron-oxo species have been implicated as key intermediates in the catalytic cycles of dioxygen activation by metalloenzymes, usually relying upon a high-spin (S=2) iron(IV)-oxo intermediate for the initial oxidation of substrate. In biomimetic studies, the nonheme iron(IV)-oxo complexes have been reported so far possess an intermediate (S=1) ground spin state, whereas only a small number of HS iron(IV)-oxo complexes have been prepared. Moreover, mechanistic comparison of nonheme IS and HS iron(IV)-oxo complexes in oxidation reaction have been rarely investigated. In this presentation the reaction mechanism and reactivity studies of IS and HS iron(IV)-oxo complexes in oxidation reaction (e.g. C-H bond activation, OAT and ET reaction) will be described.

1SBA-4 X 線自由電子レーザーを用いた時間分解結晶構造解析：酵素反応への応用
Time-resolved crystallography using X-ray free electron laser: application to enzymatic reaction

Takehiko Tosha (*RIKEN, SPring-8*)

Metalloenzymes can catalyze various kinds of chemical reactions under mild condition. Therefore, the elucidation of the mechanism of the chemical reactions catalyzed by metalloenzymes will lead to design new catalysts as well as to understand biology. Characterization of reaction intermediates in the enzymatic reaction is crucial for revealing the reaction mechanism. However, it is quite difficult to determine the structure of the short-lived reaction intermediate by conventional X-ray crystallography. Here, to overcome this issue, we developed the method for the structural determination of the reaction intermediates by time-resolved x-ray crystallography at an X-ray free electron laser facility, SACLA, using photosensitive caged substrate as a reaction trigger.

1SBA-5 QM/MM 計算で解明した鉄含有酵素の反応機構
Reaction mechanisms of iron-containing proteins elucidated using QM/MM calculations

Mitsuo Shoji[1], Sotaro Yamasaki[2], Megumi Kayanuma[1], Yasuteru Shigeta[1] ([1]*CCS, Univ. Tsukuba*, [2]*Grad. Sch. Of Pure & App. Sci., Univ. Tsukuba*)

Recently, high-resolution X-ray structures have be solved for many metalloproteins, and the fundamental basis become clear very rapidly. On the other hand for the catalytic reactions, it is still difficult for their transient and unstable states. Theoretical calculation is one promising approach to elucidate the catalytic reaction mechanisms. In this study, we discuss about the reaction mechanisms of iron-containing proteins, assimilatory nitrite reductase (aNiR) and trypanosome cyanide-insensitive alternative oxidase (TAO), elucidated using QM/MM calculations. Their energy profiles and structural changes in their micro chemical reactions are discussed.

1SCA-1 細胞運動における自発的シグナル生成の仕組み
A mechanism of spontaneous signal generation in cell migration

Satomi Matsuoka[1,2], Seiya Fukushima[1,2], Masahiro Ueda[1,2] ([1]*RIKEN, Quantitative Biology Center (QBiC)*, [2]*Osaka University, Graduate School of Frontier Biosciences*)

Cell migration emerges from intrinsic dynamics of a signaling network even without extrinsic signals. Spontaneous cell migration has been examined at different resolutions ranging from a molecule to a cell in a model organism, *Dictyostelium discoideum*, by using live-cell imaging and statistic analyses. We have revealed that a local enrichment of phosphatidylinositol-3,4,5-trisphosphate, PIP_3, on the cell membrane, which serves as an anterior signal, arises spontaneously due to a mutual inhibition relationship between PIP_3 and the phosphatase, PTEN, and an excitable property of PI3-kinase. It illustrates a design principle of the network that ensures intrinsic dynamics with stochastic generation of all-or-none signal and thereby efficient migration in random directions.

1SCA-2 連続光照射時のオオアメーバの運動
Behavior of *Amoeba proteus* on constant photo-irradiation

Yukinori Nishigami (*Department of Physics, Graduate School of Science, Kyoto University*)

Sunlight is one of the most important factors for almost all species. In addition to energy sources, the sunlight gives organisms information about environment and then they decide their behaviors to adapt to the environment. A large free-living amoeba, *Amoeba proteus*, has been used as a model system of amoeboid locomotion. Though responses to light of *A. proteus* were reported in several papers, dependence of behaviors on the constant photo-irradiation has still been unclear. Then we investigated the locomotion of *A. proteus* on the constant photo-irradiation. As a result, *A. proteus* exhibited two, active and static, modes of movement depending on color of the irradiating light. In the static mode, remarkably, oscillatory translational motion were exhibited.

1SCA-3 繊毛虫の学習能力の再考
Rethinking the learning capacity of ciliates

Itsuki Kunita (*University of The Ryukyus*)

In the 1930s and 1940s, it was reported through ethological studies that ciliates have a capacity to learn. After the 1960s, it was clarified that the mechanism by which the membrane potential changes in ciliates is essentially the same as that in nerve cells of higher organisms. Additionally, it has been elucidated that membrane potential dynamics in cilia can control ciliary movement. As a result, we are now rethinking some of the previously reported learning behaviors in ciliates, from the point of view of membrane potential dynamics. As a specific example, we introduce our research about the adaptive capacity in response to spatial expansion in ciliates, including Paramecium, and Tetrahymena.

1SCA-4 ロクロクビムシのプロボーシスの伸縮運動
Extension and Contraction of the Proboscis of a Ciliate, *Lacrymaria olor*

Ryuji Yanase (*Grad. Sch. Sci., Univ. Hyogo*)

The free-living ciliate protozoa, *Lacrymaria olor* has a proboscis for hunting prey, which rapidly extends up to 10 times longer than its original length. To reveal the extension–contraction mechanism, we conducted detailed analyses of the extension–contraction of the proboscis using several microscopic observation techniques. The results indicate that (1) ciliary movement of an oral part on the distal end of the proboscis mainly contributes to the extension, (2) the proboscis has a property like a nonlinear spring, and (3) some contractile factor which works only during contracting period exists in the proboscis. We will discuss characteristic physical properties of the proboscis of *L. olor* and propose the extension–contraction mechanism.

1SCA-5 壁面付近における繊毛虫の遊泳運動
Swimming behavior of a ciliate near a wall

Takuya Ohmura, Masatoshi Ichikawa (*Grad. Sch. of Sci, Kyoto Univ.*)

One kind of water microorganisms, ciliate, swim by ciliary beating. Swimming ciliates in nature interact with various solid boundaries, other cells, a bottom of pond or a surface of waterweed. Nevertheless, as compared with microorganisms driven by flagellar beating, there were little biophysical studies about the swimming motion of a ciliate interacting with the solid boundary. To analyze hydrodynamic effect on the swimming ciliate by a wall, we investigated their swimming near the wall by two approaches; experiment and numerical calculation. Observing Tetrahymena pyriformis, we found a novel phenomenon that the cell swam adjacent to the wall. In addition, the reproduction of the swimming with the adjacence was achieved by a developed hydrodynamic model.

1SCA-6 ラビリンチュラ類の外質ネットによる栄養摂取
Nutrition of thraustochytrids (Labyrinthulea) by their ectoplasmic nets

Daiske Honda[1], Yoko Hamamoto[2], Izumi Iwata[2] ([1]*Faculty of Science and Engineering, Konan University*, [2]*Graduate School of Natural Science, Konan University*)

The Labyrinthulea is characterized by an ectoplasmic net system. Thraustochytrids inhabit the ocean all over the world and have been recognized as important eukaryotic decomposers in the marine ecosystem. The ectoplasmic nets are superficially similar to narrow pseudopods of many protists but different in the following points: their origin from a unique organelle named the bothrosome, membrane invagination along ectoplasmic net, and absence of mitochondria and ribosomes. We revealed that Golgi body is related to the formation of the bothrosome and that actin is present in the ectoplasmic nets and in the cytoplasm around the bothrosome. When the ectoplasmic nets attached the baits, the ectoplasmic nets became massive and the structure of membrane invagination in the ectoplasmic nets were developed complexly. This suggested that the ectoplasmic nets recognized the organic matter and efficiently secrete digestive enzyme and intake nutrients at the attached area. On the other hand, the vegetative cells of *Aplanochytrium* extended the ectoplasmic nets to the living cells of diatoms, and then chloroplasts of the diatoms shrank and bleached. It was suggested that the thraustochytrids play the role as not only decomposers but also “predators”. The thraustochytrids probably intake the nutrients from the ecologically important primary producers, diatoms, in the wide sphere of radially developed ectoplasmic nets.

1SDA-1 高速原子間力顕微鏡を用いた回転軸の無い腸内連鎖球菌由来 V_1-ATPase の回転運動の解析
Analysis of Rotational Dynamics of Rotorless *Enterococcus hirae* V_1-ATPase using High-Speed Atomic Force Microscopy

Motonori Imamura[1], Kazuya Nakamoto[2], Shintaro Maruyama[2], Fumihiro Kawai[3], Ryota Iino[3], Takayuki Uchihashi[4], Takeshi Murata[2], Toshio Ando[1] ([1]*Bio-AFM FRC, Kanazawa Univ.*, [2]*Grad. Sch. Sci., Chiba Univ.*, [3]*Okazaki Inst. Integ. Biosci., IMS, NINS*, [4]*Grad Sch. Sci., Nagoya Univ.*)

High-Speed AFM (HS-AFM) has been applied to visualizing dynamic biomolecular processes in solution. Here, we used this technique to visualize the dynamics of V_1-ATPase (V_1). V_1 is a rotary motor protein, similar to F_1-ATPase (F_1). V-ATPase as a whole pumps H^+ or Na^+ across membranes using energy liberated by ATP hydrolysis. A previous HS-AFM study showed that the $\alpha_3\beta_3$ stator ring of F_1 can execute an intrinsic cooperative catalytic action (CCA) even without the γ rotor. In this study, we investigated if the A_3B_3 stator ring of V_1 would also execute a similar CCA without the DF rotor. HS-AFM observation showed that the CCA in the A_3B_3 is much weaker than that found in F_1, suggesting that the stator-rotor interaction is critical in the generation of CCA by V_1.

1SDA-2 超遠心分析によるバイオおよびナノ粒子の溶液挙動の解析
Solution behavior of bio- and nano-particles as analyzed by analytical ultracentrifugation

Fumio Arisaka (*Tokyo Institute of Technolgy*)

Analytical ultracentrifugation is one of the best theoretically understood tools of analyzing macromolecules in solution. Due to the development of instrumentation and software since 1990's, the application of the methodology is expanding in both the kind of behavior such as association and conformational change and materials. In this talk, examples of application of analyses including protein association by the method of component gradient sedimentation equilibrium (CG-SE) and analyses of emulsion dissolved in water will be introduced.

1SDA-3 Elucidation of structural dynamics of protein with binding to drugs based on kinetic and thermodynamic analysis

Satoru Nagatoishi[1,2], Kouhei Tsumoto[1,2] ([1]*The Institute of Medical Science, The University of Tokyo*, [2]*School of Engineering, The University of Tokyo*)

In drug discovery, understanding of molecular recognition between drugs and proteins often require a characterization of the binding energy with structural information and correlation of its thermodynamics. However, structural dynamics of proteins with the binding of drugs are still unclear. We focused on the binding process of the molecular recognition to discuss the structural dynamics of protein. Binding kinetic analysis was carried out to elucidate the binding process and we investigated thermodynamics of the transition state in the interaction of drugs with the target protein. Our results demonstrate that structural information for protein dynamics with binding to small molecules can provide us an important viewpoint for design and assessment of drugs.

1SDA-4 SEC-SAXS によるタンパク質複合体の溶液構造解析
Solution structure analysis of the protein complex using SEC-SAXS

Nobutaka Shimizu (*PF, IMSS, KEK*)

The biological small-angle X-ray solution scattering (BioSAXS) is a useful technique for the structure characterization of a protein in solution. Especially, BioSAXS combined with an inline size-exclusion chromatography (SEC-SAXS) has recently been utilized as an important method for the investigation of the interaction state of proteins. This method can analyze a specific structure state precisely since it isolates a target molecule just before SAXS measurement using a gel filtration column. This presentation will introduce details and several examples of SEC-SAXS analysis.

1SDA-5 高温における可逆的かつ迅速な蛋白質非天然状態の会合体形成
Reversible and rapid oligomerization of non-native proteins at high temperature

Shun-ichi Kidokoro (*Dept. Bioeng., Nagaoka Univ. Tech.*)

Calorimetry was performed to observe the thermal transition of an acidic molten globule state (MG1) of cytochrome *c* at concentrations from 0.5 to 18.2 mg/ml. DSC profiles are highly reversible and showed no scanning-rate dependence in the rage from -0.5 K/min to 1 K/min but clear protein-concentration dependence, indicating that a reversible and rapid oligomerization process occurs during the thermal transition. These DSC and PPC data were found to be well explained by a six-state model, including three monomeric states: MG1, MG2, and denatured state, and three oligomeric states: dimer, trimer, and tetramer. Their thermodynamic properites and some other examples indicating reversible oligomerization will be discussed in the presentation.

1SDA-6 ピロリ菌 CagA がんタンパク質の構造多型が極性制御因子 PAR1 b結合に及ぼす影響
Impact of structural polymorphism of the H. pylori CagA oncoprotein on binding to polarity regulating kinase PAR1b

Hiroko Nishikawa[1], Takeru Hayashi[1], Fumio Arisaka[2], Toshiya Senda[3], Masanori Hatakeyama[1] ([1]*Grad. Sch. Med., Univ. Tokyo*, [2]*Coll. Biores. Sci., Nihon Univ.*, [3]*Inst. of Mater. Struct. Sci., KEK*)

Helicobacter pylori CagA is a bacterial oncoprotein, which, upon delivery into gastric epithelial cells, binds to and inhibits the polarity-regulating kinase PAR1b via its CM motif, eliciting junctional and polarity defects in the host cell. Interestingly, a variety of CM motifs have been identified among distinct CagA variants, differing in both composition of the sequence and copy number. Through quantitative analysis of the CagA-PAR1b interaction, we found that while some CagA species have lost their ability to bind to PAR1b, others display strikingly elevated PAR1b-binding activity through multiple duplications of the CM motif. Thus polymorphism of the CM motif is a key determinant for the outcome of gastrointestinal diseases, including gastric cancer.

1SDA-7 Solution-based Analyses on Microtubule Depolymerization via Depolymerizing Machine

Tadayuki Ogawa[1], Shinya Saijo[2], Nobutaka Shimizu[2], Xuguang Jiang[1], Nobutaka Hirokawa[1] ([1]*Univ. Tokyo*, [2]*KEK-PF*)

Microtubules (MTs) are dynamic polymer structures composed of alpha-/beta- tubulin hetero dimers, which are fundamental for the cell morphogenesis and motility. MT-depolymerizing machine catalytically depolymerizes the MT using the energy from ATP hydrolysis. This talk will introduce the combination of multiple solution-based analyses on MT depolymerization, and present the efficient mechanism of catalytic MT depolymerization via depolymerizing machine.

1SFA-1 脂質二重膜がカリウムチャネル開閉に及ぼす多様な影響
Specific and non-specific actions of membrane lipids on the gating of the potassium channel

Masayuki Iwamoto, Shigetoshi Oiki (*Dept. Mol. Physiol. & Biophys., Univ. Fukui Facult. Med. Sci.*)

Lipid bilayer methods allow examination of ion channel activities in simplified membrane environment by circumventing complexity of biological membranes. We developed a novel lipid bilayer method named the contact bubble bilayer (CBB) that generate membranes of arbitrary lipid compositions in each leaflet, and hydrophobic substances can be rapidly administered via the oil-phase route during the recording of the single-channel currents. Here we present our recent results of the lipid effects on the KcsA potassium channel. Specific and non-specific effects of lipids were elucidated on the open-close transition (gating) of the KcsA channel. Molecular mechanisms underlying the lipid effects were examined.

1SFA-2 遷移パスシミュレーションによる Na^+/H^+ antiporter の輸送メカニズム
Transport mechanism of Na^+/H^+ antiporter from transition-path simulations

Kei-ichi Okazaki[1], Gerhard Hummer[2] ([1]*IMS*, [2]*MPI of Biophysics*)

Cation-proton antiporters (CPA) are secondary-active transporters involved in a wide range of cellular processes, from controlling pH and salt concentration to osmoregulation of the cell volume. Na^+/H^+ transporters exchange sodium ions (Na^+) and protons (H^+) by transporting them in opposite directions across lipid membranes, using the gradient of one ion to drive the uphill transport of the other. Here we resolve the Na^+ and H^+ transport cycle of PaNhaP, an archaeal CPA1-family Na^+/H^+ antiporter, in unbiased molecular dynamics trajectories focused on transition dynamics. By introducing a transition-path shooting algorithm, we reveal the transport mechanism of seconds-scale ion exchange processes.

1SFA-3 高速原子間力顕微鏡によるナノディスクに埋め込まれた膜タンパク質のダイナミクス観察
High-speed AFM imaging of membrane proteins in lipid nanodiscs

Mikihiro Shibata (*InFiniti, Kanazawa Univ.*)

High-speed atomic force microscopy (HS-AFM) is a powerful technique to visualize surface structures of individual proteins in action at sub-molecular resolution. HS-AFM studies performed in the last few years provided new mechanistic insight into the functional mechanism of several types of proteins. In this study, we applied HS-AFM to visualize protein dynamics of membrane proteins in the lipid membrane under near-physiological conditions. Using lipid nanodiscs, which is a synthetic model membrane system, we visualized oligomeric structures of light-driven ion-pumping microbial rhodopsins and conformational changes of ATP-binding cassette transporter. In the symposium, we will discuss our recent HS-AFM studies focused on membrane proteins.

1SFA-4 X 線自由電子レーザーで捉えたバクテリオロドプシン構造変化の三次元動画
A three-dimensional movie of structural changes in bacteriorhodopsin captured by X-ray free electron lasers

Eriko Nango[1,2], So Iwata[1,2] ([1]*RSC*, [2]*Kyoto Univ. Med.*)

Recent advent of intense, femtosecond X-ray pulses from X-ray free electron laser (XFEL) have enabled to acquire diffraction patterns from protein microcrystals before the onset of radiation damage. We observed conformational changes in bR at thirteen time-points from nanoseconds to milliseconds following photo-activation at 2.1 Å resolution using time-resolved serial femtosecond crystallography at the facility of XFEL, SACLA. The resulting cascade of structural changes throughout the protein provided unprecedented insight into how structural changes in bR conspire to achieve unidirectional proton transport.

1SFA-5 分子シミュレーションで探る膜輸送体・受容体の分子機能
Atomistically deciphering functional processes of membrane transporter and receptor with molecular simulations

Shigehiko Hayashi (*Dept. of Chem., Grad. Sch. of Science, Kyoto Univ.*)

Functional processes of membrane transporter and receptor involve dynamic and global molecular conformational changes of complex protein systems which correlate with local molecular events such as bindings of substrates and/or their chemical reactions. Hence coupling of the local events with protein global molecular dynamics underlying functional processes need to be revealed for understanding of molecular nature of protein functions. In this talk, I will present our recent development of novel molecular simulation techniques, linear response path following and QM/MM RWFE-SCF methods, to atomistically elucidate the local-global coupling in functional processes as well as their applications to ADP/ATP membrane transporter and rhodopsin membrane photo-receptors.

1SFA-6 バナナ状たんぱく質の集合による膜チューブ形成
Membrane tubulation induced by assembly of banana-shaped protein rods

Hiroshi Noguchi (*ISSP, Univ. Tokyo*)

BAR superfamily proteins have a banana-shaped domain and bend the membrane along the domain axis. We have studied tubulation by these banana-shaped protein rods using meshless membrane simulations.
The protein rods self-assemble by membrane-mediated interactions. In the case of a high rod curvature, a straight rod cluster bends into a disk-like tubule. In contrast, for low rod curvature and high rod density, the cylindrical tubules protrude from the vertices of a rod cluster network. The positive side rod curvature and addition of the laterally isotropic inclusions with positive spontaneous curvature accelerate the tubulation while the negative curvatures suppress the tubulation. Two types of the rods with opposite rod curvatures induce a striped bump structure.

1SGA-1 Development of GENESIS for high performance computing of biomolecular simulations

Jaewoon Jung[1,2], Chigusa Kobayashi[1], Yuji Sugita[1,2,3] ([1]*RIKEN AICS*, [2]*RIKEN TMS*, [3]*RIKEN QBiC*)

GENESIS (GEneralized-Ensemble Simulation System) is molecular dynamics (MD) software for biomolecular systems. It is designed to extend the time scale and available system size by efficient parallelization schemes and enhanced conformational sampling algorithms. At the current status, GENESIS is scalable more than 260,0000 cores, handling more than 100 million atom systems on K computer. GENESIS shows good parallel efficiency not only on K, but also on PC clusters with various architectures including GPU and Intel KNL. In this meeting, we show several applications using GENESIS on K computer and discuss future development of GENESIS on next-generation supercomputer.

1SGA-2 エネルギー表示溶液理論を用いた蛋白質－蛋白質複合体構造予測
Protein-protein complex structure prediction using the solution theory in the energy representation

Kazuhiro Takemura[1], Nobuyuki Matubayasi[2], Akio Kitao[1] ([1]*IMCB, Univ. of Tokyo*, [2]*Grad. Sch. Eng. Sci, Osaka Univ.*)

We analyzed binding free energy difference through molecular dynamics simulation using the solution theory in the energy representation for complex models selected by CyClus which performs a fast clustering using a cylindrical approximation of interface and improves results of rigid-body docking. Our free energy analysis using conformational energies, solute entropies, and solvation free energies improved the results of CyClus and the complex models similar to the native structure have the lowest binding free energies, suggesting that this procedure is effective in protein-protein complex structure predictions. We further improved the procedure by placing interface waters into protein-protein interface before free energy evaluations.

1SGA-3 分子動力学シミュレーションと小角 X 線散乱実験を組み合わせた蛋白質の動的構造変化の解析
Protein dynamics revealed by a combination analysis of molecular dynamics simulations and small-angle x-ray scattering experiments

Toru Ekimoto, Mitsunori Ikeguchi (*Yokohama City Univ.*)

Owing to an increment of computational capability, MD simulations become a powerful tool to elucidate protein dynamics in atomic resolution. However, a timescale is still one of the limitations, and then solution structures generated by MD are needed to be assessed by experimental results. SAXS experiments can measure solution structures without effects of crystal packing. However, SAXS data are low resolution, and then high resolution data are needed to further analyze their data. Considering demands of MD and SAXS, their combination analysis is a promising hybrid tool to obtain solution structures in atomic resolution guaranteed by experiments. In this talk, we will introduce an example of the MD-SAXS analysis for vitamin D receptor ligand-binding domain.

1SGA-4 Molecular dynamics simulations for the study of thermodynamic properties in streptavidin mutant-biotin analog systems

Keiko Shinoda, Hideaki Fujitani (*RCAST, The Univ. Of Tokyo*)

The biotin-streptavidin (SA) system is known to have a strongest noncovalent biological interaction, and has been widely used as not only a molecular detection tool in many biotechnological applications but also medical applications such as pre-targeting system. In the pre-targeting system, the SA is modified to decrease the immunogenicity, and the SA mutant binds to an artificial biotin analog while abolishing affinity for natural biotin. In this meeting, we report the effect of mutations on dynamical and structural changes of the system using a series of molecular dynamics simulations for SA or its mutants with/without biotin analog systems and evaluation the binding affinity of biotin analog by free energy calculations.

1SGA-5 創薬ビッグデータ統合システムの開発とゲノム医療への応用
Development of Next-generation computational infrastructure for drug discovery and practical application to genomic medicine

Mitsugu Araki[1,2], Yasushi Okuno[1] ([1]*Grad. Sch. Med., Kyoto Univ.*, [2]*RIKEN, AICS*)

In the initial stages of the drug discovery process, in-silico computational technologies for efficiently searching and optimizing drug candidates are strongly required. For the purpose of fast and highly accurate prediction of drug candidate molecules by exploiting the computing power of post "K", we are developing a computational infrastructure combining molecular dynamics simulations and next-generation in-silico drug discovery methods. In this symposium, I will report development of a methodology to accurately predict the protein-compound binding affinity, which is a core element technology in the infrastructure. Also, I will introduce case studies of practical application of previously-developed computational technologies to genomic medicine.

1SGA-6 機械学習による MD 計算に基づく結合ポーズ推定の高速化
Acceleration of MD-based Binding-Pose Prediction with Ligands and Proteins by Machine Learning

Kei Terayama[1], Hiroaki Iwata[2], Mitsugu Araki[4], Yasushi Okuno[3,4], Koji Tsuda[1,5,6] ([1]*Grad. Sch. Frontier Sci., Univ. Tokyo*, [2]*Found. for Biomedical Researcha and Innovation*, [3]*Grad. Sch. Med., Kyoto Univ.*, [4]*AICS, RIKEN*, [5]*AIP, RIKEN*, [6]*Center for Material Research By Info. Integration, NIMS*)

Fast and accurate prediction of protein-ligand binding structures is indispensable for structure-based drug design and accurate estimation of binding free energy of drug candidate molecules in drug discovery. Recently, accurate pose prediction methods based on short-MD simulations such as MM-PBSA and MM-GBSA have been used. However, these methods are computationally expensive. In this talk, we show that a machine learning method, called Best Arm Identification, can optimally control the number of MD runs for each binding pose to reduce total MD runs. Experimental result showed that the computational cost can be reduced substantially without sacrificing accuracy.

1SIA-1 DNA を利用した色素間エネルギー移動の詳細な解析

Analysis of energy transfer between dyes by using DNA scaffold

Hiromu Kashida[1,2] (*[1]Grad. Sch. Eng., Nagoya Univ., [2]PRESTO, JST*)

Fluorescent Resonance Energy transfer (FRET) is widely used in biotechnology. Although distance dependence of FRET is often used to measure distance, orientation dependence is not used in most cases. On the other hand, we have succeeded in observing orientation dependence of FRET by using DNA scaffold. Besides, observed FRET efficiency showed excellent agreement with Forster theory. Now, we are applying this orientation dependent FRET system to structural analyses of various nucleic acid structures. In addition, energy migration between identical chromophores can also be analyzed by using DNA scaffold.

1SIA-2 生きた脳で RNA の観測ができたら

in vivo RNA labelling reveals dynamic regulation of ribonucleic foci in living neurons

Ikumi Oomoto[1], Hiroki Umeshima[1], Yoshie Harada[1], Yong-Woon Han[1], Akimitsu Okamoto[2], **Ohtan Wang**[1] (*[1]Kyoto University, iCeMS, [2]Research Center for Advanced Science and Technology, University of Tokyo*)

RNA molecules are dynamically regulated in all cell-types, especially in highly polarized and complex brain cells. Being able to image RNA in a behaving mouse brain will provide significant insights on experience-driven transcription and spatiotemporal RNA regulation/dysregulation; however, many hurdles have to be removed before we can achieve this goal. We recently applied hybridization-sensitive fluorescent probes to imaging RNA dynamics by directly introducing oligonucleotide probes into living mouse whole brains. Although our imaging was limited to abundant RNA species such as U6 and U23 noncoding RNAs, the dynamics we observed demonstrated fundamental difference between normal tissue cells and cancer cells where RNA dynamics is conventionally studied.

1SIA-3 CUBIC: 細胞・細胞回路の網羅的解析を目的としたセロミクスパイプライン

CUBIC: a Cell-omics pipeline for comprehensive cell and cell circuit analysis

Etsuo A. Susaki[1,2,3] (*[1]Dept. Syst. Pharmacol., UTokyo Grad. Sch. Med., [2]PRESTO, JST, [3]Lab. Synthetic Biol., RIKEN QBiC*)

The multicellular organism is composed of various types of cells inside, where they connect with each other and work in a coordinated manner. In this presentation, we will introduce a comprehensive cell and cell circuit analysis pipeline termed CUBIC (Clear, Unobstructed Brain/Body Imaging Cocktails and Computational analysis), which includes an efficient and reproducible whole organ/body clearing, a rapid 3D imaging of whole organ/body, and computational image informatics. CUBIC aims to realize an -omics type approach in the cell and cell circuit layer (cell-omics) and thus can be applied to the wide range of life science and medical researches, which will facilitate our understanding of the complicated multicellular living systems.

1SIA-4 細胞内カルシウムシグナル解読への新しいアプローチ

A new approach to decoding of Ca^{2+} signals in a single cell

Hiroko Bannai[1,2], Fumihiro Niwa[3], Shigeo Sakuragi[4], Katsuhiko Mikoshiba[2] (*[1]JST PRESTO, [2]RIKEN BSI, [3]IBENS, [4]Tohoku Univ, Grad. Sch. Life Sci.*)

Calcium (Ca^{2+}) is a versatile intracellular messenger that operates in various signaling pathways leading to multiple biological outputs. The diversity of spatiotemporal patterns of Ca^{2+} signals is considered to underlie the diversity of biological outputs caused by Ca^{2+}. However, such Ca^{2+} signal pattern diversity has not been well described. Here, we propose a new method to report Ca^{2+} signals at higher sensitivity and spatial resolution. Targeting of genetically encoded Ca^{2+} sensor (GECI) to the subcellular compartments enables detection of Ca^{2+} release or Ca^{2+} influx at subcellular resolution, avoiding the diffusion of GECI and Ca^{2+}. This approach, i.e. the precise detection of local Ca^{2+} signals in a single cell, will contribute to decoding Ca^{2+} signals.

1SIA-5 アクチン線維が負の張力センサーとして働く仕組みを分子イメージングから解明する試み

Analysis of fluctuations of a single actin filament that works as a tension sensor

Hitoshi Tatsumi (*Department of Applied Bioscience, Kanazawa Institute of Technology (KIT)*)

The cells are continually exposed to various mechanical stimuli, such as, muscle contraction, ongoing blood flow, blood pressure, distension of visceral organs. Mechanical forces are sensed by mechanosensors that presumably undergo change in their enzymatic activity or interaction with signaling molecules in response to forces. However, the molecular entities and the underlying biophysical mechanisms of mechanosensing molecules are largely unknown. A recent in vitro study (Hayakawa et al., 2011, JBC) revealed that the actin filament itself functions as a mechanosensor. We have constructed a newly designed microscope to conduct the analysis of torsional fluctuations of actin filaments, which may play a significant role in mechano sensing.

1SIA-6 ゴーストサイトメトリー

Ghost Cytometry

Sadao Ota[1, 2] (*[1]Applied Chemistry Department, University of Tokyo, [2]JST, PRESTO*)

In this talk, I report development of an ultrafast and accurate fluorescence “imaging” cytometry by a single pixel detector even without producing the object’s image, named ghost cytometry. In the method, relative motion of cells flowing against a static random optical structure compressively converts their spatial information into temporal waveforms of the single pixel detector. Combining this temporal signal with the information of the random light pattern, a computational reconstruction method realizes the ultrafast, continuous, multi-color, compact, and low-cost fluorescence imager. More importantly, we enabled morphology-based cytometry at high throughput (>10,000 cells/sec).

1SLA-1 Specific and non-specific protein-protein interactions in cellular environments

Yuji Sugita (*RIKEN*)

We investigate protein-protein interactions in the cytoplasm and biological membranes using molecular dynamics (MD) simulations. In the the cytoplasm, we observed that non-specific interactions have important roles on conformational stability and protein-ligand binding and the effects are not always positive, which is different from the classical views of macromolecular crowding. We also performed all-atom MD simulations of NOR/NIR complex in the biological membrane. In this case, the complex structure is meaningful for transporting NOs, ligands to be transported from NIR to NOR. Based on these two examples, we discuss the functional roles of specific and non-specific protein-protein interactions in the cellular environments.

1SLA-2 Atomistic modeling of protein liquid-liquid phase separation

Sanbo Qin, **Huan-Xiang Zhou** (*Florida State University*)

We have developed a powerful computational method called FMAP for determining the thermodynamic conditions for liquid-liquid phase separation, where proteins separate into a dissolved and a droplet phase. FMAP involves calculating the excess chemical potentials of protein molecules over a wide range of concentrations. By using fast Fourier transform to efficiently evaluate protein-protein interactions, FMAP enables an atomistic representation of the protein molecules. Here we applied FMAP to three homologues of γ-crystalin to elucidate why minor changes in amino-acid sequence can lead to drastic differences in critical temperature for phase separation. A Ser to Trp change in the inter-domain ridge makes a prominent contribution to the disparity in Tc.

1SLA-3 Nonspecific protein-protein interactions in dense protein solutions and near membranes

Michael Feig[1,2] ([1]*MSU*, [2]*QBiC*)

Cellular environments are defined by a high degree of crowding that makes frequent non-specific protein-protein interactions unavoidable. To better understand how such interactions affect the dynamics and structure of proteins, results from recent molecular dynamics simulations of dense solutions of proteins are presented. A primary focus is the characterization of how diffusional motions are altered in crowded environments as a result of weak protein-protein interactions. Homogeneous dense proteins solutions are compared with systems that include membrane bilayers to describe the interplay of biological membranes on crowding effects.

1SLA-4 網羅的変異解析による VemP 翻訳伸長停止モチーフの同定と解析
Identification and characterization of a translation arrest motif in VemP by systematic mutational analysis

Hiroyuki Mori, Sohei Sakashita, Jun Ito, Eiji Ishii, Yoshinori Akiyama (*Inst. Front. Life Med. Sci., Kyoto Univ.*)

VemP (*Vibrio* protein export monitoring polypeptide) is a secretory protein that regulates expression of downstream genes, *V.secDF2*. When export of VemP is compromised, its translation undergoes elongation arrest near the C-terminus. Though our previous study suggests that a highly-conserved C-terminal 20-residue region of VemP contributes to the elongation arrest via specific interactions between the nascent chain and the translating ribosome, a precise role of each amino acid residue in this region in the arrest remains unclear. We constructed a reporter system in order to easily monitor the *in vivo* arrest activity of VemP. Systematic mutational analysis of the conserved region using this reporter system enabled us to identify and characterize the arrest motif in VemP.

1SLA-5 細胞内での一酸化窒素の動態
NO Dynamics in Cellular System

Yoshitsugu Shiro (*Univ. Hyogo*)

Nitric oxide (NO) is a cyto-toxic molecule. In dentrification micro-organisms, it was generated by nitrite reductase (NiR: NO2- + 2H+ + e- -> NO + H2O) and detoxified by nitric oxide reductase (NOR: 2NO + 2H+ + 2e- -> N2O + H2O). A simple question is how the NO molecule generated by a water-soluble enzyme, NiR, can be transferred to and then decomposed by a membrane-integrated enzyme, NOR, without diffusing in cell. We were successful to determine the crystal structure of the NiR/NOR protein complex. The molecular dynamic simulation and mutagenesis works supported that the complex formation is essential for the NO transfer and decomposition immediately after its generation. The molecular mechanism of the NO reduction by NOR will be presented in my talk.

1SMA-1 Ｖ１モーターの構造形成の分子機構
Molecular mechanism of the structural formation of V1 rotary motor

Takeshi Murata[1,2] ([1]*Grad. Sch. Sci., Chiba Univ.*, [2]*PRESTO, JST*)

V-ATPases function as ATP-dependent ion pumps, the hydrophilic V1 portion is known as rotary motor in which a central axis DF complex rotates inside a hexagonally arranged catalytic A3B3 complex using ATP hydrolysis energy. We previously succeeded in obtaining the crystal structures of the A3B3 complex which is a three-fold assembly of the identical A1B1 pair, but showed asymmetrical hexamer ring structure. Recently, we have elucidated the crystal structures and biochemical properties of the A-subunit, B-subunit, A1B1 complex, and A3B3 mutant. Based on these and previous findings, we propose a molecular mechanism model of the structural formation of V1 rotary motor.

1SMA-2 蛋白質膜透過駆動モーター SecDF
Protein Translocation Motor SecDF

Tomoya Tsukazaki[1], Arata Furukawa[1], Kunihito Yoshikaie[1], Takaharu Mori[2], Hiroyuki Mori[3], Yusuke V. Morimoto[4], Yasunori Sugano[1], Shigehiro Iwaki[1], Tohru Minamino[5], Yuji Sugita[2], Yoshiki Tanaka[1] ([1]*Grad. Sch. of Biol. Sci., NAIST*, [2]*RIKEN*, [3]*Inst. for Front. Life and Med. Sci., Kyoto Univ.*, [4]*Grad. Sch. of Comp. Sci. and Sys. Eng., Kyushu Inst. of Tech.*, [5]*Grad. Sch. of Front. Biosci., Osaka Univ.*)

Protein secretion mediated by SecYEG translocon and SecA ATPase is enhanced by membrane-embedded SecDF by using proton motive force. SecDF proposed to form at least two characterized transition states, termed the F and I forms. We report the structures of full-length SecDF in I form at 2.6- to 2.8-Å resolution. The structures revealed that SecDF in I form can generate a tunnel that penetrates the transmembrane region and functions as a proton pathway. In one crystal structure, periplasmic cavity interacts with a molecule which may mimic a substrate peptide. This study provides structural insights into the Sec protein translocation that allows future analyses to develop a more detailed working model for SecDF.

1SMA-3 Functional dynamics of membrane proteins revealed by NMR

Takumi Ueda, Ichio Shimada (*Grad. Sch. Pharm. Sci. The Univ. of Tokyo*)

Membrane proteins have various important functions in signal transduction, transportation, and bioenergetics, and over half of the currently available drugs target membrane proteins. Various snapshots of membrane proteins have been solved by X-ray crystallography and cryo-electron microscopy. However, these snapshots cannot explain the functions of membrane proteins, such as basal activity of GPCRs. I will talk about our study that clarifies the mechanisms underlying the functions of the membrane proteins by NMR study of their conformational equilibria.

1SMA-4 Combining XFEL crystallography and single-crystal spectroscopy for studying reaction dynamics of respiratory metalloenzymes

Minoru Kubo (*RIKEN SPring-8 Center*)

Time-resolved optical spectroscopy is useful for probing reaction dynamics of proteins, and has been extensively used for characterization of their reaction intermediates. However, the spectroscopic signals do not contain direct information on the 3D structures. Recently, X-ray free electron lasers (XFELs) have enabled time-resolved X-ray crystallography, which provides the atomic coordinates of transient protein structures during the reaction. We have combined time-resolved X-ray structural analysis with spectroscopic intermediate characterization (in crystal) at SACLA, and tracked the structural dynamics of various proteins. Here, the successful application of the technique to bovine cytochrome c oxidase and fungal nitric-oxide reductase will be presented.

1SMA-5 Structural basis of muscle force generation and regulatory mechanism by CryoEM

Takashi Fujii (*RIKEN, QBiC*)

Muscle contraction is driven by cyclic interactions of myosin in the thick filament with actin in the thin filament composed of actin, tropomyosin and troponin complex. To understand the force generation and the regulatory mechanism, it is necessary to elucidate the structure of the actomyosin complex and the thin filament at high resolution. CryoEM structural study of actomyosin rigor complex suggests how its asymmetric binding along actin filament causes directionally biased thermal fluctuations of myosin and actin to work as a Brownian ratchet. Additionally, we introduce recent advances in structural analysis of the reconstituted muscle thin filament by CryoEM. Finally, we would like to introduce our CryoEM applications for membrane protein.

1SNA-1 蛍光 X 線ホログラフィーによるヘムタンパク質の金属周辺構造観測
First X-ray fluorescence holographic imaging of iron environments in heme proteins

Ayana Sato-Tomita[1], Naoya Shibayama[1], Naohisa Happo[2], Kouichi Hayashi[3], Yuji Sasaki[4] ([1]*Div. Biophys., Jichi. Med. Univ.*, [2]*Grad. Sch. Info. Sci., Hiroshima City Univ.*, [3]*Dep. Phys. Sci. Eng., NITech*, [4]*Grad. Sch. Frontier Sci., Univ. Tokyo*)

X-ray fluorescence holography (XFH) is a model-free atomic imaging which can visualize the three-dimensional structures around specific elements. Using the developed experimental setup for the Bio-XFH [A. Sato-Tomita et al., Rev. Sci. Inst. 87, 063707, 2016], the hologram patterns (interference patterns containing both intensity and phase information necessary for image reconstruction) of human hemoglobin (Hb) and sperm whale myoglobin (Mb) crystals were recorded at the beamlines BL6C, KEK-PF and BL39XU, Spring-8. We have recently succeeded for the first time in reconstruction of atomic-images of Mb, but still struggled with Hb, due to the complexity arising from the image overlapping of orientationally different 16 subunits existing in the unit cell of the Hb crystal.

1SNA-2 High resolution and time-resolved X-ray crystallographic study on enzymatic reaction of human MTH1

Teruya Nakamura[1,2], Shaimaa Waz[2], Keisuke Hirata[2], Mami Chirifu[2], Shinji Ikemizu[2], Yuriko Yamagata[2] ([1]*Priority Organization for Innovation and Excellence, Kumamoto Univ.*, [2]*Grad. Sch. of Pharmaceut. Sci., Kumamoto Univ.*)

Human MTH1 hydrolyzes oxidative nucleotides such as 8-oxo-dGTP and 2-oxo-dATP with broad substrate specificity and prevents transversion mutations caused by their misincorporation into DNA. In order to understand the broad substrate specificity, the protonation state of Asp residues (substrate-binding residues) was examined by bond-length analysis using high resolution X-ray data (~1.0 A). Furthermore, in order to reveal the hydrolytic mechanism, the course of reaction was followed by time-resolved X-ray crystallography. Here we will discuss the unique mechanisms of broad substrate recognition and hydrolytic reaction by MTH1.

1SNA-3 時間分解分光法による ABC トランスポーターの輸送と ATP 加水分解過程の直接観察

Direct observation of allocate-transport and ATP-hydrolysis for the ABC transport by time-resolved spectroscopy

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Time-resolved spectroscopy is powerful to follow the changes in the structure and chemical property of the active sites along the reaction axis. Here, to elucidate the molecular mechanism of ABC transporters, the time-resolved visible and infrared spectroscopy are applied to the heme importer; BhuUV-T complex. The visible absorption spectrum of heme is changed by its location, which allow us to monitor the transport of the allocate. The time-resolved infrared microscopy in the SPring-8 BL43IR enabled us to follow the hydrolysis of ATP. Now, we are trying to investigate the single-turn-over of the transport by the novel microscopic infrared/visible spectrometers equipping the micro-channel flow-cells.

1SNA-4 生物学的プロトントンネリング機構解明へ～新規 ENDOR 解析法によるタンパク質構造精密解析～

Substrate Positioning of Soybean Lipoxygenase For H-Atom Abstraction by ENDOR 'Crystallography'

Masaki Horitani (*Saga Univ., Dept of Appl Biochem & Food Sci*)

Without a ground state substrate-bound structure for the prototypical nonadiabatic tunneling system, soybean lipoxygenase (SLO), it has remained unclear whether the requisite close tunneling distance occurs through an unusual ground state active site arrangement or by thermally sampling conformational substates. We introduce Mn^{2+} as a spin-probe surrogate for the SLO Fe ion. $^{1}H/^{13}C$ ENDOR then reveals the locations of linoleic acid (hydrogen donor) and water (acceptor) relative to the metal, and molecular dynamics simulations of the fully solvated SLO model using ENDOR-derived restraints give additional metrical information. This talk will introduce the developed ENDOR analytical method and discuss about the mechanism of enzymatic C-H activation by hydrogen tunneling.

1SNA-5 生自然殺害細胞内 X 線 1 分子計測

X-ray single molecular observations in living Natural killer cells

Jae-Won Chang[1,3], Masahiro Kuramochi[1,3], Kouhei Ichiyanagi[2], Yuji Sasaki[1,3] ([1]*Graduate School of Frontier Science, The University of Tokyo*, [2]*KEK*, [3]*OPERANDO-OIL*)

There are many proteins on cell membranes co-acting with other molecules. Our previous studies using Diffracted X-ray Tracking (DXT) revealed dynamics of these membrane proteins related to their functional state, that is, membrane protein is one of the most important active site of cells. Recently, we succeeded in measuring different dynamics of Interleukin-2 (IL-2) and Interleukin-15 (IL-15) bounded to same receptors on Natural Killer (NK) cells membranes using monochromatic DXT adapting Cu-Kα light at the sub-second level. There are unidentified different dynamics of IL-2 and IL-15 with their receptor which is supposed to determine the different second signals of immune systems. We will reports individual dynamics of these ligands inducing NK cells maturation.

1SNA-6 SACLA と SPring-8 により可視化された亜硝酸還元酵素のレドックス依存的な構造変化

Redox-dependent structural change in nitrite reductase visualized by SPring-8 and SACLA

Eiichi Mizohata (*Grad. Sch. Eng., Osaka Univ.*)

Metalloprotein studies with synchrotron radiation crystallography (SRX) have faced difficulties, because X-ray photoreduction changes the native structures of metal centers. Serial femtosecond crystallography (SFX) using ultrabright femtosecond X-ray free electron lasers has opened a new age of structural biology. SFX enables structure determination from microcrystals at room temperature without radiation damage of the sample. I applied SFX at SACLA to visualize intact structures of copper-containing nitrite reductase (CuNiR). On the other hand, I utilized photoreduction in SRX at SPring-8 to initiate a catalytic reaction of CuNiR and to trap enzymatically produced intermediary structures. By comparing SFX and SRX data, new insights of catalysis of CuNiR were obtained.

1SNA-7 Energetics of proton transfer in proteins

Hiroshi Ishikita (*The University of Tokyo, RCAST*)

The pKa of H-bond donor and acceptor moieties in H-bonds can be analyzed from the potential energy profiles of the H-bonds. The energy difference between the H-bond donor and acceptor moieties corresponds to the pKa difference. Calculations performed at the at the density functional theory (DFT) level are likely to stray away from correct description of geometry towards better description of energy. Therefore, H-bonds should be evaluated based on the potential-energy profiles. In particular, low-barrier H-bonds (LBHB) can be unambiguously defined by the potential-energy profile at the DFT level (irrespective of considering the nuclear Schrodinger equation), because identical pKa values of the donor and acceptor moieties is the requirement for LBHB formation.

1SAP-1 時間発展する超分子集合体

Time-dependent evolution of a metastable supramolecular assembly

Kazunori Sugiyasu (*NIMS*)

Molecular self-assembly that operates under out-of-equilibrium conditions is expected to yield nanostructures that are inaccessible through the spontaneous thermodynamic process. Moreover, time evolution, which is reminiscent of biomolecular systems, may occur under such conditions and allow the synthesis of supramolecular assemblies with enhanced complexities. Recently, we have reported the time evolution of a metastable supramolecular assembly of a porphyrin derivative. In this system, two aggeregation pathways interplayed; kinetically formed nanoparticle transformed into thermodynamically stable nanofiber over time through autocatalytic process. Based on their energy landscape, we could control the lag time of the time evolution by rational molecular design.

1SAP-2 分子の集合・離脱が駆動する神経軸索ガイダンスの分子メカニクス

Molecular Mechanics for Axon Navigation in the Brain

Naoyuki Inagaki (*Nara Inst Sci Technol*)

Neurons extend a long process, axons, to the right destinations and form complicated networks in the brain. Axonal outgrowth can be navigated by attractive chemical cues such as soluble chemicals (chemotaxis) and substrate-bound chemicals (haptotaxis), the processes called axon guidance. We are analyzing the molecular mechanics for chemotaxis and haptotaxis involved in axon guidance. We show that shootin1 functions as a clutch molecule that couples F-actin retrograde flow and the cell adhesion molecule L1-CAM at axonal tips. Shootin1 and L1-CAM are located at critical interfaces, transducing chemical signals into the forces for axonal chemotaxis and haptotaxis.

1SAP-3 How can we control swarming of self-propeled biomolecular motors

Akira Kakugo[1,2], Jakia Jannat Keya[1], Arif Md. Rashedul Kabir[2] ([1]*Graduate School of Chemical Sciences and Engineering, Hokkaido University*, [2]*Faculty of Science, Hokkaido University*)

Collective motion is a fascinating example of coordinated behavior of self-propelled objects, which is often associated with the formation of large scale patterns. In this work, we have demonstrated the collective motion of kinesin driven microtubules by regulating mutual interaction among the gliding microtubules, by employing depletion force among them. Proper regulation of the mutual interaction among the gliding microtubules through employment of the depletion force was found to allow the exhibition of collective motion and stream pattern formation by microtubules. We also discuss how collectively moving microtubule on kinesin coated elastomer substrate response to external stimuli such as mechanical stresses.

1SAP-4 アクトミオシン細胞骨格におけるモーター誘起応力の理論

Theory on motor-induced stress in an isotropic actin-myosin network

Tetsuya Hiraiwa (*Department of Physics, The University of Tokyo*)

Bodies of eukaryotic cells are covered by an actomyosin cytoskeleton, a pseudo two dimensional network consisting of actin and myosin filaments. Mechanics of this cytoskeleton governs motor-induced contractility of a cell, which plays crucial roles in dynamic behaviors of cells.
In the talk, I will talk about our theoretical work on motor-induced contractility in such cytoskeletal network [1]. I will propose a mechanical model of an isotropic stiff F-actin network with crosslinkers and explain how and when contractility occurs. Since this cytoskeleton in a living cell should be fluidic, we consider the network in which there are only few amount of crosslinkers and/or crosslinkers and filaments can turn over.
[1] T. Hiraiwa and G. Salbreux, PRL, 116, 188101 (2016).

1SAP-5 ロタキサン連結高分子系超分子における組織化制御

Dynamical Ordering of Supramolecular Architecture Comprising Rotaxane-Linked Polymers

Toshikazu Takata (*Dept. of Chem. Sci. and Eng., Tokyo Inst. of Tech.*)

Threading or penetrating structure of linear molecule into cyclic molecule called as “(pseudo)rotaxane” ensures high freedom and mobility of the two molecules because of the weak interaction between the molecules linked by mechanical bond but not covalent bond. Therefore, as proved by the works of the Nobel laureates (2016 in chemistry), rotaxane molecules can be readily applied to molecular switch and machine. Meanwhile, these rotaxane molecules has collected much interest, in particular when the component molecules tether polymer chains, since polymers can form certain assembled or ordered structures depending on their mobility.
In this paper, we would like to discuss on the two dynamical ordering systems based on the (pseudo)rotaxane linking of polymers.

1SAP-6 基板上で自発的に運動・増殖する細胞のためのミニマル粒子モデル

A particle-based minimal model for crawling and proliferating cells on substrate

Ryoichi Yamamoto[1], Simon Schnyder[2], John J. Molina[1] ([1]*Department of Chemical Engineering, Kyoto University*, [2]*Fukui Institute for Fundamental Chemistry, Kyoto University*)

Unique nontrivial collective motions can occur in several biological systems such as swimming microorganisms and migrating cells. We have been developing a simple particle-based minimal model for crawling and proliferating cells on substrate. It mimics a real mechanics of migrating/proliferating cells with the mechanisms of the contact inhibition of locomotion (CIL) and the contact inhibition (CI) of cell division in a straightforward way. The present model has been applied to simulate the collective motions of crawling cells and also growing colony composed of proliferating cells. As it will be shown in the presentation, some basic properties seen in real crawling cells have been successfully reproduced.

1SKP-1 光化学系 I-フェレドキシン電子伝達複合体の X 線構造および NMR 解析

X-ray structure and NMR analysis of the electron transfer complex between Photosystem I and Ferredoxin

Hideaki Tanaka[1,2], Hisako Kawai[1], Risa Mutton[1], Setif Pierre[3], Marc Nowaczyk[4], Matthias Rogner[4], Takahisa Ikegami[5], Genji Kurisu[1,2] ([1]*IPR, Osaka Univ.*, [2]*JST-CREST*, [3]*CEA Saclay*, [4]*Ruhr-University Bochum*, [5]*Grad. Sch. of Medical Life Science, Yokohama City Univ.*)

Photosystem I (PSI), a large protein complex of the thylakoid membrane, mediates the final step of light-driven electron transfer to the stromal electron carrier protein, Ferredoxin (Fd). Although several structures of electron transfer complexes between Fd and Fd-dependent enzymes are available, the pivotal PSI-Fd electron transfer complex is structurally unknown. Here we report the first structural description of the PSI-Fd complex from the cyanobacterium Thermosynechococcus elongates BP-1. Each Fd is recognized by a PSI protomer in a similar orientation but with different distance of Fd- and PSI-redox centres (ranging from 8.3 to 9.6 Å). In combination with nuclear magnetic resonance (NMR) analyses on Fd, our results show two different Fd-binding states.

1SKP-2 分子構造に基づく理論解析による光合成膜蛋白質における反応機構の解明
Theoretical investigation based on molecular structures reveals reaction mechanisms in photosynthetic membrane proteins

Keisuke Saito (*RCAST, The University of Tokyo*)

In photosynthesis, membrane proteins convert light energy into a proton gradient across the membrane. Three-dimensional molecular structures of these membrane proteins have been clarified in high resolutions by using various methods, such as the X-ray crystallography and the cryo-electron microscopy. Using the protein structures, we have investigated reaction mechanisms of photosynthesis by theoretical approaches including quantum-mechanical and molecular-dynamics calculations. Here, I will talk about our recent studies on proton-transfer process in photosystem II protein complex, which mediates the oxygen-evolution reaction in photosynthesis of plants and algae.

1SKP-3 The Regulatory Functions and movements of quinones: It's Insane in the Membrane!

Duncan McMillan[1], Yoshio Nakatani[2], Lars Jeuken[3], Julia Butt[4], Gregory Cook[2], Hiroyuki Noji[5] ([1]*Department of Biotechnology, Delft University of Technology*, [2]*Department of Microbiology and Immunology, University of Otago*, [3]*School of Biomedical Sciences, University of Leeds*, [4]*School of Chemistry, and School of Biological Sciences, University of East Anglia*, [5]*Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo*)

Little is known about quinone-quinol interconversions in the lipid membrane environment by respiratory enzymes. It is well known that respiratory adaptation occurs, proton-pumping enzymes are expressed under aerobic conditions while non proton-pumping enzymes under anerobic conditions. However, the role of quinones in these processes, and the reasons behind switching between ubiquinone and menaquinone is poorly understood. Here, three quinone-utilizing proteins cymA, cytochrome bo3, and NADH Dehydrogenase 2, have been explored from the model microbes S. oneidensis, E. coli and Cb. thermarum respectively. The purpose of the switch between the use of MQ and UQ upon anaerobic/aerobic conditions is explored alongside the influence of a membrane environment.

1SKP-4 X 線自由電子レーザーを用いた、チトクロム酸化酵素からの一酸化炭素解離に伴う構造変化の時分割結晶構造解析
A nanosecond time-resolved XFEL analysis of structural changes associated with CO release from Cytochrome *c* Oxidase

Atsuhiro Shimada[1], Minoru Kubo[2], Seiki Baba[3], Hideo Ago[2], Tomitake Tsukihara[4], Shinya Yoshikawa[5] ([1]*Fac. Appl. Biol. Sci., Gifu Univ.*, [2]*RIKEN, SPring-8 Center*, [3]*JASRI*, [4]*Inst. for Protein Res., Osaka Univ.*, [5]*Picobiol. Inst., Univ. Hyogo*)

Cytochrome *c* oxidase (CcO) pumps protons utilizing electrostatic repulsion between protons transferred through a water channel and net positive charges created by oxidation of heme *a* for reduction of O_2 at heme a_3 (Fe_{a3}). The channel must be timely closed after collection of pumping protons before Fe_{a3} oxidation to prevent spontaneous proton back leakage. For understanding the channel closure mechanism, opening process of the channel which occurs upon release of CO from CcO is investigated using time-resolved XFEL with nanosecond time-resolution. The opening process indicates that Cu_B senses completion of proton collection and binds O_2 prior to binding to Fe_{a3} to close the water channel using a conformational relay system among Cu_B, heme a_3 and a transmembrane helix.

1SKP-5 好熱菌由来 V 型 ATP 合成酵素の単粒子解析
Single-particle analysis of V-type ATPase/synthase from *Thermus thermophilus* by cryo-EM

Atsuko Nakanishi[1], Jun-ichi Kishikawa[1], Kaoru Mitsuoka[2], Ken Yokoyama[1] ([1]*Dept. of Life Sci. Kyoto Sangyo Univ.*, [2]*Res. Ctr. UVHEM. Univ. Osaka*)

V-type ATPase (V-ATPase) is a rotary molecular motor, which couples ATP hydrolysis/synthesis in V_1 domain with proton flow in V_o domain through the rotation of central rotor apparatus. Here, we present the structures of three rotational states of the V-ATPase from *Thermus thermophilus* by single-particle analysis using cryo-electron microscopy (cryo-EM). The obtained three structures, defines by the position of the central rotor F subunit, provided insights into how the surrounding stator subunits dynamically deform during the transition of the ATP catalytic cycle. Large cavities are observed in V_o domain, suggesting pathways of proton exit and entrance. Based on the structures, we discuss the rotary catalytic mechanism of the V-ATPase.

1SKP-6 Cryo-EM structures of the autoinhibited E. coli ATP synthase in three rotational states

Meghna Sobti[1], Callum Smits[1], Andrew Wong[2], Robert Ishmukhametov[3], Daniela Stock[1,4], Sara Sandin[2], **Alastair Stewart**[1,4] ([1]*VCCRI, Sydney, Australia*, [2]*SBS, NTU, Singapore*, [3]*Physics, University of Oxford, UK*, [4]*Medicine, UNSW, Australia*)

A molecular model that provides a framework for interpreting the wealth of functional information obtained on the E. coli F-ATP synthase has been generated using cryo-electron microscopy. Three different states that relate to rotation of the enzyme were observed, with the central stalk's epsilon subunit in an extended autoinhibitory conformation in all three states. The proton translocating subunit contains near parallel helices inclined by ~30 degrees to the membrane, a feature now synonymous with rotary ATPases. The peripheral stalk is resolved over its entire length of the complex, revealing the F1 attachment points and a coiled-coil that bifurcates toward the membrane with its helices separating to embrace subunit a from two sides.

1SLP-1 タンパク質構造・配置に対する混合溶媒効果の全原子自由エネルギー計算による解析
Mixed-solvent effect on protein configuration studied by all-atom computation of free energy

Nobuyuki Matubayasi (*Division of Chemical Engineering, Grad Sch Eng Sci, Osaka Univ*)

The configuration of protein is strongly influenced by the surrounding environment. In the present work, we address the effects of urea cosolvent and of lipid membrane from the standpoint of energetics. By conducting all-atom computation of free energy with MD simulation and a solution theory, we discuss the roles of a variety of intermolecular interaction components such as electrostatic, van der Waals, and excluded-volume in the denaturing activity of urea. The lipid-protein interaction is further treated within the framework of the solution theory by viewing the lipid and water as a mixed solvent and the protein as the solute. Water is then shown to stabilize a surface-bound state of protein due to the balance between the attractive and repulsive interactions.

1SLP-2 好アルカリ性細菌の高アルカリ性環境適応に関与するメゾレベルでの場としての細胞表層酸性高分子役割の解明

Elucidation of the role of cell surface acidic polymers as a place at meso level from alkaliphilic bacteria

Masahiro Ito (*Faculty of Life Sciences, Toyo Univ.*)

Alkaliphilic Bacillus halodurans C125 has a large amount of negative charge by acidic polymers on the cell surface when it is grown in highly alkaline pH rather than neutral pH. Alkaliphilic Bacillus pseudofirmus OF4 also has a negatively charged S-layer protein. It is expected that the ion environment near the cell surface layer will be provided with a "place at meso level" by the Donnan effect. The intracellular pH of an alkaliphile growing at external pH 10.5 is maintained at around 8.3, and the proton motive force (PMF) is only -38 mV. But, in alkaliphilic Bacillus, ATP synthesis by oxidative phosphorylation is carried out using a PMF. The actual pH near the outside of the cell membrane is expected to be lower than the external environment pH by the Donnan effect.

1SLP-3 リン脂質二重膜の構造変化に伴う水和状態の変化：テラヘルツ分光法による研究から

Changes in the hydration states of phospholipid bilayers accompanying bilayer structural changes: From the studies by THz spectroscopy

Mafumi Hishida (*Dept. Chem., Univ. Tsukuba*)

Water has been believed to be important for self-assembly of biomolecules. Strongly bound water, which form hydrogen-bond with solutes, has been investigated actively in relation to the self-assembly. It is, however, recently claimed that there are also a lot of slightly bound water, which indirectly affects the self-assembly through hydrogen-bond network. Although it had been difficult to detect the slightly bound water, recently developed spectroscopy, THz spectroscopy, have made it possible. I will present our studies of the hydration state of biomolecules, mainly phospholipid bilayers, by THz spectroscopy. Not only the amount of the slightly bound water, the change in the hydration states accompanying the structural change of the bilayers were also clarified.

1SLP-4 蛋白質―脂質相互作用と小孔形成毒素

Protein-lipid interactions in a pore-forming toxin

Kouhei Tsumoto[1], Jose Caaveiro[2] ([1]*Grad. Sch. Eng. and Inst. Med. Sci., Univ. Tokyo*, [2]*Grad. Sch. Pharm., Kyushu Univ.*)

Pore-forming toxins (PFTs) are metamorphic proteins that fold stably in water solutions as well as in cellular membranes, where they assemble to form lethal transmembrane holes producing cell death. Actinoporins are a family of potent hemolytic toxins vigorously studied as a paradigm of alpha-helical PFTs in the context of lipid–protein interactions. We have revealed for the first time the complete energetic and structural basis of the transformation of a PFT from the water-soluble to the active transmembrane state, and its reverse process. We will show that FraC, an actinoporin, undergoes a stepwise metamorphosis towards the lethal pore that is catalyzed by the physicochemical properties of the membrane and by key non-covalent interactions with specific lipids.

1SLP-5 タンパク質構造への分子環境の効果：抗原抗体界面の分子動力学計算による研究

Molecular environment effects on the protein structure: Molecular dynamics studies on the antigen-antibody interface

Takefumi Yamashita (*RCAST, Univ. Tokyo*)

It is very challenging but necessary to develop a technology artificially controlling protein properties through environmental effect. Toward this ultimate purpose, we studied local structures (hydrogen bonds, salt bridges, and so on) with the molecular dynamics (MD) simulations in the context of the environmental effect. For example, we found that the stability of the salt bridge could be explained not only by the configuration of charged residues but also by the environmental effect. Interestingly, bulky residues (e.g., Trp and Tyr) play an important role; the environmental side-chains seem to limit the range of motions of salt-bridge residues. Our results suggested that the understanding of the environmental effect is necessary to control the protein structure.

1SLP-6 NMR analysis of proteins in living cells

Hidehito Tochio (*Dept. Biophys., Grad. Schl. Sci., Kyoto Univ.*)

NMR spectroscopy to investigate protein structures and dynamics has been dedicated to analyzing highly purified samples in test tubes. Performing such studies only in test tubes, however, may overlook features that only emerge when they are in their native environment. And functioning proteins in reality often change their structural states depending on the context in which they live. Thus, if at all possible, proteins structure and function should be explored at their native environment, although it is far from an easy task. We have been working on proteins in living cells with NMR, where proteins originally produced in vitro but then artificially delivered into living cells are analyzed. In this talk, our recent study on a two-domain protein will be presented.

1SMP-1 Structural basis for the heme-dependent transcriptional regulation

Shigetoshi Aono[1,2] ([1]*Okazaki Int. Integ. Biosci.*, [2]*Inst. Mol. Sci.*)

A transcriptional regulator HrtR senses and binds a heme molecule as its physiological effector to regulate the expression of a heme-efflux system responsible for heme homeostasis in L. lactis, but its regulatory mechanisms are not clear. To elucidate the molecular mechanisms of how HrtR senses a heme molecule and regulates the gene expression for the heme efflux system, we determined the crystal structures of apo-HrtR/DNA complex, apo-HrtR, and holo-HrtR. HrtR adopts a unique mechanism for its functional regulation upon heme-sensing. Heme-binding to HrtR causes a coil-to-helix transition of the α4 helix in the heme-sensing domain, which triggers a structural change of HrtR to dissociate from the target DNA for derepression of the genes encoding a heme efflux system.

1SMP-2 光活性化アデニル酸シクラーゼの構造と機能
Structure and function of photoactivated adenylyl cyclase

Mio Ohki[2], Sam-Yong Park[2], **Mineo Iseki**[1] ([1]*Facul. Pharm. Sci., Toho Univ.*, [2]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

Photoactivated adenylyl cyclase (PAC), first identified as a photosensor in the unicellular alga Euglena, has attracted considerable attention as an optogenetic tool to control cAMP-related biological functions. In addtion, the activation mechanism of PAC has long remained unelucidated mainly because of difficulties in obtaining a sufficient amount of protein for X-ray crystal structure analysis. Recently, we found a PAC-like gene on the genome of the cyanobacterium Oscillatoria acuminata and succeeded in the crystallization of the encoded protein OaPAC expressed in E. coli. The solved structure revealed a novel coiled coil interfacing each monomer. Here, we discuss the light-activation mechanism of OaPAC on the basis of structure and site-directed mutagenasis.

1SMP-3 細菌機械受容チャネル MscL のメカノゲーティングに対する計算科学的アプローチ
Computational Approach to Mechano-Gating of the Bacterial Mechanosensitive Channel MscL

Yasuyuki Sawada[1], Masahiro Sokabe[2] ([1]*Dept Nutrition Fac Human Life Science Nagoya Univ Economics*, [2]*Mechanobiology Lab Nagoya Univ Grad Sch Med*)

The bacterial mechanosensitive channel MscL is constituted of homopentamer of a subunit with TM1 inner and TM2 outer transmembrane helix. The major issue on MscL is to understand the gating mechanism driven by membrane tension. To get insights into the detailed mechanism of the mechano-gating including the relationship between the major tension sensor F78 and the gate including G22, we performed MD simulations for opening of WT and mutant (G22N GOF, F78N LOF and G22N/F78N LOF) MscLs. As a result, the substituted amino acid residue N78 loses the stable interaction both with lipids and with the neighboring I32-L36-I40 in TM1, suggesting that F78 plays important roles both as sensing membrane tension and as transmitting the sensed force to TM1 helix which forms the gate.

1SMP-4 電位依存性ホスファターゼ VSP のカップリング機構に関する構造生物学的研究
Structural analysis of voltage-sensing phosphatase (VSP) on the electrochemical coupling

Hirotaka Narita[1,3], Naoki Kanda[1], Yasushi Okamura[2], Atsushi Nakagawa[1,3] ([1]*Inst. Protein Res., Osaka Univ.*, [2]*Grad. Sch. of Med., Osaka Univ.*, [3]*CREST, JST*)

The voltage-sensing phosphatase (VSP) consists of a transmembrane voltage sensor domain, an inter-domain linker, and a cytoplasmic region. The cytoplasmic region is a phosphoinositide phosphatase with high structural similarity to PTEN and the enzymatic activity is regulated by voltage sensor movement upon membrane potential. However, the molecular mechanism of the coupling in VSP is still unclear. Here, we investigated the effect of structural changes of the linker on substrate binding in VSP using ITC assays. Our findings suggest that conformational change in the inter-domain linker plays a key role in substrate-binding and coupling in membrane potential and phosphatase activity.

1SMP-5 電位依存性プロトンチャネル VSOP/Hv1 の電場中での動態の解析
Molecular dynamics study of kinetics of the voltage-gated proton channel VSOP/Hv1 under electric fields

Hiroko X. Kondo[1], Yasushige Yonezawa[2], Naoyuki Miyashita[3], Masayo Iwaki[4], Kohei Takeshita[5], Yuichiro Fujiwara[6], Matsuyuki Shirota[7,8,9], Kengo Kinoshita[8,9,10], Yasushi Okamura[6], Atsushi Nakagawa[5], Hideki Kandori[4], Yu Takano[1] ([1]*GSIS, Hiroshima City Univ*, [2]*Iat, Kindai Univ*, [3]*Bost, Kindai Univ*, [4]*Grad Sch Eng, Nagoya Inst Tech*, [5]*IPR, Osaka Univ*, [6]*Grad Sch Med, Osaka Univ*, [7]*Grad Sch Med, Tohoku Univ*, [8]*ToMMo, Tohoku Univ*, [9]*GSIS, Tohoku Univ*, [10]*IDAC, Tohoku Univ*)

VSOP/Hv1 is a voltage-gated proton channel that is activated by membrane depolarization. VSOP/Hv1 contains four-transmembrane segments homologous to the voltage-sensing domain of conventional voltage-gated ion channels, and its crystal structure in the Zn^{2+}-bound (inactivated) state was determined by Takeshita et al. However, the mechanism of activation of VSOP/Hv1 is still unclear. The results of FTIR spectra suggest a conformational change upon the Zn^{2+} binding, indicating structural differences between the closed state and the Zn^{2+}-bound state. To investigate the activation mechanism, we performed molecular dynamics simulations with applied voltage. We try to predict the structures in the resting and activated states and a conformational transition among them.

1SMP-6 Structural basis of redox-dependent regulation of SERCA2b

Michio Inoue[1], Nanami Sakuta[1], Satoshi Watanabe[1], Ryou Ushioda[2], Yoshiki Tanaka[3], Tomoya Tsukazaki[3], Kazuhiro Nagata[2], **Kenji Inaba**[1] ([1]*Tohoku Univ*, [2]*Kyoto Sangyo Univ*, [3]*NAIST*)

Sarco/Endoplasmic reticulum (ER) Ca2+-ATPase 2b (SERCA2b) is a ubiquitously expressed membrane protein that conducts Ca2+ uptake from the cytosol to the ER. Our recent study revealed that an ER disulfide reductase ERdj5 activates SERCA2b by reducing its luminal disulfide bond. We here determined crystal structures of oxidized and reduced forms of SERCA2b in E1-2Ca2+-AMPPCP state. Their detailed structural comparisons demonstrate slight but significant positional shifts of the luminal loops and the TM5-TM11 helices upon reduction of the luminal disulfide, leading to the altered geometry of the Ca2+-binding ligands. We discuss molecular mechanisms by which the Ca2+ transport activity of SERCA2b is regulated in a redox-dependent manner.

1SNP-1 オルガネラサイズの熱源を作り細胞機能を温熱制御する試み
Thermal Control of Cellular Functions Using Organelle-sized Heat Spots

Satoshi Arai (*Res. Inst. Sci. Eng., Waseda Univ.*)

Probably, temperature is the most significant element to affect cellular activities in living organism. If we achieve to heat up intracellular target quantitatively, it would lead to the establishment of a powerful methodology to control cellular functions according to thermodynamic law. Yet, it still remains challenging. Here we proposed a means to generate a tiny heat spot in a live cell through material science-based approach. Using fluorescent thermosensors, we imaged the temperature distribution provided by the heat spot and then discussed how cells behave in response to the temperature rise at localized area. Our study will contribute to the current argument that the heterogeneous temperature distribution exists at a single cell level.

1SNP-2 Nanostructured Smart Materials for the Remote Manipulation of Cell Behavior

Attilio Marino[1], Gianni Ciofani[1,2] ([1]*Smart Bio-Int., IIT, Italy*, [2]*Dept. Mech. Aero. Eng., Politec. Torino, Italy*)

The possibility to non-invasively modulate the cellular activity by a remote manipulation is subject of intense research efforts, that brought to the development of different stimulation approaches, based on ultrasounds (US) and on near-infrared (NIR) radiation, among others. Here we present different strategies that combine physical stimulation with the "smart" responsiveness of particular nanomaterials to foster specific cellular activation. Specifically, piezoelectric and plasmonic nanomaterials has been adopted in combination with US and NIR radiation in order to generate electrical and heat-based stimulation, respectively. Moreover, we show how to combine smart nanomaterials with cell-instructive nanostructured scaffolds for tissue regeneration and engineering.

1SNP-3 A molecular mechanism of gene regulation by matrix mechanics -A moving story of FHL2 and Force-

Naotaka Nakazawa[1], Aneesh Sathe[2], G.V. Shivashankar[2,3,4], Michael Sheetz[2,3,5] ([1]*iCeMS, Kyoto Univ.*, [2]*Mechanobiology Institute, National Univ. of Singapore*, [3]*Dept. of Biol. Sci., National Univ. of Singapore*, [4]*iFOM, Italy*, [5]*Dept. of Biol. Sci., Columbia Univ.*)

Matrix mechanics affects physiological processes through mechano-chemical signals from focal adhesion (FA) complexes that subsequently modulate gene expression. We find that shuttling of FHL2 between FAs and the nucleus depends on matrix mechanics. In particular, on soft surfaces or after the loss of force, FHL2 moves from FAs into the nucleus and concentrates at RNA polymerase II sites causing an increase in *p21* gene expression that will inhibit growth on soft surfaces. At the molecular level, shuttling requires FHL2 phosphorylation by active FA kinase (FAK). Thus, we suggest that FHL2 phosphorylation by FAK is a critical, mechanically dependent step in signaling from soft matrices to the nucleus to inhibit cell proliferation by increasing *p21* expression.

1SNP-4 Curvature-propagated mechanochemical waves in subcellular pattern formation

Min Wu, Maohan Su, Cheesan Tong, Shengping Xiao (*National Univ. Singapore*)

Oscillatory travelling waves of cortical activity, linked to actin dynamics in many cases, have been documented in a variety of single-cell systems, including various immune cell types. Occurrences of such patterns indicate the presence of local and global coupling mechanisms. However, the nature of the spatial coupling remains to be determined. My talk will focus on our recent discovery of a critical involvement of FBP17 and CIP4, two of the BAR domain superfamily proteins, in cortical actin waves. In addition, I will discuss the role of physical parameters such as membrane curvature and plasma membrane tension in the propagation of waves. A mathematical model proposing the mechanochemical basis of the experimentally observed pattern formation will also be presented.

1SNP-5 メカノトランスダクションと心筋リプログラミング、心臓再生

Mechano-transduction and Direct Cardiac Reprogramming for Heart Regeneration

Masaki Ieda (*Department of Cardiology, Keio University School of Medicine*)

Mechanical stress is critical for cardiac function and cell fate decision. However, the role of mechano-transduction in cardiac cell fate specification and heart regeneration remains undetermined. We first found that a combination of cardiac-specific transcription factors, Gata4, Mef2c, and Tbx5 (GMT), directly reprogrammed mouse fibroblasts into cardiomyocyte-like cells (iCMs) in vitro without mediating through a pluripotent state (Ieda et al. Cell, 2010). We also found that in vivo cardiac reprogramming with GMT converted resident cardiac fibroblasts into iCMs and regenerated infarct hearts in mice (Inagawa et al. Circ Res 2012, Circ Res, 2015). I will review in vivo microenvironment, mechano-transduction, and direct cardiac reprogramming in this symposium.

1SNP-6 臓器内部における末梢神経のメカノセンシング動態

Mechanosensing dynamics of peripheral nerves inside organs

Atsunori Kamiya (*NCVC*)

Mechanosensing of physical and chemical stimulations is necessary for maintaining homeostasis in cellular, organic and whole-body levels. Peripheral nerve is one of key mechanosensors. However, earlier studies addressing peripheral nerves have recorded neural activity outside organs by electrodes and limited to understand neural dynamics inside organs, that interface directly variable physical and chemical stimulations. Accordingly, I have started to visualize mechanosensing dynamics inside organs of peripheral nerves (i.e., baroreflex afferent nerves, peripheral sensory nerves). My results have revealed population coding dynamics in these nerves, that are different from earlier reported characteristics of peripheral nerve outside-organ.

1SNP-7 ゆらぎを利用した低侵襲な力測定による神経細胞オルガネラ輸送の解明

Non-invasive force measurement using fluctuation for organelle transport in neurons

Kumiko Hayashi (*Sch. Eng., Tohoku Univ.*)

Organelles are transported by motor proteins such as kinesin and dynein in living neurons. The motion of organelles was observed by fluorescence microscopy. We developed a non-invasive force measurement method based on non-equilibrium fluctuation properties of the organelle's motion. The force distribution thus measured had a several peaks, indicating the existence of multiple force producing units, which consist of motors, for the organelle transport. Cooperative transport by multiple motors is thought to realize a stable transport in neurons. We believe that the elucidation of mechanism about neuronal organelle transport is helpful for the understanding of neurodegenerative diseases.

2SAA-1 Development of techniques for imaging physiological functions toward visualization of singularity caused by minority elements

Takeharu Nagai (*The Institute of Scientific and Industrial Research, Osaka University*)

If we carefully observe the cell population that at first glance looks uniform and homogeneous, we may find small number of heterogeneous cells with a different nature. Moreover, this minority cells would sometimes significantly alter the behavior of the whole cell population. In this symposium, I would like to summarize each speaker's studies by discussing 1) possible mechanism by which variety output could be produced even in the cells with identical biomolecular reaction networks, and 2) development of techniques for imaging physiological function at wide range of spatiotemporal scale, which is indispensable for identification of minority cells.

2SAA-2 細胞集団に螺旋信号波をもたらす臨界現象
Critical transition controls the self-organized spiral nuclearion

Kazuki Horikawa (*Tokushima Univ. Biomedical Sci.*)

Spiral wave is common to excitable media, but mechanisms for the spontaneous spiral nucleation remained elusive. To ask this classical question, we performed a large-scale observation of intercellular relay of cAMP in the population of social ameba. Newly developed red fluorescent cAMP indicator allowed the analysis of signaling dynamics in 13,000-70,000 cell population with 1-cell resolution, that revealed the critical transition phenomena bringing spatially heterogeneous excitability. We will discuss how the cellular discreetness controls the spontaneous symmetry breaking in the self-organized pattern formation.

2SAA-3 Minor 要素の人為的な活性制御を可能とする受容体の配位ケミカルジェネティクス
Coordination chemical genetics of receptors for artificially regulating minority events

Shigeki Kiyonaka (*Grad. Sch. Eng., Kyoto Univ.*)

The main focus of our research is developing new methods which enable the artificial regulation of transmembrane receptors in a target cell in tissues or live animals. As one of the potential approach, we have recently developed a novel allosteric activation method of neurotransmitter receptors, termed coordination chemical genetics, which enables the selective activation of specific neurotransmitter receptors in target neurons. We expect that this method will be useful for identifying minor elements by artificially regulating signal transduction cascade in target cells.

2SAA-4 Small cells bur large impacts, revealed by extensive 2P / 8K-CMOS singularity imaging

Satoshi Nishimura (*Jichi Med Univ*)

In cardiovascular system, cell dynamics, blood flows, and force changes are always taking place, and it is unclear how these small perturbation can have large future impact, leading to pathological phenotype. We developed multi-scale imaging systems in space-and-time, to capture "singularity" point. In vivo platelet activation models, thrombus kept self-growing and collapsing. However, after emergence of minor platelet aggregations firmly attached to endothelium, thrombotic responses are dramatically enhanced by this micro core. In addition, minor endothelium injuries enhanced later inflammatory responses. In this session, I will introduce our recent imaging technologies, our applications, and future aspects for new "singularity" biology.

2SAA-5 High speed Raman imaging for chemical profiling of cells and tissues

Katsumasa Fujita (*Osaka Univ*)

Raman spectroscopy has been utilized as a power tool for detecting chemical composition in samples. Recently, this analytical capability has been applied to biological and medical research for characterizing cell or tissue by using the information of intracellular molecules. We have developed a technique to obtain the distribution of molecular vibrations rapidly in biological samples by using Raman scattering and applied to visualize the cell species and states during various cellular events. In this presentation, I will discuss the potential of Raman spectroscopy as a versatile tool for chemical profiling of biological sample, which can be realized by high-speed Raman imaging.

2SAA-6 How can one quantify singularity in cells from Single Cell Raman Imaging?

Tamiki Komatsuzaki[1,2] ([1]*Hokkaido Univ., RIES, MSC*, [2]*Hokkaido Univ., Grad. School of Life Science*)

Singularity in biology involves phase-transition-like behaviors triggered by a small set of elements in the whole system. To characterize the singularity requires spatiotemporal information of the system and some scheme to measure causality between the event in question and the set to trigger the event. Along this perspective, single cell Raman imaging contain rich information about the cell as a whole about the components that comprise the cell such as organelle and its components. Here we present our recent information theoretic approach to identify the state of cells, and address the possible generalization into spatiotemporal data set.

2SAA-7 マイノリティ細胞による自己免疫疾患発症制御機構の解明
Regulation of autoimmunity by minority cells

Taku Okazaki (*Institute of Advanced Medical Sciences, Tokushima University*)

The recent success of tumor immunotherapy targeting an immuno-inhibitory co-receptor PD-1 and the occasional development of autoimmune diseases as its adverse effect highlight the importance of inhibitory co-receptors in the regulation of tumor immunity as well as autoimmunity. The development of autoimmunity and the eradication of tumor cells are supposed to rely on a limited number of antigen specific T cells, because antigen specificity of T cells is extremely diverse. We are trying to characterize the features of individual T cell with autoreactivity in the presence or absence of inhibitory co-receptors to understand how these rare antigen-specific T cells regulate autoimmunity and tumor immunity.

2SAA-8 点描画解析プラットフォームを用いた確率的全脳マッピング
Probabilistic Mapping of Mouse Brains with Scalable and Pointillistic Analytical Platform

Tatsuya Murakami[1], Tomoyuki Mano[2,3], Shu Saikawa[3], Shuhei Horiguchi[4], Kousuke Baba[5], Mochizuki Hideki[5], Kazuki Tainaka[6], Hiroki Ueda[1] ([1]*Med., Univ. Tokyo*, [2]*Dept. Chem., Princeton Univ.*, [3]*Univ. Tokyo*, [4]*Osaka Univ.*, [5]*Med., Osaka Univ.*, [6]*Niigata Univ.*)

A three-dimensional single-cell-resolution mammalian brain atlas will accelerate systems-level identification and analysis of cellular circuits underlying various brain functions. To this end, we developed a whole-organ clearing and homogeneous expansion protocol. The expanded highly-cleared brain enabled us to construct a mouse brain atlas with single-cell annotation (CUBIC-Atlas), allowing us to directly count the number of cells in an adult mouse brain. Probabilistic activity mapping of pharmacologically stimulated mouse brains onto CUBIC-Atlas revealed the existence of distinct functional structures in the hippocampus. This pointillistic brain atlas provides a new platform for whole-brain cell profiling.

2SBA-1 トレハロースリポソームによるがん治療効果とアポトーシス
Therapeutic effects of trehalose liposomes against carcinoma along with apoptosis

Yoko Matsumoto (*Grad. Life, Univ. Sojo*)

Trehalose liposomes (DMTre) composed of DMPC and trehalose micelles have been produced. Hydrodynamic diameter of DMTre composed of 30 mol% DMPC and 70 mol% TreC14 was 100 nm with single and narrow range of size distribution, which was preserved for a period remaining stable for more than one month. The thickness of the fixed aqueous layer (TFAL) of DMTreCn was evaluated from the zeta potential and increase in TFAL values of DMTreCn was obtained in a dose-dependent manner. The remarkable inhibitory effects of DMTre on the growth of human colon, gastric, hepatocellular, lymphobrastic carcinoma, and lung carcinoma cells have been obtained. DMTre inhibited the growth of carcinoma cells leading to apoptosis in vitro and using xenograft mice model of carcinoma in vivo.

2SBA-2 天然糖トレハロースによる空間認知記憶の改善とオートファジーの関与
Trehalose intake improves spatial memory through autophagy activation in the brain of mice

Kunikazu Tanji, Yasuo Miki, Fumiaki Mori, Koichi Wakabayashi (*Dept. of Neuropathol., Inst. of Brain Sci., Hirosaki Univ. Graduate Sch. of Med.*)

Trehalose is a natural disaccharide composed of two glucose units. We applied trehalose to normal and dementia model mice to investigate effect of trehalose on abnormal protein aggregation. Consistently, trehalose increased level of the autophagosomal protein LC3, especially a lipidated form LC3-II in the mice brain. Further studies revealed that level of detergent-insoluble protein was suppressed in mice following oral administration of trehalose, despite an apparent alteration was not observed regarding abnormal protein aggregation. These results suggest that the oral intake of trehalose modulates propensity of molecules prior to aggregate formation.

2SBA-3 肺がん転移促進タンパク質 CERS6 およびそれを分子標的とした薬剤戦略
Targeting ceramide synthase 6-dependent metastasis-prone phenotype in lung cancer cells

Motoshi Suzuki (*Nagoya Univ Grad Sch Med, Mol Carcinog*)

Sphingolipids contribute to unique biological properties. We found that the ceramide synthase gene CERS6 is overexpressed and associated with lung cancer invasion. We showed that CERS6 may promote metastasis; CERS6 promoted a cell migration in vitro, as well as a RAC1-positive, C16 ceramide-dependent lamellipodia/ruffling formation and attenuation of lung metastasis in mice. We hypothesized this pathological overexpression can be utilized for cancer therapy, since excess ceramides have been known to promote apoptosis. Accordingly, a ceramide precursor DMPC induced a lethal amount of C16 ceramide accumulation. Taken together, targeting CERS6-dependent sphingolipid-metabolic homeostasis may provide a novel therapeutic strategy for lung cancer.

2SBA-4 脂質代謝酵素 PLA2 ファミリーによるリポクオリティ制御の新機軸
Novel insights into the lipoquality control by the PLA2 family

Makoto Murakami[1,2,3] ([1]*Center for Disease Biology and Integrative Medicine, Faculty of Medicine, The University of Tokyo*, [2]*Tokyo Metropolitan Institute of Medical Science*, [3]*AMED-CREST*)

The phospholipase A2 (PLA2) family comprises a group of lipolytic enzymes that hydrolyze phospholipids to yield fatty acids and lysophospholipids. The mammalian genome encodes >30 PLA2s or related enzymes, which are structurally classified into several subfamilies. PLA2s have been implicated in signal transduction, membrane homeostasis or energy production, and therefore can be regarded as key regulators of the quality of lipids (lipoquality). Disturbance of PLA2-driven lipoquality hampers tissue homeostasis and can be linked to various diseases. In this symposium, I will highlight several examples of the lipoquality control by the PLA2 family, as revealed by our ongoing studies using knockout mice for various PLA2s in combination with comprehensive lipidomics.

2SBA-5 実在形質膜をモデル化した脂質二重層膜の分子動力学計算
Molecular dynamics study of lipid bilayers modeling real plasma membranes

Yoshimichi Andoh, **Susumu Okazaki** (*Nagoya University*)

Molecular dynamics calculations of lipid bilayer modeling the real plasma membranes of murine thymocytes and hepatocytes have been performed under physiological conditions. Changes in the membrane properties induced by canceration were investigated. Our calculations clearly show disordering and fluidization of the leukemic cell membranes. In contrast, hepatic canceration causes plasma membranes to become more ordered laterally and less fluid than the normal cell membranes. The changes caused by canceration depend of the cells. The deep understanding of the membrane properties of the normal and cancered cell membranes contribute to a DDS strategy for the drug.

2SBA-6 広帯域分光を用いた二糖周辺の水の水素結合ネットワーク評価
Characterization of the hydrogen-bond network of water around sucrose and trehalose investigated with broadband spectroscopy

Keiichiro Shiraga[1], Yuichi Ogawa[2], Masahito Nakamura[3], Katsuhiro Ajito[3], Takuro Tajima[3] ([1]*RIKEN Center for IMS*, [2]*Grad. Sch. Agri., Kyoto Univ.*, [3]*Device Technology Labs., NTT*)

Modification of the water hydrogen bond (HB) network imposed by disaccharides is known to serve as a bioprotective agent, though its comprehensive understanding is still yet to be reached. In this study, we performed broadband dielectric spectroscopy of disaccharide aqueous solutions. Our result showed that disaccharides exhibit an obvious destructuring effect by fragmenting HBs and distorting the HB structure of water. At the same time, hydration water was found to exhibit slower dynamics and a greater reorientational cooperativity than bulk water due to stronger HBs. These results lead to the conclusion that disaccharides forming strong HBs structurally incompatible with native water HBs lead to the rigid but destructured HB network around them.

2SBA-7 グルコースとトレハロースの水溶液中における構造と水和に関する ab initio QM/MM-MD 法による研究
Ab initio QM/MM-MD study on conformation and hydration of glucose and trehalose in aqueous solution

Misako Aida (*Grad. Sch. Sci., Hiroshima Univ*)

Trehalose is a non-reducing disaccharide composed of two α-(D)-glucose units with 1,1-glycosidic linkage. Trehalose is known to have special properties which may induce extraordinary stabilization of biological materials, while the reason is not fully understood yet. Saccharides can take many conformations, and structures in aqueous solution must be different from those in the gas phase. Furthermore, the hydration must play an important role in the stability of conformers in aqueous solution. In this work, we aim to show whether trehalose has special characteristics which differ from glucose or not. To this end, we clarify the hydration patterns of several conformers of glucose and trehalose in aqueous solution using QM/MM-MD method.

2SCA-1 このシンポジウムの狙いについて
Introduction of hybrid/integrative structural biology

Masaaki Sugiyama (*KURRI*)

In these days, hybrid/integrative structural biology is one of key strategies to reveal functional dynamics in biomacromolecules. As an opening, the overview of the hybrid/integrative approach by quantum beam scattering techniques and NMR, and computational science, will be introduced shortly.

2SCA-2 モデル膜の熱揺らぎと機械的性質に及ぼすペプチドの効果
Effects of incorporating small peptide on collective thermal fluctuations and elastic and viscous properties in model lipid bilayers

Michihiro Nagao[1,2], Elizabeth Kelley[1], Paul Butler[1] ([1]*NIST*, [2]*Indiana U.*)

Neutron spin echo spectroscopy (NSE) provides unique insights into thermal fluctuations in model lipid bilayers, which are controlled by elastic and viscous properties of the membranes. Recently we developed a method to calculate some of these parameters from the NSE data. Here we use this novel technique to determine the mechanical properties of lipid bilayers incorporated with small peptide, gramicidin, which is known to form inorganic monovalent cation channels by creating dimers in the bilayer. The dimerization and channel formation affect the membrane dynamics to be suppressed if the concentration is high. We discuss the origin of the suppression in terms of the properties of the membranes.

2SCA-3 Protein dynamics as studied by neutron spin echo and MD simulation

Rintaro Inoue[1], Takashi Oda[2], Tomotaka Oroguchi[3], Mitsunori Ikeguchi[2], Masaaki Sugiyama[1], Mamoru Sato[2] ([1]*Research Reactor Institute, Kyoto University*, [2]*Yokohama City University*, [3]*Keio University*)

Proteins, especially multi-domain proteins, possess a structural complexity reflected in a complex dynamical behaviour. In addition to unspecific and fast stochastic local fluctuations with the timescale of picosecond, large-scale rearrangement and movements (domain motion) are often responsible for numerous protein's intrinsic functions. Hence, the experimental approaches, which can access to protein domain motion is highly demanded. Recently, it has demonstrated that neutron spin echo (NSE) is one of the candidates for detecting the domain motions in proteins. In this presentation, we have employed NSE technique and MD simulation to detect and characterize the domain motion of restriction endonuclease EcoO109I.

2SCA-4 **Protein Structural Fluctuations Investigated by X-ray Solution Scattering and Molecular Dynamics Simulation**

Tomotaka Oroguchi[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*)

The structures of proteins are fluctuating in solution and these fluctuations are essential for protein functions. Therefore, to understand mechanisms of protein functions, the experimental methods to obtain the information on protein structural fluctuations in solution are needed. For this purpose, we have developed the method using the combination of small-angle X-ray scattering (SAXS) and molecular dynamics (MD) simulations (MD-SAXS). We have applied the MD-SAXS method to study the structural fluctuations of restriction endonuclease, proliferating cell nuclear antigen and glutamate dehydrogenase. The results have demonstrated that both of the structural fluctuations and the hydration structures are indispensable to account the experimental SAXS data.

2SCA-5 **統合的な構造物学アプローチによるに糖タンパク質および糖鎖の構造ダイナミクスの解析**

Integrative structural biology approaches for understanding conformational dynamics of oligosaccharides and glycoproteins

Hirokazu Yagi[1], Saeko Yanaka[2], Rina Yogo[1,2], Tatsuya Suzuki[2], Takumi Yamaguchi[3], Masaaki Sugiyama[4], Koichi Kato[1,2] ([1]*Grad. Sch. of Pharm. Sci., Nagoya City Univ.*, [2]*Okazaki Inst. for Integra. Biosci. and Inst. for Mol. Sci., Nat. Inst. of Nat. Sci.*, [3]*Sch. Of Materials Sci., JAIST*, [4]*Research Reactor Institute, Kyoto University*)

Glycoprotein glycans exhibit conformational fluctuations because of a significant degree of motional freedom of glycosidic linkages. Each conformer among their dynamic ensemble has the potential to interact with binding partners for various biological functions. Therefore, without knowledge of their conformational dynamics, one can barely understand functional mechanisms of glycoproteins. Recently integrative structural approaches to the glycoproteins including molecular simulations has advanced our general understanding of the mechanisms underlying molecular recognition mediated by weak interactions involving conformationally flexible biomolecules. In this symposium, we will outline our hybrid approach for the structural studies of oligosaccharides and glycoproteins.

2SCA-6 **分子シミュレーションの動的解析手法によるタンパク質のダイナミクスの研究**

Investigating protein dynamics by using dynamical analysis methods of molecular simulations

Ayori Mitsutake (*Dept. Phys, Keio Univ.*)

Molecular simulation is a powerful method for describing the stability, dynamics, and function of proteins at atomic resolution. Recent technological advances allow us to perform long simulations. As longer MD simulations are performed, it is more important to develop analysis methods to investigate dynamics and kinetics. We have developed relaxation mode analysis, to investigate “dynamic” properties of structural fluctuations of proteins. In RMA, slow relaxation modes are extracted from molecular simulations. We apply RMA to four 5μs-simulations of LmrR, which consists of 210 amino acid resides. We also calculate some dynamical quantities. We investigate dynamics in this time scale by clarifying common structural changes.

2SCA-7 **中性子散乱と計算機科学の融合による蛋白質のドメインダイナミクスの解析**

Analysis of protein domain dynamics by integrating of neutron scattering and computer science

Hiroshi Nakagawa[1,2] ([1]*Japan Atomic Energy Agency, Materials Science Research Center*, [2]*JST, PRESTO*)

Elucidating domain fluctuation as a structural unit is necessary to understand the molecular basis of structural polymorphism and plasticity of proteins, which interact with various molecules. In this study, I will develop a correlative structural analytical method by integrating neutron scattering experiment data and computational analysis to obtain information on domain motion at the atomic level. By applying this technique to MurD with three domain, I will elucidate the functional domain motions.

2SDA-1 **Emergence of genetic information in information-polymer soup**

Shoichi Toyabe (*Grad. Sch. Eng., Tohoku Univ.*)

The first life form has presumably developed in the soup of information polymers. In this process, the emergence of molecular species sustaining genetic information is a crucial step. However, no scenario has clearly addressed it. We explore the templated ligation of DNA strands, which simulates the simplest and most primitive reaction of information polymers. We find that, by repeated templated ligations, DNA strands inevitably form a precursor of species, a stable and complex nonequilibrium structure replicating its genetic information. The key concept behind is the cooperative hyper-exponential growth of sequence information. We demonstrate the spontaneous symmetry breaking of sequence and the coexistence of different species in spatially resolved systems.

2SDA-2 **自己複製する鋳型高分子系において複雑な配列が選択される条件**

Conditions for selecting complex sequences in mathematical model of self-replicating template polymer system

Yoshiya Matsubara, Kunihiko Kaneko (*Grad. Sch. Arts and Sci., The Univ. of Tokyo*)

One of the major questions in the study of origin of life is the emergence and maintenance of complex catalytic polymers. To answer this question, we analyzed a mathematical model of chemical reaction system in a chemostat. In the model, long polymers work as a template in which polymers replicate through step-wise ligations of two types of monomers. We investigated the model by numerical calculation and mathematical analysis. We discovered the steady distribution of the concentration of polymers is biased to a specific sequence and it varies non-trivially with the flow speed of chemostat. The slower the flow, the more complex arrays tend to be selected. Our results show that there are kinetic conditions that favors for selecting more complex polymer sequence.

2SDA-3 染色体複製サイクルの繰り返しによる環状 DNA の試験管内自律増殖

Autonomous propagation of circular DNA molecules in vitro through a continuous repetition of a chromosome replication cycle

Masayuki Su'etsugu, Hiraku Takada (*Col. of Sci., Rikkyo Univ.*)

Propagation of genetic information is a fundamental biological property that is common to living organisms probably started with the origin of life. Here, we have reconstituted an entire replication cycle of the *Escherichia coli* circular chromosome with 25 purified proteins that catalyze initiation, fork progression, Okazaki-fragment maturation, and decatenation. Because decatenation provides supercoiled monomer DNA that are competent for the next round of replication initiation, the cycle repeats autonomously and continuously. This Replication-Cycle Reaction (RCR) propagates large circular DNA molecules exponentially in an isothermal condition. We also propose the use of RCR as a tool for bottom-up approach towards self-replicating life-like systems.

2SDA-4 Emergence of DNA-encapsulating liposomes from a DNA−Lipid blend film

Shunsuke Shimobayashi (*Department of Mathematical Science and Advanced Technology, Japan Agency for Marine-Earth Science and Technology*)

A micro-sized lipid vesicle that enclose genetic information is the universal structure that life has. Therefore, biomacromolecules that carry genetic information may have been encapsulated in the semipermeable compartment during the emergence of life or in the early stage of the cell birth. If so, how were these macromolecules encapsulated under prebiotic conditions? Here, we study the mechanism of the dehydration-rehydration process, which is considered to be one of the candidates to form such protocellular structures. By combining fluorescent observations and small-angle x-ray diffraction experiments, we reveal the effects of the macromolecule size on this process. These findings would give insights into the story of the origin of life.

2SDA-5 オンチップ人工細胞：無細胞系の遺伝子発現と幾何形状による制御

***Artificial-cells*-on-a-chip: cell-free gene expression in microwells with various geometries**

Ziane Izri[1], Ryota Sakamoto[1], Vincent Noireaux[2], Yusuke Maeda[1] ([1]*Dept. Phys., Kyushu Univ.*, [2]*Dept. Phys., Univ. Minnesota*)

In this talk will be presented a new microfluidic setup that allows the robust and flexible study of cell-free gene expression in microwells of different geometries, closed by a biological membrane, mimicking the behavior of simplified bacterial cells.
Gene expression using a cell-free transcription-translation system is performed in cylindrical femtolitre microreactors sealed by a membrane made of a mixture of phospholipids. A wide array of microreactors with different sizes can be built in the same microfluidic chip, allowing to test the effect of both the volume and the membrane surface within the same experiment. The robustness of the expression of a low number of genes has been tested against the radius and the height of the microwells, and will be discussed.

2SDA-6 細胞内外で機能する合成 RNA-タンパク質複合体の設計と構築

Synthetic RNA-protein nanostructured devices that function in vitro and in cells

Hirohide Saito, Hirohisa Ohno (*Kyoto Univ.*)

RNA-protein (RNP) complexes play an important role to construct and regulate living systems. We are interested in designing and generating synthetic RNP nanostructured devices and systems by mimicking naturally occurring RNP complexes. In this talk, I would like to introduce our updated synthetic RNA technologies. First, I will explain our "RNA switch" technologies that detect signals, control gene expression and cell function. By using these synthetic RNAs, we can precisely distinguish and control cell fate. Second, I will introduce "RNA nanomachines" that function in vitro and in living cells. Interestingly, the RNA nanomachines may function as intracellular "molecular robots", because they can sense endogenous protein/RNA signals and induce RNA conformational change to produce desired functions. Finally, I would like to discuss how to apply these synthetic RNA/RNP nanodevices to deepen understanding the origin and evolution of Life.

2SEA-1 シアノバクテリアのタンパク質時計が教えてくれること

Lessons from Cyanobacterial Circadian Clock System

Shuji Akiyama[1,2,3] ([1]*CIMoS, IMS, NINS*, [2]*SOKENDAI*, [3]*RIKEN SPring-8 Center*)

We have used cyanobacterium *Synechococcus elongatus* PCC 7942 as the model system and looked for minimal-and-slow the reaction serving as the pacemaker of in vivo transcriptional-translational oscillation rhythm. Our present results, together with other physicochemical studies, offer insight into the mechanism by which cyanobacteria on ancient Earth were able to encode the period of the Earth's rotation into their biological systems. The fact that a water molecule, ATP, the polypeptide chain, and other universal biological components are involved in this regulation suggests that humans and other complex organisms may also share a similar molecular mechanism.

2SEA-2 天然変性タンパク質とリン酸化

Protein intrinsic disorder and phosphorylation

Motonori Ota (*Sch. Info. Nagoya U.*)

Biological importance of intrinsically disordered proteins are frequently discussed in terms of their roles in protein-protein interaction network, as hub proteins. Disordered proteins are also known to be abundantly localized in nucleus, but there have been no evidence that hub proteins tend to be nucleus proteins. We revealed that the multiple localized proteins, nucleus and cytoplasm proteins, tend to be hub proteins, and among them, phosphoproteins function in transcription tend to be disordered proteins. Phosphorylation is frequently used by disordered proteins, when they change the interaction partners or subcellular locations. In addition, disordered regions and phosphorylation sites are analyzed, and their relationships will be discussed.

2SEA-3 Chemical and structural biology approaches to understand molecular mechanism underlying 24-hour period of mammalian circadian clock

Tsuyoshi Hirota (*Institute of Transformative Bio-molecules, Nagoya University*)

In mammals, circadian rhythms are generated through transcriptional regulatory networks of the clock genes. To search for novel clock modifiers, we applied chemical biology approach. From hundreds of thousands of small molecules with diverse structure, we identified a number of compounds that potently change the period of the circadian clock in human cells. We developed affinity probe in collaboration with organic chemists and purified interacting proteins which were further identified with mass spectrometry analysis. By using these compounds as probes, we revealed important regulatory mechanisms of the circadian clock. To understand the mechanism of action of these unique compounds at atomic level, we are now applying structural biology approach.

2SEA-4 Flexible time: turning of circadian period through the loop region of CRYPTOCHROME protein

Koji Ode[1,2], Hiroki Ueda[1,2] ([1]*Dept. Sys. Pharm., Grad. Sch. Med., The Univ. Tokyo*, [2]*Lab. Syn. Biol., QBiC, RIKEN*)

Mammalian cryptochrome 1 (CRY1) is a transcriptional repressor that closes a negative feedback loop to drive autonomous oscillation of circadian clock. We found that multi phosphorylation sites near the loop domain of CRY1 significantly alters the circadian period. Phosphorylation on such sites may alter the structure of loop domains through modulating the local electrostatic properties. Because cryptochrome superfamily is conserved among phyla with differentiated functions, we analyzed the sequence diversity around the loop structure to investigate whether there is an evolutional trace suggesting the functional importance of electrostatic condition around the loop, and insights gained from the phylogenic analysis was tested through the mutagenesis of mammalian CRY1.

2SEA-5 哺乳類の発生過程における 24 時間周期の形成機構
Appearance of 24 hour rhythms during the developmental process in mammals

Kazuhiro Yagita (*Kyoto Prefectural University of Medicine*)

In mammals, the circadian clock controls temporal changes of physiological functions such as sleep/wake cycles, body temperature, and energy metabolism. Although the suprachiasmatic nucleus (SCN) is a center of circadian rhythms, circadian clocks resides in peripheral cells throughout the body.
Recently, we found that circadian clock development in mammalian cells is closely correlated with cellular differentiation process. Our results suggest that the development of the mammalian circadian clock requires two steps. The first is an epigenetic and transcriptional program-mediated cellular differentiation process, and the second is the establishment of the transcriptional/translational feedback loops (TTFLs) and molecular networks of the mammalian circadian system.

2SFA-1 細胞内クラウディング環境下の蛋白質のフォールディング・ダイナミクスを NMR で観測する
NMR approaches to investigate protein folding and dynamics in the crowded intracellular environment

Yutaka Ito (*Dept. Chemistry, Tokyo Metropolitan Univ.*)

In vivo observations of 3D structures, dynamics or interactions of proteins are essential for the explicit understanding of the structural basis of their functions inside cells. In-cell NMR is currently the only approach that can provide structural information of proteins inside cells at atomic resolution.
I will report our recent developments in in-cell NMR methods, e.g. new strategy for obtaining structural information and efficient structure calculations assisted by Bayesian inference, which enable us to determine protein structures, relative orientations of domains and protein complexes in eukaryotic cells. In-cell NMR strategies for understanding protein folding stability and dynamics under intracellular crowing environment will also be discussed.

2SFA-2 長時間分子シミュレーショントラジェクトリの解析から探るタンパク質の不均一なダイナミクス
Deciphering the heterogeneous dynamics of proteins from the analysis of millisecond-long molecular dynamics simulations

Toshifumi Mori[1,2], Shinji Saito[1,2] ([1]*IMS*, [2]*SOKENDAI*)

Conformational heterogeneity has become the key to understand proteins. Recent advances in computational tools have enabled atomistic molecular dynamics simulations to reach μ~ms, thus to provide molecular insights into the heterogeneous dynamics found in state-of-the-art experiments. Yet, analyzing these high dimensional trajectories is still a challenging task.
Here we show how the temporal information the trajectories can be used efficiently to understand the underlying dynamics. With this method, we study multiple ~ms trajectories obtained by Anton to reveal the heterogeneous dynamics behind protein folding. Furthermore, we discuss how the dynamics can be analyzed in more detail using multiple variables and temporal informations.

2SFA-3 Ultrahigh-speed single-particle tracking by interferometric scattering (iSCAT) microscopy

Chia-Lung Hsieh (*Institute of Atomic and Molecular Sciences, Academia Sinica*)

Single-particle tracking (SPT) is a powerful method to study single-molecule dynamics. While fluorescence SPT has made great success in many applications, scattering-based SPT remains indispensible when high spatial localization precision and high temporal resolution are needed simultaneously. I will present an imaging-based interferometric approach, the iSCAT microscopy, which allows us to track smaller particle with shot-noise limited localization precision at ultrahigh-speed [1]. I will show an example of single-molecule dynamics in biological membranes unveiled by the iSCAT microscopy [2]. Finally, I will discuss our strategy of background correction for high-precision SPT.
References
[1] Optics Express 22(8), 9159 (2014).
[2] Scientific Reports 6:20542 (2016).

2SFA-4 ラマン散乱顕微鏡とアルキン標識による生物活性小分子のイメージングとスクリーニング

Raman scattering microscopy and alkyne-tag for imaging and screening of bio-active small molecules

Jun Ando[1,2,3,4], Katsumasa Fujita[1,2], Mikiko Sodeoka[2,3] ([1]*Dept. of Applied Physics, Osaka Univ.*, [2]*AMED-CREST, AMED*, [3]*RIKEN*, [4]*Institute for Molecular Science*)

Raman scattering microscopy directly identifies molecular species by scattered light, and visualizes its distribution in the sample. We have developed a method using alkyne as a tiny Raman tag to specifically observe bio-active small molecules in soft biological systems. Recently, we improved detection sensitivity of alkyne by using metal nanoparticles as surface-enhanced Raman scattering (SERS) agent. Due to the efficient adsorption of alkyne on the metal surface, alkyne's Raman signal is largely enhanced up to millionfold. Here, I will review alkyne-tag Raman imaging of various small molecules, and present our recent progress using alkyne-SERS, including its application to high-throughput screening of small molecules bound with proteins in complex mixtures.

2SFA-5 High-Speed AFM Observation of Domain Flexibility Related to Enzymatic Function of CRISPR-Cas9

Takayuki Uchihashi[1], Mikihiro Shibata[2,3], Hiroshi Nishimasu[4,5], Noriyuki Kodera[3,5], Seiichi Hirano[4], Toshio Ando[3,6], Osamu Nureki[4] ([1]*Dept. Phys., Nagoya Univ.*, [2]*ISFS, Kanazawa Univ.*, [3]*Bio-AFM FRC, Kanazawa Univ.*, [4]*Dept. Biol., Univ. Tokyo*, [5]*JST-PRESTO*, [6]*JST-CREST*)

Cas9 known as one of a microbial adaptive immune systems associates with dual guide RNAs and cleaves DNA complementary to the crRNA guide. Cas9-RNA recognizes a protospacer adjacent motif on the dsDNA and then cleaves the DNA strand. Previous structural studies provided mechanistic insights into the RNA-guided DNA cleavage by Cas9. However, its dynamics remains to be fully elucidated. Here, we applied high-speed AFM to visualize the conformational dynamics of Cas9 in action. The HS-AFM movies revealed that apo-Cas9 adopts unexpected flexible conformations, while Cas9-RNA forms a stable bilobed structure. Further, the HNH domain fluctuates upon DNA binding. This result would provide insight of a role of flexible structure and its fluctuation on protein functions.

2SFA-6 高速１分子イメージング解析で明らかとなったリニア分子モーター、回転分子モーターの化学力学共役機構

Chemo-mechanical coupling mechanisms of linear and rotary molecular motors revealed by high-speed single-molecule imaging analysis

Ryota Iino[1,2,3] ([1]*OIIB, NINS*, [2]*IMS, NINS*, [3]*SOKENDAI*)

We have been developing high-speed single-molecule imaging methods monitoring free, fast motions of protein molecular motors with nanometer localization precision and microsecond temporal resolution. Our methods are based on dark-field scattering imaging of gold nanoparticles and nanorods with the size of several tens of nanometers. These nanoprobes have advantages over the commonly used fluorescent dyes and quantum dots, because much stronger signals can be obtained without suffering from photobleaching and blinking. Furthermore, their small sizes make viscous drag of water almost negligible. In this symposium, I will discuss chemo-mechanical coupling mechanisms of a linear molecular motor chitinase A and a rotary molecular motor V1-ATPase revealed by our observation.

2SGA-1 リポソーム・ナノディスクの膜環境と脂質ダイナミクス

Structure and Dynamics of Lipids in Liposomes and Nanodiscs

Minoru Nakano (*Graduate School of Medicine and Pharmaceutical Sciences, University of Toyama*)

Phospholipid bilayer liposomes and nanodiscs are widely used as tools to investigate structure and function of proteins attached or incorporated into the bilayers. Physico-chemical properties of these nanoparticles have, however, not been well understood. We have revealed by several approaches that dynamic behavior of lipids in these particles differs depending on surroundings where the lipids are located, e.g., phospholipids and cholesterol in nanodiscs are more tightly packed and hence more entropically forced to dissociate from the bilayer than those in liposomes. I will introduce our resent progress of the evaluation of these lipid assemblies.

2SGA-2 脂質ナノディスク形成のための膜活性ポリマーのデザイン

Molecular design of membrane-active polymers for lipid nanodisc formation

Kazuma Yasuhara, Masaya Inoue, Jin Arakida, Jun-ichi Kikuchi (*Graduate School of Materials Science, Nara Institute of Science and Technology*)

For the structural and functional analysis of membrane proteins, there is a great need for the development of molecular platforms that mimic the local environment of biomembranes. We have designed amphiphilic polymethacrylate derivatives that spontaneously form discoidal lipid membranes through the fragmentation of a lipid bilayer. Screening of the polymer library revealed that membrane disruption activity of the polymer depends on the structural characteristics of the polymers such as amphiphilicity and molecular weight. It was clarified that the addition of the designed polymer with an optimized structure to liposomes spontaneously form nanometer-sized nanodiscs in which the characteristics of lipid bilayer was maintained.

2SGA-3 脂質ータンパク協同性による上皮成長因子受容体の膜近傍ドメイン二量体形成機構

Lipid-protein cooperativity in the regulation of juxtamembrane domain dimer formation in epidermal growth factor receptor

Ryo Maeda[1], Takeshi Sato[2], Kenji Okamoto[1], Yasushi Sako[1] ([1]*Cellular Informatics Lab., RIKEN*, [2]*Kyoto Pharmaceutical Univ.*)

Transmembrane (TM) helix and juxtamembrane (JM) domains (TM-JM) bridge the extracellular and intracellular kinase domains of single-pass membrane proteins including epidermal growth factor receptor (EGFR). It has been proposed that dimerization of TM-JM plays a crucial role for regulation of EGFR kinase activity and phosphorylation of Thr654 on JM conversely leads to desensitization. While interactions of JM with membrane lipids are thought to be important for TM-JM dimerization, conformational mechanisms underlying the dimer formation remain unclear. Here, combining single-molecule FRET imaging and nanodisc techniques, we analyzed how JM conformations are dynamically regulated by membrane lipids molecules, especially PIP2, and a threonine phosphorylation in JM domain.

2SGA-4 High-speed AFM observation of membrane protein embedded in Nanodisc

Takamitsu Haruyama[1], Yasunori Sugano[1], Yoshiki Tanaka[1], Hiroki Konno[2], Tomoya Tsukazaki[1] ([1]*Grad. Sch. of Biol. Sci., NAIST*, [2]*Bio-AFM FRC, Inst. of Sci. & Eng., Kanazawa Univ.*)

High-speed AFM (HS-AFM) permits direct observation of membrane proteins at high spatiotemporal resolution under physiological condition. Purified membrane proteins for AFM imaging are usually solubilized by detergents or reconstituted into liposomes. However, these methods sometimes cause loss of activity during preparation and problematic imaging of the small membrane proteins due to randomly distribution and orientation in a lipid bilayer. Here, we applied Nanodiscs, which consist of membrane proteins, membrane scaffold proteins and lipids, to HS-AFM observation of membrane proteins. Nanodiscs can keep membrane proteins stable and active at the single molecule level, which enables us to detect microscopic fluctuations of soluble domains of membrane proteins by HS-AFM.

2SGA-5 GraDeR: 遊離界面活性剤無膜タンパク質の調整方法
GraDeR: micelle free membrane protein preparation

Christoph Gerle (*IPR, Osaka Univ.*)

The presence of free detergent is a nuisance for many experimental approaches used to advance our understanding of membrane biology. We have developed a novel approach for the complete & mild removal of free detergent from LMNG (MNG-3) stabilized integral membrane proteins by density gradient centrifugation termed GraDeR. Thus far GraDeR worked on all membrane proteins tested and I would like to use the session for discussing which experimental approaches might benefit from its use.

2SGA-6 リポソーム中の膜タンパク質機能構造を捉えるクライオ電子顕微鏡単粒子解析法
CryoEM single particle analysis for functional structure of membrane proteins in liposomes

Hideki Shigematsu (*RIKEN CLST*)

Many of recent challenges in cryoEM single particle analysis of membrane proteins to overcome technical issues and hypothetical questions to obtain close to native state of membrane protein structure, not only many detergents but amphiphilic molecules, nanodiscs are utilized to achieve high resolution structural analysis.
Here we present a sub-nanometer cryo-EM structure of the Kv1.2 channel complex in a lipid bilayer, obtained from protein reconstituted into liposomes. Using this system, we expect that voltage-gated channels can be subjected to physiological membrane potentials and ion gradients.

2SIA-1 メカノバイオロジー: これまでの成果とこれからの課題
Mechanobiology: Past achievements and future issues

Masahiro Sokabe (*Mechanobiology Lab, Nagoya Univ Grad Sch Med*)

Mechanobiology is an emerging field aiming at understanding roles and mechanisms underlying the action of forces in organisms, in which cell mechanosensing is central. Over the past decade, it has been revealed that cells have a variety of mechanosensing machineries that can sense not only stresses in cells but also stiffness and topography of surrounding micro-environments, thus contributing to the regulation of fundamental cell functions such as proliferation, differentiation and migration. One of the pressing issues in this field is to elucidate detailed molecular and biophysical mechanisms underlying the cell mechanosensing. This requires cutting edge technologies able to measure and manipulate quantitatively the stress and strain in cells and tissues.

2SIA-2 Mechanobio-materials manipulating motility and functions of stem cells

Satoru Kidoaki (*IMCE, Kyushu Univ.*)

Biomaterials to manipulate the stem cell mechanobiology have drawn much attention in the basic researches of stem cell biology in this decade. To systematically control the mechanobiological behaviors of stem cells, we have developed the sophisticated design of micromechanical field of cell culture matrix using the photolithographic microelasticity-patterning of hydrogels. In this presentation, we introduce the potential of elastically-patterned gel with microscopic heterogeneous distribution of matrix stiffness to manipulate to motility and function of stem cells. Especially, we show new methodology of mechanosignal input to the cells that employ spontaneous movement and translocation of cells among different region of elasticity.

2SIA-3 メカノバイオロジーのための形状記憶型動的培養基盤
Shape Memory-based Dynamic Culture Platforms for Mechanobiology

Koichiro Uto (*ICYS, NIMS*)

Cells reside in a highly dynamic extracellular matrix microenvironment, where biochemical, physicochemical, mechano-structural cues are displayed in a spatiotemporal fashion. To recapitulate this, complex microenvironments and dynamic culture platforms have emerged as powerful tool to probe and direct active changes in cell function. Here, I briefly overview the cell manipulation technologies based on spatiotemporally tunable biomaterials with a focus on shape-memory polymers.

2SIA-4 遺伝子発現制御に対するアクチンの役割を理解するための微細構造化細胞培養基材の開発
Microtopographical cell culture substrate to understand the role of actin cytoskeleton for regulation of gene expression

Masashi Yamazaki[1], **Hiromi Miyoshi**[1,2] ([1]*Grad. Sch. System Design, Tokyo Metropolitan Univ.*, [2]*PRIME, AMED*)

A growing number of the researchers have demonstrated that the actin cytoskeletal forces is related to cell fate, specifically proliferation and differentiation, although the detailed mechanism remains to be clarified. It is known that the actin filaments connect to the intranuclear chromatin fibers through inner nuclear membrane proteins. We hypothesized that the mechanical forces transmitted to the nuclear interior will affect the intranuclear distribution of chromatin fibers, which could change the transcriptional activities. To test the hypothesis, we are developing a cell culture substrate with micro-/nano-structures to define the spatial distribution of the actin cytoskeleton with submicrometer resolution through a response of cells to geometrical patterns.

2SIA-5 Live-cell imaging of actin dynamics in cortex and lamellipodium by high-speed atomic force microscopy

Yoshitsuna Itagaki[1], Yanshu Zhan[1], Aiko Yoshida[1], Nobuaki Sakai[2], Yoshitsugu Uekusa[2], Masahiro Kumeta[1], **Shige H. Yoshimura**[1] ([1]*Grad. Schl. Biostudies, Kyoto U.*, [2]*R&D Group, Olympus Corp.*)

Dynamic network of actin filaments plays major roles in cell morphology, motility, and mechano-sensing and -responses. Here, we visualized actin filaments in living cells without labeling and staining by using high-speed atomic force microscopy, and analyzed its dynamics in the cortex and lamellipodium. In the cortex, actin filaments are synthesized beneath the plasma membrane and eventually descend into the cytoplasm. In lamellipodia, polymerization occurs at the edge of the cell, and drives retrograde flow of the network. Inhibition of polymerization/depolymerization cycle inhibited such retrograde flow in both places, but inhibition of Arp2/3 complex and formin affected only lamellipodia, indicating that the actin polymerization is initiated by different mechanisms.

2SIA-6 細胞の力学：単一細胞から多細胞へ
Cell Mechanics: from single cell to multi-cellular dynamics

Hirokazu Tanimoto[1,2], Kyogo Kawaguchi[1,3], Masahito Uwamichi[1], **Masaki Sano**[1] ([1]*Dept. Phys. Univ. Tokyo*, [2]*Inst. Jacques Monod*, [3]*Sys. Bio. Harvard Univ.*)

Cell migration is a highly complex process that integrates many spatial and temporal cellular events. In general, motile cells are able to migrate spontaneously in a seemingly random manner even in the absence of external stimuli. To understand how cell produces seemingly random motion and crawls on the substrate by deforming its shape, we developed a multipole expansion analysis of traction force distribution exerted by individually migrating cells and looked at correlations to their motion. We found a simple law between force distribution and migration. Some relations to a recent theoretical approach will be discussed. Recent development in understanding collective behavior of multi-cellular dynamics will be explained.

2SKA-1 配列空間における蛋白質フォールディング
Protein folding in the sequence space

Akira R. Kinjo (*Inst. Protein Res., Osaka Univ.*)

What separates foldable proteins from unfoldable polypeptides is the pattern of amino acid sequences. By changing the sequence pattern rather than environmental variables, can we observe a “folding transition” in the sequence space? By using Monte Carlo simulations of a statistical mechanical model of protein sequence alignment (https://goo.gl/XPt2W0) that integrates long-range interactions and variable-length insertions, I demonstrate the existence of a cooperative two-state transition between natural-like sequences and random sequences. The results suggest that, if some selective pressure is imposed on one or a few key residues, the evolution of the entire protein sequence to form a family (or unique fold) can be greatly accelerated.

2SKA-2 Toward a Quantitative Description of Microscopic Pathway Heterogeneity in Protein Folding

Athi N. Naganathan (*IIT Madras*)

How many structurally different microscopic routes are accessible to a protein molecule while folding? We answer this fundamental question by analyzing 100,000 folding events generated from a statistical mechanical model incorporating detailed energetics from more than a million conformational states on five single-domain proteins. We find that a minimum of ~3-200 microscopic routes, with a diverse ensemble of transition-path structures, are required to account for the total folding flux. The partitioning of flux amongst the numerous pathways is observed to be subtly dependent on the experimental conditions that modulate protein stability, topological complexity and the structural resolution at which the folding events are observed.

2SKA-3 Structural features of the urea denatured apomyoglobin using molecular modeling and experimental data

Yasutaka Seki (*Molecular Biophysics, Kochi Medical School, Kochi University*)

The unfolded protein in solution consists of an ensemble with a great number of conformations. As an experiment gives only a piece of structural information of the unfolded protein, it is necessary to integrate diverse experimental data for elucidating its structural features. We developed a computational method for generating conformations of unfolded protein. It enables us to generate a large number of conformations very rapidly by avoiding atomic collisions efficiently. Using our method, we have tried to find an ensemble which best reproduces experimental data obtained from both residual dipolar couplings of NMR and solution X-ray scattering. As a result, it was clarified that the urea-unfolded apomyoglobin has structural features.

2SKA-4 Structural Proteome to Targetability Estimation: Novel Concepts in Drug Discovery

Nagasuma Chandra (*Indian Inst. Sci.*)

Target identification is a critical step in modern drug discovery. Identifying the right target however is by no means simple, since a variety of factors need to be considered simultaneously. One main problem is that most candidates exhibit adverse drug effects due to off-target interactions. We have developed new methods in the laboratory in the area of structural systems biology which present a rational approach to prioritize targets, explore poly-pharmacological targets, understand drug pharmacodynamics, obtain lead clues and obtain shortlists for exploring drug repurposing. A case study with tuberculosis proteome will be presented, illustrating how such knowledge can be used in the discovery of new, safer drugs.

2SKA-5 Data integration and statistical/*ab initio* modelling towards rational drug discovery

Kenji Mizuguchi (*NIBIOHN*)

Data integration is key to establishing systems approaches to drug discovery. Using our TargetMine system, an integrated data warehouse for target prioritization, we have identified genes/proteins that would play key roles in infectious and pulmonary diseases and subsequently verified these hypotheses by direct experimentation. Based on these standardized databases, statistical models can be built for predicting protein structure, function and interaction, typically with machine-learning techniques. Also, often required are mathematical (ab initio) models based on some forms of first-principle equation, for complementing the data-driven approaches. In this talk, I will discuss these issues, with specific applications in target discovery and pharmacokinetic modelling.

2SKA-6 Cis proline-specific protein structure and dynamics

Gautam Basu (*Bose Inst.*)

The amino acid proline imposes unique constraints on proteins due to its cyclic sidechain and the lack of an amide hydrogen atom. Specifically, the replacement of the amide hydrogen atom with the delta carbon atom makes Xaa-Pro segments in proteins prone to occupy the cis-peptidyl-prolyl conformation which can yield rare but functionally important structural and dynamical consequences. I will discuss a new cisPro containing helix N-cap motif, occurrence of Gly-cisPro united residue in beta-sheets, effect of non-contiguous aromatic residues in modulating the cisPro conformation and the direct observation of concerted backbone-sidechain dynamics in a designed peptide involving the Pro (i) omega backbone angle and the X1 sidechain angle of Trp (i+2) residue.

2SLA-1 超解像光学顕微鏡法 PALM によって明らかになった軸索輸送における非定型微小管
Opening talk: visualizing unconventional biological component using super-resolution photo-activated localization microscopy

Shiori Toba[1,2] ([1]*Osaka City Univ. Grad. Sch. of Medicine*, [2]*Present Address: Hirosaki Univ. of Health and Welfare*)

Optical microscopy enables us to visualize the various behavior and conformation of biological components. In this symposium, we will present recent imaging technologies, including super-resolution, adaptive optics, digital holography, and image processing. Our findings using super-resolution photo-activated localization microscopy (PALM) provide clues about the functional relevance of synuclein proteins, microtubules, and cytoplasmic dynein for intracellular transport. Based on our observations, we hope to discuss these recent developments and their significance. We believe this symposium will encourage further applications of these techniques to increase the experimental output.

2SLA-2 新規光技術を用いた二光子励起顕微鏡の機能向上
Improvements of two-photon excitation microscopy by utilizing novel optical technologies

Kohei Otomo[1,2] ([1]*RIES, Hokkaido Univ.*, [2]*Grad. Sch. IST, Hokkaido Univ.*)

Two-photon excitation laser scanning fluorescence microscopy (TPLSM) has been widely used as an analytical method for direct visualization of dynamical molecular and cellular phenomena. This is because of its superior penetration depth and less invasiveness in specimens owing to its near-infrared excitation laser wavelength compared with the wavelength of single-photon excitation based systems. In this presentation, our improvement studies for TPLSM by utilizing novel optical technologies, e.g. high-peak-power semiconductor lasers for deeper penetration depth, spatial light modulators for applying stimulated emission depletion microscopy and a spinning disk confocal scanner for higher temporal resolution are introduced.

2SLA-3 補償光学：光の乱れの補正による深部生細胞イメージング
Adaptive optics: Towards deep imaging of living cells by active correction of optical disturbance

Yosuke Tamada (*Div. Evol. Biol., Natl. Inst. Basic Biol.*)

Live-cell imaging is the technique to observe the dynamics of molecules or structures in living cells using fluorescent probes and an optical microscope. In live-cell imaging, the images degrade according to the depth inside living cells and tissues, which contain many kinds of structures with different refractive indices. When light goes through such structures, the light is disturbed, causing the image degradation. Adaptive optics (AO) is one of the prospective solutions for this problem. AO measures the disturbance on light, and actively regulates the spatial light modulator to correct the disturbance. Here, I would like to introduce our current research to apply AO to deep live-cell imaging, and summarize the trend of the research of AO microscopy in the world.

2SLA-4 SIM/STORM イメージングの使命と将来の展望
Missions and the future of SIM/STORM super-resolution microscopy

Wataru Tomosugi (*Nikon Corporation*)

Many of key biological phenomena are triggered by interactions of central-dogma players such as proteins, DNA and RNA. These events take place at a single-molecule level and occur in smaller area than diffraction limit of light microscopy. A mission of super-resolution microscopy is to visualize such triggering events directly. Here, I will first describe the essential principles of SIM and STORM to understand how these technologies can go beyond diffraction limit and then will show some representative images of biological samples from SIM and STORM. I will also introduce in-depth technical tips to acquire better super-resolution images from the points of view of system setting and sample preparation. Finally I will discuss the future prospects of SIM and STORM.

2SLA-5 能動学習を用いた生物画像の効率的自動分類
Efficient Automatic Classification of Biomedical Images Using Active Learning Algorithm

Natsumaro Kutsuna[1,2], Yuki Shimahara[1,2], Seiichiro Hasezawa[1,2] ([1]*Lpixel Inc.*, [2]*Grad. Sch. Front. Sci., Univ. Tokyo*)

Advances in bioimaging techniques have yield massive images into the biology. Automatic classification of images is a key to the solution of the problems accompanied by the flood of image data. However, preparation of correct and massive training images is one of bottle-neck for accuracy and rapid development of machine learning software. To brake the bottle-neck, we develop new machine learning algorithm based on active learning approach. In the proposed algorithm named CARTA, multiple query images are shown at once and they are sorted and tiled in line reflected with their similarity. Compared with supervised learning, the CARTA rapidly increased their accuracy from the limited number of annotated mages.

2SLA-6 ディジタルホログラフィとバイオイメージングへの応用可能性
Digital holography and its applicability to biology

Tatsuki Tahara[1,2] ([1]*Kansai University*, [2]*PRESTO, JST*)

Digital holography is an interferometric imaging technique without an imaging lens and has performed simultaneous imaging of multidimensional information such as three-dimensional (3-D) structure, dynamics, quantitative phase, multiple wavelengths, and state of the polarization of light. A variety of applications have emerged from the holographic motion-picture recording ability. In this review, we introduce recent progress in multidimensional sensing by using digital holography, including 3-D motion-picture recording of multiple specimens simultaneously, quantitative phase imaging, multimodal imaging, multiwavelength imaging with holographic multiplexing, and 3-D imaging of natural light with a single-shot exposure.

2SLA-7 Closing remarks: Advanced bioimaging techniques for biophysics

Yoshiyuki Arai (*ISIR, Osaka Univ*)

Bioimaging has become an indispensable tool to elucidate the biological phenomena quantitatively at living conditions. In this session, we have introduced and discussed the advanced imaging techniques such as, superresolution imaging, adaptive optics, machine learning for the image analysis, and digital holography. Although each technique includes advanced technology, they would be introducible for our biophysical experiments practically. We believe each technique must be more important for future biophysics.

2SMA-1 はじめに
Introduction

Kunio Miki (*Graduate School of Science, Kyoto University*)

This symposium aims to review and discuss recent development of high-resolution and high-precision crystallography for structural biology by means of synchrotron X-ray and by conventional utilization of neutron diffraction. Recent ultra-high resolution X-ray structures enabled us to perform charge density analysis to obtain information of outer-electron distribution of protein molecules. Determination of hydrogen positions by neutron is going to become a more conventional method in protein crystal structures. Development of high-performance beamlines suitable for such analyses is important in both X-ray and neutron works. Speakers talk about current status of high-resolution and high-precision structure analyses by X-ray and neutron protein crystallography and discuss their cooperative and complementary usage in current and future sciences.

2SMA-2 緑色蛍光タンパク質の X 線および中性子線解析
X-ray and neutron diffraction analyses of green fluorescent protein

Kazuki Takeda (*Grad. Sch. Sci., Kyoto Univ.*)

Hydrogen atoms and valence electrons define the chemical property of proteins. However, it is difficult to investigate with the conventional protein crystallography. We have performed detailed crystallographic analyses of green fluorescent protein (GFP) from Aequorea victoria. X-ray data sets were collected using high-energy synchrotron X-rays. The structures of T203I (in the A form), S65T (in the B form) and E222Q (in the B form) variants are determined at 0.95, 0.85 and 0.77 Å respectively. In addition, neutron data at 1.6 Å were also collected using a large crystal of the perdeuterated S65T variant. At the symposium, functional implications will be discussed based on fine structural information such as hydrogen positions and valence electronic distribution.

2SMA-3 Experimental environments for high-resolution diffraction data collection at SPring-8

Takashi Kumasaka, Kazuya Hasegawa (*Protein Crystal Analysis Division, Japan Synchrotron Radiation Research Institute (JASRI)*)

The high energy storage ring of SPring-8 is suitable to produce high-energy X-ray, which is useful for ultra-high resolution data collection. We have been developing the experimental station for high-energy X-ray at the beamline BL41XU, SPring-8. The beamline has now been operated with two modes: normal mode (6.5 to 17.7 keV) and high energy mode (20 to 35 keV). In 2014, we installed new instruments for the high-energy X-ray; a compound refractive lens focusing X-ray to 12 x 3 μm in size, and a CMOS detector, which has a thick CsI phosphor (300 μm) for high quantum efficiency even in higher energy. Using the environment, we successfully collected the diffraction data of triclinic HEW lysozyme crystals beyond 0.65 Å resolution.

2SMA-4 電子伝達タンパク質の高分解能中性子結晶構造解析 High-resolution neutron crystal structural studies of electron transfer proteins

Taro Tamada (*QuBS, QST*)

Neutron crystallography is a powerful technique to obtain accurate positions of hydrogen atoms in protein structures. Recently, we have performed high-resolution neutron crystal structure analyses of high-potential iron-sulfur protein (HiPIP) and NADH-cytochrome b5 reductase (b5R). We succeeded in data collection of these proteins at higher resolution, 1.1 Å (HiPIP) and 1.4 Å (b5R), using pulsed neutron beams at BL03 (iBIX) beamline in MLF/J-PARC. Joint neutron and X-ray crystallographic refinement is in progress, but we have already observed protonation statuses of polar residues located in molecular surface and orientation of water molecules. Furthermore, we confirmed some characteristic hydorogens which have unideal geometries.

2SMA-5 Challenging to visualize ammonia transposition in a channel of amidotransferase GatCAB using neutron macromolecular crystallography

Min Yao[1,2], Long Li[2] ([1]*Faculty of Advanced Life Science, Hokkaido University*, [2]*Graduate School of Life Science, Hokkaido University*)

Neutron macromolecular crystallography (NMC) is regarded as a complementary method of X-ray macromolecular crystallography to visualize hydrogen atoms as well as nitrogen atoms in protein structural analysis even at typical (1.5 - 2.5 Å) resolutions, but requires huge crystal. By using NMC, we tried to visualize the ammonia transposed through an intramolecular channel (30 Å in length) of amidotransferase GatCAB (MW=119 kDa) which converts mischarged Glu-tRNA^{Gln} to Gln-tRNA^{Gln}. We attempted many crystallization methods, and finally grew huge crystals of GatCAB up to > 3 mm^3 successfully. The neutron diffraction data sets were obtained on beamline FRM II of MLZ, Germany, and the structure was solved. We will introduce the details in this presentation.

2SMA-6 Neutron protein crystallography with single-crystal neutron diffractometer iBIX at pulsed neutron source MLF, J-PARC

Katsuhiro Kusaka[1], Taro Yamada[1], Naomine Yano[1], Takaaki Hosoya[1], Takashi Ohhara[2], Ichiro Tanaka[1], Masaki Katagiri[1] ([1]*Frontier Research Center of Applied Atomic Sciences, Ibaraki University*, [2]*J-PARC Center, JAEA*)

Single crystal neutron diffraction is one of the powerful tools to obtain the structure information including the hydrogen atoms. The high performance time-of-flight single crystal neutron diffractometer iBIX (IBARAKI biological crystal diffractometer) was developed at next generation neutron source (Materials and Life science experimental Facility MLF, J-PARC) to elucidate the hydrogen, protonation and hydration structures of biomacromolecules in various life processes. In the end of 2012, iBIX could be started to user experiments for biomacromolecules after upgrading the detectors. We will report the development status and future prospects of iBIX and recent scientific outcomes which make the most of the merit of the neutron diffraction experiment by iBIX.

2SNA-1 形態形成における確率過程 Stochastic process in multicellular morphogenesis

Tatsuo Shibata (*RIKEN QBiC*)

It has been studied extensively in single cellular organisms that gene expressions and signal transduction activities are driven by stochastic processes. For instance, in a decision-making process of cells, bistable systems can provide two stable states, among which cells make a decision induced by a noise that arises from various sources within cells. Such cell-autonomous noise-driven processes are also present in developing tissues to generate stochastic fate decision. Morphogenesis of multicellular tissue is also a stochastic process. For instance, it has been reported that at the cell-cell junctions the length and the myosin activities exhibit temporal fluctuations during morphogenesis. In this talk, I will present how tissue morphogenesis can take advantage of stochasticity in cells to achieve tissue-autonomous plasticity keeping the mechanical integrity.

2SNA-2 Molecular mechanism to generate heterogeneous gene expression in mouse ES cell population

Hitoshi Niwa (*IMEG, Kumamoto University*)

Mouse ES cells maintains pluripotency in continuous self-renewal. Major proportion of ES cells can exhibit pluripotent character after single cell injection into blastocyst that results in chimeric embryo formation. Therefore, ES cell population is quite homogeneous in their pluripotent phenotype. In contrast, the gene expression pattern in each cell is obviously heterogeneous. It was reported that many pluripotency-associated transcription factors show various degree of heterogeneity in ES cell population cultured in FCS-containing medium. We have analyzed the molecular basis of the heterogeneity and found multiple mechanisms underlying it. We will discuss about the multiple topics and try to get the whole picture of the molecular mechanism.

2SNA-3 マウス着床前発生において細胞はどのように分化するか？
How do cells differentiate during preimplantation mouse development ?

Toshihiko Fujimori (*Div. of Embryology, NIBB*)

During mouse preimplantation development a zygote undergoes cleavage and increases its cell number followed by the two rounds of cell differentiation. The trophectoderm (TE) will contribute to the placenta while the inner cell mass (ICM) cells give rise to the epiblast (EPI) and primitive endoderm (PrE) . EPI cells will form the embryo proper, whereas the PrE cells will generate extraembryonic tissues. We analyzed the differentiation of these three cell types by tracking cellular behaviors and gene expression. TE cell specification was depending on the position of cells while segregation of EPI and PrE lineages was not depending on the cellular positions. We found that even during these early stages, cells show plasticity of specification.

2SNA-4 組織恒常性を支える幹細胞の動的不均一性をマウス精子形成に学ぶ
Dynamical heterogeneity of the stem cell pool underlying the homeostatic sperm production in mice

Shosei Yoshida (*National Institute for Basic Biology*)

Historically, tissue homeostasis is thought to be achieved by the robust behavior of individual stem cells, as elegantly shown in tissues including Drosophila germlines. Here, stem cells are tethered to anatomically defined niche and undergo invariable asymmetric divisions. However, in the mouse testis, spermatogenic stem cells (SSCs) are not clustered to particular regions, but actively migrate between differentiating progenies, and undergo stochastic self-renewal and differentiation. So, although individual SSCs behaviors are dynamic, variable and unpredictable, their self-renewal and differentiation are perfectly balanced at the level of population. I will discuss our latest knowledge about the population dynamics of SSCs underlying the robust tissue homeostasis.

2SNA-5 機械学習によるデータ駆動型サイエンス：現状と展望
Machine learning for data-driven scientific discovery: state-of-the-art and future perspective

Ryo Yoshida (*Inst. Stat. Math.*)

We are now facing a revolutionary period. In recent years, drastic advances in machine learning algorithms in recent years have brought innovative thinking and scientific methods in various fields. This talk highlights the essence and scientific relevance of advanced machine learning methods along with successful applications across some of the primary focus areas of our studies on biology (Toyoshima et al., PLoS Compt Biol, 2016; Tokunaga et al., Bioinform, 2014) and materials science (Ikebata, et al., J Comput Aided Mol Des, 2017). The focus of this talk is on the Bayesian inverse problem and a rational experimental design technique based on reinforced learning methods aimed at the "extrapolative prediction".

2SNA-6 脳発生過程における神経幹細胞の動的多様性
Dynamic heterogeneity of neural stem cells in brain development

Fumio Matsuzaki (*RIKEN Center for Developmental Biology*)

In the development of folded brain (gyrencephalic), multiple heterogeneous types of neural stem cells are formed in a single cell lineage, in contrast to the ordinary neural stem cell lineage in vertebrates. These neural stem cells are hight dynamic, and can be interchangeable with each other, forming an extremely diverse cell lineages from one lineage to another. While this neural stem cell system appears to contribute very much to form a large and complex brain, we do not know about any rules that control the cell number of a single lineage nor about how the entire number of neurons and their subtypes are regulated. We address these problems by comparing the bran development between the ferret and mouse.

2SAP-1 生命システムにおける状態・形・少数性の問題
State, Shape, and Small-Number Issues in Biological Systems

Yuichi Togashi (*Grad. Sch. Sci., Hiroshima Univ.*)

There are a variety of macromolecules in the cell. They move and react with each other. However, their behavior cannot be fully described by classical reaction-diffusion models. Firstly, many macromolecules, particularly molecular machines, have internal conformational states related to their operation. Secondly, they work in a crowded environment in the cell. Even in passive processes, the situation is far from free diffusion, and their size and shape may matter. Finally, the copy number of such macromolecules is typically low, sometimes on the order of 1 molecule per cell. We theoretically study how these characteristics may affect overall behavior of the system. In this talk, we introduce some simple models and discuss their relevance to actual biological systems.

2SAP-2 Collective motion switches directionality of molecular motor along filament

Nen Saito (*Grad. Sch. Sci., Univ. Tokyo*)

Despite the conventional view that the directionality for a given molecular motor is constant in the absence of an external force, a recent experiment showed that the directionality of a kinesin motor switches as the number of motors bound to a microtubule increases.
Here, we introduce a theoretical model of a microtubule-sliding assay in which multiple motors interact with the filament. We show that, due to the small-number effect, the directionality of the motor changes (e.g., from minus- to plus- end directionality), depending on the number of motors. A possible role of the switch in the directionality for the mitotic spindle formation will be discussed. This phenomenon represents a good example of how number (not concentration) regulates robust biological functions.

2SAP-3 Information thermodynamic study of biochemical clock

Sosuke Ito[1], Pieter Rein Ten Wolde[2] ([1]*Hokkaido University, RIES*, [2]*FOM Institute AMOLF*)

When we consider a biochemical system in a small cell, the effect of thermal noise is not negligible. Thermodynamics of information (information thermodynamics) is useful to discuss a precise mechanism of the biochemical system in a small cell.
In this talk, we discuss an application of information thermodynamics to the biochemical clock such as the Kai clock proteins in cyanobacteria. We made a simple model of a biochemical clock, and discuss the information-thermodynamic efficiency of a precise measurement of time.

2SAP-4 シロイヌナズナ遺伝子発現揺らぎの新規モデル分布
Novel statistical model of fluctuating gene expression levels of Arabidopsis thaliana

Akinori Awazu[1], Atsushi Nagano[2] ([1]*Dept. of Math. and Life Sci., Hiroshima Univ.*, [2]*Faculty of Agriculture, Ryukoku Univ.*)

Gene expression levels exhibit stochastic variations among genetically identical organisms under the same environmental conditions. In this study, using RNA-seq data of Arabidopsis thaliana, the characteristics of gene-dependent distribution profiles of the gene expression levels were analyzed. These distribution profiles could be suitably fitted by a novel distribution function named Gauss-Power mixing distribution, which was derived from a simple model of the stochastic transcription network containing the feedback loop. The present fitting function predicted that the gene expression levels showing the distributions with long tail tend to be strongly influenced by the feedback in transcription network.

2SAP-5 E-Cell System: from a single molecule to a whole cell

Kazunari Kaizu, Masaki Watabe, Kouichi Takahashi (*RIKEN Quantitative Biology Center (QBiC)*)

A cell is a complex, heterogeneous and multiscale system, where a few number of molecules can even dictate the fate of the whole cell. To fill the gap between a molecule and a cell in time and space, we have developed E-Cell system, the integrated platform for cell simulations. The latest version of E-Cell system provides multiple algorithms, which enable us to model cellular systems at the single molecule resolution. In addition, microscope simulations make direct comparison possible between the cell model and experimental measurements. Here, we show a computational framework and its application to prove and validate the theory of single-molecule biochemistry. Also, we demonstrate a whole cell simulation of *Escherichia coli* at the single nucleotide level.

2SAP-6 スパインにおける小体積効果：Robust, Sensitive で Efficient な情報伝達
Small-Volume Effect Enables Robust, Sensitive, and Efficient Information Transfer in the Spine

Masashi Fujii (*Grad. Sch. Sci., Univ. Tokyo*)

The spine of a neuron is so small that it can contain only small numbers of molecules and reactions inevitably become stochastic. Why is the spine so small? We found the advantages of smallness of spine from the viewpoint of information transfer. Despite such noisy conditions, the spine exhibits robust, sensitive and efficient features of information transfer. We also show the quantitative analysis which these features are realized by the smallness of the spine; i.e. the small-volume effect enables robust, sensitive and efficient information transfer. In this presentation, we propose that the small-volume effect is the functional reason why the spine has to be so small.

2SAP-7 A quantitative view of the biosphere: from the most abundant taxa to the most abundant proteins

Yinon Bar-On, Rob Phillips, Ron Milo (*Weizmann Inst. Sci.*)

A census for biomass on Earth is key for understanding the structure and dynamics of the biosphere. Similarly, a census of the mass of proteins that drive global elemental cycles can help us understand the constraints that they experience in the wild. Yet, a global quantitative view of how the biomass of different taxa compare with each other, and which proteins are most abundant in nature is still lacking. We harness recent advances in global sampling techniques to assemble the overall biomass composition of the biosphere. We establish a census of the biomass of all the kingdoms of life. Using this census of biomass, we estimate the global abundance of ubiquitous proteins throughout the biosphere. From these analyses, we highlight several key take-home insights.

2SGP-1 はじめに：高分子混雑の世界
Introduction: the world of macromolecular crowding

Miho Yanagisawa (*Tokyo Univ. Agri. Technol.*)

In this symposium, we focus on macromolecular crowding of live cells. Biopolymers such as proteins are present in very high concentrations in cells, which greatly affect the behavior of biopolymers. Although these effects, so-called "macromolecular crowding" are attracting attention, many of them are unknown due to the complexity. At this symposium, 4 experimental and 2 theoretical researchers introduce the world of cells and/or cell-mimicking systems dominated by macromolecular crowding, especially about biological reactions, diffusion of DNA or proteins, and the stabilities.

2SGP-2 回転および並進拡散計測による細胞内分子クラウディング状態の評価

Evaluation of molecular crowding based on the rotational and translational diffusion measurement in living cells

Johtaro Yamamoto (*Fac. Adv. Life Sci.*)

Rotational and translational diffusion of GFP was successfully analyzed in living cell by polarization-dependent fluorescence correlation spectroscopy (Pol-FCS). Furthermore, Pol-FCS measurement of GFP in polymer gels suggested that the ratio of relaxation time between rotational and translational diffusion reflects the extent of intermolecular space/gap around target molecule. The results indicated that the Pol-FCS provides information of molecular crowding in living cells. In this work, we discuss different crowding state in the different cell lines by comparing the rotational and translational diffusion. Finally, Pol-FCS will be applied to clarify the state of molecular crowding in cytoskeletal network of cells and polymer gels as a model of crowding.

2SGP-3 混雑化で生み出される人工細胞内の Min システム反応拡散波

A localization wave of proteins reconstituted in artificial cells with crowding environments

Kei Fujiwara (*Dep. Biosci. and Info., Keio University*)

We will present the behavior of a bacterial protein localization wave driven by reaction-diffusion dynamics in artificial cells. MinD and MinE, a deterministic system for the cell division plane of bacteria, change their localization like waves by reaction-diffusion dynamics. We found that this wave does not emerge in artificial cells composed of bacterial polar lipids, suggesting MinD and MinE are not enough for the generation of the protein localization wave in cell-sized spaces. Focusing on the influence of macromolecular crowding on reaction and diffusion, we found a very high concentration of a macromolecule to the system triggers Min wave in artificial cells. Min waves in artificial cells characteristic behaviors suitable for cell growth.

2SGP-4 Brownian motion in dense DNA solutions

Yoshihiro Murayama (*Tokyo Univ. of Agri. and Tech.*)

On Brownian motion in dense DNA solutions such as an inside of nucleus, not only viscosity but also elasticity becomes important. We have investigated Brownian motion of a micron-sized particle in long-DNA (48 or 166 kbp) solution. In both short and long time scales DNA solution acts as a viscous fluid, while in medium time scale it acts as a viscoelastic fluid. In the medium time scale, the exponent of mean square displacement is less than 1, which means that the motion is restricted by the time scale dependent elasticity. Our results obtained with different lengths DNA show that the disappearance of the elasticity in long time scale is not explained by disentanglement of macromolecules.

2SGP-5 不均一な環境下での異常拡散

Anomalous diffusion in heterogeneous environments

Takuma Akimoto (*Tokyo University of Science*)

Diffusion is a key phenomenon in biological reactions. In living cells, there are many macromolecules which provide heterogeneous environments due to macromolecular crowding. In this talk, I will introduce several heterogeneous environments and discuss diffusion of a biological molecule in these environments. Using stochastic models and molecular dynamics simulations, I will present that the mean square displacement (MSD) does not increase linearly with time (anomalous diffusion) and the time-averaged MSDs show aging (it depends on the measurement time) and ergodicity breaking (it is not equal to the ensemble average). The role of anomalous diffusion in cells will be discussed.

2SGP-6 高分子混雑環境下での蛋白質 NMR 緩和解析

NMR relaxation analysis of the protein under macromolecular crowding environment

Hideyasu Okamura[1], Takanori Kigawa[1,2] ([1]*RIKEN QBiC*, [2]*Department of Computer Science, Tokyo Institute of Technology*)

Macromolecular crowding environment in biological cells is significantly different from the experimental condition performed in diluted solutions. The model-free analysis for NMR relaxation data is one of the most powerful methods for obtaining the dynamic information of proteins. However, the application of the conventional model-free analysis to macromolecular crowding environment has proven problematic. To solve this problem, we have newly extended the conventional model-free formalism to be applicable to such situations. This extension explain the NMR relaxation data obtained under macromolecular crowding environment in a straightforward way. Then, the resulting data illuminates physical feature of macromolecular crowding environment.

2SGP-7 細胞混雑中の蛋白質と代謝物のダイナミクス: 全原子分子動力学法による理論的研究

Dynamics of Proteins and Metabolites in Cellular Crowding Environment: Theoretical Study with All-atom Molecular Dynamics Simulation

Isseki Yu[1,2], Po-Hung Wang[2], Michael Feig[3], Yuji Sugita[1,2] ([1]*RIKEN iTHES*, [2]*RIKEN Theoretical Molecular Science Lab.*, [3]*Michigan State University*)

Inside of a cell is highly crowded with a large number of macromolecules together with solvents and metabolites. How variable interactions within dense cellular environments may affect the structure and dynamics, and ultimately function is one of the most fundamental questions in life science. We constructed full atomistic model of the cytoplasm of bacteria and various levels of protein crowding models. Using these model, we performed all-atom molecular dynamics (MD) simulations. Influence of crowding and non-specific interaction between macromolecules on the translational/rotational motion of proteins are analyzed. Anomalous diffusion and the localization of metabolites, such as ATP and amino acids, on the macromolecule surface are also investigated.

2SKP-1 タンパク質微小結晶構造解析の将来に向けて
Towards the next generation protein micro-crystallography at SPring-8 and SACLA

Masaki Yamamoto (*RIKEN RSC*)

Macromolecular crystallography coupled with a highly brilliant X-ray beam from advanced SR and X-ray Free Electron Laser (XFEL) continues to shine light on many challenging and scientifically important problems. Recently, the structural determination of membrane proteins has been accelerated by the use of micro-focus beamlines. BL32XU at SPring-8 is a beamline dedicated for protein micro-crystallography. The beamline can provide a 1-10 micron beam facilitating the determination of high impact protein structures. In 2012 XFEL/SACLA was open for users. We are developing femtosecond crystallography using a fixed-target and several type of sample injectors. We will present the current state and future of protein micro-crystallography at SPring-8 and SACLA.

2SKP-2 Structure and function of the polymyxin-resistance-associated response regulator PmrA

Chwan-Deng Hsiao (*Institute of Molecular Biology, Academia Sinica*)

Two-component systems (TCSs) are adopted in bacteria, archaea, certain lower eukaryotes and higher plants to couple environmental stimuli with adaptive responses. TCSs are absent in mammals, so they are attractive targets for drug development. In this study, we used PmrA/PmrB TCS to study its structure and function. PmrA, an OmpR/PhoB family response regulator (RR), takes part in the TCS that manages genes for antibiotic resistance. Phosphorylation of OmpR/PhoB RR induces the formation of a symmetric dimer in the N-terminal receive domain, promoting 2 C-terminal DNA-binding domains to recognize the promoter DNA to elicit adaptive responses. We report the function for interacting with RNA polymerase holoenzyme and the crystal structure of the PmrA-DNA complex.

2SKP-3 二重殻構造を持つイネ萎縮ウイルスの構造構築機構
Structure assembly mechanism of a double-shelled virus, Rice dwarf virus

Akifumi Higashiuira, Yusuke Nakamichi, Kenta Tsutsumi, Naoyuki Miyazaki, Kenji Iwasaki, **Atsushi Nakagawa** (*Inst. Protein Res., Osaka Univ.*)

Rice dwarf virus (RDV), a causal agent of rice dwarf disease, is a member of the genus Phytoreovirus in the family Reoviridae. A viral particle consists of two concentric layers of proteins that encapsidate double-stranded RNAs. The core particle contains transcriptional complexes composed of P1, P5 and P7 proteins with a thin layer that is consisted of 120 copies of P3 protein. The outer layer is composed of 780 copies of P8 protein, with a small number of P2 and P9 proteins. The total molecular mass of an each particle is about 75 MDa.
Atomic structure of a virus particle and our recent results of structural studies of intermediate structures of particle assembly and a major viroplasm protein, Pns12, suggested the hierarchical organization of virus particle assembly.

2SKP-4 A structural proteomic approach to understand cobra venom actions beyond neurotoxicity of the bitten victims

Wen-Guey Wu (*Institute of Bioinformatics and Structural Biology, National Tsing Hua University, Taiwan*)

Despite of the general belief that cobra venom actions mainly induce neurotoxicity of the bitten victims, recent clinical evaluation of cobra snakebites by Naja atra indicates a localized swelling and tissue necrosis as the most common symptom with less than 5% of the supposed block of neuromuscular junction. We hypothesize that the metabolic products of the endogenous purinergic signaling pathway may play a significant role in the severe tissue necrosis. By using both the structural proteomics and cell signaling processes of glycosylated high molecular weight (HMW) toxins from Taiwan cobra, we illustrate how the cobra venom could act through HMW venom toxins.

2SKP-5 統合構造生物学と生理学のための最新 NMR
Advanced NMR for Integrated Structural Biology and Physiology

Chojiro Kojima[1,2] ([1]*Grad. Sch. Eng., Yokohama Nat. Univ.*, [2]*Inst. Protein Res., Osaka Univ.*)

NMR is a powerful tool in structural biology, and easily combined with other tools, such as X-ray. We have developed NMR methods to determine high resolution NMR structure, and to monitor protein-protein interactions. For example, fully automated NMR structure determination tool is developed for conventional targets. For tough targets, selective 13C/15N labeling and chemical modification are used to monitor protein-protein interactions by NMR combining with X-ray. New method for physiology is also developed. In this presentation, these NMR methods are demonstrated with its biological application.

2SKP-6 Circular permutation: Database, Prediction and Design

Ping-Chiang Lyu (*Institute of Bioinformatics and Structural Biology, National Tsing Hua University*)

Circular permutation (CP) is a protein structural rearrangement phenomenon, through which nature allows structural homologs to have different locations of termini and thus varied activities, stabilities and functional properties. It can be applied in many fields of protein engineering. The limitation of applying CP lies in its technical complexity, high cost and uncertainty of the viability of the resulting protein variants. We have previously reported the CPSARST to be an efficient database search tool and designed a comprehensive method for predicting viable CP cleavage sites in proteins. Here we also report the prediction and redesigning of a carbohydrate-binding module family 21 protein (CBM21) to test our tool.

2SLP-1 細胞における温度動態：観察と意義
Thermal dynamics in individual cells: observation and significance

Yasuo Mori (*Kyoto Univ., Grad. Sch. Engineering*)

Recent developments in biometric technologies have enabled observation of thermal changes at single-cell and subcellular levels. In this symposium, I first explain imaging probes (ts-GFPs) we invented on the basis of GFP fluorescence and coiled-coil structure of the Salmonella protein TlpA to detect thermal changes in living cells in vitro and in vivo, and try to validate our observation of subcellular heterogenity of thermal distribution. More specifically, fluctuation of heat generation associated with lipid droplets as well as thermal elevation in the nucleus are displayed and their significance are discussed. In addition, an interesting relationship between thermal and redox regulation of protein function is discussed in terms of TRP cation channels, which show unique sensitivities to changes in thermal and redox status.

2SLP-2 マウス体内時計の温度応答
Temperature-responses of the circadian clock oscillation in mice

Yoshitaka Fukada (*Dept. Biological Sciences, School of Science, The Univ. Tokyo*)

The periods of the circadian clock are kept constant within a range varying from 21 to 27 hours. The variation depends on species and ambient conditions, where it is resistant to changes in environmental temperature with a Q10 value of 0.8-1.2. This amazing property of the circadian clock was originally recognized as temperature independence. The circadian oscillation was not slowed down but rather slightly accelerated by lowering temperature in some condition. The overcompensation phenomenon suggested the existence of a temperature compensation mechanism. Our cell-based screening of genetic perturbation and chemical treatment raised the possibility that a mixed combination of signaling pathways is important for temperature-responses of the circadian clock in mice.

2SLP-3 16S rRNA 遺伝子の GC 含量と原核生物の生育温度との関係
Relationship between guanine-plus-cytosine content of 16S rRNA genes and growth temperature of the prokaryotic hosts

Yu Sato[1], **Hiroyuki Kimura**[2] ([1]*Grad. Sch. Sci. Technol., Shizuoka Univ.*, [2]*Res. Inst. Green Sci. Technol., Shizuoka Univ.*)

16S rRNA genes are a good marker for phylogenetic analysis of prokaryotes because they are highly conserved in all prokaryotes. On the other hand, it has reported that the 16S rRNA gene sequence is naturally inscribed with the thermal features of the prokaryotic host. This observation was based on a high correlation between the growth temperatures of prokaryotes and the guanine-plus-cytosine contents (P-GC) of the16S rRNA genes: thermophiles generally have high P-GC of 16S rRNA genes, whereas mesophiles and psychrophiles have low P-GC of 16S rRNA genes. Here, we introduce the microbial molecular thermometer to calculate growth temperatures of prokaryotes. We also present physiological advantage of halophilic archaea that harbors different P-GC of 16S rRNA genes.

2SLP-4 細胞内微小空間における温度と分子の相互作用
Interaction between temperature and molecules in intracellular microenvironments

Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Graduate School of Pharmaceutical Sciences, The University of Tokyo*, [2]*JST, PRESTO*)

Temporal and spatial temperature change in living cells as visualized by fluorometric thermometry have attracted great attention in recent years. Recently, we monitored transient heating inside of cells and revealed distinctive intracellular heat dynamics, proving the existence of unique chemical environments within cells. Additionally, we found local thermogenesis-mediated acute translation reprogramming via RNA granule formation, proving the contribution of intracellular temperature change to cell functions. These facts imply an intriguing concept: local temperature and macromolecules have a mutually influential relationship, which may account for the unique thermal dynamics of, and thermal signaling that occurs within, intracellular microenvironments.

2SLP-5 温度応答性超分子を用いたがん集積システムの開発
Development of a tumor-accumulation system using temperature-responsive supramolecule

Satoru Karasawa[1,2,3], Takeru Araki[3], Kazuteru Usui[3], Shuhei Murayama[4], Ichio Aoki[4] ([1]*Univ. Showa*, [2]*JST PRESTO*, [3]*Grad. Sch. Pharm. Univ. Kyushu*, [4]*Ins. QST*)

It is well known that the temperature of tumor tissues is higher that of healthy tissues. Taking advantage of this temperature difference between the tissues, we investigated the accumulation of the temperature-responsive molecules, EgXs, in tumor tissues. EgXs are composed of a fluorophore, alkylureabenzene, and OEG chains. OEG plays a significant role in water solubility and thermal responsiveness. EgXs exhibit "lower critical solution temperature (LCST)", in which the molecules assemble abruptly in response to heat. In addition, the LCST depends on OEG length. Accordingly, if LCST values are maintained at tumor temperature, EgXs are capable of accumulating into the tumor tissues, thus enabling the confirmation of the degree of accumulation by fluorescence imaging.

2SMP-1 エンドサイトーシス関連細胞質タンパク質の構造から迫るクラスリン重合機構
Insights into clathrin assembly from the structures of cytosolic endocytic proteins

Atsushi Shimada[1,2] ([1]*Med. Inst. Bioreg., Kyushu Univ.*, [2]*RIKEN SPring-8 Center*)

The internalization of extracellular molecules through clathrin-mediated endocytosis (CME) is crucial in many physiological responses in eukaryotes, such as receptor internalization, nutrient uptake, and synaptic vesicle recycling. CME starts with the assembly of clathrin into the clathrin lattice on the membrane. During clathrin assembly, clathrin does not directly interact with the membrane and requires a number of cytosolic regulatory proteins for higher-order assembly on the membrane. In this symposium, I discuss the mechanism of clathrin assembly based on the structural and functional data on some of these regulatory proteins.

2SMP-2 Dynamic remodeling of Dynamin complexes during membrane fission

Tetsuya Takeda[1], Daiki Ishikuro[2], Huiran Yang[1], Toshiya Kozai[2], Kaho Seyama[1], Yusuke Kumagai[2], Hiroshi Yamada[1], Takayuki Uchihashi[4], Toshio Ando[2,3], Kohji Takei[1] ([1]*Grad. Sch. Med. Dent. Pharm. Sci., Okayama Univ.*, [2]*Coll. Sci. Eng., Kanazawa Univ.*, [3]*Bio AFM, Kanazawa Univ.*, [4]*Dept. Phys., Nagoya Univ.*)

Dynamin is a mechanochemical GTPase essential for membrane fission in endocytosis. Dynamin forms helical complexes at the neck of endocytic pits and their structural changes upon GTP hydrolysis drive membrane fission. However, precise mechanisms of the Dynamin-mediated membrane fission remain to be elucidated.
In this study, we analyzed dynamics of Dynamin complexes during membrane fission using EM and HS-AFM. Interestingly, the Dynamin helices were dynamically remodeled to form clusters upon GTP hydrolysis and membrane fission occurred at the flanking “bare” membrane regions.
Thus, our new approaches using HS-AFM demonstrated dynamics of Dynamin complexes during membrane fission for the first time proposing a novel mechanism of the Dynamin-mediated membrane fission.

2SMP-3 エンドサイトーシス型受容体 ApoER2 のリガンド結合状態の結晶構造
Crystal structure of the endocytic receptor ApoER2 in the ligand-bound state

Terukazu Nogi (*Grad. Sch. Med. Lif. Sci., Yokohama City Univ.*)

Apolipoprotein E receptor 2 (ApoER2) is a cell-surface receptor belonging to the low-density lipoprotein receptor (LDLR) family. ApoER2 is implicated not only in lipoprotein uptake, but also in signal transduction during brain development through capture of the extracellular protein reelin. We have determined a crystal structure of full-length ApoER2 ectodomain in complex with a signaling-competent fragment of reelin. Although LDLR was thought to adopt the extended conformation to capture the ligand, the ligand-bound ApoER2 ectodomain assumes a contracted conformation by engaging reelin through multiple binding interfaces. Our structure is expected to provide important clues for understanding the ligand capture and release mechanism in the LDLR family.

2SMP-4 Mechanisms of *trans*-synaptic adhesion for inducing synapse formation

Shuya Fukai (*IMCB, Univ. Tokyo*)

Synapse formation is initiated by *trans*-synaptic adhesion mediated by receptor-like adhesion molecules called synaptic organizers. One of the two major presynaptic organizers is the type IIa receptor protein tyrosine phosphatase, which includes LAR, PTPσ and PTPδ. Using crystallographic, biophysical and cell biological techniques, we have elucidated the mechanisms of selective pairing between PTPδ and postsynaptic organizers, IL-1RAcP, IL1RAPL1 and the Slitrk family protein. Recently, we determined crystal structures of *trans*-synaptic adhesion complexes between PTPδ and other postsynaptic organizers. Based on the newly determined structures and structure-based mutagenic analysis, we reveal new structural aspects of *trans*-synaptic adhesion for inducing synapse formation.

2SMP-5 The spatial distribution of the BAR domain proteins on the membrane

Shiro Suetsugu (*NAIST*)

Dimeric proteins containing Bin-Amphiphysin-Rvs167 (BAR) domains sculpt membranes. Depending on concave or convex surface of the dimeric proteins for membrane binding, they form membrane invaginations or protrusions, respectively. BAR domain proteins assemble to oligomer of defined organization, which surrounds the membrane structures in vitro. However, the assembly had not been clarified in cells. Here, we utilized the super-resolution analysis to reveal the sheet-like assembly of BAR domain containing protein. The BAR domain proteins were localized close to each other, forming the protein sheet. The observed concentration of the protein was ~1 molecule/20 nm3. Therefore, the highly concentrated BAR domain proteins function for the plasma membrane morphogenesis.

2SMP-6 Molecular mechanisms involved in the reassembly of the actin cortex in membrane blebs

Junichi Ikenouchi (*Dept. Biol., Facl. Sci., Kyushu Univ.*)

Actin filaments usually lie beneath the plasma membrane. When the plasma membrane detaches from actin filaments, spherical protrusions of the membrane form, which are called membrane blebs. Membrane blebs are initiated as a rapid protrusion of the plasma membrane driven by the intracellular hydrostatic pressure after local disruption of membrane-actin cortex interactions. Thereafter, actin filaments polymerize beneath the protruded membrane to halt bleb expansion and retract protruded membrane. It remains unknown how such reassembly of actin cortex is regulated. I will introduce our recent findings about the molecular mechanisms involved in the regulation of dynamic interplay between membrane and actin filaments.

2SMP-7 Role of plasma membrane tension in cell migration and invasion

Kazuya Tsujita (*Biosignal Research Center, Kobe University*)

It is well established that actin-driven cell membrane shape changes like protrusions are vital for cell movement. These actin-associated membrane protrusion structures are known as lamellipoda, filopodia, and invadopodia, which are intrinsically affected by a mechanical property of the plasma membrane (PM), namely membrane tension. We and others have shown that PM tension plays an important role in cell shape changes and cell movement. In my talk, I will introduce our approaches that can address the mechanisms underlying the regulation of PM tension. I will also discuss our recent findings of how PM tension regulates cell migration and invasion.

2SMP-8 Actin polymerization in contact with the plasma membrane may be a Brownian ratchet-based information collector

Naoki Watanabe[1,2], Kazuma Koseki[2], Daisuke Taniguchi[2] ([1]*Kyoto Univ. Grad. Sch. Biostudies*, [2]*Kyoto Univ. Grad. Sch. Med.*)

Actin generates force for cell protrusion. The force-polymerization relationship at the interface with the plasma membrane is theorized by Brownian ratchet mechanisms, yet its evidence remains elusive. The ratchet and pawl cannot move in one direction without energy supply. Information to change kinetic barriers according to the particle's position may also drive the ratchet in one direction. Using Single-Molecule Speckle microscopy, we found that immediately after cell stretch, actin assembly increases specifically at the lamellipodium tip. The rate of actin assembly increased with increasing stretch speed, as simulated by the Brownian ratchet model. Thus, actin polymerization at the cell edge may function as a Brownian ratchet-based force sensor for cell protrusion.

2SNP-1 スパースモデリングに基づく計測データ解析 Measurement data analysis based on sparse modeling

Toshiyuki Tanaka (*Graduate School of Informatics, Kyoto University*)

On the basis of the framework of sparse modeling, novel methods for analyzing measurement data have been developed in various fields, and they have been promoting changes in methologies of measurements. In this talk, focusing on compressed sensing, one of the representative approaches in sparse modeling, we review some topics regarding progresses in measurement data analysis via sparse modeling.

2SNP-2 位相的データ解析とその応用 Topological Data Analysis and its Applications

Kenji Fukumizu (*ISM*)

Topological data analysis (TDA) is a methodology for extracting topological and geometrical features from complex geometric data structures. Persistent homology provides a multiscale descriptor for the topology of data, and has been recently applied to data analysis. I will introduce a machine learning framework of TDA with vectorization by kernel methods, which enables systematic use of standard data analysis to TDA. I will show some applications of TDA to phase transitions of amorphous solid and times series of protein data.

2SNP-3 ディープラーニングを用いた医用 CT 画像のテクスチャ識別 Texture classification on Medical CT image using Deep Learning

Hayaru Shouno (*University of Electro Communications*)

Deep convolutional neural networks (DCNNs) is a kind of neural network, which can learn feature representation provided from the large amount of training dataset. In order to apply a DCNN into the field of medical imaging, which has not so much large dataset, we investigate a transfer style learning method. The transfer method requires small amount of medical image dataset and large amount of other labeled image dataset. We introduced a simple method, that is, the initial state of the DCNN has already been trained with large amount of natural images. Then we train the DCNN with diffuse lung disease (DLD) pattern for fine-tuning. In the result, we found the transfer-style learning shows higher performance rather than that of the DCNN trained with only DLD dataset.

2SNP-4 シミュレーション／データ両駆動型データ同化の創出へ Towards a generation of the simulation-/data-driven data assimilation

Hiromichi Nagao[1,2] ([1]*ERI, UTokyo*, [2]*IST, UTokyo*)

Data assimilation (DA), which the modern weather forecasting bases, integrates simulation models and observation data based on Bayesian statistics. DA is spreading its applicability to wide variety of scientific fields in which simulations play important roles, such as seismology and materials science. Since the current DA strongly depends on a given model, it never extracts phenomena that the model does not assume even when data contain them. For further extension of DA to scientific fields like biology in which observations are much more essential than simulations, a new DA that can perform data-driven modeling such as sparse modeling is required. We introduce our recent DA studies and struggles towards a generation of the simulation-/data-driven DA methodology.

2SNP-5 低感度 NMR スペクトルから情報を得るための安定同位体標識法の in-cell NMR への応用 How to cope with noisy NMR spectra; application of a novel isotope labeling strategy to in-cell NMR

Takuma Kasai[1,2], Kae Higuchi[1], Kohsuke Inomata[1], Takanori Kigawa[1,3] ([1]*RIKEN QBiC*, [2]*PRESTO, JST*, [3]*Sch. Comput., Tokyo Inst. Tech.*)

NMR is useful for analyses of protein structures, dynamics, and interactions; however, in difficult situations such as in-cell NMR, signal assignments are difficult due to enhanced relaxation. Our isotope labeling strategy, SiCode (Stable isotope encoding), helps assignments by amino-acid typing with a few labeled samples. SiCode is based on a concept that amino-acid information is encoded by labeling ratio and is decoded from observed spectra. To achieve high noise tolerance, we improved both encoding and decoding. For encoding, the labeling pattern was optimized so that the samples can hold maximum information. For decoding, a model-based decoding was introduced to obtain information even from noisy spectra by searching the best parameters to explain observed spectra.

2SNP-6 統計的画像処理による超解像顕微鏡法
Super-resolution imaging by statistical image data processing

Yasushi Okada[1,2] ([1]*Quantitative Biology Center, RIKEN*, [2]*Dept. Physics, Univ. Tokyo*)

The image of fluorescent microscope is sum of the signals from a finite number of fluorescent molecules in the view field. Thus, the goal of the superresolution techniques can be regarded as to determine their positions as precisely as possible. Many techniques have recently been proposed to improve the precision in measurement by using special optics or special dyes. Meanwhile, several data processing approaches have also been proposed. Since both approaches are independent, their combination will give us even better results. In this talk, we will review these technologies based on our own results.

3SAA-1 散乱光で細胞・分子の状態を測る
Light scattering microscopes to quantify the cellular and molecular states

Taro Ichimura, Junichi Kaneshiro, Arno Germond, Tomonobu Watanabe (*RIKEN QBiC*)

Light scattered from living cells and molecules tells us the cellular and molecular status by its polarization, phase, spectrum, and radiation pattern, depending on optical process chosen from many options. The biologically significant information can be extracted from the light in analytical or statistical methods. In this presentation, we will introduce biological applications of some kinds of light scattering microscopes, including Raman scattering for cellular state measurement and second harmonic generation for molecular structure measurement. The principles of the optical processes and methodologies for grabbing the information will be discussed.

3SAA-2 光第二高調波イメージングの細胞生物学研究への応用
Application of SHG imaging to cell biology

Mutsuo Nuriya[1,2] ([1]*Department of Pharmacology, Keio University School of Medicine*, [2]*Graduate School of Environment and Information Sciences, Yokohama National University*)

Second harmonic generation (SHG) imaging visualizes SHG signals originating from materials that distribute in a non-centrosymmetric manner. This requirement is best fulfilled in the lipid-water interface of plasma membrane. Indeed, when cells are stained with amphiphilic dyes, SHG can specifically highlight plasma membrane and sensitively report its changes. Importantly, use of the SHG-specific dye allows simultaneous and independent acquisitions of SHG and fluorescence signals from various fluorescence reporters, realizing the multimodal two-photon imaging. Thus, SHG imaging is well suited and readily applied to various cell biology researches.

3SAA-3 Quantitative and multimodal phase imaging for analysis of cellular characteristics

Nicolas Pavillon, **Nicholas Smith** (*Osaka Univ, IFReC*)

To probe the functions of living cells, the typical approach is: identify targets, label by dyes, and then image to elucidate the role of those targets. Instead, by label-free imaging via quantitative phase microscopy, we observe overall cell morphology. While not as specific as a labels, some morphological features of cells indicate highly useful information. Observation of cell cycle, activation state, or discrimination between different cell types can be measured by digital holographic microscopy. Additionally, using Raman analysis, in parallel with the phase imaging, we can gain information on the chemical makeup of the cells and how it varies depending on cellular features. These measurements can be performed non-invasively on single cells, with high throughput.

3SAA-4 非ラベル分子の画像化のための位相敏感広帯域 CARS 分光
Phase-sensitive multiplex-CARS spectroscopy for label-free molecular imaging

Takayuki Suzuki[1], Yuki Obara[2], Kazuhiko Misawa[2] ([1]*Grad. Sch. Sci., Meiji Univ.*, [2]*Grad. Sch. Eng., Tokyo Univ. of A&T*)

There has been growing importance in observing the density distribution of molecules in order to identify their species. To find target molecules in the observation area, one conventionally uses fluorescence or index molecules as labels. Such methods, however, limit subject molecules and fields.
We have developed a method for efficient phase modulation for phase-sensitive coherent anti-Stokes Raman scattering (CARS) spectroscopy which reveals intrinsic molecular vibrational spectra. We also demonstrated two-dimensional density mapping of small molecules, which are difficult to label, by referring to their intrinsic vibrational spectra. Here, by using time-resolved technique, we suppressed intense background noise generated from water.

3SAA-5 誘導ラマン散乱顕微法による高速代謝物イメージング
High-speed imaging of metabolites with stimulated Raman scattering microscopy

Yasuyuki Ozeki (*Department of Electrical Engineering and Information Systems, University of Tokyo*)

Raman scattering microscopy is recently regarded as a powerful tool for detecting molecular vibrational signature with subcellular spatial resolution. Among several methods of Raman scattering microscopy, those based on stimulated Raman scattering (SRS) have several advantages including high-speed image acquisition and straightforward spectral analysis. In fact, we have demonstrated high-speed hyperspectral SRS microscopy at a frame rate of 30 frames per second or higher. In this talk, I'd like to discuss the advantages of high-speed imaging capability with SRS by introducing our recent results on single-cell metabolite analysis of microalgae.

3SAA-6 光熱変換顕微法による生物組織の高感度・高分解光吸収イメージング

Photothermal microscopy for high sensitivity and high resolution absorption contrast imaging of biological tissues

Jun Miyazaki (*Fac. Sys. Eng., Wakayama Univ.*)

Photothermal (PT) microscopy is an efficient method for visualizing the distribution of non-fluorescence endogenous chromophores in in biological specimens. To achieve fast imaging as well as to avoid thermal damage on the sample, it is necessary to improve the signal-to-noise ratio. We developed a high-sensitivity PT microscope by implementing a new detection scheme into a laser scanning microscope. Furthermore, with an apodizing filter, spatial resolution was twice as high as that of the conventional microscopy. This system demonstrated label free 3D imaging of mitochondria in skeletal muscle cells. Simultaneous PT and fluorescence imaging of mouse brain tissue was also conducted to visualize both neurons expressing YFP and endogenous non-fluorescent chromophores.

3SBA-1 高 LET 重イオン線によってヒト正常線維芽細胞に誘導されるバイスタンダーシグナル伝達と細胞死の機構解明

High-LET heavy-ion-induced bystander signalling and cell death in normal human fibroblasts

Masanori Tomita (*Radiat. Safety Res. Cent., CRIEPI*)

A radiation-induced bystander response is known as a cellular response induced in non-irradiated cells that received bystander signals released from the irradiated cells. Bystander response induced by high-linear energy transfer (LET) heavy ions at low fluence is an important health problem for astronauts in space and patients received hadron therapy. Normal human fibroblasts irradiated with high-LET heavy ions showed the cell killing effect at low doses higher than estimated by a linear extrapolation from high doses. Additionally, we found that Akt- and NF-κB-dependent signalling pathways and nitric oxide were involved in high-LET heavy-ion-induced bystander signalling. The difference in the bystander response between heavy ions and X-rays will also be discussed.

3SBA-2 高 LET 放射線による DNA 酸化損傷の生成とその分布観察

Observation of DNA oxidative damage induced by high LET radiation

Atsushi Ito (*Sch. Eng. Tokai Univ.*)

The biological effects of radiation are generally understood by direct action via direct ionization of biomolecules and indirect action via oxy-radicals generated by radiolysis of water. High LET (Linear Energy Transfer) radiation such as heavy-charged ion particles has a unique track structure which consists of a core region with high ionization density and a penumbra region where secondary electrons mainly contribute to energy deposition, with relatively low LET nature. The biological effects of high LET radiation should be characterized based on such a track structure. In this study, we detected oxidative DNA damage induced by OH radicals and obtained distribution of the damage in mammalian cells and thin DNA sheet using immunofluorescence method.

3SBA-3 Analysis of the modification of cell death by energy deposition to a local site in a cell

Munetoshi Maeda (*Proton Medic. Res. Gr., WERC*)

It is generally accepted that the biological effects of radiation, such as cell death, are mainly caused by unrepaired DNA damage in the cell nucleus. Meanwhile, recent studies have revealed the new phenomena which could not be explained only by this theory. Using a beam size-changeable synchrotron X-ray microbeam cell irradiation system developed at the KEK, we demonstrated that the death of irradiated and bystander cells was clearly higher following nucleus-only irradiation with low-dose X-ray microbeams than after whole-cell targeting. Our results clearly indicate that the existence of radiation-responsive mechanisms in the cytoplasm. Intracellular communication between the nucleus and cytoplasm may plays an important role in modification of the cell mortality.

3SBA-4 Computational analysis of bystander signaling in cellular population irradiated with microbeam

Yuya Hattori[1], Akinari Yokoya[2], Daisuke Kurabayashi[1], Ritsuko Watanabe[2] ([1]*Dept. of Sys. & Ctrl. Eng., Sch. of Eng., Tokyo Tech.*, [2]*Quantum Beam Science Research Directorate, QST*)

Even when only a limited number of cells in a population are irradiated with spatially limited ionizing radiation, such as microbeam, unexposed cells could also be affected by receiving certain intercellular signals from the irradiated cells. This "bystander effects" has been intensively studied from the point of view of low-dose radiation risk. To investigate detailed mechanism of the unique non-targeting effects, we analyzed the characteristics of the bystander signaling among the cells using a mathematical model, which consists of several simple functions describing bystander signal production, DNA damage induction, or cell death. Linear and non-linear characteristics of bystander signaling were revealed by fitting model to experimental results in a previous report.

3SBA-5 マイクロビーム照射とシミュレーションを用いた線虫の筋運動に対する放射線影響の解析

Analyses of radiation effects on muscular movements in *Caenorhabditis elegans* using microbeam irradiation and simulation-based approach

Michiyo Suzuki[1], Yuya Hattori[2], Tetsuya Sakashita[1], Yuichiro Yokota[1], Yasuhiko Kobayashi[1], Tomoo Funayama[1] ([1]*Dept. of Radiat. Appl. Biol. Res., QST-Takasaki*, [2]*Dept. of Sys. & Ctrl. Eng., Sch. of Eng., Tokyo Tech*)

To better understand the effects of radiation on critical functions such as stimulation resonses and/or motor control, we use the nematode *Caenorhabditis elegans* which is a good in vivo model system for examination of behaviors. In this presentation, we will give an outline of the radiation effects on rhythmic movements of *C. elegans*. Especially, we will refer to heavy-ion microbeam irradiation and show the effects of region-specific irradiation. In addition, we will introduce our simulation-based approach that aims to estimate the mechanisms of radiation effects on oscillation generation of muscular movements at cell level, and discuss about further studies to understand the detailed mechanisms underlying the temporary changes of the movements following irradiation.

3SBA-6 メダカ胚で観察された重イオン局所照射によって誘発される照射野以外への影響

Abscopal activation of microglia in embryonic fish brain following targeted irradiation with heavy-ion microbeam

Takako Yasuda[1], Shoji Oda[1], Tomoo Funayama[2], Hiroshi Mitani[1] ([1]*Grad. Sch. Frontier Sci., Univ. Tokyo*, [2]*TARRI, QuBS, QST*)

We locally irradiated the optic tectum (OT) of medaka embryonic brain, using a collimated carbon-ion micro beam at the facility of QST, and investigated the dynamics of microglial activities induced after irradiation. The microglial activation includes two steps in the phagocytotic process, and the early and the later step was indicated by the specific two biomarkers, respectively. Targeted irradiation of the limited area induced L-plastin expression only in the microglia that was located in the irradiated area. Subsequently, ApoE expression in microglia was induced, not only in the target irradiation area of OT, but also in the nonirradiated area of OT. These findings strongly suggest that the abscopal activation of brain immune system can be induced after irradiation.

3SBA-7 生物影響からみた光子放射線と粒子放射線の違いー評価と防護ー

Differences between photon and particle radiations in terms of their biological effects: Evaluation and protection

Tetsuo Nakajima (*Dept of Radiation Effects Research, NIRS, QST*)

We have opportunities exposed to many kinds of radiations, which are not only photon radiations like X-rays but also particle radiations such as protons, neutrons or heavy-ion beams in medical treatments or space long-term missions etc. To understand radiation exposure risk about each of them is important in our modern society. Here, some examples to explore useful biological markers for evaluating radiation effects will be introduced. Particularly, differences in biological effects between photon and particle radiations might be possibly detected due to linear energy transfer (LET) or particle fluence. In addition, to explore radio-protective agents which are easily taken and have no side effects will be also shown.

3SCA-1 F 型結晶構造から明らかとなったアクチン重合と ATP 加水分解機構

ATPase mechanism and dynamic assembly of actin revealed by the F-form crystal structures

Shuichi Takeda[1], Akihiro Narita[1], Toshiro Oda[2], Kotaro Tanaka[1], Ryotaro Koike[3], Motonori Ota[3], Ikuko Fujiwara[4], Nobuhisa Watanabe[5], Yuichiro Maeda[1] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*Univ. Tokaigakuin*, [3]*Grad. Sch. of Info. Sci., Univ. Nagoya*, [4]*FRIMS., NITech*, [5]*SRRC., Univ. Nagoya*)

Actin is an ATPase and the nucleotide hydrolysis is greatly accelerated by polymerization that is accompanied with a conformational change of the molecule from the monomeric G-form to the filamentous F-form. We solved a crystal structure of actin in complex with a gelsolin superfamily protein fragmin. In this atomic structure, four actin molecules adopt a double-stranded F-actin-like orientation, with the conformation of the two barbed end subunits in the “F-form”. Furthermore, with the aid of a fragmin domain, we obtained ~1.3 Å resolution crystal structures of the F-form actin with AMPPNP, ADPPi and ADP states. Based on these new structures, we will discuss the molecular details of the ATP hydrolysis that is fundamental to the dynamic nature of actin filaments.

3SCA-2 Struture and mechanism of dynein motors

Takahide Kon (*Dept. of Biol. Sci., Grad. Sch. of Sci., Osaka Univ.*)

Dyneins are microtubule-based motor complexes of 1,000-3,000 kDa that power a wide variety of biological processes within eukaryotic cells, including ciliary beating, cell division, cell migration, and intracellular trafficking. The large size and complexity of dynein molecules have made elucidating their mechanisms a challenging task. In this presentation, I will discuss how dynein generates force and movements, based on recently obtained results through a combination of approaches including X-ray crystallography, MD simulations, cryoEM and single-molecule analysis.

3SCA-3 回転分子モーターの分子動力学シミュレーション

Molecular dynamics simulations of molecular rotary motors

Mitsunori Ikeguchi (*Yokohama City Univ.*)

F_1-ATPase and V_1-ATPase are molecular rotary motors driven by ATP hydrolysis. We have investigated the rotation mechanism of the rotary motors using molecular dynamics (MD) simulations. To elucidate the rotation mechanism of V_1-ATPase on the basis of the recently determined structure, we conducted multiscale MD simulations of V_1-ATPase. First, all-atom MD simulations were carried out to analyze the thermal fluctuations in the hydrolysis-waiting state. Then, the coarse-grained (CG) MD simulations were performed, and the 120-degree rotation of V_1-ATPase was successfully observed in the CG MD simulations. From the simulations, the key events during the rotation were identified.

3SCA-4 Design of circadian clock of cyanobacteria by dual ATPases in KaiC

Takao Kondo (*Nagoya Univ*)

The period length and its temperature compensation are key features for the circadian rhythms to coordinate metabolism of life on the Earth. We found that ATPase activity of KaiC protein is extremely weak (15 ATP/day) but highly temperature compensated. Moreover, even without KaiA and KaiB, this activity is proportional to frequency of KaiC phosphorylation rhythm. We analyzed activities of two ATPases under various biochemical and genetic conditions and propose that CI ATPase would be responsible for passive physical constants that define circadian period by a harmonic fashion. CII ATPase would function as oscillator that drives and sustains the robust oscillation.

3SCA-5 ABC トランスポーターは ATP 結合と加水分解のエネルギーを多剤排出にどのように利用するのか

How ATP binding cassette (ABC) transporter harnesses the energy of ATP binding and hydrolysis to multidrug export

Hiroaki Kato[1,2] ([1]*Grad. Sch. Pharm. Sci., Kyoto Univ.*, [2]*RIKEN/SPring-8*)

ABC multidrug transporters play an important role in cancer drug resistance, in protection against xenobiotics, and in the drug disposition through cellular and tissue barriers. They export structurally diverse hydrophobic compounds from the cell, driven by ATP binding and hydrolysis. Crystal structures of the ABC multidrug transporter from Cyanidioschyzon merolae in both inward- and outward-open states provide us how the transporter pumps a large variety of chemicals unidirectionally. The structural comparison also assumed the free energy transduction process that ATP binding stores the free energy in the strain of the transmembrane domains in the outward-open state and ATP hydrolysis ensures the specific rate to return the inward-open conformation.

3SDA-1 Structural analysis of the centromere specific nucleosome

Hiroaki Tachiwana[1,2], Midori Suzuki[3], Yoshimasa Takizawa[4], Matthias Wolf[4], Hitoshi Kurumizaka[2] ([1]*Japanese Foundation for Cancer Research, Cancer Institute*, [2]*Faculty of Science & Engineering, Waseda University*, [3]*Graduate School of Advanced Science & Engineering, Waseda University*, [4]*Okinawa Institute of Science and Technology Graduate University*)

Centromeres are specific region of chromosomes, which ensure equal chromosome segregation in mitosis. The histone H3 variant, CENP-A, is a key protein for the centromere. However, little is known about how CENP-A is involved in the centromeric chromatin formation. We have reported that a nucleosome containing human CENP-A has different structural feature from that of canonical nucleosomes indicating that the CENP-A nucleosome contributes to organization of the centromeric chromatin structure. To verify our hypothesis, we further analyzed structural features of CENP-A nucleosome in the reconstituted tri-nucleosomes. Together with our biochemical and Cryo-EM studies, I would like to discuss the centromeric chromatin structure with the CENP-A nucleosome.

3SDA-2 単一ヌクレオソームイメージングが明かすクロマチンダイナミクスと転写

Single nucleosome imaging reveals global chromatin stabilization upon transcription

Kayo Hibino[1,2], Ryosuke Nagashima[2], Kazuhiro Maeshima[1,2] ([1]*NIG*, [2]*SOKENDAI*)

Chromatin dynamics such as local fluctuation and long-range movement are involved in RNA transcription, which specifies cell fates. However, how the chromatin dynamics can be modulated by extracellular environmental changes remains unclear. Here, using single nucleosome imaging techniques, we have investigated the chromatin dynamics in human epithelial RPE-1 cells in serum-starved G0 quiescent state. Unexpectedly, we found that their local chromatin dynamics greatly increased and an active RNA pol II significantly decreased in the quiescent situations. These results suggest that large transcription machinery can stabilize chromatin upon transcription and that the untranscribed chromatin becomes more dynamic in a “ready-to-go” state for next transcriptional activation.

3SDA-3 Relationship between kinetics of higher-order genomic structure and transcriptional activity

Hiroshi Ochiai[1,2] ([1]*PRESTO, JST*, [2]*Grad. Sch. Sci., Hiroshima Univ.*)

It has become clear that long-range interaction between genomic loci is involved in gene expression regulation. It is also considered that such genomic interaction restricts chromatin movement within the nucleus. However, studies using exogenous reporter genes have shown that there is a correlation between transcriptional activation and mobility of the gene locus, contradicting the above discussion. To understand gene regulatory mechanisms within the restricted nuclear space, I explored the transcription and nuclear dynamics of many endogenous genes in mouse embryonic stem cells. In this presentation, I will report on the results and discuss the relationship between kinetics of higher-order genomic structure and transcriptional activity.

3SDA-4 Transcription dynamics in living Drosophila embryos

Takashi Fukaya, Tyler Heist, Michael Levine (*Lewis-Sigler Institute for Integrative Genomics, Princeton University*)

Intermittent bursts of de novo transcription are a general property of gene regulation in eukaryotes. Using newly developed MS2/PP7 live imaging method, we have previously shown that dynamic cis-interactions between enhancers and promoters control the level of gene activities by modulating transcriptional bursting in early fly embryos.
Recently, we have successfully visualized trans-homologue enhancer-promoter interactions in living embryos. Evidence is provided that insulators mediate homologue paring and inter-allelic enhancer-promoter interactions to drive transcriptional bursting in trans. Surprisingly, a single enhancer can drive synchronous bursts from two promoters separated in two alleles, suggesting concomitant recruitment of Pol II clusters in cis and trans.

3SDA-5 リボソーム RNA 遺伝子の核内動態： DNA 複製阻害タンパク質 Fob1 と DNA 損傷チェックポイントタンパク質に依存した核膜孔との結合

Fob1-dependent binding of ribosomal RNA genes to the nuclear periphery in budding yeast

Chihiro Horigome[1], Eri Unozawa[1,2,3], Takamasa Ooki[1], Takehiko Kobayashi[1,2,3] ([1]*Inst. Mol. Cell. Biosci., Univ. Tokyo*, [2]*NIG*, [3]*SOKENDAI*)

The ribosomal RNA genes (rDNA) in budding yeast are organized into a single tandem array of about 150 repeats. Fob1 unidirectionally inhibits replication fork progression at the replication fork barrier and induces DNA double-strand break (DSB) in the rDNA. The DSB leads to unequal sister-chromatid recombination and hence rDNA instability.
We performed chromatin immunoprecipitation assay to determine the localization of rDNA within the nucleus. We showed that rDNA binds to the nuclear pore in a manner dependent on Fob1 and DNA damage checkpoint kinases Mec1/Tel1. Furthermore, nuclear pore plays an important role in the rDNA stability. We speculate that Fob1 sequesters rDNA at the nuclear periphery to inhibit aberrant recombination events.

3SDA-6 ３次元ゲノム構造の多階層的理解～ヌクレオソームレベルから全染色体レベルまで～
Understanding 3D genome structure in mulitiscale from the nucleosome to whole choromosome level

Yuichi Taniguchi (*Quantitative Biology Center, RIKEN*)

Determining global and local rules that govern the structure of genome-wide, hierarchical chromatin architecture remains a critical challenge in biology. However, structures throughout the hierarchy at the smallest, or nucleosome scale, remain poorly understood. Here, we couple sequencing technology and molecular dynamics simulation to unveil the 3D spatial distribution of nucleosomes with their genome-wide orientations in chromatin. The method, called Hi-CO, revealed distinct structured folding motifs lower in the hierarchy across the yeast genome. The results revealed genome-wide, but local characteristic structural motifs that couple to specific epigenetic events.

3SDA-7 キャプチャー Hi-C を用いたゲノム間相互作用解析
Genome wide interaction analysis using Capture Hi-C

Shuichi Tsutsumi[1], Atsushi Okabe[2], Hiroyuki Aburatani[1] ([1]*Genome Sci. Div., RCAST, Univ. Tokyo*, [2]*Mol. Onc., Grad. Sch. of Med., Univ. Chiba*)

Gene activities are controlled by a combination of proximal and distal regulatory elements that interact with each other despite their genomic distances. A large number of enhancer regions have been annotated, but the principles defining the relationships between these regulatory elements and distal target genes remain unknown

To investigate globally how active enhancers dynamically interact with their target genes, we used Hi-C and Capture Hi-C assay in p53-positive HCT116 cells treated with 5-FU. Two thousands of TAD were found and more than 181,000 significant interactions were found ($p < 10^{-4}$). Active enhancers have a tendency to interact with active promoters. For Capture Hi-C, our pipelines are able to find feasible genomic interactions.

3SDA-8 Bridging the gap between the dynamics and organization of chromatin domains by mathematical modeling

Soya Shinkai[1,2], Tadasu Nozaki[3], Kazuhiro Maeshima[3], Yuichi Togashi[2] ([1]*RIKEN QBiC*, [2]*RcMcD, Hiroshima Univ.*, [3]*Natl. Inst. of Genet.*)

The genome is not only one-dimensional information of DNA sequences, but is three-dimensionally and hierarchically organized into chromatin in the cell. In the hierarchical chromosome organization, different types of submegabase-sized chromatin domains were uncovered by chromosome conformation capture methods. Genome functions are regulated within and across the domains according to their organization, whereas the chromatin itself is highly dynamic. However, the details of such dynamic organization of chromatin domains in living cells remain unclear. To unify chromatin dynamics and organization, we recently developed a mathematical model. Here, we will show the implication of our mathematical model and analysis to single-nucleosome movement in living human cells.

3SFA-1 Single-Molecule Detection of Biomolecules and Protein Conformational Dynamics

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Soluble and membrane proteins efficiently function accompanying dynamic conformational changes under their inherent environments. Detection of these changes are thus the heart of understanding of their true mechanisms, and optical microscopes can be the tool to dissect real-time conformational dynamics. We have developed techniques to quantify angle changes of single fluorophores attaching to mobile helices in single proteins immobilized on the glass. For domain dynamics, high-speed AFM is also useful to visualize membrane proteins, especially packed in highly-organized structures such as nanodisc compartment. Properties of motor proteins and membrane proteins, e.g., kinesin-microtubule system, ATP synthase and Ca^{2+}-ATPase, will be demonstrated in the talk.

3SFA-2 小胞型ヌクレオチドトランスポーターのアロステリック制御
Allosteric regulation of vesicular nucleotide transporter

Hiorshi Omote (*Okayama University Grad. School of Med., Dent. and Pharm. Sci.*)

Vesicular nucleotide transporter (VNUT) is a member of the SLC17 transporter family. This family contains vesicular glutamate transporters (VGLUTs), sialin and type I Na+/Pi co-transporters. All of these transporters exhibit membrane potential driven organic anion transport activity. Very interestingly, these transporters require Cl- as an allosteric activator. Hill coefficients of Cl- activation of VGLUT and VNUT are 3~4, indicating multiple Cl- binding site in a functional unit and cooperative interaction between binding sites. Various keto acids suppress activation by Cl-. We investigated molecular mechanism of Cl- activation through biochemical way using purified transporters.

3SFA-3 Single molecule analysis of membrane transport proteins using artificial cell-membrane microsystems

Rikiya Watanabe (*Department of Applied Chemistry, The University of Tokyo*)

The maintenance of an appropriate intracellular environment, a constant challenge for all living organisms, is maintained by membrane transport proteins. To understand their mechanisms, we developed a novel artificial cell-membrane microsystem (ALBiC) that forms femtoliter chambers, each sealed with an artificial cell-membrane. Due to the small volume of chambers, ALBiC can enhance the detection sensitivity by 106 fold, demonstrating the single-molecule analysis of transmembrane transport. Moreover, we reproduced the asymmetric phospholipid distribution on ALBiC, allowing the single-molecule analysis of phospholipid scrambling. Thus, our new platform, ALBiC, holds promise for understanding the mechanism of various membrane transport proteins.

3SFA-4 ギャップ結合チャネルのクライオ電子顕微鏡単粒子解析
Single particle cryo-EM of a gap junction channel

Atsunori Oshima[1,2] ([1]*CeSPI, Nagoya Univ.*, [2]*Dept. Pha., Nagoya Univ.*)

Gap junction channels directly connect the cytoplasm of two adjacent cells, and play critical roles in many biologically important processes, including cardiac and nervous system development, fertility, immunity, and electrical synapse formation.
We show the single particle cryo-electron microscopy structures of wild type INX-6 gap junction channels at atomic resolution. We found that the arrangements of the INX-6 monomeric structure are highly similar to those of Cx26, despite the lack of significant sequence similarity. Our observations suggest that the INX-6 cytoplasmic domains are cooperatively associated with the N-terminal funnel conformation, and an essential linkage of the N-terminal with channel activity is presumably preserved across gap junction families.

3SFA-5 Ca^{2+}-ATPase の E1/E2 転移における大規模構造変化の分子動力学法シミュレーション
Molecular dynamics simulations for conformational changes on E1/E2 transition of Ca^{2+}-ATPase

Chigusa Kobayashi[1], Yasuhiro Matsunaga[1,2], Jaewoon Jung[1,3], Yuji Sugita[1,3,4] ([1]*RIKEN, AICS*, [2]*JST, PRESTO*, [3]*RIKEN, TMS*, [4]*RIKEN, QBiC*)

Ca^{2+}-ATPase is a representative protein of P-type ATPases, which transports Ca^{2+} across membrane against a large concentration gradient. Biochemical and structural studies suggest that the large conformational changes of the protein has important roles in the Ca^{2+} transport. It is, however, difficult to simulate this transition due to its slow time-scale. To overcome this difficulty, we have developed a high-performance MD simulation package, GENESIS. In this study, we applied a rare event sampling method (string method) implemented in GENESIS to the structural transition of Ca^{2+}-ATPase. We discuss rearrangements of the transmembrane helices coupled with large-scale cytoplasmic domain movements.

3SFA-6 Mechanics of Single Protein Molecules

Matthias Rief (*Technischen Universität München, Physik-Department*)

Proteins are amazing molecular machines that can fold into a complex three dimensional structure in a self-organization process called protein folding. Even though powerful structural methods have allowed us taking still photographs of protein structures in atomic detail, the knowledge about the folding pathways and dynamics as well as material properties of those structures is rather limited. Over the past 15 years, our group has developed single mechanical methods to study the dynamics and mechanics of protein structures. In my talk I will discuss how these methods can be used to investigate and control the conformational mechanics of individual proteins. Examples include protein folding as well as protein-protein interactions and enzyme mechanics.

3SGA-1 分子シミュレーションによるヌクレオソームと転写因子の動態研究
Dynamics of nucleosomes and transcription factors studied by molecular simulations

Shoji Takada (*Biophys. Sci. Kyoto Univ*)

In eukaryotic genome, nucleosomes can be major bottlenecks for transcription factors (TF) to find their cognate sites. While nucleosomes are intrinsically stable, they are known to be dynamic and can move either spontaneously or driven by remodeler, which can affect the TF binding. Using high-throughput experimental data, we developed a new protein-DNA interaction model that account for specific interactions accurately, and applied it to simulate nucleosome sliding dynamics, TF binding dynamics, and their mixtures. We found that nucleosome sliding is highly sequence dependent and can be versatile. TF search dynamics can be hampered by many local traps and the distinction between sequence-independent electrostatic interactions and sequence specific interactions.

3SGA-2 methyl CpG 結合ドメインタンパク質の分子基盤研究
Structural biochemistry of methyl CpG binding domain containing proteins

Mariko Ariyoshi (*Grad. Sch. Frotier Bio.*)

Eukaryotic genome is wrapped around histone octamers and folded into a higher-order chromatin structure. Together with histone modification and histone variants, DNA methylation provides epigenetic mechanisms to alter chromatin structural and functional states linking to various gene regulation mechanisms. The Methyl CpG binding domain (MBD) family proteins play key roles in coordinating crosstalk between DNA methylation, histone modifications and chromatin organization required for accurate gene regulation. Of theses MBD proteins, SETDB1/2 histone methyltransferases possess unique MBD properties. The molecular basis of this unique MBD will be presented here based on our recent structural biochemical study.

3SGA-3 高速 AFM による天然変性タンパク質の構造動態解析
Structural dynamics analysis of intrinsically disordered proteins by high-speed AFM

Noriyuki Kodera[1], Daisuke Noshiro[1,2], Sujit Dora[1], Toshio Ando[1,2] ([1]*Bio-AFM FRC, Kanazawa Univ.*, [2]*CREST, JST*)

IDPs (intrinsically disordered proteins) are disordered entirely or partly but function as hubs of cellular signaling and regulation in transcription, translation and cell cycle. Their structure is highly flexible and dynamically samples a multitude of conformational states. Therefore, structural analysis of IDPs is considerably difficult. Here, through the HS-AFM observations of several IDPs, we demonstrate that HS-AFM allows us not only to determine the number of amino acids contained in disordered regions of IDPs but also to identify other regions undergoing order-to-disorder transitions at the accuracy of a few residues level.

3SGA-4 Chromosome association of noncoding RNA during homologous chromosome pairing in fission yeast meiosis

Da-Qiao Ding[2], Tokuko Haraguchi[1,2], **Yasushi Hiraoka**[1,2] ([1]*Graduate School of Frontier Biosciences, Osaka University*, [2]*National Institute of Information and Communications Technology*)

In meiosis, pairing and recombination of homologous chromosomes are necessary for accurate segregation of chromosomes. We examined involvement of noncoding RNA in homologous chromosome pairing in the fission yeast Schizosaccharomyces pombe. In S. pombe, the sme2 locus shows extraordinarily robust pairing; the sme2 gene encodes a meiosis-specific noncoding RNA, and accumulation of the sme2 RNA transcript at the sme2 locus is essential for the robust pairing. We identified a group of sme2 RNA-associating proteins that are involved in chromosome association of RNA. Genome-wide search identified chromosomal loci for RNA association besides the sme2 locus. We propose that chromosome associated RNA plays a role in recognition of homologous chromosome for pairing.

3SGA-5 シーケンシングと分子動力学計算の組み合わせによるクロマチン 3D 構造解析
3D chromatin structure revealed by the combination of sequencing analysis and molecular dynamics simulation

Masae Ohno[1], Tadashi Ando[2], Yuichi Taniguchi[1] ([1]*QBiC, RIKEN*, [2]*Dept. of Appl. Elec., Tokyo Univ. of Science*)

In eukaryotes, all DNA-templated events, including gene regulation, are mediated by chromatin, which is composed of repeating units of nucleosomes. Although higher-order chromatin structure have been well studied, but little is known about local nucleosome folding. Here, we developed a new chromatin structure analysis, called Hi-CO, by coupling sequencing technology and molecular dynamics simulation. Using this method, we determined 3D yeast chromatin structure with nucleosome level resolution. This genome-wide nucleosome folding structure demonstrates basic structural motifs in chromatin. We also found that these structural motif are associated with epigenomic profile. Our method and results can provide novel aspects of nucleosome folding in chromatin fiber.

3SGA-6 高解像度 Hi-C データを活用した遺伝子発現制御の理解
Understanding gene regulation by using high-resolution Hi-C data

Mikita Suyama (*Medical Institute of Bioregulation, Kyushu University*)

Hi-C data is a rich source of information about the conformation of chromosomes. To provide an easy access to the high-resolution Hi-C data, we developed a web tool, ChromContact (http://bioinfo.sls.kyushu-u.ac.jp/chromcontact/). One of the possible applications of ChromContact is investigating novel long-range promoter-enhancer interactions. We successfully applied the web tool to interpret a novel phenotype, which might be caused by a mutation in the enhancer region. We are also analyzing the Hi-C data obtained from F1 hybrid mice to understand spatial organization of chromosomes by discriminating homologous chromosomes. From this analysis, we found an interesting phenomenon that homologous chromosomes can interact with each other in the nucleus in interphase.

3SGA-7 The phase-separation principle of human genome architecture

Shin Fujishiro, Masaki Sasai (*Dept. Comp. Sci. & Eng., Nagoya Univ.*)

The 3D organization of mammalian genome should be closely related to the epigenetic state of chromatins. Although this relation has been analyzed by several simulation studies, the principle that governs the 3D organization is still unclear. We developed a computational model of human genome by modeling chromosomes as chains of soft-core beads, whose softness is defined by the epigenetic state of the corresponding part, while no specific interaction is assumed among beads. With this bottom-up approach, the experimentally observed contact maps and nuclear lamina interactions were well reproduced, which suggested that a major determinant of the 3D genome organization is the spontaneous phase separation of heterochromatin-like and euchromatin-like regions in the nucleus.

3SIA-1 Biobit の可能世界
Possible world of Biobit

Yuzuru Husimi (*Japan Science and Technology Agency*)

Evolutionary molecular engineering has provided various tools to explore the functionality of the possible world in some polymer sequence spaces. It also has provided the evolvability view point of life, regarding the origin of life as the emergence of “encoded digital information” in our Universe. Because this encoded digital nature was based on the specific interaction between molecules, it did not reach the level of the ideal symbol (bit) manipulation. We would like to call this information processing “Biobit” manipulation. The real world of Biobit on the Earth is a tiny portion in the possible world of Biobit. It invented, however, the bit manipulation and the concept of Qubit through the biological and cultural evolution.

3SIA-2 VHH ファージライブラリーからの有用な抗体の迅速単離と試験管内抗体進化
Rapid isolation of valuable antibodies from VHH phage display libraries and in vitro antibody evolution

Akikazu Murakami[1], Maiko Yoshida[1,2], Narutoshi Tsukahara[3], Takachika Azuma[2], Hidehiro Kishimoto[1] ([1]*Grad. Sch of Med., U-Ryukyus*, [2]*Antibody Engineering Research Center Inc.*, [3]*Innovex Science Co., Ltd.*)

The antigen-binding fragment of heavy-chain antibodies consists of a single domain known as VHHs. Because of the many favourable properties, they have become widely used in research and are beginning to show commercial potential. We constructed semi-synthetic VHH phage display libraries having more than 40 billion clones and isolated hundreds of clones against more than 30 different antigens. Most of the clones have the favourable properties but some of them are not. Therefore, we established two kind of methods to obtain useful VHH clones. One of the optimized method is panning and the other is in vitro evolution of the unfavourable VHH clones. With those optimized methods, valuable VHH clones can be isolated within 15 days constantly.

3SIA-3 網羅的配列解析による抗体ファージライブラリーからの抗原特異的抗体の効率的な選別

Efficient selection of antigen-specific antibodies from phage library using high throughput sequencing

Yuji Ito (*Grad. Sch. Sci. and Eng., Kagoshima Univ.*)

Phage library system is a powerful tool in finding specific functional molecules from molecular library. Biopanning used in this system is a process to select efficiently the phages which display functional molecules. However, this process harbors the time-consuming and laborious steps of cloning several hundreds of phages and binding screening for them. The recent use of high-throughput sequencing (HTS) on NGS have enabled to save such labors and to find a variety of binders. In this presentation, we will report the application of HTS for identification of antigen-specific binders from human scFv and alpaca VHH antibody phage libraries. We hope to discuss about the possibility of this technique in design of new artificial functional biomolecules “neo-biomolecules”.

3SIA-4 アミノ酸の種類が制限された cDNA ディスプレイライブラリからのポリメラーゼリボザイムに対するコファクターペプチドの試験管内淘汰

In Vitro selection of cofactor peptides of polymerase ribozyme form a cDNA display library composing of limited set of amino acids

Shigefumi Kumachi (*Epsilon Molecular Engineering Inc.*)

RNA world has been accepted as a promising hypothesis in the origin of life on the earth. On the other hand, how, and why RNA world move into RNP world has been remained as an open question. The hypercycle theory is a hypothesis proposed as giving a clue toward the origin of translation system. Furthermore, a virus-like member that consists of proto-mRNA and its coding peptide could introduce Darwinian evolution (1). This theory suggests that the first encoding peptide could emerge as a cofactor of replication ribozymes. Therefore, we demonstrated the selection of cofactor peptides activating a polymerase ribozyme. In this presentation, the selected peptide which activating a polymerase ribozyme will be discussed.

(1) Nemoto N and Husimi Y. J Theor Biol 176, 67-77 (1995)

3SIA-5 Evolutionary Engineering and Characterization of Membrane Proteins Using Liposome Display

Tomoaki Matsuura (*Dep. Biotechnol, Grad. Sch. Eng., Osaka Univ.*)

An in vitro translation (IVT) system has been used for various applications including in vitro protein evolution. As protein synthesis with IVT is disconnected from cell growth, a wide range of proteins can be targeted. We previously report the development of a method, named liposome display, for evolving the properties of membrane proteins entirely in vitro. This method, which involves in vitro protein synthesis inside cell-sized liposomes, was applied to evolve the pore-forming activity of α-hemolysin, a membrane protein derived from Staphylococcus aureus, EmrE multidrug transporter from Escherichia coli and others. The results of the in vitro membrane protein evolution will be presented.

3SIA-6 Rapid adaptation of RNA bacteriophage to environmental changes

Akiko Kashiwagi (*Fac. Agr and LifSci, Hirosaki Univ.*)

Determining the mechanisms underlying adaptation of living organisms to a new environment contributes to obtaining crucial insights into evolutionary biology. To elucidate this mechanism, we have used experimental evolution systems with Escherichia coli and RNA bacteriophages Qβ. Because of the short generation time and small genome size, we can trace and analyze the adaptation processes over many generations in short periods and can understand the relationships between genetic and phenotypic changes easily.

I will show and discuss the adaptation process of Qβ in the following two system, i) Coevolution with E. coli and Qβ, and ii) Thermal adaptation of Qβ.

PLoS Genetics, e1002188, (2011), Journal of Virology,11459, (2014), Frontiers in Microbiology, 124, (2015).

3SIA-7 バクテリア 16S rRNA の進化中立性の実験的検証

Comparative RNA function analysis reveals primarily neutral evolvability of bacterial 16S rRNA genes

Kentaro Miyazaki[1,2] ([1]*AIST*, [2]*Univ Tokyo*)

The bacterial ribosome consists of 3 rRNAs and 57 proteins, which plays a crucial role in protein biosynthesis. Because of the structural and mechanistic complexity, it is believed that each ribosomal component coevolves to maintain its function (Jain et al., 1999). However, we have shown that an active ribosome whose 16S rRNA has been substituted with that from foreign bacteria can be genetically reconstituted in E. coli (Kitahara et al., 2012) even with those from a different phylum, Acidobacteria. We experimentally showed that 334 different nucleotides between the genes were predominantly neutral mutations.

3SIA-8 Evolution and function of OEC-family proteins in chloroplasts

Kentaro Ifuku (*Grad. Sch. Biostudies, Kyoto Univ.*)

The photosynthetic oxygen-evolving reaction is the basis for the light-to-chemical energy conversion and catalyzed by photosystem II (PSII). The oxygen-evolving complex (OEC) proteins are membrane-extrinsic subunits of PSII and optimizes oxygen evolution. It is known that the composition of OEC proteins are largely differed among photosynthetic organisms. In addition, multiple isoforms and homologs for OEC proteins have been found in the chloroplasts. We have reported that OEC-family proteins have various roles in photosynthetic electron transfer. Our results suggest that functional diversification of OEC family proteins during evolution would be important to regulate efficient photosynthesis in changing environments.

3SIA-9 進化分子工学と極限環境生物
Evolutionary Engineering and Extremophiles

Tairo Oshima (*Inst. Environ. Microbiol., Kyowa-Kako*)

In general, an environmental factor had been changed gradually in laboratory experiments in Evolutionary Engineering to create a biopolymer with a desired biochemical property. However, such “evolution” is called “microevolution”. My proposal is to investigate molecular mechanisms of “macroevolution” in laboratory using knowledge about extremophiles. If molecular mechanisms of microevolution and of macroevolution are essentially different, and if we succeed to clarify the differences, we can open a new frontier in Evolutionary Engineering. For instance, I wish to encourage young researchers to carry out experiments to create a thermophile from a mesophile in a laboratory.

3SKA-1 ハプト藻に存在するハプトネマの急速コイリング運動における微小管ダイナミクス
Microtubule dynamics for rapid coiling movement of haptonema in the haptophyte algae

Mami Nomura[1], Kohei Atsuji[1], Keiko Hirose[2], Kogiku Shiba[1], Kazuo Inaba[1] ([1]*Shimoda Marine Research Center, University of Tshukuba*, [2]*Biomedical Research Institute, National Institute of Advanced Industrial Science and Technology*)

The haptonema is a motile machinery of haptophytes, composed of six or seven singlet microtubules as long as ~150 micrometer. It plays multiple roles including prey capture and gliding migration. The most notable movement of haptonema is rapid “coiling”, which occurs in several milliseconds by mechanical stimuli. The coiling is inhibited by paclitaxel (taxol), suggesting that microtubule dynamics is involved in the mechanism. To understand the mechanism of coiling, we have studied the structure and protein composition of the haptonema. TEM observation of demembranated haptonema showed that one or two microtubules wind around the others in a helical path. A proteomic analysis identifies 25 proteins that are potentially involved in this microtubule dynamics.

3SKA-2 螺旋形細菌レプトスピラの遊泳と滑走のメカニズム
Swimming and gliding mechanisms of the spirochete *Leptospira*

Shuichi Nakamura (*Grad. Sch. Eng., Tohoku Univ.*)

Leptospira is a coiled shaped bacterium that has two flagella between the outer membrane and peptidoglycan; one flagellum is attached to each end of the protoplasmic cylinder (PC). Both ends of the cell body are rotated by rotations of flagella, and the PC is believed to be rotated by countertorque of the flagella. *Leptospira* not only swims in liquid but also glides on surfaces, but the mechanism by which cell-body rotations are converted to two distinct translational motilities. To date, we have been investigating correlative cell-body rotations in swimming cells, the relationship between translation and cell rotation, and so on. In the symposium, based on our experimental results, I will propose hypothetical mechanisms of swimming and gliding of *Leptospira*.

3SKA-3 Structure, mechanics, and shape dynamics of Spiroplasma

Hirofumi Wada (*Department of Physical Sciences, Ritsumeikan University*)

We will discuss on the unique motility of Spiroplasma, in terms of their structure, mechanics, kinematics and dynamics. We will first discuss their helical cell shape from the viewpoint of elastic composites, then estimate the cell's elastic modulus combining theory and micromanipulation experiments (work with Miyata Lab in Osaka city univ.). To study the dynamics, we will get back to the paradigmatic "bistable helix" model (R. E. Goldstein et al, 2000) and confirm via numerical simulations a scaling prediction on the kink speed, which however seems to contradict recent experiments. We will define major issues regarding the enigmatic motility of Spiroplasma, envision how future experiment and theory may advance our understanding on this problem.

3SKA-4 Mechano-electrical communications in actin filament

Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

Mechanical stimulus applied to an actin filament alters the affinity with actin-binding proteins (ABPs), and clarifying this mechanosensing mechanism is the key challenge in mechanobiology. We here conducted the molecular dynamics simulation of an actin filament to study the response to applied tension, and found that the tension changes the electrostatic potential on the filament surface, indicating that the piezoelectric allostery [Ohnuki et al., Phys. Rev. E (2016)] is inherent in actin. The piezoelectricity is induced by the intra-filament electrostatic communication through the electrostatic bond (ionic and hydrogen bond) network. We further discuss how the piezoelectricity alters the inter-molecular electrostatic communication with ABPs.

3SKA-5 Hypervariation in primary and quaternary structures of ParMs, prokaryotic actin-like polymerizing motors

Robert C. Robinson[1,2] ([1]*Institute of Molecular and Cell Biology*, [2]*RIIS, Okayama Univ.*)

Elongating filaments systems, such as actin, are polymerizing motors that drive movement in many biological processes. The actin filament is astonishingly well conserved across a diverse set of eukaryotic species. In contrast, bacterial actin-like proteins have diverged to the extreme. My laboratory is interested in understanding how the force and structure generated from these varied polymerization systems are integrated into different biological processes. In particular in prokayotes, we focus on the ParCMR plasmid segregation machineries. The motor proteins (ParMs) have hypervariable sequences that translate into the conserved actin fold, which in turn assembles to form highly variable filament architectures.

3SKA-6 クライオ電子顕微鏡で解き明かす細菌べん毛モーター回転子の立体構造と回転対称性

Structure and rotational symmetry of the rotor of the bacterial flagellar motor revealed by electron cryomicroscopy

Akihiro Kawamoto[1], Tomoko Miyata[1], Miki Kinoshita[1], Tohru Minamino[1], Takayuki Kato[1], Keiichi Namba[1,2] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ*, [2]*QBiC., RIKEN*)

The bacterial flagellum is a motility nanomachine with a rotary motor and a helical propeller. The MS ring of the flagellar basal body is the rotor composed of a single membrane protein, FliF, and acts as the base for flagellar assembly and motor rotation. The MS ring structure previously analyzed by electron cryomicroscopy (cryoEM) and image analysis showed the 26-fold rotational symmetry. However, the resolution was limited to show the structural detail to confirm it. We report a high-resolution cryoEM structure of the *Salmonella* MS ring at 3.9 Å resolution, which clearly shows the 34-fold rotational symmetry in the S ring region, disproving a widely believed hypothesis on the symmetry. We will discuss the mechanism of torque transmission in the flagellar motor.

3SKA-7 べん毛軸構造蛋白質の構造と集合体形成

Structure and assembly of bacterial flagellar axial proteins

Katsumi Imada (*Grad. Sch. Sci., Osaka Univ.*)

The bacterial flagellum is a motile organelle made of thousands of protein subunits. The filamentous part extended from the cell surface is called the axial structure, which consists of the rod, the hook, the junction, the filament, and the cap complex, from the proximal to the distal end. While they share a common basic architecture, each part shows quite distinct mechanical property to achieve its function. Recently, we have determined high-resolution crystal structures of the distal rod protein, the junction proteins and the cap protein. In combination with previously determined structures, we have constructed a model of the axial structure. We will discuss the molecular mechanism and architecture of the flagellar axial structure on the basis of the model.

3SLA-1 AL アミロイドーシスにおけるアミロイド形成の引金 - 診断と阻害戦略への展望

Triggers of amyloid formation in AL amyloidosis - perspective for development of diagnosis and inhibition strategy

Daizo Hamada[1,2,3] ([1]*Grad Sch Eng, Kobe Univ*, [2]*CASS, Kobe Univ*, [3]*RIKEN SPring-8*)

Amyloid light chain (AL) amyloidosis is a protein-misfolding disease characterised by accumulation of immunoglobulin light chains into amyloid fibrils that induce tissue damage and multiple organ failure. Biophysical techniques have been employed to investigate the mechanism of protein unfolding prior to amyloid formation. The studies identified specific sequence patterns in the molecular surface on the variable domain that promotes the protein unfolding either by decreasing the stability of the native monomer or by shifting the homodimer-monomer equilibrium toward monomerisation. Fluctuation analysis revealed structural feature of partially unfolded state that serves for designing methodologies of amyloid inhibition and diagnosis of AL amyloidosis.

3SLA-2 Ras がん遺伝子産物を分子標的としたがん治療薬のインシリコ創薬

In silico discovery of anti-cancer drugs targeting the Ras oncoproteins

Tohru Kataoka (*Grad Sch Med, Kobe Univ.*)

Ras, the products of the ras oncogenes, are the most promising targets for anti-cancer drug development. Nevertheless, there is no effective molecular targeted therapy for it. Although recent success in drug discovery using SBDD has boosted hopes for its application to anti-cancer drug development, Ras are refractory to this approach because they lack “druggable” surface pockets. Recently, by X-ray crystallography and NMR, we solved a novel tertiary structure of the GTP-bound form of Ras, which corresponded to a novel conformation possessing surface pockets suitable for drug binding. This led us to apply SBDD to target Ras by utilizing the structural information on these surface pockets. I will talk about the successful discovery of novel Ras inhibitors.

3SLA-3 Computational approach for understanding protein-aggregation diseases

Sihyun Ham (*Dept of Chem, Sookmyung Women’s Univ.*)

We here unveil a crucial role of hydration water in ruling the aggregation propensity of proteins both in vitro and in vivo. The protein overall hydrophobicity, defined solely by the hydration free energy of a protein in its monomeric state sampling its equilibrium structures, was shown to predominantly dictate the protein aggregation propensity in aqueous solutions. We also find striking discrimination by the hydration water of positively and negatively charged residues depending on the protein net charge in regulating the solubility of a protein, which establishes novel design strategies for the biotechnological generation of aggregation-resistant proteins as biotherapeutics.

3SLA-4 動的構造解析による多剤耐性転写制御因子の非特異的かつ高親和性な結合メカニズムの解明

Promiscuous high-affinity recognition of a multidrug resistance transcriptional regulator revealed by structural dynamics analyses

Koh Takeuchi[1], Misaki Imai[1,2], Yuji Tokunaga[1], Ichio Shimada[3] ([1]*AIST, Molprof*, [2]*JBIC*, [3]*The Univ of Tokyo, Grad Sch Pharma Sci*)

Multidrug resistance (MDR) transcriptional regulators (TR) serve as sensors in MDR systems. The MDR TRs are known to bind structurally unrelated toxic compounds with high affinity, however, the molecular mechanism for the multidrug recognition remains unclear. Here, we structurally and dynamically characterized a MDR TR, LmrR, in the apo and compound-bound states, by solution NMR. The analyses revealed that LmrR binds to multiple compounds by conformational selection mechanism and the compound binding induces the enhancement of ps-ns dynamics to allosteric sites, which entropically contribute for its high-affinity interaction. The data show how LmrR can dynamically exert its functions through promiscuous multi-target interactions.

3SLA-5 熱測定によるアミロイド疾患の診断を目指した研究
Calorimetric approach for investigating disease-related amyloidogenesis

Young-Ho Lee (*Inst of Protein Res, Osaka Univ.*)

Protein misfolding and aggregation have been recognized as a main cause for more than 40 protein misfolding diseases including neurodegenerative diseases and amyloidoses. Although much has been revealed on the mechanism of the formation of amyloid fibrils and their structures using several biophysical methods, more convincing and informative approaches for the examination of the principle and inhibition of amyloid formation is still required. I herein show how isothermal titration calorimetry (ITC) can be effectively used for the thermodynamic characterization of amyloidogenesis of several aggregation-prone proteins. The application of ITC to a practical assay for amyloid formation and inhibition will be also discussed based on our recent studies.

3SMA-1 原子分解能をめざしたクライオ電子顕微鏡の技術開発
Towards atomic resolution structural analysis by electron cryomicroscopy

Keiichi Namba (*Grad Schl Frontier Biosci, Osaka Univ*)

Electron cryomicroscopy and single particle image analysis has become a powerful tool in structural biology. Crystallization is not required, and there is no upper limit in the molecular size. Only a few tens of micrograms of specimen in solution is sufficient for structural analysis. The recent tremendous technical progress has been made possible mainly by a high-resolution CMOS image detector. Its high-speed image acquisition allows image blurring by specimen drift, charging and ice deformation to be eliminated by motion correction to achieve near atomic resolution. However, there is still a possibility of further technical developments in electron optics of the microscope towards atomic resolution structural analysis. Such possibilities will be discussed in detail.

3SMA-2 近原子分解能クライオ電子顕微鏡単粒子解析に向けたデータ測定及び画像処理条件の最適化
Studies on Data Acquisition Conditions and Image Processing for Near-atomic Resolution Cryo-EM Single Particle Analysis

Takeshi Yokoyama (*CLST., RIKEN*)

Single particle electron cryo-microscopy (cryo-EM) is a powerful tool to determine the structures of macro-molecular complexes in frozen-hydrated state. Recent technological advancements in both electron microscopy and image processing programs allowed us to investigate the structure of smaller molecules and boosts the attainable resolution toward near-atomic resolution. In Riken Yokohama campus, three transmission microscopes are operating for the attempt to determine the large variety of macro-molecular complex structures. In this presentation, we show recent our investigation for the optimization of image acquisition condition and image processing. In addition, some test case of reconstruction will be shown.

3SMA-3 SACLA を用いたタンパク質の時間分割構造解析
Time-resolved x-ray crystallography at SACLA

So Iwata[1,2] ([1]*Grad. Sch. Med., Univ. Kyoto*, [2]*SPring-8 Center, RIKEN*)

At the Japanese XFEL facility, SACLA, we are currently developing a data collection system focusing on dynamic crystallography putting a particular effort on membrane proteins. An experimental system for pump-probe experiments based on serial femtosecond crystallography using a viscous material injector has been developed. For the first target, we chose a light-driven proton pump, Bacteriorhodopsin (bR). Time-resolved serial femtosecond crystallography was applied to visualize conformational changes in bR from nanoseconds to milliseconds following photoactivation. The resulting cascade of structural changes throughout the protein shows how motions are choreographed as bR transports protons uphill against a transmembrane concentration gradient.

3SMA-4 XFEL によって明らかになった光化学系 II 水分解触媒の中間体構造と反応機構
Structure of an intermediate S-state of photosystem II and the mechanism of water-splitting revealed by XFEL

Jian-Ren Shen (*Res. Inst. for Interdiscip. Sci., Okayama Univ.*)

Light-induced water oxidation in photosystem II is catalyzed by a Mn4CaO5-cluster, which proceeds with the Si-state cycle (i = 0-4). The structure of the Mn4CaO5-cluster at its dark-stable S1-state has been solved at atomic resolutions using synchrotron radiation X-rays as well as XFEL. In order to reveal the mechanism of water-splitting and oxygen evolution, it is essential to analyze the structures of the intermediate S-states. We analyzed its structure in the S3-state induced by 2-flashes illumination using time-resolved serial femtosecond crystallography with the XFEL pulses at SACLA. Our structure showed that a new oxygen atom was inserted to a position close to an oxo-bridged oxygen O5, which leads to the generation of molecular oxygen between O5 and O6.

3SMA-5 Computational tools to characterize structure and dynamics of biomolecular systems from single molecule experiments

Florence Tama[1,2,3] ([1]*RIKEN AICS*, [2]*Nagoya University, Physics*, [3]*ITbM-WPI*)

Cryo-EM single particle analysis provides valuable structural information on biomolecular complexes and can now achieve very high resolution. XFEL is also emerging as a new experimental approach to image biomolecules but technical challenges remain. Both experimental methods generate significant number of data, i.e. 2 dimensional images of molecules in real space or Fourier space. In order to extract information from these data, computational tools need to be developed. We will present some of our recent developments aimed at understanding structure and dynamics from cryo-EM and XFEL experiments.

3SMA-6 電子顕微鏡法のための画像解析と構造決定法の紹介
Image analysis and structural reconstruction for electron microscopy

Takuo Yasunaga (*Dept. of Biosci. Bioinfo., Sch. of Comp. Sci. Sys. Eng., Kyutech*)

Three-dimensional (3D) electron microscopy is one of the most powerful techniques to elucidate the relationship between structure and functions of biomacromolecules and architecture in cells or in vitro. Many software tools have been developed for 3D reconstruction, image processing/analysis for 2D images and 3D volumes: Relion2 and Frealign, etc. are de facto standards for single particle analysis, whereas eTomo etc. are ones for electron tomography. We have also been developing an environment for image processing and analysis of electron micrographs called as Eos/PIONE. Recent topics are implementation techniques like segmentations from 3D maps and modelling using molecular dynamics etc. I will here introduce topics in these field including our approach.

3SNA-1 Keto-enol tautomerism of Gln on BLUF domain

Shota Ito (*Nagoya Inst. Tech.*)

BLUF (sensor of blue-light using FAD) domain is a photoreceptor domain that binds flavin (FAD) as a chromophore. Conserved Gln and Tyr residue near FAD is prerequisite for the photoreaction and light-induced hydrogen bonding network changes must be important for signal transduction by light.
To clarify hydrogen bonding network around Gln, Tyr and FAD, light-induced chemical structural changes of these residues were analyzed by FTIR spectroscopy using specific amino acid isotope labeled proteins, which labeling efficiency was estimated by MALDI-MS analysis. Based on the results from our FTIR spectroscopy and QM/MM calculation and those from other groups, keto-enol tautomerism of Gln and its hydrogen bonding network changes and its role will be discussed.

3SNA-2 核酸分子におけるケト-エノール互変異性
Keto-enol tautomerism in nucleic acids

Hiroyuki Kamiya (*Grad. Sch. Biomed. Hlth. Sci., Hiroshima Univ.*)

Among the canonical nucleobases, G, C, and T/U contain keto group(s). The Watson-Crick type base pairs are formed by hydrogen bonds between the major base tautomers. When the minor enol tautomer in template DNA or incoming deoxyribonucleotides are present in the active site of DNA polymerase, incorrect pairs would be formed. In addition, damaged nucleobases are generated by mutagens and some of the modified bases display altered keto-enol tautomerisms and cause mutagenesis.
I would show (i) the presence of an incorrect Watson-Crick type G:T base pair in the active site of DNA polymerase, (ii) misincorporation of the 2-hydroxyadenine nucleotide with the keto-enol tautomerism, and (iii) mutations induced by 8-hydroxyguanine (7,8-dihydro-8-oxoguanine) in the lecture.

3SNA-3 タンパク質環境における互変異性に関する計算科学的研究
Computational Studies on tautomerism in protein environment

Yasuteru Shigeta[1], Katsumasa Kamiya[2], Mitsuo Shoji[1] ([1]*Center for Computational Sciences, University of Tsukuba*, [2]*Center for Basic Education and Integrated Learning*)

Aldehydes and ketones exist as equilibrium mixtures of two different structures called keto- and enol-forms in solution. In general, simple aldehydes and ketones are preferentially present in the keto-form (existence ration: 99.99%>: 0.01%

3SNA-4 植物の葉の香りを決めるケトエノール互変
Keto-enol tautomerism determining plant leaf fragrance

Yasuo Yamauchi (*Grad. Sch. Agr. Sci., Kobe Univ.*)

Green leaf volatiles (GLVs) are C6 compounds characterizing plant fragrance. Among them, (*E*)-2-hexenal is the sole GLV having α,β-unsaturated bond and acts as an oxidative stress response signaling chemical, but an enzyme biosynthesizing (*E*)-2-Hexenal had not been identified. Our groups first purified the enzyme, (*Z*)-3:(*E*)-2-hexenal isomerase, and found that the isomerases are widely distributed among the plant kingdom. A suicidal substrate, (*Z*)-3-hexyn-1-al irreversibly inactivated the isomerase, indicating that catalytic mechanism is a keto-enol tautomerism mediated by His residue. Overexpression of the isomerase in tomato caused drastic increase of (*E*)-2-hexenal in total volatiles, suggesting that the isomerase is one of the determinant of plant smell.

3SNA-5 Keto-enol tautomerism of curcumin upon binding to amyloid fibrils

Daijiro Yanagisawa (*Mol. Neurosci. Res. Ctr, Shiga Univ. Med. Sci.*)

Curcumin binds to amyloid fibrils and inhibits the elongation of the fibrils. Curcumin and its derivatives with keto-enol tautomerism showed high binding activity to amyloid fibrils, while the binding activity of the keto form analogue was found to be much weaker. Some curcumin derivatives existed predominantly in the enol form during binding to amyloid fibrils, suggesting that the enolization of curcumin is crucial for binding to fibrils. Curcumin derivatives with keto-enol tautomerism displayed intense fluorescence upon binding, and inhibited the formation of amyloid aggregates. The tautomeric structure may be a novel target for the design of curcumin derivatives that can be used both for therapy and for amyloid detection in Alzheimer's disease.

1B1320　ウサギ骨格筋線維の X 線赤道反射に対するミオシン阻害剤の効果

Effects of myosin inhibitors on the X-ray equatorial reflections of rabbit skeletal muscle

Hiroyuki Iwamoto (*SPring-8 JASRI*)

The effects of small-molecule myosin inhibitors (blebbistatin, benzenetoluene sulfonamide, and butanedione 2-monoxime) on the X-ray equatorial reflections were studied by using skinned rabbit psoas muscle fibers. In the presence of these inhibitors, the 1,1/1,0 intensity ratio increased upon calcium activation (pCa = 4.0), indicating that the actomyosin association is not inhibited. In control, the myofilament lattice spacing was substantially reduced upon activation. On the contrary, in the presence of the inhibitors, the lattice remained constant or even expanded. The results suggest that the radial force to shrink the lattice is characteristic of the active cross-bridges. The results support the idea that the inhibitor keeps myosin in the attached weak-binding form.

1B1332　ミオシン分子の巧みな集団運動によって心筋細胞の高速振動周期は一定に調節される

Constant beating frequency of sarcomeres in cardiomyocytes regulated ingeniously by collective motion of myosin molecules

Seine Shintani[1,2], Takumi Washio[3], Hideo Higuchi[1] ([1]*Dept. of Phys., Univ. of Tokyo*, [2]*JSPS Research Fellow*, [3]*Dept. Human and Eng. Env., Univ. of Tokyo*)

Although the study of the muscle contraction mechanism under the maximum activation condition is well understood, unresolved issues remain about contraction under important intermediate activation conditions during heartbeat. In fact, we found that cardiomyocytes spontaneously beat the temperature of beating cardiomyocytes to 38 to 42 °C., while cardiomyocytes continue their spontaneous beat and simultaneously perform rapid oscillations of natural period. This feature that makes it possible to maintain the oscillatory state including the maintenance of the period and to respond to the change in the calcium concentration can be called beating-homeostasis. I found that hierarchy of myosin and sarcomere produced this property by co - creation of experiment and simulation.

1B1344*　心筋ミオシンの自発的振動の解明

spontaneous oscillation of cardiac myosins

Yongtae Hwang, Hideo Higuchi, Motoshi Kaya (*Univ. of Tokyo Dep. Science*)

Heart is the most important organ, which contracts periodically to circulate blood flow. It has been generally recognized that such periodical contraction is driven by the periodical changing of calcium concentration. However, recent studies suggested that cardiac myosin ensemble may oscillate spontaneously, independent of calcium concentration. Therefore, we investigated force generation of cardiac myosin ensembles using optical tweezers. Our current results frequently showed “go back and forth” stepwise actin displacements. Dwell times between two consecutive steps appeared to be independent of loads. These phenomena are different from skeletal myosin ensembles and thus, may be a key feature for spontaneous oscillation in cardiac myosins

1B1356*　アクチンの切断は動的ネットワークの収縮を誘起する

The fragmentation of actin filaments induces the contraction of the active network

Kyohei Matsuda, Takuya Kobayashi, Mitsuhiro Sugawa, Yoko Y. Toyoshima, Junichiro Yajima (*Graduate School of Arts and Sciences, The University of Tokyo*)

Actomyosin contraction with passive cross-linkers is driven by self-organization of active actin networks below low ATP concentration. At this ATP concentration, myosin filaments gained processivity and severed actin filaments. However, it is not clear how the processivity and severing phenomena relates contraction of active networks. Using in vitro reconstitution assay, we found that the severing activity of an actin related protein caused a trigger of contraction of actomyosin network. We thus propose a model of the active network contraction that the network with passive cross-linkers contracts below the physiological ATP concentration when the connectivity of the network decreases due to the fragmentation of actin filaments by myosin.

1B1408*　細胞質ダイニンのマルチスケールシミュレーション：全原子から連続体へ

Multiscale Simulations of Cytoplasmic Dynein: From All-atom to Continuum Mechanics

Shinji Iida[1,3], Benjamin Hanson[3], Narutoshi Kamiya[2], Genji Kurisu[1], Takahide Kon[3], Haruki Nakamura[1], Sarah Harris[4] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sch. SS., Univ. Hyogo*, [3]*Grad. Sch. Sci., Osaka Univ.*, [4]*Sch. Phys. Astro., Univ. Leeds*)

All-atom molecular dynamics (MD) can also be used to parametrize coarse-grained (CG) models. One such model is Fluctuating Finite Element Analysis (FFEA), a simulation technique which represents large, globular proteins as continuum mechanical objects moving under the influence of thermal noise. Our aim is to illustrate that this kind of multiscale modelling allows us to accurately track the dynamics of macromolecules. All-atom MD simulations of Dictyostelium discoideum dynein were performed, from which the effective Young’s modulus was calculated and used to initialize a low resolution continuum representation. FFEA simulations were then performed using this CG model and were shown to successfully reproduce the relevant dynamics.

1B1426*　キネシンネックリンカーによる発生力は小さい

Neck linker of kinesin is low force generator

Yuichi Kondo, Hideo Higuchi (*Grad. Sch. Sci., Univ. of Tokyo*)

To understand mechanism of force generation caused by conformational change of neck linker, displacement of single molecules of one- and double-headed kinesins were measured under assisting and hindering loads at AMPPNP state. Kinesins took ~5-nm displacement toward both directions. The rate of the plus end motion (neck linker docking) decreased with load and became equal to that of minus end at ~3 pN. The results indicate that the displacement and force generated by docking of neck linker is 5 nm(~60 % of kinesin step size, 8.2 nm) and 3 pN (~40% of stall force). Neck linker docking explains only a part of the force generation of kinesin.

1B1438* **N 末端側 β バレルヘッドバンドが V_1-ATPase の非対称性を産み及び協同性を付与する**

An N-terminal β-barrel head-band gives rise to the asymmetrical motor structure of V_1-ATPase and promotes cooperativity

Shintaro Maruyama[1], Kano Suzuki[1], Hikaru Sasaki[1], Kenji Mizutani[2], Yasuko Saito[3], Fabiana Lica Yakushiji[1], Yoshiko Ishiduka-Katsura[4], Mikako Shirouzu[4], Shigeyuki Yokoyama[5], Ichiro Yamato[1,3], Takeshi Murata[1,6] ([1]*Grad. Sch. Sci., Univ. Chiba*, [2]*Grad. Sch. Med. Life. Sci., Univ. Yokohama City*, [3]*Grad. Bio. Sci. & Tech., Tokyo Univ. of Science*, [4]*DSSB, RIKEN*, [5]*Struct. Biol. Lab., RIKEN*, [6]*JST, PRESTO*)

V-ATPase works as a cation pump coupled with ATP hydrolysis. The hydrophilic domain, A_3B_3 complex, is a rotary motor composed of three units of A_1B_1 heterodimer forming a ring. We mutated the β-barrel region and determined the three dimensional structures of the mutant A_3B_3 complex. In the absence of bound nucleotides, the mutant A_3B_3 had a more symmetrical open structure than the wild-type. In the presence of AMP-PNP, it had a closely packed spiral structure with a disrupted crown. We conclude that the crown is the major determinant of the motor asymmetrical ring shape of V_1-ATPase. We further discuss how the motor is constructed asymmetrically, and how it works cooperatively by transitioning between various meta-stable asymmetrical structures.

1B1450* **結晶構造との対応付けを目指したミトコンドリア F_1-ATPase の回転解析**

Single-molecule analysis of bovine mitochondrial F_1-ATPase for direct assignment of crystal structures and rotational pausing states

Ryohei Kobayashi, Hiroshi Ueno, Toshiharu Suzuki, Mayu Hara, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

F_1-ATPase (F_1), the best-characterized molecular motor, has been extensively studied by both single-molecule studies and structural analysis. However, the model F_1's for single-molecule studies and structural analysis have been different. So, the correlation between crystal structures and rotational pauses has been still unclear. Here, we conducted single-molecule rotation assay of bovine mitochondrial F_1 (bMF_1), which is abundant structural information. We found two pauses during 120 degrees rotation at saturating ATPγS condition. The observation indicates that two or more elementary reactions of ATP hydrolysis after substrate binding occur at different angular positions, one of which is probably the ATP cleavage waiting state. We are now identifying them carefully.

1B1502* **腸内連鎖球菌由来の回転分子モーター V_1-ATPase のサブステップと化学力学共役機構**

Substeps and chemo-mechanical coupling scheme of rotary molecular motor *Enterococcus hirae* V_1-ATPase

Tatsuya Iida[1,2,3], Yoshihiro Minagawa[4], Hiroshi Ueno[4], Fumihiro Kawai[3], Takeshi Murata[5], Ryota Iino[1,2,3] ([1]*SOKENDAI (The Grad. Univ. for Adv. Stud.)*, [2]*Inst. for Mol. Sci.*, [3]*Okazaki Inst. for Integr. Biosci.*, [4]*The Univ. Tokyo*, [5]*Chiba Univ.*)

A rotary molecular motor V-ATPase is an ion pump driven by ATP-hydrolysis. To understand the chemo-mechanical energy conversion mechanism, we conducted single-molecule analysis of V_1 moiety of *E. hirae* V-ATPase. We found that 120° steps per ATP-hydrolysis were further divided into 35° and 85° substeps. At low [ATP], pause duration before 35° step was dependent on [ATP], indicating ATP-binding (k_{on} ~ 1.0×10^7 $M^{-1}s^{-1}$). At high [ATP], two time constants (0.5, 0.7 ms) independent of [ATP] were obtained. At all [ATP], pause duration before 85° step (2.5 ms) was independent of [ATP]. These time constants correspond to ATP-hydrolysis, Pi- or ADP-release dwell. With the results of an arginine-finger mutant, we discuss a chemo-mechanical coupling scheme model including substeps.

1B1514* **DNA ナノチューブに沿って一方向に移動する生体分子モーターの設計**

Engineered biomolecular motor that directly moves along DNA nanotubes

Ryota Ibusuki[1], Kazuhiro Oiwa[1,2], Hiroaki Kojima[2], Ken'ya Furuta[2] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*Adv ICT Res Inst, NICT.*)

The mechanism of biomolecular motors generating directional motion along cytoskeletal filaments have been a long-standing question. To address this, one needs to investigate the relationship between unidirectional motion and asymmetric structures of the motor-filament interface. However, these filaments can easily be destabilized by mutation, making it difficult to study the above relationship. Here we overcome this limitation by creating novel motors that directly move along synthetic DNA nanotube. The novel motors constructed from dynein and DNA-binding proteins robustly translocated 10-helix DNA nanotubes. Our strategy opens the way to systematic studies on the mechanisms of motors, and to nanotechnological applications using the powerful DNA-based molecular toolbox.

1B1532* **電圧駆動型モータータンパク質プレスチンの細胞外ループが、作動電圧域を調節する**

Characteristic extracellular loops of prestin modulate its voltage operating point

Makoto Kuwabara[1], Koichiro Wasano[2], Satoe Takahashi[2], Tomotaka Komori[1], Sotaro Uemura[1], Tomohiro Shima[1], Kazuaki Homma[2] ([1]*Dep. of Biol. Sci., Grad Sch. of Sci., The Univ. of Tokyo*, [2]*Feinberg Sch. of Med., Northwestern Univ.*)

Prestin (SLC26A5) is quite unique among the SLC26 family members in that it displays voltage-dependent motor activity (electromotility). However, it is conceivable that a common molecular mechanism underlies the diverse physiological functions of SLC26 proteins given the high degree of amino-acid sequence similarity. Here we show the cells expressing pendrin (SLC26A4) also displaying a sign of electromotility. Futher, the extracellular loops of prestin play significant roles in determining the voltage operating point, and that pendrin electromotility becomes evident when one of the extracellular loops is replaced with that of prestin. Our result suggests that the fundamental structural component responsible for electromotility is shared among the SLC26 family members.

1B1544* **Motor evolved from F-ATPase for *Mycoplasma mobile* gliding**

Takuma Toyonaga[1], Takayuki Kato[2], Akihiro Kawamoto[2], Keiichi Namba[2,3], Makoto Miyata[1,4] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Grad. Sch. Front. Biosci., Osaka Univ.*, [3]*QBiC, RIKEN*, [4]*OCARINA, Osaka City Univ.*)

M. mobile, a fish pathogenic bacterium, glides on solid surfaces with a unique mechanism. The gliding machinery is constituted from surface legs and internal filaments including gliding motors evolved from F-ATPase. Previously, we visualized the 3D structure of the motor by single-particle electron cryomicroscopy. Two hexamers similar to F1-ATPase were paired by a frame and attached with eight arm-like extentions. In the present study, we analyzed the image of internal filaments obtained by negative-staining electron microscopy. The filaments were aligned at regular intervals with bridging structures, suggesting that the filaments form a sheet by the arms of the motor. The sheet formation may contribute to the directionality and cooperativity of leg movements.

1B1556*　拡散係数の増大を用いた F_1-ATPase の遷移率の解析
Analyzing the Transition Rate of F_1-ATPase from Enhanced Diffusion

Ryota Shinagawa, Kazuo Sasaki (*Grad. Sch. Eng., Univ. Tohoku*)

The effective rotational diffusion coefficient *D* of the rotor's angle of F_1-ATPase without ATP is enhanced by the external torque *N* applied to it and has peaks at the appropriate magnitude of *N*. This phenomenon called diffusion enhancement occurs in the system with an angle dependent periodic potential and *N*. The position of peaks teaches us about the information on the periodic potential (R. Hayashi *et al*., PRL (2015)).
In this study, we calculated *N* dependence of *D* by numerically solving Fokker-Planck equation in the model with the transition by ATP hydrolysis and synthesis to obtain the information on the potential and transition. It is revealed by the calculation that *D(N)* has peaks whose dependence on ATP concentration has the information on transition rate.

1B1608　シアノバクテリアは光の向きを認識して IV 型線毛を非対称に分布する
Asymmetric distribution of type IV pili triggered by directional light in unicellular cyanobacteria

Daisuke Nakane, Takayuki Nishizaka (*Dept. Phys., Gakushuin Univ.*)

The type IV pili (T4P) system is a super-molecular machine observed in prokaryotes. Cell repeats the cycle of extension, surface attachment and retraction of T4P fibers to move over surfaces, like a spider-man. Here we demonstrated the sequential process of T4P dynamics from stimulus to taxis at the single-cell level in a model cyanobacterium *Synechocystis* sp. PCC6803, which can recognize light direction. We directly visualized that T4P filaments dominantly appeared from the side of the cell opposite the illumination. This asymmetric activation is regulated on a timescale of minutes, and the process was transitioned between three sequential phases. These findings provide clues toward a general regulation mechanism of the T4P system.

1C1320　分子拡散に対するミクロ空間に閉じ込めと高分子混雑の相乗効果
A synergistic effect of macromolecular crowding and biomimetic confinement on molecular diffusion

Chiho Watanabe, Miho Yanagisawa (*Grad. Sch. Eng., Tokyo Univ. Agri. Tech.*)

Macromolecular crowding and micrometric confinement by lipid membrane are essential characteristics for cells that each has been considered as a factor to induce slow molecular diffusion. However, their synergistic effect has been elusive. Using biomimetic droplets containing maclomolecular solution, we have recently found a synergistic effect of them to accelerate molecular diffusion at the center of the droplet. In order to reveal the mechanisms of the accelerated molecular diffusion, we measured the molecular diffusion parameters near from the confinement interface by fluorescent correlation spectroscopy (FCS). The result will be discussed at the presentation.

1C1332*　DNA 人工細胞骨格によるリポソームの力学的補強
DNA cytoskeleton for stabilizing artificial cells and the mechanical reinforcement

Chikako Kurokawa[1], Kei Fujiwara[2], Masamune Morita[5], Ibuki Kawamata[4], Yui Kawagishi[4], Atsushi Sakai[1], Yoshihiro Murayama[1], Shin-ichiro Nomura. M[4], Satoshi Murata[4], Masahiro Takinoue[3], Miho Yanagisawa[1] ([1]*Department of Applied Physics, Tokyo University of Agriculture and Technology*, [2]*Department of Bioscience and Informatics, Keio University*, [3]*Department of Computer Science, Tokyo Institute of Technology*, [4]*Department of Robotics, Tohoku University*, [5]*Advanced Industrial Science and Technology, Biomedical Research Institute*)

Liposome has used as artificial cells. However, the liposome is fragile due to the absence of cytoskeleton. To solve this problem, we constructed an artificial cytoskeleton with DNA nanotechnology. The designed DNA oligomers form a Y-shaped nanostructure and connect to each other with their complementary sticky ends to form networks. By electrostatic interaction between the cationic lipid and the DNA, we successfully created DNA shell underneath the membrane. We confirmed that the DNA shell improved the mechanical stability by using micropipette aspiration and AFM and prevented membrane rapture against external osmotic shock. These results demonstrate that DNA shell is a novel stabilizer of the lipid membrane like cytoskeleton in cells.

1C1344*　選択的抗がん作用をもつトレハロース脂質含有リポソームの物性の計算化学的解析
Molecular dynamics analysis of physical properties of mixed liposomes containing trehalose surfactant with selective anticancer effect

Takashi Kagamiya (*Center for Biol. Res. & Inform., Tokyo Tech*)

It has been reported that a mixed liposome (DMTre) composed of DMPC and trehalose surfactant (TreC14) shows selective anticancer effect and the effect becomes enhanced with increasing TreC14 content. In addition, the physical property of DMTre such as the thickness of fixed aqueous layer was also shown to largely change with increasing TreC14 content, which may be relevant to the anticancer effect. In this study, to elucidate the origin of such TreC14-induced physical property changes of DMTre, we performed all-atom MD simulations for several DMTre liposomes with different contents of TreC14. As a result, it was revealed that TreC14 partly recombines its hydrogen bond partner from surrounding lipid molecules to water molecules, as the TreC14 increases.

1C1356*　電子線による高精細バーチャル電極ディスプレイを用いた膜ドメインと膜形態の動的制御
Dynamic Control of Membrane Domains and Morphology Using an Electron-beam Induced Fine Virtual Cathode Display

Hiroki Miyazako, Takayuki Hoshino (*IST, UTokyo*)

Physical and chemical properties of lipid membranes depend on external environmental factors such as pH and ionic strength. To understand relationships between such environmental factors and spatiotemporal dynamics of lipid membranes, we have developed a fine virtual cathode display using an electron beam. In this study, we have achieved detachment and lateral migration of supported lipid bilayers on the virtual cathode by changing pH and ionic concentration around the virtual cathode. Moreover, the growth of lipid rafts in DOPC/DPPC/cholesterol mixtures was observed during the lateral migration of the bilayers. We also confirmed reversible deformation of stacking lobe structures on supported lipid bilayers. The detailed mechanism of these phenomena will be discussed.

1C1408 細菌の膜小胞取り込みに寄与する表面電位と膜弛緩性
Contribution of surface potentials and membrane looseness on bacterial uptake of membrane vesicles

Yosuke Tashiro, Kotaro Takaki, Yusuke Hasegawa, Hiroyuki Futamata (*Grad. Sch. Intgr. Sci. Technol., Shizuoka Univ.*)

Membrane vesicles (MVs) are small liposome-like structures secreted from many microbes and have a role of delivering their content to other microbial cells. Although MVs play important roles in bacterial communication, little is understood about the mechanism on bacterial uptake of MVs. Here we show that two parameters are associated with the uptake of MVs using a Gram-negative bacterium *Buttiauxella agrestis*. A low electrostatic repulsion between cells and MVs increased at the initial stage of the MV-attachment on cells. Furthermore, the uptake of MVs was enhanced by the depletion of membrane-peptidoglycan linking protein, suggesting that looseness of outer membrane is important for the uptake of MVs.

1C1426 高速原子間力顕微鏡（高速 AFM）による細菌が生産する膜小胞の物性解析
Physical heterogeneity of bacterial membrane vesicles revealed by high-speed AFM

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Bacterial membrane vesicles (MVs) are released from bacterial cells to extracellular milieu. It is generally accepted that MVs transport chemical signals for cell-cell communication and/or DNA, RNA for lateral gene transfer to other cells. However, the molecular mechanism of the transport of cargo by MVs remains unclear. In this study, we observed MVs, which were produced by an Gram-negative pathogenic bacterium, *Pseudomonas aeruginosa*, using a high-speed AFM that is capable of imaging biological molecules at high resolution under physiological conditions. The observed MVs ranged from 10 to 100 nm in height. Phase shift imaging visualized the physical properties of the surface of the MVs, and indicated that they were physically heterogeneous.

1C1438 肺サーファクタントタンパク質 B の N 末端セグメントにより起こる脂質単分子膜の崩壊現象
Collapse in lipid monolayers induced by N-terminal segments of lung surfactant protein B

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Lung surfactant is a lipid-protein complex at the air-water interface of the alveolus. Its primary function is to reduce the surface tension. The reduction makes the process effortless during the process of inhalation and this property prevents the lungs from collapse during exhalation. The surfactant protein B (SP-B) is mainly involved in enhancing the surface activity of the surfactant film during compression and expansion. However, the function of SP-B in the monolayer or replacement surfactants is not well understood. Here we observed the morphology and collapse transitions in the model surfactant monolayers induced by N-terminal segments of SP-B, using isotherms, surface elastic modulus and fluorescence microscopy. The details of the results will be discussed.

1C1450 ラクトフェリシン B 由来の抗菌活性を持つヘキサペプチドの大腸菌細胞質への侵入
Entry of Antimicrobial Hexapeptide Derived from Lactoferricin B into Single cells of *E. coli* without Damaging their Membranes

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Short peptides derived from Lactoferricin B (LfcinB) have antimicrobial activity, but its mechanism is not well understood. Last year, we reported that rhodamine B-labeled LfcinB (4-9) (Rh-LfcinB (4-9)) entered single GUVs without leakage of AF647. Here we investigated the interaction of Rh-LfcinB (4-9) with single cells of *E. coli* containing calcein. We found that the fluorescence intensity due to Rh-LfcinB (4-9) at the central region of *E. coli* cells became larger than that at their rim without leakage of calcein, indicating that Rh-LfcinB (4-9) entered their cytoplasm without pore formation. Interaction of Rh-LfcinB (4-9) with DNA increased its fluorescence intensity greatly. Based on these results, we discuss the mechanism of its antimicrobial activity.

1C1502* 外側と内側の単分子膜の脂質の充填がマガイニン２の脂質膜中のポア形成に影響を与える
Effect of Asymmetric Packing of Lipids in Outer and Inner Monolayer on Magainin 2-Induced Pore Formation in Lipid Bilayer

Moynul Hasan[1], Mohammad Abu Sayem Karal[1], Victor Levadny[1,2], Masahito Yamazaki[1,3,4] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Rus. Acad. Sci.*, [3]*Res. Inst. Ele., Shizuoka Univ.*, [4]*Grad. Sch. Sci., Shizuoka Univ.*)

We investigated the effect of asymmetric packing of lipid in two monolayers on the rate constant of magainin 2 (mag)-induced pore formation, kp. Firstly, we prepared GUVs composed of PG/PC/lyso-PC (LPC) in inner monolayer and PG/PC in outer monolayer, which had different lipid packing in both monolayers. This was confirmed by several experiments such as the fluorescence intensity of their membranes due to the fluorescent analogue of LPC. Next, we investigated the interaction of mag with these GUVs, and found that kp decreased with increasing LPC concentration in the inner monolayer. This result can be quantitatively explained by our theory on kp: the higher packing of the inner monolayer decreases its stretching on the binding of magainin 2, which decreases kp.

1C1514 Formation mechanism of “lipid raft” in cell membranes

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Phase separation in giant lipid vesicles that mimic cell membranes is of great interest to cell biologists and biophysicists, because it may explain the formation mechanism of the nano-sized functional heterogeneities in cell membranes. However, micro-sized domains are formed in such lipid vesicles, and the size discrepancy is unsolved. Here, we experimentally show that micro-sized domains are reduced up to nano-sized by being exposed to externally added glycolipids, with two-step morphological transformations. Moreover, we numerically confirm such reductions using a TDGL model, which describes phase separation and elastic membrane. Finally, we conclude that the spontaneous curvature due to lipid asymmetry plays a critical role in determining the lipid raft size.

1C1532* **パターン化人工膜を用いた光シグナル伝達中における脂質ラフトの機能解析**

Role of lipid rafts in phototransduction studied with a micropatterned model membrane

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Phototransduction is believed to be regulated by lipid rafts. We quantitatively evaluated the affinity of the membrane proteins involved in the phototransduction to lipid rafts (raftophilicity) by using a model membrane having patterned liquid-ordered and liquid-disordered bilayers. The raftophilicity of photoreceptor rhodopsin (Rh) was heighted upon light-dependent dimerization, whereas rhodopsin kinase had a low raftophilicity, indicating that the phosphorylation of Rh should be hindered by the presence of raft. Furthermore, we obtained the raftophilicity of G-protein transducin, phosphodiesterase, and S-modulin. We discuss on the implication of the obtained results together with the results in disk membrane and kinetic simulations.

1C1544 **パターン化人工膜を利用した NAP-22 の膜結合と凝集挙動解析**

Membrane binding and aggregation of neuronal acidic protein of 22kDa (NAP-22) studied with a patterned model membrane

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NAP-22 is a neuron-enriched membrane protein, whose function remains unknown. It associates with a lipid membrane with a myristoyl chain, but its binding and aggregation behaviors on cell membranes are not fully understood. We studied the binding and aggregation on a patterned model membrane having defined compositions and geometries. We found that acidic lipids such as phosphatidylserine (PS) promoted membrane binding and aggregation. The enhancement was also found on the detergent resistant membrane, but not on its lipid extracts, suggesting the involvement of protein components. The systematic studies using a model membrane give insight into the nature of NAP-22 binding and aggregation, and should help to elucidate its roles in neurons.

1C1556* **Two-in-one biohybrid microfluidic system for detection and elimination of staphylococcus**

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In this study, we developed a multi-functional biohybrid microfluidic system that can detect bacteria with antibacterial activity. Microfluidic channels in the device were coated with polydiacetylene (PDA) vesicles that have color transition property upon external stimuli. Moreover, PDA vesicles functionalized with lysostaphin (LST) that has antibacterial function to staphylococcus. PDA-LST coated microfluidic channels were designed as fish gill mimicking structure to increase efficiency of enzymatic reaction for LST with staphylococcus in fluid flow. 80 % of staphylococcus in fluid was immortalized by LST, inducing color transition of PDA vesicles on the microchannels. We expect that our system can be applied to a number of biomedical and industrial applications.

1C1608* **DNA Hairpin Based Spore Detection through α-Hemolysin Nanopores**

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Nanopore- and aptamer-based stochastic sensor enables rapid and sensitive detection of targets. However, they have limited applications because most of the aptamers are not able to make recognizable signal differences with and without the aptamers bound to the targets when they translocate through the nanopores. To overcome the current limitations, we designed the DNA hairpin that is complement to the aptamers. We subsequently extracted unbounded hairpins by centrifugation and counted them by detecting their unique translocation signals. We applied our method to detect Bacillus spores, resulting in the detection limit as low as 12 CFU/mL. Since hairpin DNA structure can be designed depending on target aptamers, our system is applicable to any target specific aptamers.

1D1320* **ハナガサクラゲ由来の耐酸性・単量体型 GFP**

Acid-tolerant monomeric GFP derived from jellyfish Olindias formosa

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Fluorescent protein (FP) has made a great contribution to visualize molecular and cellular processes. However, most FPs lose fluorescence at pH lower than their neutral pKa, and this has hampered their application in acidic organelles (pH = 4.5-6.0). Here we developed an acid-tolerant monomeric GFP 'Gamillus' from jellyfish Olindias formosa with excellent brightness, maturation speed and photostability. Results of X-ray crystallography suggest that the acid-tolerance is attributed to stabilization of deprotonation on chromophore phenyl ring in broad pH range by forming unique trans configuration. We demonstrated that Gamillus serves as a universal molecular tag, suitable for imaging in acidic organelles through autophagy-mediated molecular tracking to lysosomes.

1D1332* **複数の自由行動マウスにおける脳活動計測が可能な化学発光膜電位指示薬の開発**

Development of a chemiluminescent voltage indicator applicable to a brain activity recording in freely-behaving multiple mice

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Here, we present the world's first chemiluminescent voltage indicator, named LOTUS-V composed of a voltage-sensing domain fused with a chemiluminescent protein and a yellow fluorescent protein. LOTUS-V allowed long-term drug evaluation in cardiomyocytes derived from induced pluripotent stem cells by means of substrate perfusion, and showed full compatibility with multiple optogenetic stimulation in pheochromocytoma cells. Furthermore, we could perform an easy and less invasive brain activity recording in freely-behaving multiple mice without complex optics arrangement and fiber insertion. Thus, LOTUS-V not only serves technological innovation in wide field of life sciences but also stands alone among the various techniques for brain activity recording.

1D1344* **細胞内グルタチオンの求核付加・解離平衡に基づく超解像蛍光イメージングプローブの開発**

Development of spontaneously blinking fluorophores based on nucleophilic addition of intracellular glutathione for superresolution imaging

Akihico Morozumi[1,4], Mako Kamiya[2,5], Shin-nosuke Uno[1], Keitaro Umezawa[1], Toshitada Yoshihara[3], Seiji Tobita[3], Yasuteru Urano[1,2,4] ([1]*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*, [2]*Grad. Sch. of Med., The Univ. of Tokyo*, [3]*Grad. Sch. Sci. Tech., Gunma Univ.*, [4]*AMED CREST*, [5]*JST PRESTO*)

Single-molecule localization microscopy (SMLM) provides super-resolution images by repeated precise localization of individual fluorophores which are induced to blink. However, to cause blinking of conventional fluorophores generally requires intense laser irradiation and chemical additives, limiting the live-cell applications. Here, we propose a novel blinking mechanism based on nucleophilic addition and dissociation of intracellular glutathione (GSH). Based on this strategy, we succeeded in developing two fluorophores which show spontaneous and appropriate blinking to allow live-cell SMLM without intense laser irradiation or any additives. At present, these fluorophores are being applied to some experiments including two-color SMLM in mammalian and bacterial cells.

1D1356* **新規微分干渉顕微法を用いた生細胞ヘテロクロマチンにおける物質密度のイメージング**

Density imaging of heterochromatin in live cells using orientation-independent-DIC microscopy

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It is an established view that heterochromatic regions in cell nuclei are highly dense. But how really dense are they? What are they like in live cells? To investigate the heterochromatic regions, we observed the mouse pericentric heterochromatin foci, a good model heterochromatin, using the orientation-independent-DIC microscopy system, which can analyze density in live cells. Strikingly, we found that density of the foci in live cells is only about 1.6-fold higher than that of surrounding euchromatin region while their DNA density stained by fluorescent DNA dye was more than 5-fold higher. This result suggests that the heterochromatic regions are not necessarily dense as we have ever expected. A possible heterochromatin environment will be discussed.

1D1408* **Development of Bioluminescent Low Affinity Ca2+ Indicators Applicable to Analyze Ca2+ Dynamics in Endoplasmic Reticulum**

Nadim Hossain Md[1], Kazushi Suzuki[1,2], Megumi Iwano[2], Tomoki Matsuda[1,2], Takeharu Nagai[1,2] ([1]*Graduate School of Engineering, Osaka University*, [2]*The Institute of Scientific & Industrial Research (ISIR), Osaka University*)

To study SR/ER Ca2+ dynamics, genetically encoded calcium indicators (GECIs) with low Ca2+ affinity have already been reported. Recently our group reported bioluminescent protein based GECI with high Ca2+ affinity GeNL(Ca2+). To expand their detectable Ca2+ range to more higher concentration for imaging in SR/ER, we have successfully developed a cyan color variant with low affinity named CeNL(Ca2+). In addition, an orange color variant with middle affinity, OeNL(Ca2+) developed. We performed simultaneous three color imaging of intracellular Ca2+ dynamics in mammalian cells expressed in ER localized CeNL(Ca2+), mitochondria localized OeNL(Ca2+) and nucleus localized GeNL(Ca2+). SR Ca2+ dynamics in C2C12 myoblasts cells has successfully been monitored by CeNL(Ca2+).

1D1426 **Single-cell quantitative analysis of ATP concentration by fluorescence lifetime imaging microscopy**

Hideki Itoh[1], Satoshi Arai[2], Thankiah Sudhaharan[1], Tetsuya Kitaguchi[3], E. Birgitte Lane[1] ([1]*Inst. of Med. Biol. (Imb), Agcy. for Sci., Tech. and Res. (A*STAR), Singapore*, [2]*Res. Inst. Sci. Eng., Waseda Univ., Japan*, [3]*WASEDA Biosci. Inst. Singapore (WABIOS), Singapore*)

Adenosine triphosphate (ATP) is an essential molecule for all living organisms, providing energy currency for cell processes. We have developed novel genetically-encoded fluorescent ATP indicators whose fluorescence lifetime changes with ATP concentration, and are using fluorescence lifetime imaging microscopy (FLIM) to measure these changes. Because the FLIM readout is an absolute value, the ATP concentration of specific organelles in single cells can be quantified without losing spatial resolution. We show the use of this technique in cell biology to demonstrate the relationship between energy metabolism and cell type or cell cycle.

1D1438 **熱産生する褐色脂肪細胞における Ca^{2+} を伴う 3 相のミトコンドリア pH 変化**

Triphasic mitochondrial pH changes associated with Ca^{2+} for heat production in stimulated brown adipocytes

Madoka Suzuki[1,2] ([1]*PRESTO, JST*, [2]*Res. Inst. Sci. & Eng., Waseda Univ.*)

Brown adipocytes (BAs) are endowed with a high metabolic capacity for energy expenditure due to their high mitochondria content. While mitochondrial pH is dynamically regulated in response to stimulation and in return affects various metabolic processes, how the pH is regulated during thermogenesis is unknown. Here, we report a triphasic mitochondrial pH change in BAs upon stimulation, demonstrated using a mitochondrial targeted pH-sensitive protein, mito-pHluorin. In comparison to a thermosensitive dye [*Sci. Rep.*, **7**, 1383 (2017)], we reveal that phases 1 and 2 of the pH increase precede thermogenesis, while phase 3, characterized by a pH decrease, occurs during thermogenesis. We suggest that this pH increase may play a role in the potentiation of thermogenesis.

1D1450* **ヒト 2 型自然リンパ球の 1 細胞実時間イメージングによる 2 型サイトカイン応答観察に基づいた新規アレルギー診断の可能性**

Potentiality for novel allergy diagnosis by real-time single-cell secretion imaging of human type 2 innate lymphoid cells

Kaede Miyata[1], Yoshitaka Shirasaki[1,2], Nobutake Suzuki[1], Rie Baba[3], Hiroki Kabata[3], Mai Yamagishi[1,2], Osamu Ohara[2], Koichi Fukunaga[3], Kazuyo Moro[2], Sotaro Uemura[1] ([1]*Graduate School of Tokyo*, [2]*Institute of Physical and Chemical Research, IMS.*, [3]*Division of Pulmonary Medicine, Keio University*)

We developed a new tool for a parallel measurement platform for real-time single-cell secretion imaging with a multi-reservoir integrated nano litter-well array chip.

Here, we monitored type 2 cytokine responses, a putative trigger of an allergy from rare human type 2 innate lymphoid cells obtained from peripheral blood. We found that early stage responses within 24 hours were dominantly detected for the allergic background donor, while later stages were not. Subsequent recovery of cells based on secretion activity enabled us to perform phenotype-specific single-cell RNA-Seq, elucidating different pattern of expression profiles in type 2 secretion response related genes. Therefore, this new tool is expected to contribute to a personalized diagnosis for an allergy.

1D1502*　生理的条件下の細胞形態変化に伴う ATP レベル変動の定量的解析

Spatiotemporal quantification of native ATP dynamics during changes in cellular morphology

Rika Suzuki, Kohji Hotta, Kotaro Oka (*Grad. Sch. Sci and Tech., Keio Univ.*)

Although ATP is a major energy source of cells, ATP dynamics under physiological conditions without extensive stimulations has not been understood well. In this study, a simultaneous imaging and image processing analysis allowed us to observe and quantify relationships between ATP levels and cellular morphological changes under physiological conditions. We found that microtubule dynamics cause cellular shape change accompanying an increase in ATP level. Also, spatiotemporal quantification of the length of actin rich-protrusion and ATP levels suggested that they are influencing each other. This work demonstrates that cellular motility and morphology are regulated by ATP-related cooperative function between microtubule and actin dynamics.

1D1514*　独立成分解析（ICA）を利用したマウス全脳の匂い BOLD 応答検出

Detection of the odor BOLD response in the mouse whole brain, using independent component analysis (ICA)

Hirotsugu Funatsu, Fuyu Hayashi, Sosuke Yoshinaga, Naoya Yuzuriha, Shunsuke Kusanagi, Mitsuhiro Takeda, Hiroaki Terasawa (*Fac. Life Sci. Kumamoto Univ.*)

BOLD analysis is the main method to track real-time odor responses in rodent brains. Mice have smaller brains and are more susceptible to peripheral hemodynamic changes than rats, which make it harder to obtain sufficient BOLD signals. We revealed the real-time odor response in the mouse whole brain by using periodic stimulation and ICA. Isoamyl acetate (banana-like odor) activated the dorsal olfactory bulb, as in the previous rat study[1], the piriform cortex on the olfactory pathway, and the posterior lateral hypothalamus, known as the feeding center. These signals were maximal at 8±2 sec after the stimulations, similar to the human canonical hemodynamic response function.

[1] Martin, C. *et al.*, NeuroImage **36**, 1288—1293 (2007)

1D1532*　過渡的刺激に対する２型自然リンパ球（ILC2）の確率的な分泌応答

Stochastic Secretion Response to Transient Stimulus of Type-2 Innate Lymphoid Cells (ILC2)

Kazuki Yoda, Nobutake Suzuki, Sotaro Uemura, Yoshitaka Shirasaki (*Grad. Sch. Sci., Univ. Tokyo*)

Our real-time single-cell secretion imaging method (Shirasaki et al. 2014) clarified that individual type-2 innate lymphoid cells (ILC2) started secreting at very different times one by one after being stimulated with interleukin (IL)-2 and 33.

To understand the mechanism underlying this fluctuation, we analyzed the secretion responses against different duration of stimulus. The shorter transient stimulus resulted in the smaller number of secreted cells and the shortened distribution of secretion onset. In addition, continuous stimulus was required to maintain the secretion activity level.

Our results suggest that each individual ILC2 slowly and stochastically responds to IL-2/33 stimulus but suspends its secretion activity when the stimulus disappears.

1D1544*　一粒子輝度イメージングによるグルココルチコイド受容体二量体の生細胞内時空間分布解析

Shot noise free number and brightness analysis visualizes spatio-temporal distribution of glucocorticoid receptor dimer in living cells

Ryosuke Fukushima[1], Jotaro Yamamoto[2], Masataka Kinjo[2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

Glucocorticoid receptor (GR) belongs to nuclear receptor superfamily. GR has dynamic properties such as nuclear translocation by ligand binding and assembly to DNA as a dimer. This is well-known scheme; however, it is still mystery whether GR forms monomer or dimer during the translocation.

To visualize spatio-temporal distribution of monomer/dimer GR, we developed a method to generate particle brightness map using confocal laser scanning microscopy operating with two detector system to eliminate noise signals. The time series of the brightness map revealed GR translocates as a monomer and then dimerizes in nucleus. The result was confirmed with dimerization deficient mutant. This would be the first step towards understanding of GR dynamic mechanism in living cell.

1D1556*　顕微ラマン分光法によるバクテリアー細胞の代謝活性測定

Single bacterial cell analysis of metabolic activity by Raman microspectroscopy

Yota Kato[1], Hiroshi Ueno[1], Hiroyuki Noji[1,2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*ImPACT, JST*)

The individuality of bacterial metabolic activity is thought to be a key for their adaptation against ever-changing environment. Persister cell is one of such adaptation strategies. In this study, we combined D_2O labeling with Raman microspectroscopy to measure metabolic activity of single cells. In the presence of D_2O, active cells incorporated D to generate C-D bonds in fatty acids or carbohydrates via anabolism, which gave a distinct peak in Raman spectra. Cells treated with antibiotics showed lower C-D peak intensities than untreated ones, suggesting that the C-D signal can be the indicator of metabolic activity. We also measured the C-D signal of a bacterial population while observing cell divisions with attempt to quantify metabolic activity of persister cells.

1D1608*　高速 AFM が大腸がん細胞における核膜孔の選択的なゲートの喪失を明らかにした

Loss of Nuclear Pore Selective Barrier Revealed by High-Speed Atomic Force Microscopy in Colorectal Cancer Cells

Mahmoud Shaaban Mohamed[1,2,3,4], Akiko Kobayashi[1,2,3,4], Azuma Taoka[4], Takahiro Watanabe-Nakayama[2], Yosuke Kikuchi[4], Masaharu Hazawa[1,2,3,4], Toshinari Minamoto[5], Yoshihiro Fukumori[4], Noriyuki Kodera[2], Takayuki Uchihashi[2], Toshio Ando[2], Richard Wong[1,2,3,4] ([1]*Cell-Bionomics Research Unit, Kanazawa Univ.*, [2]*Bio-AFM Frontier Research Center, Kanazawa Univ.*, [3]*Lab of Mol. Cell Biol. Institute of Science and Engineering, Kanazawa Univ.*, [4]*Institute of Science and Engineering, Kanazawa Univ.*, [5]*Division of Translational and Clinical Oncology, Cancer Res. Inst., Kanazawa Univ.*)

Nuclear pore complexes (NPCs) are the gates embedded in the nuclear envelope (NE), acting as regulators of transport between the cytoplasm and the nucleus. Some of nucleoporins composed of intrinsically disordered phenylalanine-glycine strings (FG-Nups), playing a key role in transport selectivity. The dynamic FG-Nups protein molecules are imperceptible in vivo. We show that high-speed atomic force microscopy (HS-AFM) can directly visualize nanotopographical changes of the nuclear pore central channel in colorectal cancer cells. Furthermore, using MLN8237, an apoptotic inducer, we revealed the loss of nucleoporins, particularly the FG-Nups barrier. These findings not only illuminate the potential application of HS-AFM as an intra-cellular nanoendoscopy.

1E1320* 水-タンパク質間相互作用のための連続体モデルによる分散力エネルギー計算
Continuum-model-based Dispersion Energy Calculation for Protein-Water Interaction

Dan Parkin, Yukinobu Mizuhara, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

The generalized Born (GB) model is widely used to calculate protein-protein interaction (PPI) in water, where water is treated as a continuum medium. Previously, we reported over-destabilization of PPI in GB models and provided a means to improve the electrostatic component of the desolvation penalty upon binding. Calculation of non-electrostatic energy change upon binding, however, has yet to be improved: it is over-stabilized without properly considering the desolvation penalty due to the dispersion force interaction between water and protein. In this study, we demonstrate that the application of the GB-like continuum model is useful as well to improve the non-electrostatic component of desolvation penalty upon binding.

1E1332 気液界面におけるタンパク質の変性
Protein Unfolding at the Air-Water Interface

Yohko Yano[1], Etsuo Arakawa[2], Wolfgang Voegeli[2], Chika Kamezawa[2], Tadashi Matsushita[3] ([1]*Department of Physics, Kindai University*, [2]*Department of Physics, Tokyo Gakugei University*, [3]*Photon Factory, Institute of Materials Structure Science, KEK*)

Many proteins lose their biological activity after exposure of their solutions to the air-water interface. This is due to adsorption and unfolding processes resulting from the amphiphilic nature and comformational stability of globular proteins. In the present work, we investigated the early stage of protein adsorption at the air-water interface using a recently-developed simultaneous multiple angle-wavelength dispersive X-ray reflectometer. This has enabled us to obtain the electron density profile of the adsorbed protein molecules with an acquisition time of 1 second. We will discuss the driving force behind adsorption-induced protein unfolding for three globular proteins, lysozyme, Myoglobin and BSA.

1E1344 Unexpected heterogeneity and slow dynamics of simple poly-alanine peptides detected by single molecule fluorescence spectroscopy

Supawich Kamonprasertsuk[1,2], Hiroyuki Oikawa[1,2], Satoshi Takahashi[1,2] ([1]*Institute for Multidisciplinary Research for Advanced Materials, Tohoku University*, [2]*Department of Chemistry, Graduate School and Faculty of Science, Tohoku University*)

Unfolded polypeptides are mixtures of heterogeneous conformations assumed to interconvert within microseconds. However, we showed that the unfolded ubiquitin demonstrates much slower dynamics. In this study, we investigated alanine-based model polypeptides using the single molecule fluorescence spectroscopy having the time resolution of ~100 μs. A sample showed broad distribution of the FRET efficiency, suggesting the heterogeneous conformation and slow dynamics. Another sample showed two peaks likely corresponding to the helical and unstructured states, suggesting the energy barrier between them. Thus, even alanine-based polypeptides showed heterogeneity and slow dynamics.

1E1356 二次元蛍光寿命相関分光法によるシトクロム *c* のフォールディング過程の部位選択的な観測
Site-selective observation of folding dynamics of cytochrome *c* by two-dimensional fluorescence lifetime correlation spectroscopy

Miyuki Sakaguchi[1], Masaru Yamanaka[2], Shun Hirota[2], Kunihiko Ishii[1,3], Tahei Tahara[1,3] ([1]*Msl, RIKEN*, [2]*Grad. Sch. Mat. Sci., NAIST*, [3]*RAP, RIKEN*)

Two-dimensional fluorescence lifetime correlation spectroscopy (2D FLCS) enables us to visualize structural heterogeneity and dynamics of fluorescently labeled molecules with microsecond time resolution. In this study, acid-induced unfolding dynamics of horse cytochrome *c* is analyzed by 2D FLCS under an equilibrium condition. We examined three fluorophore labeling sites, namely 50th, 83rd, and 104th positions in the sequence. For all the samples, an unfolded and a partially folded conformational ensembles were detected. Their interconversion was observed to be longer than a millisecond. This result indicates that the early stage of folding occurs not in a stepwise manner but in a globally cooperative way.

1E1408* Oct4 の 2 つの DNA 結合サブドメインを結ぶ linker 領域の構造多様性
Structural variety of the linker connecting two DNA-binding subdomains of Oct4

Tomonori Hayami[1,2], Shoji Takada[3], Kota Kasahara[4], Haruki Nakamura[1], Junichi Higo[1] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sch. Fro. Bio., Osaka Univ.*, [3]*Dept. Biophys., Grad. Sch. Sci., Kyoto Univ.*, [4]*Dept. Bioinfo., Col. Life Sci., Ritsumeikan Univ.*)

Oct4 is a transcription factor protein related to stem cell's pluripotency. An Oct4 DNA-binding domain consists of two DNA-binding subdomains connected by a linker, which is crucial for reprogramming.
We obtained a conformational ensemble of the linker by performing virtual-system coupled adaptive umbrella sampling (V-AUS), and obtained several free-energy landscapes at 300 K.
A free-energy landscape showed that the linker alone prefers compact conformations, although structures similar to the X-ray structure exist in extended conformations. Another landscape showed many low free-energy clusters, whose conformations are helical or hairpin-like. We consider that this conformational variety of the linker allows Oct4 to make various protein-protein interactions.

1E1426* フィブリノーゲンによるアミロイド線維形成阻害機構の解明
Investigation of inhibition mechanism of fibrinogen in the amyloid fibrillation

Taiki Akai, Naoki Yamamoto, Eri Chatani (*Grad. Sch. of Sci., Kobe Univ.*)

Amyloid fibrils are abnormal protein aggregates and associated with a number of pathological diseases. To understand amyloid fibrillation under a condition coexisting with other proteins, like in vivo, we investigated effects of fibrinogen (Fg) on amyloid formation of an insulin-derived peptide fragment, B chain. As a result, Fg inhibited the fibrillation by trapping intermediates, which was revealed by analyses of CD, AFM, and DLS. Moreover, the inhibition effect of Fg occurred even when Fg was added after the intermediates were formed. From a 1H-NMR measurement, which suggested that Fg weakly interacted with the intermediates and stabilized them, it was indicated that Fg prevents subsequent formation of fibrils by attaching to the surface of the intermediates.

1E1438* **プリオンアプタマーはアルツハイマー病に関与するプリオン蛋白質と Aβ オリゴマーの複合体の形成を阻害する**

An anti-prion aptamer inhibits the formation of prion protein-amyloid β oligomer complex that is related to Alzheimer's disease

Mamiko Iida[1,2], Tsukasa Mashima[1,2], Yudai Yamaoki[1], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Inst. of Adv. Energy, Kyoto Univ.*, [2]*Grad. Sch. of Energy Sci., Kyoto Univ.*)

Amyloid beta (Aβ) oligomers may play a crucial role in Alzheimer's disease. Recent studies proposed that Aβ oligomers bind to prion protein (PrP), which is anchored on a cell membrane, causing Alzheimer's disease. Here, we demonstrate that an RNA molecule, R12, that tightly binds to PrP, can disrupt the interaction of the Aβ oligomer with PrP. Fluorescence intensity of thioflavin S decreased in the presence of either PrP, mutant of N-terminal half of PrP or even a fragment peptide of PrP, indicating that PrP interacts with Aβ and inhibits fibrillization of Aβ. Upon the addition of R12, however, the intensity was restored to the same level as was observed in the absence of PrP. This indicates that R12 can bind to and snatch away PrP in the PrP- Aβ oligomer complex.

1E1450* **Photo cross-linking and MS analyses of the amyloid β-peptide oligomers**

Mai Kawashita[1], Shintaro Yoshida[1], Sosuke Yoshinaga[1], Mitsuhiro Takeda[1], Ayumi Tanaka[1], Takashi Hamaguchi[1], Hitomi Yamaguchi[1], Shigeto Iwamoto[1], Takashi Saito[2], Yoshihiko Takinami[3], Toshiyuki Kohno[4], Takaomi C. Saido[2], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*RIKEN, Inst. Phys. Chem. Res.*, [3]*Bruker Daltonics*, [4]*Kitasato Univ. Sch. Med.*)

The deposition of senile plaques is observed in the brains of Alzheimer's disease (AD) patients. Aβ oligomers, formed in the process of senile plaque production, are thought to be neurotoxic in AD. Therefore, for a radical cure of AD, it is essential to clarify the oligomerization mechanism of Aβ. Solid-state NMR studies previously elucidated that the Aβ fibrils have parallel or antiparallel β-sheet structures. In this study, to reveal the intermolecular binding pattern of the Aβ oligomers, we performed an MS analysis of a minimal oligomer unit, an Aβ dimer, which was generated by photo cross-linking a mixture of stable isotope labeled and unlabeled Aβ. We will describe the type of β-sheet that is quantitatively predominant in the Aβ oligomers.

1E1502 **アミロイド分解能を有する人工ペプチドの設計**

Designing artificial peptides that have ability to hydrolyze amyloid fibrils

Yoshihiro Iida, Atsuo Tamura (*Grad. Sch. Sci., Univ. Kobe*)

Amyloid fibrils are misfolded and self-assembled aggregates of proteins approximately 10 nm in diameter and several micrometers in length. Amyloidosis is the extracellular deposition of these insoluble protein fibrils, leading to tissue damage and disease. To remedy amyloidosis, one of the most effective ways is to hydrolyze amyloid fibril directly. We thus tried to design short peptides having hydrolysis activity against amyloid fibrils. As a strategy for the design, we made peptides to have the catalytic triad on a helix. It has been shown that the designed peptide takes the alpha-helical conformation and can hydrolyze amyloid fibrils. It is concluded that the designed peptide can be regarded as a hydrolase which is capable of hydrolyzing amyloid fibrils.

1E1514 **再設計法と新規設計法による膜貫通アルファヘリックスペプチドバレルの開発**

Redesign and de novo design of transmembrane alpha-helical peptide barrels

Ai Niitsu[1,2], Kozhinjampara R. Mahendran[3], Andrew R. Thomson[4], Hagan Beyley[3], Yuji Sugita[1], Derek N. Woolfson[2] ([1]*Wako Inst, RIKEN*, [2]*Univ. Bristol*, [3]*Univ. Oxford*, [4]*Univ. Glasgow*)

Successful rational designs of membrane proteins not only add new structural motifs to the protein engineering field but also deliver sequence-structure relationships to understand protein folding. However, membrane protein design has been hindered by the poorer understandings of membrane protein structures than those for water-soluble proteins due to the limited high-resolution structural information. Here, we design, synthesize and characterize peptide-based, membrane-spanning alpha-helical barrels. We demonstrate new designs derived from two different approaches: 1) the redesign of a natural membrane-spanning domain of the alpha-helical barrel protein Wza; and 2) the computational de novo design of transmembrane coiled coil-based alpha-helical barrels.

1E1532* **Rational design of a novel affinity ligand for antibody purification by controlling the pH-sensitive antibody interaction**

Yoshiki Oka[1], Taihei Sawada[1], Takahiro Watanabe[1], Hisashi Kudo[1], Manami Wada[1], Hidenobu Kawai[1], Mari Chang[2], Yuuki Hayashi[1], Munehito Arai[1,2] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Dept. Phys., Univ. Tokyo*)

Protein A (PA) is frequently used as an affinity ligand for purification of antibodies (Ab). However, acidic pH is required to dissociate Ab from PA, which may cause aggregation of Ab. To dissociate Ab at more neutral pH, we designed a novel affinity ligand, FPA, which is a fusion of PA and the coiled-coil region of c-Fos. FPA associates Ab at pH 7 and dissociates them at acidic pH by forming a homodimeric coiled-coil. Here, we rationally introduced multiple mutations into the c-Fos region of FPA, to stabilize the homodimer by electrostatic attraction. We succeeded in creating the FPA mutant that dissociates Ab at pH 5.47. We will also report the affinities of the wild-type and mutant FPAs with Ab measured by isothermal titration calorimetry.

1E1544 **メニーコアプロセッサ向け蛋白質・リガンドドッキングエンジン sievgene_M の開発**

Development of protein-ligand docking engine sievgene_M for manycore processors

Takanori Sugihara[1,2], Takashi Kurosawa[2,3], Hironori Nakamura[4], Tadaaki Mashimo[2,5], Yoshifumi Fukunishi[2,6], Haruki Nakamura[2,7] ([1]*JBIC*, [2]*N2PC*, [3]*Hitachi Solutions East Japan, Ltd.*, [4]*Biomodeling Research Co., Ltd.*, [5]*IMSBIO Co., Ltd.*, [6]*AIST/molprof*, [7]*Inst. for Protein Research, Osaka Univ.*)

We propose a method to accelerate in-silico screening and decrease the cost required to discover pharmaceutical candidate compounds. We implement a multithreaded version of the protein-ligand docking engine sievgene for better parallel performance.

In drug development, it is quite important to decrease labor to find candidate compounds. Usually, experimental methods are used for ligand screening. In those methods, we can analyze target protein-ligand systems in detail but the cost increases in proportional to labor.

In-silico screening is a useful automated method based on high-performance computing. In this method, we can evaluate economically millions of protein-ligand interactions for short time. We explain a method to parallelize sievgene with manycore processors.

1E1556* **Analysis of protein pockets using a fast and efficient comparison method with a reduced vector representation**

Tsukasa Nakamura[1], Kentaro Tomii[1,2,3] ([1]*CBMS, GSFS, Univ. Tokyo*, [2]*AIRC, AIST*, [3]*BRD, AIST*)

Analyzing interactions between proteins and small molecules is important to predict the ligands which bind to parts of putative ligand binding pockets. Such analysis demands a fast and efficient method. Methods have been developed for representing a binding pocket with one reduced vector. However, some possible caveats must be associated with existing methods. To overcome them, we defined the similarity among all triangles which are producible under our labeling method, and developed a method to represent a binding pocket with a reduced vector using multidimensional scaling based on those triangles. Our method shows higher performance than existing methods, and could obtain the classification results of pockets, corresponding to the conformational diversity of ligands.

1E1608* **Phase transition in a single giant DNA molecule: Differences between 1-propanol and 2-propanol aqueous solutions**

Yue Ma, Yuko Yoshikawa, Koichiro Sadakane, Takahiro Kenmotsu, Kenichi Yoshikawa (*Graduate School of Life and Medical Sciences, Doshisha University*)

In order to understand polarity of alcohol solutions' influences on genome-sized DNA's structure, we performed a comparative study between 1- and 2-propanols. For DNA molecules in different concentrations of 1-propanol solutions, two minima of average length appear at 60% (v/v) and 80% (v/v). In 2-propanol solutions, the average long-aixs length of DNA decreased and transited from elongated coil state to folded globule is generated around 70-75% (v/v). Above 75% (v/v), DNA maintained as folded globule and the average length of DNA molecules remains essentially the constant. The observed large difference of the effect of propanol isomers on the DNA conformation will be discussed in relation to the nano-structure of alcohol solution.

1F1320* **光依存性内向きプロトンポンプ *Po*XeR の X 線結晶構造解析**
Crystal structure of *Po*XeR, a light-driven inward proton pump

Tatsuya Ikuta, Ryuichiro Ishitani, Osamu Nureki (*Grad. Sch. Sci., Univ. Tokyo*)

PoXeR is a natural light-driven inward proton pump derived from deep-ocean marine bacterium Parvularcula oceani. Although PoXeR pumps protons, it has the highest homology to a sensory rhodopsin, which does not transport any ions. For its remarkable function, the transport mechanism should be unique and different from that of bacteriorhodopsin. We established the purification and crystallization method of PoXeR and determined the crystal structure at 1.9 Å resolution. In the structure, we confirmed water molecules and lipids, but the structure does not contain retinal, which should be covalently bound to opsin. We discuss the structural difference between PoXeR, bacteriorhodopsin, and sensory rhodopsin.

1F1332* **Crystal structure of mammalian Claudin3 in complex with a toxin**

Shun Nakamura[1], Katsumasa Irie[1,2], Hiroo Tanaka[3], Atsushi Tamura[3], Sachiko Tsukita[3], Yoshinori Fujiyoshi[2] ([1]*Grad. Sch. Pharm., Univ. Nagoya*, [2]*CeSPI, Univ. Nagoya*, [3]*Grad. Sch. Med., Univ. Osaka*)

Claudins (Cldn) are the major components of tight junctions (TJ), form strands (TJ strand) that mediate cell adhesion and play a role as paracellular permselective barrier. Each Cldn subtype interacts with specific subtypes through the extracellular domain (ECD). Here we report the crystal structure of mammalian Cldn3 in complex with a toxin at 3.3 Å resolution, which shows that the third transmembrane helix (TM3) bends more than those of other structure-determined subtypes and renders ECD more inclined. Freeze-fracture electron microscopy shows that the mutations which alter the flexibility of TM3 change the shape of TJ strands. It is suggested that the angle of extracellular part of TM3 is one of the determinants for the Cldn-Cldn interaction.

1F1344* **Ca^{2+}/Zn^{2+}結合型ヒト S100A3 蛋白質四量体の X 線結晶構造解析に向けての研究**
The studies for X-ray crystallographic analysis of the Ca^{2+} and Zn^{2+} bound human S100A3 protein tetramer

Kenji Ite[1], Kenji Kizawa[2], Kenichi Kitanishi[1], Masaki Unno[1,3] ([1]*Grad. Sch. Sci. Eng., Ibaraki Univ.*, [2]*Kao Corp.*, [3]*IFRC, Ibaraki Univ.*)

S100A3 protein consists of total 101 amino acids including four arginine residues (Arg3, Arg22, Arg51, and Arg77) per a molecule. Peptidylarginine deiminase type III (PAD3) converts a symmetric pair of Arg51, but not other arginines, to citrullines on dimeric S100A3 in the presence of Ca^{2+}. This specific citrullination of the S100A3 dimer causes assembly of a homotetramer, and thereby cooperatively increases its affinity for Zn^{2+} and Ca^{2+}. In this study, we found that a mutant R51Q of S100A3 thoroughly mimics its citrullinated form. The R51Q mutant transformed to the tetramer in the presence of Ca^{2+} and Zn^{2+} ions at lower concentrations compared to R51A mutant previously reported. We also conducted structural analysis of the R51Q mutant in presence of these ions.

1F1356* **銅輸送チャネルにおける金属結合モチーフの構造変化と、それに伴う脂質二重膜への埋没**
Structural change of the metal binding motif of copper transporter induces the embedding of the motif into lipid bilayer

Mariko Okada[1], Takashi Miura[2], Takakazu Nakabayashi[1] ([1]*Grad. Sch. Pharm. Sci., Tohoku Univ.*, [2]*Dept. of Pharm. Sci., Int'l Univ. of Health and Welfare*)

The copper transporter (Ctr) proteins of fungi harbor a Cys/Trp motif as a Cu(I) binding site in their extracellular N-terminal domains. In this presentation, we report that the Cu(I) complexation with the Cys/Trp motif is accompanied not only by the structural change of the peptide backbone but also the embedding of the motif into phospholipid bilayer. The interaction of the peptide with lipid bilayer was analyzed using REES (red-edge excitation shift), which is a unique method to detect the fluorophore embedded in viscous media such as lipid bilayer. We also performed the measurement of Stern-Volmer quenching of fluorescence and CD spectra, and then discussed the correlation between the structural change of the peptide backbone and the embedding into lipid bilayer.

1F1408*　高速 AFM 観察で明らかにされた α7 ホモ 14 量体の α6 による解体過程

High-speed AFM reveals disassembly process homo-tetradecamer of proteasomal α7 subunit induced by interaction with α6 subunit

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The eukaryotic 20S proteasome is a cylindrical structure in which two hetero-heptemeric α-rings and two hetero-heptemeric β-rings are stacked into an αββα arrangement. Whereas there are some assembly chaperones involved in the formation of the eukaryotic proteasome, the α7 subunit, which is one of the component of α ring, is known to self-assemble into a double ring structure of homo-tetradecamer made of two layers of the α7 heptameric ring. The previous study using mass spectrometry revealed that the α7 tetradecamer is disassembled upon the addition of α6, giving rise to a 1:7 hetero-octameric α6-α7 complex. However, the detailed mechanisms remain unclear. Here we revealed the disassembly mechanisms of the α7 double ring induced by the interaction with α6 using HS-AFM.

1F1426*　コンピュータシミュレーションによるリゾチームと α ラクトアルブミンのモルテングロビュール状態の構造探索

Exploring Structures of the Molten Globule State of Lysozyme and αLactalbumin by Computer Simulations

Masahiro Shimizu, Yuko Okamoto (*Dept. Phys., Sch. Sci., Univ. Nagoya*)

In this study, we investigated the structures of the molten globule state of lysozyme and αlactalbumin. We performed Umbrella Sampling and Replica Exchange Umbrella Sampling simulations with the radius of gyration as a reaction coordinate to sample the conformational space. We used structural data of canine milk lysozyme, human αlactalbumin and goat αlactalbumin. We performed PCA and clustering about the REUS trajectory around the minimum value of the potential of mean force. In consequence, we got representative structures. These structures agreed with the characteristics of the molten globule state reported by many earlier studies. We conclude that it is possible to describe the structures of the molten globule state of a protein by computer simulations.

1F1438*　乾燥過程における G3LEA モデルペプチドの生体膜保護に関する計算化学的研究

Molecular dynamics study of the protective function of G3LEA model peptide on dried POPC bilayer

Yuta Takahashi, Tadaomi Furuta, Minoru Sakurai (*Center for Biol. Res. & Inform., Tokyo Tech*)

We focus on Group 3 late embryogenesis abundant (G3LEA) proteins known as a protectant against desiccation stress. Our previous studies have shown that a model peptide (PvLEA-22), two tandem repeats of an 11-mer motif, found in G3LEA proteins, possesses a function of protecting liposome from desiccation stress. However, the underlying mechanism is still unclear. In this study, we performed MD simulations to elucidate the interaction of PvLEA-22 with POPC lipid bilayer during drying process. It was shown that the hydrogen bonds between PvLEA-22 and POPC increase on dehydration and then the order parameters of the lipid aliphatic chain atoms are maintained to be as in the water rich system. This is one possible mechanism by which G3LEA peptides protect dried liposome.

1F1450*　時計タンパク質 KaiC のリン酸化と ATP 加水分解による構造変化メカニズム

Conformational change by phosphorylation and ATP hydrolysis in the cyanobacterial circadian oscillator KaiC

Katsuaki Oyama[1], Chihiro Azai[2], Kazuki Terauchi[1,2] ([1]*Graduate School of Life Sciences, Ritsumeikan University*, [2]*College of Life Sciences, Ritsumeikan University*)

The cyanobacterial circadian clock can be reconstituted in vitro by mixing three clock proteins, KaiA, KaiB and KaiC. The circadian oscillator KaiC consists of two homologous domains CI and CII in N- and C-terminal parts, respectively. CII domain carries the Ser and Thr residues showing phosphorylation circadian rhythm. Previously we resolved two conformational states of KaiC in BN-PAGE, and we found that the conformational changes of KaiC were driven by ATP hydrolysis in the CI domain. In this study, we purified the CII domain of KaiC, and found that KaiC-CII hexamer was converted into monomer accompanying change in phosphorylation states. We will discuss the mechanism of KaiC conformational changes in the KaiABC oscillator.

1F1502*　Computational investigation of conformational dynamics in Tom20/mitochondrial targeting signal complex

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Tom20 is a major component of TOM (translocase of outer mitochondrial membrane) complex which imports mitochondrial proteins into mitochondria. It recognizes and binds to presequences in mitochondrial targeting signals. Earlier experimental studies strongly indicated dynamic-equilibrium between Tom20/presequence complexes. Hence, the co-crystallization of this complex required a non-physiological disulfide bond linker. Two such complexes (A and Y) are being studied here which differ by one amino acid. Molecular dynamics (MD) and replica-exchange MD (REMD) simulations of these tethered complexes have been performed and showed narrow conformational space for Y. Crystal MD simulations will be performed to correlate dynamics and crystal contact-free space (CCFS) data.

1F1514*　分子動力学法による野生型・変異型エリスロポエチン受容体の動的解析

Dynamical analysis of wild type and mutant erythropoietin receptors by molecular dynamics simulations

Naoyuki Karasawa, Ayori Mitsutake, Hiroshi Takano (*Grad. Sch. Sci. Technol., Keio Univ.*)

A dynamical analysis method, relaxation mode analysis (RMA), has been developed for molecular dynamics simulations of protein systems. Recently, the applicant developed an improved version of RMA for large polymer systems, and found that the method extracts slow and rare structural transitions effectively. In this study, we selected a 596-residues protein trimer, an erythropoietin (EPO) and its receptors, as a target protein. EPO receptors have conserved motifs, which are referred to as WSAWS motifs. These motifs have been shown to be related to the receptor activation. We performed 3-μs molecular dynamics (MD) simulations of wild type and mutant receptors in explicit water. We will present the results of analysis of the trajectories by using the improved RMA method.

1F1532* **抗原ペプチドの硫酸化がペプチドー抗体間相互作用に与える影響の熱力学的解析**

Thermodynamic analysis of the effect of sulfation on a peptide-antibody interaction

Kazuhiro Miyanabe[1], Hiroki Akiba[2], Yuichiro Takamatsu[3], Takefumi Yamashita[3], Caaveiro Jose[4], Kouhei Tsumoto[1] ([1]*Sch. Eng., Univ. Tokyo*, [2]*NIBIOHN*, [3]*RCAST, Univ. Tokyo*, [4]*Grad. Sch. Pharm. Sci., Kyushu. Univ*)

To access how sulfation affects the dynamics of peptide-protein interactions, we studied an interaction between an anti-peptide antibody and the peptide antigen with or without a sulfatation. X-ray crystallography of the sulfated peptide-antibody complex was almost identical to that of the non-sulfated peptide-antibody complex. In contrast, isothermal titration calorimetry demonstrated that the affinity of the sulfated peptide was increased with the reduction of unfavorable entropy change. Interestingly, molecular dynamics simulations showed that the sulfation changed the secondary structure of the peptide before binding. Our results suggested that the sulfation affected the dynamics of the peptide before binding and hence minimized the loss of entropy upon binding.

1F1544* **Structure-based analyses of the interaction between the chemokine receptor-regulator FROUNT and novel anti-inflammatory compounds**

Soichiro Ezaki[1], Sosuke Yoshinaga[1], Norihito Ishida[1], Mitsuhiro Takeda[1], Kaori Yunoki[1], Yuya Terashima[2], Etsuko Toda[2], Kouji Matsushima[2], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*Grad. Sch. Med., Univ. Tokyo*)

Leukocyte chemotaxis is induced when chemokines bind to their receptors, which exist in the migration tip during inflammation. We previously identified the cytoplasmic regulator, FROUNT, which binds to the chemokine receptor CCR2, and obtained compounds (A and B) that inhibit the FROUNT—CCR2 interaction. The aim of this study is to optimize the compounds, based on the structural information of FROUNT—CCR2. We performed NMR titration analyses using FROUNT and compound A or B. Although their chemical structures are different, the binding regions on FROUNT were similar. Furthermore, their binding regions on FROUNT were in close proximity to the CCR2-binding region. We discuss whether the compounds function by allosteric inhibition, based on an NMR relaxation analysis.

1F1556 **Laser processing of protein crystals for native SAD data collection**

Ayaka Harada[1], Naohiro Matsugaki[1,2], Yoshiaki Kawano[3], Masaki Yamamoto[3], Toshiya Senda[1,2] ([1]*KEK, PF, Structural Biology Research Center*, [2]*The Grad. Univ. for Advanced Studies, School of High Energy Accelerator Science*, [3]*RIKEN/SPring8*)

Native SAD phasing uses anomalous scattering signals from light atoms such as sulfur and phosphorus in protein crystals. Here, we present a method minimizing the X-ray absorption; the solvent portion of a mounted frozen crystal is removed or the mounted crystal is spherically shaped by the deep UV laser processing technique. Diffraction data for native SAD phasing were collected with crystals in two times before and after the laser processing using X-ray of 3.7 keV and 4.5 keV at BL-1A of Photon Factory. The data statistics of the laser-processed crystals were much better: the values of I/sigma(I) and SigAno were significantly increased. The improvements are expected to work advantageously in phase determination by native-SAD method.

1G1320 **線虫 *C. elegans* の低温耐性から見た不凍タンパク質の機能解析、および生体内 X 線一分子観察**

In vivo* X-ray single molecule observation and functional analysis of antifreeze proteins for cold tolerance in *C. elegans

Masahiro Kuramochi[1], Chiaki Takanashi[1], Hiroshi Sekiguchi[2], Motomichi Doi[3], Sakae Tsuda[4], Yuji C Sasaki[1] ([1]*Grad. Sch. Front. Sci., Univ. Tokyo*, [2]*JASRI*, [3]*Biomedical R.I., AIST*, [4]*Bioproduction R.I., AIST*)

Antifreeze proteins (AFPs) can inhibit ice recrystallization in cells, and work as biological antifreeze materials in polar fishes. However, it is not clear how the single molecules of AFPs in living animal tissues function and affect the cold tolerance behavior. Here we evaluated that the cold tolerance behavior in the transgenic worm expressing AFPs. To monitor the AFP molecular dynamics in *C. elegans* tissues, moreover, we apply the Diffracted X-ray Tracking (DXT) capturing the single molecular dynamics at picometre and nanosecond accuracy to *C. elegans* tissues and cells. These analyses using *C. elegans* are provide us much insight for biological interpretation at the relationship between the single molecular dynamics and animal behaviors.

1G1332 **A mechanism of enzymatic activation of Cu/Zn-superoxide dismutase by its copper chaperone**

Yoshiaki Furukawa, Mami Fukuoka (*Dept. of Chemistry, Keio Univ.*)

Cu/Zn-superoxide dismutase (SOD1) is a metalloenzyme that disproportionates a superoxide radical. For enzymatic activity, SOD1 requires the binding of a copper ion and a zinc ion. A native SOD1 isolated in vivo is known to be fully metallated: i.e. one copper and one zinc ion per a SOD1 molecule. In contrast, reconstitution of SOD1 in vitro often results in the binding of sub-stoichiometric amounts of the metal ions; therefore, it remains obscure how SOD1 is fully metallated in vivo. Here, we have developed a new method to estimate the amounts of copper and zinc ions bound in SOD1 and proposed that proper zinc binding to SOD1 is required for binding the stoichiometric amounts of copper ions.

1G1344 **Pin1 の酵素反応におけるタンパク質ダイナミクスの重要性**

Crucial role of enzyme dynamics in the catalytic reaction mechanism of Pin1

Toshifumi Mori[1,2], Shinji Saito[1,2] ([1]*IMS*, [2]*SOKENDAI*)

Conformational flexibility is fundamental to proteins, and is also a key for functioning. Yet, how protein dynamics play a role in catalysis remains highly controversial. Moreover, most studies have focused on static and ensemble-averaged properties, while the dynamics has been overlooked.
To this end, here we study the Pin1 peptidyl-prolyl isomerase to understand the static and dynamic mechanism of the enzymatic reaction. We find that (1) the isomerization of the ligand occurs very rapidly within a few ps, (2) excited configuration state of Pin1 plays a fundamental role, and (3) the transition path is direction-dependent and possesses directionality. The findings are general and is expected to apply to broader enzymatic reactions.

1G1356*　ラン藻由来炭化水素合成関連酵素の活性と可溶性の向上
Improving activity and solubility of cyanobacterial enzymes for hydrocarbon biosynthesis

Hisashi Kudo, Yuuki Hayashi, Munehito Arai (*Dept. Life Sci., Univ. Tokyo*)

Both acyl-(acyl carrier protein) reductase (AAR) and aldehyde deformylating oxygenase (ADO) are key enzymes for cyanobacterial synthesis of hydrocarbons that can be used as biofuels. Because these enzymes have very low catalytic activities, it is important to identify the residues essential for the activities. Here, by introducing amino-acid substitutions, we identified the residues essential for the solubility and activity of AAR. Moreover, by introducing multiple amino-acid substitutions, we succeeded in creating the AAR mutants that can produce high amounts of aldehydes. We also investigated the residues essential for the activity and solubility of ADO, which converts aldehydes into hydrocarbons. We believe that these data are useful for improving biofuel production.

1G1408*　生細胞直接円偏光二色性測定によるシトクロム c 内多核ヘムの配置変化の追跡
Circular Dichroism Spectroscopy of Living Microbe Reveals Redox-Triggered Conformational Change of Heme Cofactors in Cytochromes c

Yoshihide Tokunou[1], Punthira Chinotaikul[1], Shingo Hattori[2], Kazuhito Hashimoto[3], Kazuyuki Ishii[2], Akihiro Okamoto[3] ([1]*Department of Applied Chemistry, School of Engineering, The University of Tokyo*, [2]*Institute of Industrial Science, The University of Tokyo*, [3]*National Institute for Materials Science*)

In this study, we developed the method to directly apply circular dichroism (CD) spectroscopy to living Shewanella oneidensis MR-1, which reflect the dynamics of cytochromes c complex located at outer-membrane (OMCs) in vivo. Once the OMCs is reduced by metabolic electrons, the CD amplitude increased over twice, indicating that electron injection into OMCs triggers conformational change of heme cofactors from oxidized state. Notably, the CD amplitude of reduced OMCs in living MR-1 was distinct from purified OMCs in reduced state, strongly suggesting that non-equilibrium condition in life further arrange the conformation of OMCs. In the presentation, we will discuss about conformation of hemes using CD spectrum of OMCs deletion mutant and TD-DFT calculation.

1G1426*　基質 DNA の長さ、濃度、及び標的配列位置が APOBEC3F の脱アミノ活性に及ぼす影響
Influences of length and concentration of the DNA substrate, as well as the location of the target sequence, on deamination by APOBEC3F

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APOBEC3F (A3F) deaminates cytosine to uracil in single-stranded (ss) DNA and is recognized to have an anti-HIV-1 activity. We analyzed the effects of the ssDNA length and concentration, as well as the target location, on the deamination of the C-terminal domain (CTD) of A3F. When ssDNA concentration is low, A3F-CTD prefers to react with longer ssDNAs over shorter ones. This length-dependency reverses when the ssDNA concentration is high. Examination of location-dependency showed that A3F has no polarity for deamination preference, which is different from the characters of well-studied A3G. These unique properties of A3F-CTD can be rationally interpreted by considering the positive and negative effects of neighboring DNA regions on search of the target site by A3F-CTD.

1G1438*　(6-4)光回復酵素の光反応過程における基質特異性に関する赤外分光研究
FTIR study of photoreaction of Xenopus (6-4) photolyase on substrate specificity

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(6-4)photolyase ((6-4)PHR) is a flavoprotein that repairs the (6-4) photoproduct. (6-4)PHR can repair both T(6-4)T and T(6-4)C, where the OH and NH_2 groups are bound at C5 position of 5' side, respectively. We have reported light-induced difference Fourier-transform infrared (FTIR) spectra in the photoreaction processes of *Xenopus* (6-4)PHR. Here, we compared the FTIR spectra for T(6-4)T and T(6-4)C to investigate the structural perturbation and the transfer of different functional groups. In addition, time-dependent illumination measurements of enzyme and substrate with different stoichiometries were used to distinguish signals between protein and DNA.

1G1450*　3D-RISM 計算での溶媒分布と MD から導く EcoRV の DNA 切断反応における水分子と Mg2+の役割
Role of Mg2+ ion and water in DNA hydrolysis by EcoRV, studied by 3D-RISM and MD

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Our goal is to elucidate the role of Mg2+ ion and water in DNA hydrolysis by homodimeric restriction enzyme EcoRV. We found the position called site IV† by us in the X-ray complex structure 1rvb from the calculated distribution of Mg2+ ion by using 3D-RISM. MD simulations with the initial structure having two Mg2+ ions at site I* and IV† were used to obtain an equilibrium complex structure, where the scissile phosphate was rotated to orient the O-P direction toward the water nucleophilie. The final MD structure is similar to the X-ray BamHI-DNA complex structure (2bam). Furthermore, we have obtained a trigonal bipyramidal structure, which is an intermediate structure in associative reaction mechanism, by QM/MM MD simulation.

1G1502　An arginine side chain in the (6-4) photolyase governs formation of a robust repair-active complex with UV-damaged DNA

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The (6-4) photolyase is a flavoprotein that repairs UV-induced DNA damage using blue light in sunlight. The key process for its photorepair is the electron transfer from the excited state of flavin to the lesions. For the efficient electron transfer, the lesion should be flipped out of the DNA duplex and properly accommodated into the active site.
In this study, we mutated amino acid residues of Xenopus (6-4) photolyase, which were located proximal to the lesions, and comprehensively characterized their binding and photorepair abilities. We found that a mutation of arginine into alanine significantly reduced binding and photorepair abilities. Theoretical calculation supported the presence of the electrostatic interaction between arginine and DNA.

1G1514 RecA Nucleoprotein Filament Formation on SSB-wrapped DNA Includes RecA-SSB Interaction

Hung-Yi Wu, Chih-Hao Lu, **Hung-Wen Li** (*National Taiwan University*)

RecA recombinase catalyzes homology pairing and strand exchange reactions in homologous recombinational repair. RecA must first compete with single-stranded DNA binding proteins (SSB) for ssDNA substrates to form nucleoprotein filaments. It has been suggested that RecA assemble mainly by binding onto free ssDNA not covered by SSB. Using the tethered particle motion method, we monitored individual RecA assembly on SSB-wrapped ssDNA in real-time. Nucleation times of RecA E38K assembly showed no apparent difference of different ssDNA lengths (60-100 nts) wrapped by one SSB. Our data have shown an unexpected RecA assembly mechanism in which direct RecA-SSB-ssDNA interaction exists. Thus, a direct RecA-SSB interaction should be included in RecA regulatory mechanism.

1G1532 テロメア長短縮をもたらす TLS/FUS 蛋白質とテロメア DNA および TERRA のグアニン四重鎖との複合体に関する NMR 解析
NMR studies for the complex of TLS/FUS protein and G-quadruplexes of telomeric DNA and TERRA, which induces telomere shortening

Keiko Kondo[1], Tsukasa Mashima[1,2], Takanori Oyoshi[3], Riki Kurokawa[4], Naohiro Kobayashi[5], Takashi Nagata[1,2], Masato Katahira[1,2] ([1]*Institute of Advanced Energy, Kyoto University*, [2]*Graduate School of Energy Science, Kyoto University*, [3]*Department of Chemistry, Shizuoka University*, [4]*Research Center for Genomic Medicine, Saitama Medical University*, [5]*Institute for Protein Research, Osaka University*)

Translocated in liposarcoma protein (TLS/FUS) binds to the G-quadruplexes of telomeric DNA (Telo) and telomeric repeat-containing RNA (TERRA), which leads to telomere shortening. However, the structural basis for the DNA/RNA recognition by TLS is yet to be elucidated. Phe and Tyr residues in RGG3 motif in the C-terminal region of TLS is essential for the recognition of Telo and TERRA, respectively. NMR analyses of the ternary complex confirmed the preferential binding of Phe and Tyr residues to Telo and TERRA, respectively. While in the binary complexes, RGG3 was found to interact with either Telo or TERRA by using both Phe and Tyr residues. We propose that Phe and Tyr residues have a dual role in engaging DNA and/or RNA G-quadruplex depending on the context.

1G1544 The mechanism of R42me2a promoting the transcription

Zhenhai Li, Hidetoshi Kono (*QST*)

The post-translational modifications (PTMs) on histone proteins regulate the gene expression. The PTM in the DNA entry/exit region, R42 asymmetric dimethylation (R42me2a) promotes gene expression. However, the mechanism is still unclear. To address this mystery, we carried out comprehensive molecular dynamics (MD) simulations on a single nucleosome with/without R42me2a. The MD simulation suggested that R42me2a will greatly reduce the interaction of H3 histone and DNA duplex. In addition we proposed a DNA sliding model. Based on the theoretical model and MD simulation results, we predict that the loss of the interaction of these amino acids to DNA duplex would significantly enhance the nucleosome unwrapping at the entry/exit region by using Monte Carlo methods.

1G1556 Modeling Sequence-Specific Protein-DNA Interaction from High-Throughput Experiments

Cheng Tan, Shoji Takada (*Graduate School of Science, Kyoto University*)

Recent high-throughput experimental techniques such as protein-binding microarrays have provided comprehensive information about the specificity for DNA-binding proteins, expressed in form of the Position Weight Matrix (PWM). Here we developed a new method of coarse-grained modeling of the sequence-specific protein-DNA interactions based on PWM and PDB structure. Applying it to several DNA-binding proteins in molecular dynamics simulations, we illustrated the ability of our model to capture the most subtle features in protein-consensus DNA recognition. Besides, our model can also be extended to study the dynamics of protein binding to weaker motifs, such as the reorientation of proteins and protein charge distribution dependent energetic frustration.

1G1608 Proteomic analysis of the lncRNA-protein complexes in colon cancer cells

Lumi Negishi, Kenzui Taniue, Yoshihiro Kawasaki, Kosuke Matsumura, Akiko Takahashi, Tetsu Akiyama (*IMCB., Univ. Tokyo*)

Long noncoding RNAs (lncRNAs) play critical roles in various biological processes, including proliferation, development and tumorigenesis. We have previously shown that the lncRNAs *MYU*, *GSEC* and *UPAT* are required for the proliferation and tumorigenicity of colon cancer cells. In the present study, we perform LC-MS/MS analysis and show that *MYU*, *GSEC* and *UPAT* interact with hnRNP-K, DHX36 and UHRF1, respectively. *MYU* interacts with hnRNP-K to stabilize CDK6 expression, and thereby promotes the G1-S transition of the cell cycle. *GSEC* inhibits the helicase activity of DHX36. *UPAT* inhibits ubiquitination and degradation of the epigenetic factor UHRF-1. These results clearly show that proteomic analysis provides novel insights into the functions of lncRNAs.

1H1320 Actin polymerization signal emitted at the raft nanodomains of the clusters of the anthrax-toxin-receptor complex: a single-molecule study

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The binding of a key subunit of the anthrax toxin for toxin internalization by the cell, called protective antigen (PA), to its cellular receptor (CMG2) induces the clustering of the PA-receptor complex, which is the first step for the toxin invasion into the cell. Here, using single molecule tracking, we found that PA-receptor complex clusters (PARCC) dynamically recruit gangliosides, raftophilic molecular species, with their exponential residency times of 0.2~0.5 s (which prolong with an increase of the cluster size), suggesting that PARCC induces raft-like domains. This further induced dynamic recruitment of N-WASP and Arp2/3, molecules involved in actin polymerization with similar residency times. Such actin polymerization might be involved in PARCC internalization.

1H1332 Functional signaling-fluorescent fusion protein for the dynamics of signaling pathway in E.coli

Ryota Shiono, Akihiko Ishijima, Hajime Hukuoka (*Grad. Sch. Frontier Biosci., Osaka Univ*)

Recently, we suggest the dynamic change in CheY-P concentration due to the receptor's activity directly regulates the rotational direction of motors. To validate this hypothesis, we focused on the localization of CheY to receptor because localization of CheY is influenced by the activity of CheA and CheW in cell pole. However, our previous CheY-GFP having 6 amino acid linker (L6) did not cause switching coordination between motors. Therefore, we searched amino acid linkers to develop full functional CheY-FP. The CheY-L3-FP did not work, however, the CheY-L10-FP generated the switching coordination, indicating this construct have function. We would like to simultaneously observe the change in CheY localization and in the rotational direction of motors as the next step.

1H1344 高速 AFM によるダイナミン 1ーアンフィファイジン複合体の動態観察
High-Speed AFM imaging of dynamics of Dynamin1-Amphiphysin1 complexes

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Dynamin is a mechanochemical GTPase required for membrane fission in endocytosis. Dynamin forms a higher ordered "helical" structure which cuts membrane in a GTP hydrolysis-dependent manner. However, precise mechanism of membrane fission by Dynamin remains to be elucidated.
In this study, we applied high-speed atomic force microscopy (HS-AFM) to analyze the Dynamin-mediated membrane fission. Using cell-free system consisting of liposomes and proteins, we succeeded in observing membrane tubulation and fission process, and found a novel dynamics such as diffusion and clustering of Dynamin complexes on lipid membrane tubules. In the presentation, we will discuss relationship between mechanisms of the Dynamin-mediated membrane fission and clustering of Dynamin complexes.

1H1356 高速 AFM による生細胞表面の分子イメージング
Molecular imaging on living bacterial cell surface by high speed AFM

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High speed atomic force microscopy (HS-AFM) is powerful tool which visualize the dynamic molecular process in physiological condition. Recently, this technique has also been applied for molecular imaging on living cell surface [1, 2]. However, the spatiotemporal resolution of HS-AFM for cell surface imaging is not sufficient compared with that of purified protein.
In this study, we developed new HS-AFM scanner with both coarse and fine motion, and applied it for observing bacterial cell surface. High resolution AFM images showed partly regular arrangement of outer membrane porin trimers. This technique will be useful to investigate dynamic molecular architectures on a living cell surface.
[1] Yamashita et. al, (2012) J. Mol. Biol. [2] Oestreicher et. al, (2015) Micron

1H1408 First evaluation of permeabilities across the actin-based compartment barriers in the plasma membrane

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Previously, we showed that all diffusing molecules in the plasma membrane undergo short-term confined diffusion within ~100-nm compartments delimited by actin membrane skeleton mesh and long-term intercompartmental hop movements, by analyzing single-molecule trajectories of a 25-μs resolution. However, our analysis of the trajectories failed to provide the permeability of the compartment barrier, a critical parameter for hop diffusion. Here, by using the analytical solution of diffusion equation in the presence of equally-spaced equipotential barriers, we were able to obtain compartment sizes and macroscopic diffusion coefficients that agreed with our previous results, showing the method worked well. The method provided the permeability, which we needed for years.

1H1426* メカノストレスによる歯周組織リモデリング機構の解明
Effects of Mechanical Stress on Remodeling of Periodontal Ligament

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Periodontal ligament (PDL), which connects the teeth to the alveolar bone, is always exposed to mechanical stress such as occlusal force at biological range (~MPa). However, the mechanism of remodeling of PDL in a molecular level is poorly understood. Here we study the effect of pressure on PDL fibroblasts. We used high hydrostatic pressure microscope to observe PDL fibroblasts under high pressure in real time. As a result, high hydrostatic pressure (> 20 MPa) contracts PDL fibroblasts and actin stress fibers. Furthermore, contracted cells restart spreading on the surface after high pressure releasing process. Our data suggest excessive occlusal force induces the collapse of PDL and occlusal force at biological range affects homeostasis of PDL.

1H1438 加圧・脱圧による芽胞ジピコリン酸の流出：高圧 NMR によるリアルタイム観測
How can pressure release DPA from bacterial spores? A study by high pressure NMR

Kazuyuki Akasaka[1], Akihiro Maeno[2], Kenji Kanaori[3], Akira Yamazaki[4] ([1]*Kyoto Prefectural University of Medicine*, [2]*Kansai Medical University*, [3]*Kyoto Institute of Technology*, [4]*Echigoseika Co.*)

A bacterial spore protects itself with an unusually high concentration (~10 per cent) of dipicolinic acid (DPA), the release of which is crucial for its inactivation. We have monitored the process of pressure-mediated DPA release from spores of Bacillus subtilis natto directly and in real-time with high-pressure NMR upon pressurizing to or depressurizing from 200 MPa at 20 degrees C. After releasing DPA, the spores become easily inactivated at temperatures much below 121 degrees C. The success of the present experiment opens a new avenue for investigating not only the state of bacterial spores, but of biological cells in general directly at the molecular level.

1H1450 光照射によるインアクティブな珪藻細胞の刺激
Stimulation of inactive diatom cells by light irradiation

Umemura Kazuo[1], Shunsuke Kondo[1], Yoshikazu Kumashiro[2], Shigeki Mayama[3] ([1]*Tokyo Univ Sci*, [2]*Tokyo Women's Medical University*, [3]*Tokyo Gakugei University*)

Simulation of living diatom cells by light irradiation was investigated. Small colonies in a microchamber were irradiated under the following three wavelengths and brightness conditions: (1) 400-440 nm/68500 lux, (2) 470-490 nm/50900 lux, (3) 520-550 nm/383000 lux. The same cell was continuously observed for 600 s although the irradiation was started at t = 100 s and stopped at t = 200 s. Although the diatom cells were activated and glided in the microchamber by the irradiation, it was not continued when the irradiation was stopped in the case of condition (1). Instead, the gliding was continued even after stopping the irradiation in the conditions (2) and (3). Our data revealed that stimulation of diatom cells was affected by the irradiation conditions.

1H1502* 滑走するヒト肺炎原因菌 *Mycoplasma pneumoniae* の“あし”P1 adhesin
P1 adhesin, the leg for gliding of *Mycoplasma pneumoniae*

U Matsumoto[1], Akihiro Kawamoto[2], Takayuki Kato[2], Yoshito Kawakita[1], Tsuyoshi Kenri[3], Shigetaro Mori[3], Keiichi Namba[2,4], Makoto Miyata[1,5] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Grad. Sch. Front. Biosci., Univ. Osaka*, [3]*Dept. Bacteriology II, NIID*, [4]*QBiC, RIKEN*, [5]*OCARINA, Osaka City Univ.*)

Mycoplasma pneumoniae glides through repeated binding of sialylated oligosaccharides on host cells by P1 adhesin, a 170 kDa “leg” protein. A recombinant P1 adhesin (rP1) consisting of domains I+II of three was analyzed. rP1 showed specific binding activity on sialic acids in bead assay. A 3D image with 9 Å resolution was reconstructed from 174,848 particle images of rP1 by cryo-electron microscopy, showing a novel shape as a sialic acid receptor (the first three authors contributed equally). We found a conserved region of about 60 amino acids featured by three highly conserved amino acids based on the amino acid sequences of p1 8 alleles and 70 orthologs. Studies on the position of conserved region on the 3D structure and the assembly of the P1 complex are under way.

1H1514* 非熱的に駆動された細胞内部の混み合いガラス状態
Molecular crowding glass driven by metabolic activity in cells

Kenji Nishizawa, Daisuke Mizino (*Dept. of Phys., Kyushu Univ.*)

Intracellular molecules are crowding and driven by metabolic activity. We therefore investigated the effects of molecular crowding and activity on cell mechanics. At first, we prepared cell extract. Viscosity of cell extracts rapidly increased as the protein concentration becomes higher. Furthermore, viscosity in living cells were measured with changing the volume fraction of intracellular macromolecules by increasing the osmotic pressure of the culture media. These behaviors between viscosity of cell extracts and that in living cells shows apparent different character. We think that this difference originate from metabolic activity in cells. Viscoelastic properties in activity deficient cells were measured to study the effect of activity on cell mechanic.

1H1532* NF-κB 転写因子の細胞質 - 核内移行の一細胞動態はその発現量によって自己制御される
Single-cell cytoplasmic-nuclear shuttling of transcription factor NF-κB is auto-regulated by the expression level

Yu Miyamoto[1], Tetsuro Ariyoshi[2], Takehiko Inaba[3], Kazunari Iwamoto[4], Koji Hase[1], Yasushi Sako[3], Yasushi Okada[2], Mariko Okada[4] ([1]*Keio Univ. Parmacy*, [2]*RIKEN QBiC*, [3]*RIKEN Wako*, [4]*Osaka Univ. Protein Research*)

Stimulus-dependent NF-κB nuclear translocation is essential for the target gene expression. Our previous study suggested that cellular NF-κB abundance might affect oscillatory dynamics of the translocation. In this study, using single-cell fluorescence microscopy, we studied how the differences in NF-κB abundance regulate the nuclear translocation in model immune B cells. When mEGFP-tagged NF-κB was overexpressed about 50-fold greater than endogenous levels, it translocated to the nucleus on stimulation, and rarely returned to the cytoplasm. However, when mEGFP-NF-κB was expressed almost the same levels as endogenous levels, nucleocytoplasmic shuttling was clearly observed. These results indicate that the abundance of NF-κB is pivotal to determine NF-κB dynamics.

1H1544* 誘引場への追従性能と細胞の前後極性から理解する好中球様 HL60 細胞の走化性運動
Chemotactic analysis of neutrophil-like HL60 cells based on cells' persistent polarity and immediate responsiveness to chemoattractant

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Neutrophils chemotaxis is thought to be dictated by a mechanism that senses difference in the chemoattractant concentration across the cell body. However, concentration differences in space is dynamically changing in vivo such as inflammation. Therefore, it is important to characterize neutrophils' chemotactic ability under dynamic chemoattractant gradient. Here, we show that neutrophil-like HL60 cells exhibit forward movement and concomitant Akt-PH and Cdc42-GTP translocation only in the rising phase of a propagating fMLP gradient. Furthermore, based on pharmacological experiments, there seems to be different roles of Rho GTPase at the leading edge, one that detects temporal change of chemoattractant gradient and the other that contributes to front-rear polarity.

1H1556* 植物細胞内でシロイヌナズナアクチンアイソフォーム（ACT2, ACT7）は異なった局在を示す
Arabidopsis vegetative actin isoforms, ACT2 and ACT7, show distinct localization in a living plant cell

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Flowering plants express multiple actin isoforms and several studies suggest that individual actin isoforms perform distinct roles. Little is known, however, about the subcellular localization of actin isoforms. Here, we constructed plasmids for the transient expression of individual Arabidopsis actin isoforms fused with a fluorescent protein, and successfully observed filaments in living Nicotiana benthamiana mesophyll cells. Surprisingly, two major vegetative actin isoforms (ACT2 and ACT7) tended to polymerize into different types of filaments. ACT2 formed longer and thinner filaments than ACT7, suggesting that different functions of actin isoforms, at least in part, depend on differential localization. We will present results of further detailed observations.

1H1608*　大腸菌走化性受容体クラスターにおける状態発振モデルの作成

Computational simulation of spontaneous transition between active and inactive in whole chemoreceptor array in *E. coli*

Tatsuki Hamamoto[1], Takashi Sagawa[2], Shin Koguchi[3], Hajime Fukuoka[1,3], Akihiko Ishijima[1,3] ([1]*Sch. Eng. Sci., Osaka Univ*, [2]*NICT*, [3]*Grad. Sch. Frontier Biosci., Osaka Univ*)

Recent our studies suggested the receptor array repeatedly change between active and inactive states without extracellular stimuli. To explain this behavior, we constructed the computational model for receptor array's activity. Each receptor has active or inactive states, and both states has also methylated or not. We considered high cooperativity in receptor array; both active to inactive and inactive to active transition were affected by surrounding other receptors states. Our model showed that the receptor array repeatedly changed between active and inactive states spontaneously and well fitted the average CW and CCW duration time. This model represents the inhibition of the cooperative manner by the insertion of receptor mutant, which was shown in experimentally.

1I1344*　海洋性真核藻類がもつ光駆動カチオンチャネル *Gt*CCR4 の分光解析

Spectroscopic analysis of a light-gated cation channel *Gt*CCR4 from marine algae

Yumeka Yamauchi[1], Masae Konno[1,2], Shota Ito[1], Satoshi Tsunoda[1,2,3], Keiichi Inoue[1,2,3,4], Hideki Kandori[1,2] ([1]*Life Sci. Appl. Chem., Grad. Sch. Eng., NIT*, [2]*OBTRC, NIT*, [3]*PREST, JST*, [4]*FRIMS, NIT*)

Microbial rhodopsins are membrane proteins with retinal as a chromophore. Light-driven archaeal proton pumps have a characteristic DTD motif. One aspartic acid functions as a proton donor and the other serves as an acceptor to realize unidirectional ion transport. Recently, some channelrhodopsins containing the DTD motif (DTD-CCRs) were found from cryptophyta *Guillardia theta* (*G. theta*). We studied molecular properties of another DTD-CCR from *G. theta* (*Gt*CCR4). Electrophysiological measurements showed that *Gt*CCR4 worked as a light-gated cation channel. Flash photolysis and low-temperature FTIR analyses suggest that the channel mechanism of DTD cation channel differs from that of CCRs from *Chlamydomonas reinhardtii*. We will discuss molecular mechanisms of *Gt*CCR4.

1I1320*　新たに発見された光駆動型外向きプロトンポンプ DTS ロドプシンの機能解析と分光研究

Functional analysis and spectroscopic study of newly discovered light-driven outward proton pump DTS rhodopsins

Chihiro Kataoka[1], Keiichi Inoue[1,2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*PRESTO, JST*)

Genomic analysis revealed new types of proton pump rhodopsins from various bacterial species. Here, we newly studied report a group of rhodopsins with "DTS motif", in which the acidic residue of proton donor of typical proton pump rhodopsin is replaced with a serine. The ion-transport property and the mechanism were not revealed for these rhodopsins. Thus, we studied their ion-transport functions and the mechanisms by functional assay and spectroscopic methods. The pump activity measurement showed that DTS rhodopsin has a proton pump function. The results of flash photolysis indicate that it takes up proton directly from cytoplasmic side to the retinal Schiff base. We investigated several mutants of DTS rhodopsin and the results willould be shown in the presentation.

1I1356　KR2 の Na^+輸送経路に位置する水分子の構造変化

Structural Changes of Water Molecules in the Na^+ Transport Pathway of KR2

Sahoko Tomida[1], Shota Ito[1], Keiichi Inoue[1,2], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*PRESTO, JST*)

KR2 is a light-driven Na^+ pump containing the unique NDQ motif, where Q123 is located near the intracellular entrance of the Na^+ transport pathway. Hydrophobic mutation on Q123 showed decreased Na^+ transport activity, suggesting that it constitutes important hydrogen-bonding structure for Na^+ transport, though its structural information remains unclear. In this study, we applied low-temperature light-induced different FTIR spectroscopy at 77 K to study structural changes between the dark state and the K intermediate. We analyzed structural changes of retinal, peptide backbone and protein bound water molecules to obtain the insight of hydrogen bonding network around Q123. Role of water molecules near Q123 for Na^+ pump will be discussed.

1I1332*　FTIR study of the T94I rhodopsin mutant in night blindness

Akiko Enomoto[1], Kota Katayama[1], Hiroo Imai[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*Primate Res. Inst., Kyoto Univ.*)

Rhodopsin is the photosensitive protein, which binds 11-cis-retinal. In the dark, rhodopsin is stabilized in an inactive state, and activated by light to initiate our vision. Therefore, the increase of the rate of dark activation in rhodopsin reduces the photosensitivity resulting in night blindness. T94I is also known as night blindness causing mutation, and this exhibits high rate of retinal thermal isomerization and dark activation. In the present study, to elucidate the molecular mechanism eliciting these properties, we measured light-induced difference FTIR spectra of T94I. We found the alteration of hydrogen bonding network around retinal, suggesting that this change induced a structural fluctuation of retinal binding pocket leading dark activation of rhodopsin.

1I1408　低温赤外分光法を用いた(6-4)光産物の修復中間体の測定

Low-temperature FTIR study of the repair processes by Xenopus (6-4) photolyase

Daichi Yamada[1], Junpei Yamamoto[2], Tatsuya Iwata[3], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*Grad. Sch. Eng. Sci., Osaka Univ.*, [3]*Fac. Pharm. Sci., Toho Univ.*)

(6-4) photolyases ((6-4) PHRs) are DNA repair enzymes that specifically revert UV-induced (6-4) photoproducts into normal bases to maintain genetic integrity. (6-4) PHRs catalyze a hydroxyl and amino group transfer for thymine and cytosine, respectively, to which various mechanisms have been postulated. Here, we attempted to monitor the repair intermediates by use of low-temperature FTIR spectroscopy. We successfully obtained light-induced difference spectra, which differ from the repair spectrum measured at room temperature. The obtained temperature-dependent spectra presumably include structural information during repair. Molecular mechanism of the repair by (6-4) PHR will be discussed based on the first structural information of the repair intermediates.

1I1426* 過渡回折格子法を用いた光センサータンパク質 EL222 の DNA 結合反応測定
Transient grating method revealed a DNA binding process of a light sensor protein EL222

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EL222 is a light dependent transcriptional regulator protein containing a light sensing domain (LOV) and a DNA binding domain (HTH). While previous reports suggested that the light stimulation of EL222 enhances the DNA binding, the reaction dynamics has not been revealed. In this study, we investigated the reaction dynamics of the DNA binding process by using the transient grating method. We detected the binding process as a reduction of the diffusion coefficient and determine the reaction rate constants. Interestingly, the reaction rate constant of the DNA binding step was independent of the sequence of the DNA fragments. This result indicates that the dissociation rate is a dominant factor for determining the affinity to the target DNA.

1I1438 光回復酵素/クリプトクロムファミリーにおける FAD 酸化還元制御メカニズム研究
The redox control mechanism of FAD in Photolyase/ Cryptochrome family

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Photolyase/cryptochrome family proteins are FAD-binding proteins that perform different functions in different organisms, despite structural homology. Their different functions are related to the redox states of FAD, which are controlled by protein environments. Our FTIR study showed that the hydrogen bond between the FAD N5-H group and the proximal Asn is strongest in the semiquinone form, presumably stabilizing the radical state. 1 In this study, we performed FTIR analysis of cryptochrome-DASH to examined the hydrogen bonding environment because the anionic fully-reduced form is quite stable. Mechanism of the redox control of FAD will be discussed on the basis of the present spectroscopic observations.

[1] Wijaya et al., J. Am. Chem. Soc. 138, 4368 (2016)

1I1450 分光法と QM/MM 計算を用いた Photoactive Yellow Protein 活性部位の構造解析
Active Site Structures of Photoactive Yellow Protein Revealed by Spectroscopy and QM/MM Calculations

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We have used quantum mechanical/molecular mechanical (QM/MM) methods to predict several spectroscopic data for photoactive yellow protein (PYP). PYP is a bacterial blue-light receptor and contains *p*-coumaric acid as a chromophore. We have computed the NMR, UV-vis, and vibrational spectroscopic data for PYPs from *Halorhodospira halophila* and *Rhodospirillum centenum* on the basis of the crystal structures. The computed spectroscopic data agree well with the corresponding observed data. These results indicate that spectroscopic investigations combined with QM/MM calculations provide detailed structural information on the active site of photoreceptor proteins.

1I1502* Acquirement of the water splitting ability and uni-directionality of the electron transfer pathway in O_2-evolving photosystem II

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Type II photosynthetic reaction centers (RC), including bacterial reaction centers (bRC) and photosystem II (PSII), convert light energy into electrochemical energy.
In both RCs, redox active cofactors are arranged along the pseudo-C2 axis, which apparently show two electron transfer pathways, A- and B-branches. However, only A-branch is electron-transfer active.
Solving the Poisson-Boltzmann equation based on the crystal structures (1, 2), we calculated the redox potential values of chlorophylls in both RCs. Our results show that uni-directional electron transfers occur in both RCs but in different mechanism, which were highly associated with the ability/ inability in splitting water molecules.

(1) Fujii et al., PDB ID: 3I4D (2010)
(2) Umena et al., Nature, 473, 55 (2011)

1I1514* フェムト秒過渡吸収分光による光化学系 II dimer のサブユニット間エネルギー移動ダイナミクスの解明
Intersubunit Energy Transfer Dynamics of Photosystem II Dimer Revealed by Femtosecond Transient Absorption Spectroscopy

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Photosystem II (PSII) is one of the representative natural systems of the membrane-protein complex, which plays a crucial role in primary processes in photosynthetic reaction. PSII consists of antenna polypeptides and D1/D2 reaction center (RC) polypeptides. Although the typical PSII takes a dimeric form, detailed functionalities of the dimer have not yet been elucidated. In the present work, we have investigated the role of the dimer by comparing the dynamics of PSII monomer and dimer by means of femtosecond transient absorption (TA) spectroscopy.

1I1532* The pH-Dependent Optical Property of Chlorophyll c bound to the Light-Harvesting Complex from a Diatom, Chaetoceros calcitrans

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Chlorophyll (Chl) c is one of the pigments bound to the major photosynthetic pigment-protein complex of diatom, FCP. Its energetic involvement to the light harvesting system, however, hasn't been clarified yet. Recently, we revealed that the optical properties of isolated Chl c in aqueous ethanol are affected by the protonation of its acrylate moiety. In this study, we examined these effects of Chl c when it is bound to the FCP. Changes in absorption, circular dichroism and fluorescence excitation spectra of the FCP purified from diatom, Chaetoseros calcitrans, were precisely compared in the buffering solution having different pH values. From the observation, we concluded that the acrylate moiety of Chl c keeps free acid from even bound to the FCP protein.

1I1544* 光依存的に環状ヌクレオチド分解活性を示す新規酵素型ロドプシン

A novel enzyme rhodopsin with light- dependent cyclic nucleotide phosphodiesterase activity

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We recently reported on a novel type of microbial rhodopsin containing C-terminal cyclic nucleotide phosphodiesterase (PDE) domain which degrades the ubiquitous second messengers cGMP and cAMP. Though Rh-PDE is constitutively active in the dark, illumination increased its hydrolytic activity toward both cGMP and cAMP, when studied in heterologous expression systems. Thus Rh-PDE may hold promise as a potential optogenetic tool for light control of intracellular cyclic nucleotides, for example, to study cyclic nucleotide-associated signal transduction cascades. However improving feasibility of Rh-PDE for optogenetics application is required. We here attempted to minimize constitutive activity and to change substrate specificity of Rh-PDE by mutation studies.

1I1556* タンパク質間 NO 転移反応を用いた SNO タンパク質の合成及びその機能の光制御

Photocontrol of SNO protein modified by protein-to-protein transnitrosylation

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We report a novel method to synthesize nitrosylated proteins using nitrosylated metallothionein (SNO-MT) and its application to photo-control of structure and sugar-binding activity of human galectin-1 (hGal-1) with NO dissociation. hGal-1 has sugar-binding activity and we succeeded in preparing nitrosylated hGal-1 (SNO-hGal-1) in which S-H bonds of Cys are nitrosylated by SNO-MT with high purity. When UV or green light is irradiated to SNO-hGal-1, intramolecular S-S bonds are generated by NO photodissociation and structural changes consecutively occurs to the oxidized hGal-1 whose sugar-binding activity is 1/10 or less than that before photoirradiation. Cell aggregation formed by SNO-hGal-1 is also shown to be photo-controlled to be monomer species by NO dissociation.

1I1608 光制御型 bZIP モジュール Photozipper の構造変化の分子機構

Molecular mechanisms for the conformational switching of a light-regulated bZIP module, Photozipper

Osamu Hisatomi (*Grad. Sch. Sci., Osaka Univ.*)

An engineered light-activatable bZIP module named “Photozipper (PZ)” consists of a bZIP domain and a LOV domain of aureochrome-1. Blue light triggers conformational change of LOV domain, which induces dimerization and subsequent DNA-binding of PZ. To elucidate the molecular mechanism of PZ, we prepared about 40 site-directed mutants in which amino acids in the LOV domain were substituted. Substitutions of hydrophobic residues on the β sheet surface of LOV core region significantly affected the dimerization and DNA-binding of PZ mutants. Photosignal received by LOV core is likely propagated through the conformational change of hydrophobic surface on the β sheet.

1J1320 時計タンパク質概日リズムを表現する素過程ベースの反応モデル

An elementary-process-based reaction model of the circadian rhythm of clock proteins

Shin-ichi Koda[1,2], Shinji Saito[1,2] ([1]*IMS*, [2]*SOKENDAI*)

Clock proteins of cyanobacterium, KaiA, KaiB, and KaiC, show a periodic phosphorylation with 24-hour period in the presence of ATP. To elucidate circadian rhythms in biological systems, several mathematical reaction models of the Kai proteins have been proposed so far. However, these models are vastly simplified so as to extract universality among general biological oscillations, and there are only a few models explaining how elementary processes and reactions in Kai proteins create the circadian rhythm. The present study, on the other hand, constructs a reaction model of Kai proteins by choosing some important elementary processes from experimental results and combining them, and discusses an origin of the periodic phosphorylation.

1J1332* Kai タンパク質間相互作用のリン酸化状態依存性による概日周期の安定性への影響

The influence of phosphorylation states dependence of Interaction between Kai proteins on stability of the circadian cycle

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The circadian rhythm in cyanobacteria is generated by an oscillator composed of three Kai proteins (KaiA, KaiB and KaiC). The Kai system is unique because the self-sustainable oscillation of KaiC phosphorylation can be reconstructed in vitro only by incubating Kai proteins and ATP. Recently, we found that the affinity between KaiC and KaiA depends on the phosphorylation state of KaiC through single-molecule and real-time observation with HS-AFM. We studied a role of phosphoform-dependent differential affinity (PDDA) of KaiA for KaiC on the circadian rhythm by using employed Monte Carlo simulation. The simulation results suggested that PDDA broadens the concentration range of Kai proteins and can explain how the oscillation is resilient to intrinsic and extrinsic noise.

1J1344 空間形状による Min たんぱく質の非線形波のコントロール

Geometric control of wave instability in Min oscillations

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Emergence of patterns in biological systems has attracted much attention among broad areas in science to understand the generic mechanism of biological functions associated with these patterns. The Min systems have been studied intensively due to their robust realisation both in vivo and vitro systems. Stimulated by these experiments, theoretical models using nonlinear reaction-diffusion equations have been proposed. Nevertheless, the theoretical understanding of Min pattern is still incomplete. In particular, a generic view of geometric effects on the pattern is required to answer whether travelling or standing (pole-to-pole) wave is chosen. Here, we consider waves on curved surface and show pole-to-pole oscillation is stabilised for an elongated shape.

1J1356* **ナノスケールでの化学的非平衡性を利用し、規則運動するｃｍサイズの液滴：生物が動く仕組みの実空間モデル**
How to generated regular motion from nano-scaled fluctuating chemical machinery: Real-world modeling of motors in living organisms

Shiho Sato, Hiroki Sakuta, Kenichi Yoshikawa (*Grad. Sch. Life and Medical Sciences, Doshisha Univ.*)

Regardless the recent development on the biophysical studies of biological motors, the underlying mechanism of the generation of macroscopic controlled motion from nm-sized motor proteins is remains still in a primitive stage. Here, we report a simple real-world model of self-propelled cm-sized active matter driven by chemical potential under isothermal condition. It will be shown that certain modes, such as orbital motion and back-and-go motion, is generated by choosing suitable boundary conditions. We have performed the experiment with cm-sized oil droplet floating on an aqueous phase. We may discuss the mechanism of the emergence of a well-controlled self-propelled motion in relation to the macroscopic regular motion driven by large number nm-sized working proteins.

1J1408* **力学-化学ハイブリッドモデルによる細胞集団形成ダイナミクス解析**
Dynamic analysis of collective cell migration by mechanochemical hybrid model

Moegi Marumoto[1], Masaya Hagiwara[2] ([1]*Grad. Sch. Sci., Osaka Pref. Univ.*, [2]*N2RI, Osaka Pref. Univ.*)

We have achieved to develop a mathematical model of collective cell migration considering not only mechanical but also chemical interaction during tissue formations. Reaction-diffusion model was employed to simulate morphogen distributions, while spring-damper model was used to consider cell-cell mechanical interactions caused by cadherin adhesions. The developed model reached well agreement with in-vitro experimental results using normal human branch epithelial (NHBE) cells whose initial conditions were controlled by photolithography. This model can simulate both collective and individual cellular dynamics at the same time. It revealed that chemical interaction drives directional collective cell migration while mechanical interaction regulates cellular behavior.

1J1426 **Numerical simulations of one dimensional cell crawling and traction force analysis**

Hsuan-Yi Chen[1,2] ([1]*Natl. Cent. Univ., Taiwan*, [2]*Academia Sinica, Taiwan*)

We present a novel model which includes cell membrane, actin polymerization, cytoskeletal flow, myosin contractility, and cell-substrate bonds to study the crawling motion of a cell in a one-dimensional environment. Our numerical simulations show that, depending on the property of the cell-substrate bonds, a cell has rest, periodic migratory, unidirectional movement, or pulsatory movement states.
Analysis of traction force applied by the substrate shows that as the motility state of the cell changes, the force dipole and force quadrupole change continuously or discontinuously. In particular, force quadrupole remains zero in the rest state and points in the direction opposite to cell movement when the cell moves.

1J1438 **ネットワークのデザイン原理と構成要素の応答性**
Network Designing and Response Sensitivity of Components

Masayo Inoue[1], Kunihiko Kaneko[2] ([1]*IMS, Meiji*, [2]*Univ. of Tokyo*)

In general, the network property is affected by the properties of its components and therefore the appropriate structure would be different depending on the components. We studied how characteristic structure of an evolved network differ according to the response sensitivity of its components. We investigated the responses of gene regulatory networks containing many genes that have undergone numerical evolution to achieve the one-to-one correspondences between an input and the output. Three different types of networks evolved depending on the gene sensitivity. Each type showed difference in behaviors of components and also some network properties such as robustness. These results have significant implications in designing biological networks.

1J1450 **Lag Phase, Stationary Phase の理論モデル**
Transitions among Log, Dormant, and Death Phases: Proposition of a simple model and quantitative characterization of dormancy and lag time

Yusuke Himeoka, Kunihiko Kaneko (*Tokyo Univ. Department of Arts and Sciences*)

Quantitative growth laws have been uncovered for log phase. However, theories for other phases such as lag and stationary phases are underdeveloped, and a simple model that exhibits the transition among these phases has to be constructed.
In the present study, we propose a simple model consisting of four chemical components. With the decrease of the external concentration of substrate, the model is shown to exhibit the transitions in growth, i.e., lag, log, stationary, and death phases.
Additionally, we found that the lag time needed for growth recovery after starvation follows the square root of the starvation time and is inversely related to the maximal growth rate. The distribution of lag time is also obtained from stochastic simulation.

1J1502 **Generalized-Ensemble Simulations of Membrane Proteins**

Te-Lun Mai[1], Chi-Ming Chen[2] ([1]*Genomic Research Center, Academia Sinica, Taiwan*, [2]*Department of Physics, National Taiwan Normal University*)

Membrane proteins, which play key roles in living cells, have both scientific and clinical importance, and more than half of know drugs are targeting on these proteins. In this work, adopting a two-stage folding of helix-bundle membrane proteins, we first proposed an algorithm to identify transmembrane (TM) segments of these proteins, and then combined molecular dynamics simulations and a fold identification algorithm to fold the structures of TM helices. Subsequently, a coarse-grained model was constructed to study the folding of polypeptide chains in membrane. By using the replica-exchange Monte Carlo simulation to search their native conformations, we found that this approach can provide comparable structures with experimental results.

1J1514* **コレラ菌走化性受容体 Mlp24, Mlp37 のリガンド認識機構の差異**

Distinct mechanisms of ligand recognition between Mlp24 and Mlp37, chemoreceptor proteins of *Vibrio cholerae*

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Toxigenic *Vibrio cholerae* has at least 45 genes for methyl-accepting chemotaxis protein-like proteins (MLPs). Among them, Mlp24 is involved in the production of cholera toxin, and Mlp37, the closest homolog of Mlp24, mediates taxis to taurine, a major constituent of human bile. Although Mlp24 and Mlp37 show very similar overall structures, the affinity to their ligands is different each other. Moreover, the ligand binding affinity of Mlp24 is affected by calcium ion, whereas that of Mlp37 not. To understand the mechanisms that cause the affinity difference, we determined the structures of the ligand binding domains of Mlp24 and Mlp37 in complex with Ser or Arg. The structures revealed that calcium ion is involved in the binding pocket structure of Mlp24.

1J1532* **ATR-FTIR 分光測定によるヒト苦味受容体 TAS2R16 のリガンド結合機構の構造解析**

Structural analysis of ligand binding in human bitter taste receptor by ATR-FTIR spectroscopy

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We perceive bitter compounds using bitter taste receptors, which belong to a GPCR family. Human TAS2R16 is known to be activated by salicin and its glucopyranoside derivatives (Imai et al., Biophys. Physiobiol. 2016). Our goal is to elucidate the molecular mechanism of G-protein activation followed by ligand recognition. In this study, human TAS2R16 was purified after heterologous expression in mammalian or yeast cells. The lipid reconstituted sample was subjected to ATR-FTIR measurements, which could identify molecular vibrational changes caused by ligand-protein interaction. Based on the results, molecular structural changes by ligand-binding of hTAS2R16 will be discussed in relation to physiological data and putative model structures.

1J1544 **グルタミン酸受容体を介した植物の長距離 Ca^{2+} シグナル**

Glutamate receptor channels essential for a long-distance Ca^{2+} waves in plants

Masatsugu Toyota[1,2] ([1]*Saitama University*, [2]*University of Wisconsin-Madison*)

Plants, unlike animals, do not have a nervous system, but they can sense local environmental stimuli (i.e., mechanical wounding), transmit this information rapidly throughout the plant body and activate defense responses. Using genetically-encoded Ca^{2+} indicators, we have visualized the plant-wide spatial and temporal dynamics of cytosolic Ca^{2+} waves in response to wounding in Arabidopsis. Mechanical wounding in a leaf induced rapid Ca^{2+} and Glu increases in the wounded region, but only the Ca^{2+} increase was propagated to distant target leaves via activation of GLUTAMATE RECEPTOR LIKE (GLR) family of Ca^{2+}-permeable channels. GLRs appear to act as wound sensors to trigger propagation of a plant-wide Ca^{2+} signal in plants.

1J1556 **神経グロビンによる知覚変化の情報処理機構**

Information processing mechanism underlying a perceptual change by a neuroglobin

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Neural circuits encode environmental information that is represented by neural response patterns, and animals can use this neural coding for their behavior. We found that a neuroglobin (GLB-5), one of O2-binding haem proteins expressed in neural circuits, alters the worms to prefer broader range of oxygen concentrations. Quantitative imaging experiments indicated that GLB-5 confers a sigmoidal O2 response curve in a major O2 sensory neuron (URX). Our computational model based on experimental data suggested that the relationship between URX and reversal behaviour is sufficient to explain a worm's preference behaviour and its alteration by GLB-5. Thus, our results demonstrated the information processing mechanism underlying the change in a worm's preference behavior.

2B1355 骨格筋ミオシン分子動態の直接可視化に基づく協同的な力発生の解明
Understanding of cooperative force generation among skeletal myosins based on direct observation of individual myosin dynamics

Motoshi Kaya, Hideo Higuchi (*Dept Physics, Univ of Tokyo*)

We have recently found coordinated force generation among myosin molecules and revealed the molecular properties to enhance a chance of such efficient collective force generation. However, our findings were based on the analyses of actin displacements, which imply a coupling effect of myosin motors. Thus, in order to gain further insight into mechanism of cooperative force generation among myosins, dynamics of myosin molecules must be directly observed. In this study, individual myosins are labeled by gold nanoparticles (GNPs) so that scattered images of individual GNPs can be recorded by a high-speed camera at 10000 frames/s. We will provide details of individual myosin dynamics during acto-myosin interactions in the response to different loads.

2B1407 ダイニン - ダイナクチン相互作用について
Interaction of dynactin complex with dynein

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Dynactin is a principal regulator of the microtubule motor cytoplasmic dynein. Recently, elaborate and complicated roles of dynactin for dynein motor activity have been intensively studied, however, the structure of dynein-dynactin complex was obtained only with an additional protein, BICD2, known as a cargo adaptor. In this study, we investigated the dynein-dynactin interaction with or without other adaptors. We found that dynactin stably bound to dynein without any additional proteins and that the negatively stained EM images of the dynein-dynactin complex showed more diverse forms than the reported image of the complex including BICD2. The relationship between structure and function of the complex will be discussed.

2B1419 Yeast cytoplasmic dynein's small group takes a biased random walk toward the left-right

Mitsuhiro Sugawa[1], Shin Yamaguchi[1], Hiroaki Takagi[2], Mitsuhiro Iwaki[3], Keitaro Shibata[1], Yoko Y. Toyoshima[1], Junichiro Yajima[1] ([1]*Graduate School of Arts and Sciences, The Univ. of Tokyo*, [2]*Department of Physics, Nara Medical University*, [3]*QBiC, RIKEN*)

Yeast cytoplasmic dynein (CD) walks processively toward the minus end of a microtubule (MT) and move laterally toward both the right and the left, switching between the MT's protofilaments. We focused on motility of CD's small group in which several CDs were linked with each other via a probe and found biased random walk in the left-right direction. Time series analyses for the acquired trajectories and Monte Carlo simulation suggest that dynein arrangement in a small group and steric hindrance of neighbor dynein molecules should constrain directionality of stepping to the right or left, while the randomness should be due to number fluctuation and changes in arrangement of dynein molecules in a small group because of their binding-dissociation events on the MT.

2B1431 単頭ダイニンのステップサイズと微小管結合時間の測定
The step size and microtubule-binding time of single-headed dynein

Yoshimi Kinoshita[1], Taketoshi Kambara[1,2], Kaori Nishikawa[1], Motoshi Kaya[1], Hideo Higuchi[1] ([1]*The University of Tokyo*, [2]*RIKEN, QBiC*)

Cytoplasmic dynein is a molecular motor moving along the microtubules for transporting vesicles in cells. To understand the molecular mechanism of dynein related with its conformational changes, we measured the step motion of single-headed dynein by optical tweezers. The displacement dynein drives microtubules decreased from about 8 nm to 0 nm as ATP concentration decreased, indicating that the step size of dynein driven by the swing of the linker is about 8 nm. To support the ATP-dependent displacement, we analyzed the microtubule-binding time of dynein, which also decreased as ATP concentration decreased. We determined the main chemical cycle and reaction rates of dynein.

2B1443 Plus-end directionality present in kinesin conserved catalytic motor core

Masahiko Yamagishi, Junichiro Yajima (*Grad. Sch. Arts and Sci., The Univ. of Tokyo*)

Kinesin is a molecular motor moving along microtubules. While N-kinesins having motor domain at N-terminus and C-kinesins having motor domain at C-terminus have similar catalytic motor core structure, N-kinesins and C-kinesins move towards the plus-ends and the minus-ends of microtubules, respectively. The origin of these directionalities is not clear. Here we engineered either N- or C-kinesin monomers that can be anchored via their N- or C-termini, leaving the opposite terminal regions mechanically disconnected from the surface. We found that a conserved catalytic motor core of both N- and C-kinesins has a default plus-end directionality and that proper function of neck-helix and neck-mimic are required to achieve the minus end directionality for C-kinesins.

2B1455 キネシンのエネルギー論
Nonequilibrium energetics of kinesin

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Kinesin is a molecular motor that carries cellular cargos along microtubules. Although its working mechanism has been understood, little is known on the quantitative energetics of walking kinesin as nonequilibrium open systems. Here, we measured the nonequilibrium energy flow of single-molecule walking kinesin via an attached probe particle using optical tweezers. The sum of the heat dissipation estimated from the violation of the fluctuation-response relation and the output power was inconsistent with the input free energy rate, implying that internal dissipation is dominant. By combining Langevin dynamics and a 2-state Markov model that satisfies local detailed balance conditions, we discuss energy flow and heat dissipation from the kinesin motor.

2B1513 **高圧力で誘起される磁性細菌の遊泳運動能**
Pressure-induced activation of the swimming motility of magnetotactic bacterium

Masayoshi Nishiyama[1], Ruan Juanfang[2,3], Yuji Shimogonya[3], Takayuki Kato[2], Toru Minamino[2], Keiichi Namba[2], Takuji Ishikawa[3], Akitoshi Seiyama[1], Long-Fei Wu[4], Yoshie Harada[1,2] ([1]*Kyoto University*, [2]*Osaka University*, [3]*Tohoku University*, [4]*Aix-Marseille University*)

We studied the swimming motility of marine bacterium MO-1 cells at high-pressure. Application of pressure could shift cells from the non-motile to smooth-swimming state at a certain period. The transient activation of the cell motility could be explained by that applied pressures have two opposite actions to the motility machinery in MO-1 cells. The first would be activation of the motility machinery. Applied pressure could force to start the motility machinery that does not work any reason. About 80% of MO-1 cells on maximum started to swim smoothly in solution at 60-100 MPa. The second would be inactivation. Applied pressure is essentially harmful against motor function. These two conflicting actions could be working on the motility machinery in different way.

2B1525 **金ナノプローブで明らかになった霊菌 Serratia marcescens 由来キチナーゼ A の 1 nm ステップ運動と運動律速段階**
One nanometer steps and the rate-limiting step of Serratia marcescens chitinase A resolved by gold nanoprobe

Akihiko Nakamura[1,2], Ryota Iino[1,2,3] ([1]*Okazaki Inst. for Integr. Biosci.*, [2]*SOKENDAI*, [3]*Institute for Molecular Science*)

Serratia marcescens chitinase A (SmChiA) is a linear molecular motor moving on crystalline chitin with cycle of decrystallization of polymer chain, hydrolysis, and product release. Here we visualized steps and pauses of SmChiA with gold nanoparticle as a probe. Step sizes were 1.1 nm and -1.3 nm for forward and backward steps respectively, consistent with the length of product chitobiose (~1 nm). Distribution of pause before forward step was fitted by a consecutive reaction with time constants of 20.1 ms and 2.7 ms. In D_2O, these time constants changed to 24.5 ms and 11.0 ms, indicating the shorter component corresponds to hydrolysis. We concluded that decrystallization is the rate-limiting by comprehensive analysis of pauses before forward, backward and recovery steps.

2B1537 **腸球菌 V-ATPase 膜内在ローターリングの阻害剤結合型の X 線結晶構造解析**
Crystal structure of inhibitor bound membrane rotor ring of Enterococcus hirae V-ATPase

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V-ATPases are ion transport molecular motors found in various organelle membranes and cell membranes. Na+-transporting V-ATPase enables E. hirae to grow in high salt and high pH condition. Previously, we have identified several inhibitors through the screening from chemical library. They not only inhibited the ATPase activity of E. hirae V-ATPase but also inhibited the growth of E. hirae in high salt and high pH condition. These inhibitors seem to bind to membrane rotor ring of V-ATPase. We expressed V-ATPase in E. coli and purified to the rotor ring. We crystalized it with inhibitors and determined the structure in high resolution. In order to create better inhibitor based on the structure, we are elucidating the interaction of rotor ring and the inhibitors.

2B1549 **How fast can bacteria grow their flagella?**

Chien-Jung Lo (*Department of Physics, National Central University*)

Bacterial flagella are self assembled filaments for swimming. We develop in vivo single cell fluorescent imaging to monitor flagellar growth. We found the flagellar growth rate is length-dependent. We model it as a 1D Injection Diffusion process. Our results shed new light to the large extracellular structure assembly. eLife e22140.

2B1601 **角度分割・時分割 X 線結晶構造解析による、哺乳類 F1-ATPase のリン酸解離駆動の回転力発生機構の分析**
Molecular mechanism of Phosphate-driven rotation of mammalian F1 by the angle-divided and time-resolved X-ray crystallographic studies

Toshiharu Suzuki[1,2,3], Kunio Hirata[4], Eiki Yamashita[5], Naoya Iida[6], Toshiya Endo[2], Toru Hisabori[3], Masasuke Yoshida[2], Hiroyuki Noji[1] ([1]*Shool of Eng. Univ of Tokyo*, [2]*Dept of Mol Biosci, Kyoto-Sangyo Univ*, [3]*CLS, Tokyo Inst of Tech*, [4]*SPring8 Center, RIKEN*, [5]*Inst for Protein Res*, [6]*Dept of Physics, Waseda Univ*)

Recently we have established an X-ray crystallography system for bovine F_1-ATPase and determined snapshot structures to explain how the rotation is driven by phosphate-binding/releasing. The structures well support the rotation scheme of human F_1 previously determined by single molecule analysis, and additionally reveal a crucial role of "Arginine finger" in a catalytic site to couple the binding/releasing event with the rotation. We have further developed angle-divided and time-resolved crystallography systems. The latter system identified many rotation intermediate structures after removing thioPi, some of which were very similar to those obtained by the conventional method, suggesting that our analysis correctly reflects rotation intermediates.

2B1613 **Biophysical Characterization of the Chemomechanical Coupling of F_1 ATPase of *Paracoccus denitrificans***

Mariel Zarco Zavala[1], Duncan G.G. Mcmillan[2], Toshiharu Suzuki[1], Hiroshi Ueno[1], Rikiya Watanabe[1], Francisco Mendoza Hoffmann[3], José J. García Trejo[3], Hiroyuki Noji[3] ([1]*Department of Applied Chemistry, Graduate School of Engineering, The University of Tokyo*, [2]*Department of Biotechnology, Delft University of Technology*, [3]*Department of Biology, Chemistry Faculty, National Autonomous University of Mexico*)

Paracoccus denitrificans (Pd) is a free living bacterium phylogenetically related to protomitochondria. Its F_1-ATPase has a tightly regulated hydrolytic activity, which is controlled by a unique α-proteobacteria inhibitor, named the ζ subunit. This protein is structurally different to the bacterial (ε) and mitochondrial (IF_1) regulators, but appears to functionally resemble both. Here, we have studied PdF_1 rotatory dynamics and obtained preliminary results of the effect of the ζ subunit on the rotatory behaviour of PdF_1. The characterization of PdF_1-ATPase rotatory catalysis will provide insight into the adaptations of ATPase regulatory machinery upon endosymbiosis.

2C1355 Characterization of prokaryotic voltage-gated calcium channel

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Prokaryotic cation channels greatly contributed to the elucidation of the molecular basis of principle function of ion channels because of their simple structure. However, endogenous prokaryotic voltage gated calcium channel has not been identified yet.
We newly cloned calcium selective voltage gated channel from *Meiothermus ruber* and named it CavMeiR. CavMeiR is homologues to NavBac but its selectivity filter sequence is different from that of calcium selective mutant of NavBac, which has twelve acidic residues. CavMeiR has eight acidic residues in the tetrameric symmetrical filter, which is similar to mammalian calcium channel. It suggested that CavMeiR has novel permeation mechanism for calcium ion.

2C1431 高速 AFM による K+チャネル KcsA とポア結合性サソリ毒ペプチド Agtx2 の一分子結合動態解析

HS-AFM revealed single-molecule blocking dynamics of a scorpion toxin on the KcsA potassium channel

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Agitoxin-2 (AgTx2) is a small protein (38 a.a.) extracted from scorpion venom, and blocks K+ channels through docking to the external surface of the channel. In this study, we observed the binding dynamics of AgTx2 to the KcsA channel using HS-AFM. The KcsA channel was reconstituted into the membrane with its extracellular side oriented upward, which was imaged as a square shape for the homo-tetrameric KcsA. When an AgTx2 was bound to the channel surface, the channel shape changed from square to round accompanied with the elevated height. We analyzed a time course of the binding transitions, and found that there are two bound states with high and low affinity. We will discuss underlying structural changes of the KcsA channel relevant to the high and low affinity states.

2C1407 電位依存性プロトンチャネルの亜鉛阻害におけるヒスチジンとカルボン酸の役割

The role of histidine and carboxylate residues for zinc inhibition in the voltage-gated proton channel Hv1/VSOP

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The voltage-gated proton channel (Hv1/VSOP) is inhibited by Zn^{2+}. X-ray crystallography proposed that a Zn^{2+} ion is ligated by carboxylate (E115, D119) and histidine (H136, H189) residues in the extracellular region although the detail coordination geometry is uncertain [Takeshita et al. (2014) Nat. Struc. Mol. Biol., 21, 352.]. In this study, Zn^{2+}-induced molecular vibrational changes in Hv1/VSOP were measured by ATR-FTIR. The effects of single/multiple mutations of the putative ligand amino acids on the IR bands, which were associated with Zn^{2+}-binding, were examined. Based on the results, the inactivation mechanism will be discussed in relation to the atomic structural and electrophysiological studies.

2C1443 アルギニンペプチド修飾型エクソソームのマクロピノサイトーシス誘導と効率的な細胞内移行

Exosomal membrane modification with arginine-rich peptides for enhanced macropinocytotic uptake of exosomes

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Exosomes are secreted cellular vesicles, which encapsulate biofunctional molecules such as microRNAs and enzymes [1]. Exosomes have pharmaceutical advantages such as a lack of immunogenicity and utilization of cell-to-cell communication pathways; thus, exosomes are highly anticipated as next-generation tools for the intracellular delivery. We found that macropinocytosis is important for the cellular exosome uptake pathway [2]. Furthermore, we recently developed arginine-rich peptide-modified exosomes, which can actively induce macropinocytotic uptake and effective intracellular delivery [3, 4]. [1] Katsuda, T. Proteomics 14, 412 (2014), [2] Nakase, I. Sci. Rep. 5, 10300 (2015), [3] Nakase, I. Sci. Rep. 6, 34937 (2016), [4] Nakase, I. Sci. Rep. 7, 1991 (2017).

2C1419 光駆動型ナトリウムポンプロドプシンは異なる２つのイオン輸送モードを持つ

Two distinct ion transporting modes of sodium pumping rhodopsin, NaR

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Sodium pumping rhodopsin, NaR is a light-driven ion pump that transports Na^+ in the presence of Na^+ and H^+ in the absence of Na^+. It is not well understood how the ion selectivity is regulated in NaR. To elucidate the mechanism behind this, we studied ion pumping properties of FdNaR (NaR identified from *Flagellimonas sp_DIK*) by electrophysiological method. We systematically replaced ionic conditions of the intercellular- and the extracellular-side independently and investigated the pumping current and kinetics. We found two different pumping modes are switched by the sodium binding in the extracellular binding pocket. The FdNaR transports not only Na^+but also H^+ under physiological conditions.

2C1455 微細加工基板上の自立脂質二分子膜における浸透圧変化と相分離

Phase separation of freestanding planar bilayer lipid membrane on Si microwell under osmotic pressure change

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Artificial bilayer lipid membranes (BLMs) are simple models of cellular systems under physically and chemically controlled conditions. In this study, we investigated the phase separation at freestanding BLMs over Si microwells. Since the liquid disordered (Ld) phase is preferable at the freestanding BLMs, the liquid ordered (Lo) phase cannot exist stably. We propose controlling the phase separation by applying osmotic pressure. The osmotic pressure changes the shape of the freestanding BLMs and causes the lateral migration of lipids. As a result, the Lo phase is formed in the freestanding BLMs. Phase separation control will be applied to a protein assay system, because the Lo phase plays a very important role in the localization and function of membrane proteins.

2C1513 **Negative chemotaxis molecular robots migrated by osmotic pressure difference**

Kan Shoji, Ryuji Kawano (*Dept. Biotech. and Life Sci., TUAT*)

Micro robots which were mimicked living cells and assembled from molecules have been reported and have attracted as an intracorporeally robots. However, although motor proteins are easily driven at the protein level, it is difficult to scale up to cell size by integrated many proteins. Therefore, in this study, we propose the giant liposome-based microrobot which can be driven by osmotic pressure difference: we named this biomimetic robot as “Lipobot”. The lipobot can sense the ion concentration difference and migrate autonomously by negative chemotaxis. We believe that the concept of the lipobot will become a big breakthrough for a driving mechanism of microrobots which can drive in living system.

2C1525 **アクチン線維封入巨大リポソームの光刺激による可逆的な形態制御**

Light-induced and reversible morphological control of F-actin-encapsulating giant liposomes

Masahito Hayashi[1], Shunsuke Tanaka[2], Kingo Takiguchi[2] ([1]*RIKEN BSI*, [2]*Grad. Sch. Sci., Nagoya Univ.*)

We have reported that F-actin-encapsulating giant liposomes (FAGLs) showed spindle-like shape due to the nature of F-actin as liquid crystal. Here, we devised the optical control system for reversible morphological change of FAGLs by using fluorescently labeled F-actin. If exposed to strong excitation light, FAGLs changed their shape from spindle-like to spherical within 30 sec. After then, upon turning off the light, the FAGLs' shape recovered to spindle-like within several minutes. The morphological change was accompanied with the length change of tubular membrane extending from apexes of the spindle. The cycle of morphological change repeated more than five times. The light-induced morphological change involved the cycle of severing and annealing of F-actin.

2C1537 **人工 RNA 複製系を用いて試験管内で宿主・寄生体の進化的軍拡競争を観察する**

Evolutionary arms races between artificial host-parasite RNA replicators in vitro

Taro Furubayashi[1], Yohsuke Bansho[1], Norikazu Ichihashi[2] ([1]*Grad. Sch. of Frontbio, Osaka Univ*, [2]*Grad. Sch. of InfoTech, Osaka Univ*)

Parasites such as viruses are most universal and abundant biological entities on earth and must have been strong evolutionary driving forces for host organisms through “evolutionary arms races”. Despite lots of indirect evidences, nobody has directly observed the evolutionary arms race processes, therefore its generality and significance on evolution is still unclear.

To investigate host-parasite arms race phenomena, we constructed an experimental model based on an artificial RNA replication system, where host-parasite coevolution is possible. We observed complex oscillations in the population dynamics of host and parasite RNA during coevolution experiments, and combined with following sequence analyses, we confirmed that host-parasite arms races actually occurred.

2C1549 **マイクロデバイスと大腸菌の融合を利用した新規人工細胞系の開発**

Development of a new artificial cell system based on the fusion of micron-scaled device and *E. coli*

Yoshiki Moriizumi[1,2], Kazuhito Tabata[1,2,3], Rikiya Watanabe[1,3,4], Tomohiro Doura[5], Mako Kamiya[3,5], Yasuteru Urano[5,6,7], Hiroyuki Noji[1,2] ([1]*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*ImPACT, Cab. Office*, [3]*PRESTO, JST*, [4]*PRIME, AMED*, [5]*Grad. Sch. Med., Univ. Tokyo*, [6]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [7]*CREST, AMED*)

Can a living cell born via the encapsulation of whole cellular cytoplasm into a cell-sized compartment? To answer this important question in the field of an artificial cell, we constructed a new artificial cell system, named as ‘a hybrid cell’, by fusing *E. coli* protoplasts to arrayed lipid bilayer chambers, ALBiCs, whose orifice are sealed with lipid bilayer. We found that the hybrid cell has the translation and transcription activity, which suggests the viability of the hybrid cell. We also observed membrane morphological changes in some hybrid cells. Even though such phenomena were quite rare events, it suggests the possibility for the hybrid cell to be a self-replicating autonomous artificial cell in the future.

2C1601 **バクテリアの長期定常期における密度依存的なリサイクリング活動**

Density-dependent recycling in the long-term stationary phase of bacterial populations

Sotaro Takano[2], Bogna J. Pawlowska[3], Ivana Gudelj[3], Tetsuya Yomo[4], **Saburo Tsuru**[1] ([1]*Univ. Biol. Inst., The Univ. of Tokyo*, [2]*Life and Env. Sci., Univ. of Tsukuba*, [3]*Biosci., Univ. of Exeter*, [4]*Inst. of Biol. and Inf. Sci., East China Normal Univ.*)

How do organisms survive for a long term after exhaustion of resources? After the majority of Escherichia coli cells died by starvation, a small proportion of the cells remained viable for months (long-term stationary phase). Here, we used this model system and verified the significance of social recycling of dead cells for long-term survival. We also show that the survivors restrained their recycling according to the cell density and did not use all available nutrients released from dead cells, which may be advantageous under starvation conditions. These results indicate that not only the utilization of dead cells but also restrained recycling coordinate the effective utilization of limited resources for long-term survival under starvation.

2D1355 **スマートフォン顕微鏡イノベーション**

Smartphone Microscope Innovation

Kuniaki Nagayama[1,2], Sumito Shirane[2] ([1]*Nagayama Microsc. Lab., LisCo*, [2]*Life Is Small. Co*)

A "Leeuwenhoek type" smartphone microscope was invented in July 2013. It is an extremely small compound microscope uniquely using the front camera of smart-devices. It seemingly looks like a toy but has a great potential deserving “biophysics innovation”. Numerous microscopic species from transmission type to fluorescence method that make the possibility manifest has been developed in the past 3 years. We started up a venture LisCo (Life is small. Company, http://lis-co.co.jp/)in July last year as an open innovation how minimal microscopes renovate conventional methods and detonate new business in various fields. Exemplifying various microscope applications, the background of R & D, history of commercialization and the business model itself of LisCo will be reported.

2D1407 高速 AFM による抗体 IgG のリアルタイム観察と挙動解析
High-Speed AFM revealed dynamic behavior of antibody

Norito Kotani, Yoko Kawamoto-Ozaki, Kumaresan Ramanujam, Ryo Nakatsuka, Takashi Morii, Takao Okada (*Research Institute of Biomolecule Metrology*)

IgG exhibit mechanisms which increase their affinity to antigens. To understand the mechanisms in detail, we analyzed IgG in liquid by High-Speed Atomic Force Microscopy (HS-AFM). HS-AFM is the only method which can visualize the dynamic behavior of IgG in solution.
IgG was observed as Y shaped structure where each of the two Fab regions were distinguished clearly and Fab regions swang by thermal fluctuation. We traced each of the locations of two Fabs and Fc, and measured the distances between every region. The movements showed hinge regions flexibility. Furthermore, we estimated mechanical aspects of IgG hinge regions. We suggest that the observations by HS-AFM could provide a new method to measure the flexibility of the hinge in the antibody.

2D1443 高速 AFM による立体パターン基板を用いたタンパク質の動態観察
HS-AFM Observations of Protein Dynamics on 3D-patterned Substrate

Akane Goto[1], Mikihiro Shibata[2,3], Ayumi Sumino[2,3], Noriyuki Kodera[3] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ*, [2]*InFiniti., Kanazawa Univ*, [3]*Bio-AFM. FRC., Kanazawa Univ*)

High-speed atomic force microscopy (HS-AFM) is a powerful technique to visualize dynamic process of biomolecules under the physiological conditions. However, biomolecules were usually absorbed on a flat 2D substrate for HS-AFM observations. Some biological molecules do not function on the flat 2D surface because of a steric disturbance. To expand biological applications of HS-AFM, we try to fabricate 3D-patterned substrates having grooves and holes in the size of nanometer. 3D-patterned substrates will enable us to observe a dynamics of membrane proteins and DNA binding proteins without any restriction from substrates. In the presentation, we would like to show fabrication process of 3D-patterned substrate and its applications to imaging of dynamic biomolecules.

2D1419 High-speed atomic force microscopy (HS-AFM) revealed dynamic structural changes of Bacteriophage T4 sheath

Hiroki Watanabe[1], Shuji Kanamaru[2], Takayuki Uchihashi[3] ([1]*RIBM*, [2]*Dept. of Life Sci. and Tech., Tokyo Institute of Technology*, [3]*Dept. of Phys., Nagoya Univ.*)

Bacteriophage T4 is a member of *Myoviridae*, which has a long and contractile tail. It has been known that a sheath which is outer layer of the phage tail, can be contracted by exposing the phage to urea. As previously reported, the sheath structure had been investigated in detail at the angstrom-scale by various methods such as cryo-EM or X-ray structural analysis. However, there are no techniques which can directly observe the structural changes of the sheath during the contraction. Here, we applied HS-AFM to the phage particle to visualize the structural changes and investigate the contraction speed. As a result, the speed was estimated at 140.4 ± 1.0 nm/sec and 285.4 ± 4.2 nm/sec. Moreover, it was indicated that the tail sheath contraction proceeded as step-wise.

2D1455 高速 AFM による脂質膜の曲率に依存したタンパク質-脂質膜の相互作用の直接観察
Direct observation of proteins-lipid membrane interactions depending on the physical shape of lipid membrane by high-speed AFM

Takahiro Toyoda[1], Akane Goto[1], Ayumi Sumino[2,3], Mikihiro Shibata[2,3], Noriyuki Kodera[3] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*InFiniti., Kanazawa Univ*, [3]*Bio-AFM FRC, Kanazawa Univ.*)

It has been recently illustrated that some proteins associate with and/or dissociate from lipid membranes by recognizing the membrane's shape or curvature. Direct observations of these phenomena at sub-molecular level by high-speed AFM would promote a better understanding of the underlying mechanisms. Last year, we reported that an AFM substrate with vast number of submicrometer-sized holes and convex parts can be fabricated using a nano-sphere imprinting method, and that lipid molecules diffuse at different speed according to the membrane shape. Currently, we are improving the fabrication method for the substrate and also attempting to directly visualize the membrane-shape dependent behaviors of integral and/or peripheral membrane proteins.

2D1431 高速 AFM による天然変性タンパク質 CAMP の構造動態観察
Structural dynamics of the intrinsically disordered protein CAMP revealed by high-speed AFM

Tomoyuki Narita[1], Masanori Ikeda[2], Kozo Tanaka[2], Noriyuki Kodera[3] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*Dept. Mol. Oncol., Inst. Dev. Aging Center, Tohoku Univ.*, [3]*Bio-AFM FRC, Kanazawa Univ.*)

CAMP (Chromosome Alignment-Maintaining Phosphoprotein) is involved in proper kinetochore-microtubule attachment for accurate chromosome segregation. CAMP is a 812 aa zinc-finger protein containing large intrinsically disordered region that includes three characteristic repeat motifs termed the WK, SPE and FPE motifs. The immunofluorescence assay determined the region of CAMP responsible for chromosome and spindle localization. However, the overall molecular structure of CAMP remains entirely elusive. Here, we directly observed CAMP by high-speed AFM. The molecule takes the shape of two small globular domains linked by a long, flexible string-like structure. Impacts of phosphorylation on the CAMP shape and the binding manner with other proteins are also revealed.

2D1513 生細胞のクロマチン構造の超解像イメージング
Dynamic organization of chromatin domains revealed by super-resolution live-cell imaging

Tadasu Nozaki, **Kazuhiro Maeshima** (*NIG*)

The eukaryotic genome is organized within cells as chromatin. For proper information output, higher-order chromatin structures can be regulated dynamically. How such structures form and behave in various cellular processes remains unclear. Here, by combining super-resolution imaging (photoactivated localization microscopy) and single nucleosome tracking, we developed a nuclear imaging system to visualize the higher-order structures along with their dynamics in live mammalian cells. We demonstrated that nucleosomes form compact domains with a peak diameter of 160 nm in live cells and move coherently. Notably, we observed the domains during mitosis, suggesting that they act as building blocks of chromosomes and may serve as information units throughout the cell cycle.

2D1525 **G タンパク質共役型受容体（GPCR）と G タンパク質の二色一分子観察をもとにした GPCR の活性化状態評価**
Evaluation of G-protein coupled receptor (GPCR) signaling activity based on dual color single molecule imaging of GPCR and G-protein

Tomoki Nishiguchi, Hideaki Yoshimura, Takeaki Ozawa (*Grad. Sch. Sci., The Univ. Tokyo*)

G protein coupled receptors (GPCRs) recognize specific stimulants and activate G-proteins inside the cells, resulting in various biological phenomena. Therefore, monitoring of GPCR signaling dynamics is important for biological research. Here, we established a method to detect heterologous activation states of GPCRs in living cells with single molecule imaging. G-proteins and GPCRs were labelled with TMR and SeTau, respectively, and monitored under total internal reflection fluorescent microscopy (TIRFM). As a result, ligand stimulation and inhibitor treatment caused changes in fluorescence intensity, location, and mobility of the spots. The results suggested that the single-molecular physical properties would be useful to assess the signaling efficiencies of GPCRs.

2D1537 **高光度化学発光タンパク質ナノ-ランタンを用いた走化性タンパク質の新規観察法**
Novel imaging method for chemotaxis protein using a super-duper chemiluminescent protein, Nano-lantern

Shintaro Aso[1], Masahiro Nakano[2], Hajime Fukuoka[1], Takeharu Nagai[2], Akihiko Ishijima[1] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [2]*ISIR, Osaka Univ.*)

Fluorescent imaging is powerful tool for studying bacterial chemotaxis. However, cells tend to response to blue light as a repellent and are sometimes damaged by blue light. Then we try to use Nano-lantern(NL) which emits light utilized bioluminescence and the emission doesn't require excitation light. First, we succeeded observing the emission of NL in cytoplasm at single-cell level. Next, we could observe the localization of NL-CheW at cell pole when the expression level was relatively higher than that of physiological condition. Now, we are optimizing the expression level of NL-CheW, which is able to detect the emission and confer normal chemotaxis. Besides, to improve the emission intensity of NL-CheW, we are searching amino acid linkers between NL and CheW.

2D1549 **Trafficking of endocytic vesicles in live cancer cells**

Seohyun Lee[1], Kohsuke Gonda[2], Motoshi Kaya[1], Hideo Higuchi[1] ([1]*Dept. of Physics, Graduate School of Science, The University of Tokyo*, [2]*Dept. of Medical Physics, Graduate School of Medicine, Tohoku University*)

Vesicle transport in intracellular area of a live cell contains essential information of cellular activity. Here, three dimensional movement of a membrane protein PAR-1 during its endosomal trafficking in a live cancer cell is imaged and reconstructed, based on ratiometric dual focus method. In order to secure stable tracking system, the position of stage is maintained by position feedback using capacitive sensor, against thermal fluctuation. As a result, time lapse fluorescent imaging revealed three kinds of distinct movement patterns of PAR-1 transport in the initial stage of endocytosis: planar movement on the membrane, internalization with irregularly changing velocities, and recycling to the membrane.

2D1601 **Linking Raman spectroscopy and gene expression profiles for genotype-phenotype prediction**

Arno Germond[1], Takaaki Horinouchi[1], Chikara Furusawa[1,2], Toshio Yanagida[1], Taro Ichimura[1], Tomonobu M. Watanabe[1,3] ([1]*RIKEN, Quantitative Biology Center (QBiC)*, [2]*Universal Biology Institute, The University of Tokyo*, [3]*Graduate School of Frontier Bioscience, Osaka University*)

Molecular vibrational spectra and gene expression profile present two facets of a same biological system: the phenotypic/observable information (Raman spectrum) and the internal information (gene expression). By integrating high dimensional datasets, namely Raman spectral data and RNA-seq data, using a mathematical model, we demonstrate the possibility to relate a set given gene with a given set of wavelengths. This approach allowed to identify specific molecular functions and gene networks underlying each cell-type or cell-state, which is not possible by using the methods independently. This study paves the way toward the monitoring the expression of specific genes of single cells on a microscope stage, without any labeling nor destructive treatment.

2D1613 **遺伝子コードされた超音波エコーイメージング造影剤の開発**
Development of genetically-encoded contrast agent for ultrasonography

Ryota Mizushima[1], Kanako Inoue[2], Atsuko Iwane[1], Tomonobu Watanabe[1] ([1]*RIKEN-QBiC*, [2]*Uhvem, Osaka Univ*)

Ultrasonography is one of the most frequently used imaging modality in clinical medicine. It has advantages in non-invasive and real time imaging capabilities with deep soft tissue access, however, its applications were limited for basic biomedical research due to lack of genetically-encoded molecular reporters like GFP in optical imaging. To expand the applicability, we have developed a new class of reporter genes function in sound imaging modality exploiting bacterial gas vesicle genes derived from a certain cyanobacteria. We will present the methodology of expressing gas vesicles in mammalian cells and validation of strong ultrasound scattering induced by gas vesicles expressed in cells, which enables intracellular contrast enhancement in ultrasonography.

2E1355 **実時間選択的回収による免疫細胞の網羅的遺伝子発現解析**
Single-cell transcriptome analysis of stimulated immune cells with real-time collection

Yumiko Tanaka[1], Yoshitaka Shirasaki[1,2], Mai Yamagishi[1,2], Kaede Miyata[1], Nobutake Suzuki[1,2], Osamu Ohara[2], Kazuyo Moro[2], Sotaro Uemura[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*IMS., RIKEN*)

Stimulated immune cells start cytokine secretion and the cytokine mRNA expression levels are known to be heterogeneous. We found that their secretion onset timing was widely fluctuated, suggesting various secretion state among the cells. We developed a novel system that directly collects in real-time each single-cells based on the secretion activity. Using this system, we collected cells just after their secretion onset and performed further quantification of their cytokine mRNA levels, resulting in uniform expression levels among collected cells. Now, we expanded to perform transcriptome analysis of the cells collected at their secretion onset and found several genes uniformed at the secretion onset besides the genes relevant to the cytokine secretion.

2E1407 走査型イオンコンダクタンス顕微鏡による一次繊毛のナノスケール形状測定

Measuring nanoscale morphology of primary cilia using scanning ion-conductance microscopy

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Primary cilia are sensory organelles whose dimensions and location are related with cell growth and quiescence. We employed hopping mode scanning ion-conductance microscopy (SICM) to visualize the topography of primary cilia from two different cell types. We successfully distinguished between surface cilia that project outward from the cell surface and subsurface cilia that were trapped below the cell surface by combining SICM with fluorescence imaging. The nanoscale structure of a single primary cilium, which can not be easily identified using a confocal fluorescence microscope, was observed in SICM images. We have also analyzed ion current signals during scanning and found that the set point current is important for detecting all parts of a long cilium by SICM.

2E1419 夾雑物存在下でマイクロ RNA を電気測定により検知する技術の開発

Detection of target microRNA in a crude sample by electrical measurement

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MicroRNA is a biomarker for cancers. We here report a system to detect the microRNA within a crude sample. The microRNA applied in the system forms a duplex with a complementary oligo-DNA. This oligo-DNA is anchored to a magnetic bead, and is consequently entrapped by a magnetic field. The duplex is then cleaved by a duplex-specific nuclease, and the fragmented DNA is released from the magnetic entrapment. The released DNA fragment is detected by electrical measurement, by using the alpha-hemolysin and droplet-contact method. Label-free, and noise-free detection was demonstrated by testing a target microRNA. This device will be useful for non-purified samples, thus will offer a possible application for the onsite diagnosis in future.

2E1431 in vitro 三次元培養における計測制御プラットフォームの構築

In vitro 3D culture platform for environmental control and imaging

Masaya Hagiwara[1], Rina Nobata[2], Tomohiro Kawahara[3] ([1]*N2RI, Osaka Pref. Univ.*, [2]*Osaka Pref. Univ.*, [3]*Kyushu Inst. of Tech.*)

In vitro three dimensional culture is essential to analyze morphogenesis, molecular interaction, and the underlying system of pattern formation. However, the observation of developed 3D structure becomes often difficult especially if the size of the sample is relatively large. Besides, culture environments in 3D is poorly controlled while thousands of microfluidic chips are available in 2D culture. In order to overcome these problems, we have developed 3D culture platform consisting two types of hydrogel. The platform allows us to image the samples from 6 sides and it enables high-resolution imaging with low magnification lens (4x, 10x). In addition, the platform can easily integrate with microfluidics technologies to control the environments surrounding samples.

2E1443 バイオメディカルアプリケーションのための 8 タップ電荷変調画素に関する研究

An 8-tap Time Resolved CMOS Lock-In Pixel Imager for Biomedical Applications

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An 8-tap time-resolved CMOS lock-in pixel imager with a lateral electric field charge modulator (LEFM) for biomedical applications is developed and demonstrated through the device simulation and measurements. The photo-signal generated in photodiode (PD) is quickly transferred to the eight storage-diodes (SDs), which are controlled by LEFM, and the transferred signal is read out by the low noise column circuits. The 8-tap CMOS lock-in pixel imager is developed by 0.11um 1P4M CIS process technology. The 8-tap lock-in pixel sensor has been successfully operated and has achieved a short intrinsic response of 780ps at 374nm.

2E1455 A mechanical model for diversified insect wing margin shapes

Yukitaka Ishimoto[1], Kaoru Sugimura[2] ([1]*Akita Pref. U.*, [2]*iCeMS, Kyoto U.*)

While the basis of the diversity of insect wing margin shapes remains unknown, smoothly curved margin is the most frequently found and implies the existence of a highly organised, multicellular mechanical structure. Here, we developed a mechanical model for diversified insect wing margin shapes, where non-uniform bending stiffness of the wing margin is considered. We showed that the model could reproduce diverse shapes. Besides, the inference of the spatial distribution of the stiffness indicates a common feature among insects. The effect of the intrinsic tension of the wing blade is also studied, and a hybrid model with the vertex model is constructed. The results indicate that the stiffness of the wing margin can play a pivotal role in shaping insect wings.

2E1513 アレルゲン免疫療法の理論的解析

Mathematical study of allergen immunotherapy

Akane Hara[1], Yoh Iwasa[2] ([1]*Grad. Sch. Sys. Life Sci. Kyushu Univ.*, [2]*Dept. Biol., Fac. Sci., Kyushu Univ.*)

Allergen immunotherapy is a treatment method for pollen allergy, in which administration of a small dose of pollen for several years can suppress allergic symptoms on later exposure to environmental pollen. We developed a simple mathematical model for differentiation of Th2 cells (trigger of allergy) and Treg cells (suppressor of allergy). We found: [1] for the therapy to be successful, Treg cells must has a low decay rate, contrary to the assumption adopted in past models; and [2] therapy with gradually increasing pollen dose is effective in suppressing allergy whilst minimizing the symptom caused by therapy itself. Since intestinal microbiome is known to affect the allergic symptoms, we also study coupled immune-enterobacteria dynamics.

2E1525 **機械学習を用いた大腸菌走化性受容体に作用する誘引物質の予測**

Prediction of attractants for the chemoreceptors of *Escherichia coli* using machine learning

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Escherichia coli cells swim in favorable directions by sensing environmental signals. Major attractants include L-aspartate and L-serine, which are recognized by the chemoreceptors Tar and Tsr, respectively. The structural bases of aspartate and serine recognition have been extensively studied, but these chemoreceptors can sense larger but distinct sets of amino acids and analogues. To predict amino acids or analogues which were recognized by the chemoreceptors, we constructed a model based on machine learning. Setting 10 physicochemical properties of molecules, our model succeeded in predicting attractants and non-attractants with 92% accuracy. The key parameter for this prediction was found to be the maximal value of negative electrostatic potentials.

2E1537 **二者の同調歩行における歩行パターン分析：受動と能動の中間的状況における身体性の拡張**

Analysis for the changes in the gait patterns in paired walking: Expanded bodily self by the ambiguity of passive/active leadership

Mai Minoura[1], Yukio-Pegio Gunji[1], Tomohiro Shirakawa[2] ([1]*School of Fundamental Science and Engineering, Waseda University*, [2]*Department of Computer Science, School of Electrical and Computer Engineering, National Defense*)

Synchronized human walking is a situation that makes it possible to observe interpersonal coordination. In order to analyze the result of ambiguity of passiveness and activeness of our bodily self, we analyzed how the walking patterns are changed depending on the leader/follower role settings in paired walking. As a result, we found that there was a change in the walking patterns when the subjects had “weak” leadership, which was not observed when the leader/follower was explicitly defined. This suggests that the situation with passive/active ambiguity may cause the change in bodily control and bodily self.

2E1549 **Surfactant role on microbead manipulation by saw-tooth shaped electrode**

Marcos Masukawa, Masahiro Takinoue (*Tokyo Institute of Technology, Takinoue Lab*)

We induced attachment, trapping, flow and oscillation of polystyrene microbeads in liquid paraffin. To induce different phenomena, we used a saw-tooth shaped micropatterned electrodes connected to DC voltage and varied the concentration of surfactant. Based on fluorescence measurements, we believe the inverted micelles formed by the surfactant adsorb to the particle surface, furthermore, the inverted micelles seem to be able to stabilize charge and modify the electrical conductivity and dielectric constant of the medium. The ability to continuously modify these constants grants control on the microbead dynamics. As a result, understanding electrodynamics of inverted micelles might be fundamental for the development of new actuators such as micropumps, traps and sorters.

2F1355 **Structural analysis of Chrimson, a red-light activated channelrhodopsin**

Kazumasa Oda, Satomi Oishi, Reiya Taniguchi, Tomohiro Nishizawa, Ryuichiro Ishitani, Osamu Nureki (*Grad. Sch. Sci., Univ. Tokyo*)

Channelrhodopsin (ChR) is a light-gated cation channel derived from algae, which conducts cations when illuminated by particular wavelength light. ChR consists of seven-transmembrane helices and all-trans retinal attached via a Schiff base. ChR variants with different absorbance peaks are widely used as tools for optogenetics. Among them, most red-shifted variant derived from Chlamydomonas noctigama, named Chrimson, offers the advantages in the noninvasive applications for pigmented tissues. However, the molecular mechanism for the extremely red-shifted absorption of Chrimson has not been yet understood. Here, we report crystal structure of Chrimson, which reveals the molecular determinant for the red-shifted absorption.

2F1407 **A novel enzyme which folds into active form only with its counterpart**

Kohei Sawada[1], Atsushi Minami[2], Taro Ozaki[2], Hiroyuki Kumeta[3], Tomohide Saio[2], Koichiro Ishimori[2], Min Yao[3], Hideaki Oikawa[2], Katsumi Maenaka[1], Toyoyuki Ose[1,3] ([1]*Faculty of Pharm. Sci, Hokkaido Univ.*, [2]*Faculty of Sci, Hokkaido Univ.*, [3]*Faculty of Adv. Life Sci., Hokkaido Univ.*)

Ionophore polyethers, one of the major groups of natural polyketides, have an unique polyether skeleton composed of tetrahydrofuran and tetrahydropyran rings. The unified biosynthetic model for polyether construction proposed comprises sequential epoxidation of polyene precursor followed by epoxide opening cascades of the resultant polyepoxide. We characterized proteins responsible for the final step of monensin biosynthesis. There is a pair of homologous ORFs named *monBI* and *monBII*; we discovered synergistic effect that MonBII works as catalyst only in the presence of MonBI. Crystal structures and ^{1}H-^{15}N HSQC spectrum of the proteins clearly show MonBII is able to fold into active form with the help of MonBI.

2F1419 **NMR characterization of the substrate-binding domains of protein disulfide isomerase using paramagnetic effects**

Methanee Hiranyakorn[1,2], Saeko Yanaka[1,2], Maho Yagi-Utsumi[1,2], Koichi Kato[1,2] ([1]*Inst. Mol. Sci, Natl. Inst. Nat. Sci.*, [2]*SOKENDAI*)

Protein disulfide isomerase (PDI) is a multidomain enzyme that functions as an essential folding catalyst in the endoplasmic reticulum through its thiol/disulfide exchange activities. In this enzyme, the b' and a' domains provide substrate-binding sites and undergo a dynamic domain rearrangement between open and closed forms, depending on the redox states of the catalytic a' domain. In this study, we analyzed PDI b'-a' domains using NMR spectroscopy assisted by paramagnetic effects including paramagnetic relaxation enhancement and pseudo contact shift. Our NMR data revealed that mutational perturbations at the microenvironment in the a' active site induced gross rearrangements of the b' and a' domains, offering insights into the functional mechanisms of this enzyme.

2F1431 X 線自由電子レーザー回折像を用いた巨大生体分子三次元構造の復元

Three-dimensional structure reconstruction of large biological molecule from diffraction images obtained by XFEL using computer simulation

Miki Nakano[1], Osamu Miyashita[1], Slavica Jonic[2], Astushi Tokuhisa[1], Florence Tama[1,3,4] ([1]*RIKEN AICS*, [2]*IMPMC, Sorbonne Univ. CNRS, UPMC Univ Paris 6, MNHN, IRD*, [3]*Grad. Sch. Science, Nagoya Univ.*, [4]*ITbM, Nagoya Univ.*)

3D structural analysis for single particles using X-ray free electron laser (XFEL) enables us to observe hard-to-crystallize biomolecules in a state close to nature. In order to restore 3D structures of the molecule from the diffraction images obtained by XFEL experiments, estimation of laser beam incidence angles to the molecule for each image and phase retrieval are required. We are developing a program package for XFEL analysis based on XMIPP, which is commonly used for image processing of single-particle 3D cryo electron microscopy. We restored 3D structure of ribosome from 2D diffraction images created by simulation. We discuss the requirements for the experimental conditions to obtain the diffraction images to restore the molecular structure at certain resolution.

2F1443 Efficient strategy to retrieve potential 3D models directly from a small amount of single particle projection data

Sandhya Tiwari[1], Florence Tama[1,2,3], Osamu Miyashita[1] ([1]*RIKEN AICS*, [2]*ITbM, Nagoya University*, [3]*Dept. of Physics Nagoya University*)

As single particle methods develop, we require computational tools to aid 3D reconstruction. We propose a strategy for finding potential 3D models from a small number of 2D data by searching a 2D image library. The library contains projection images simulated from single particle Electron Microscopy (EM) data that are resized to the same volume to reduce redundancy in the number of shape types. For 3 test cases, 5 input images per target were searched against a library of images from 250 random EM models. We found that successful retrieval of 3D models were dependent on the complexity of the target shape and the composition of the image library. Our approach can be used across various experimental techniques and to estimate the mixing of states in single particle data.

2F1455 光回復酵素と DASH 型クリプトクロムにおける紫外線損傷二本鎖 DNA の結合に寄与する因子の特定

Identification of the factors that contribute to binding UV-damaged duplex DNA for Photolyase and Cryptochrome-DASH

Ryuma Sato, Yasuteru Shigeta (*Center for Computational Sciences, University of Tsukuba*)

DNA is damaged by ultraviolet light irradiation, and the damaged DNA is one of the causes of skin cancers. The photolyase (PHR) has the DNA repair function. Although the cryptochrome-DASH (CRY-DASH) has similar structure to PHR, it has no DNA repair function. However, the reason why CRY-DASH does not have the repair function is not clarified, yet.

We performed the molecular dynamics simulation for PHR and CRY-DASH that bound to the UV-damaged duplex DNA. We found that the binding structure of CRY-DASH is less stable than that of PHR and identified the surface amino acids which contribute to binding. We also investigated CRY-DASH mutants substituted to the identified amino acids in order to make CRY-DASH acquire the repair function.

2F1513 荷電性アミノ酸の粗視化モデルの開発

Development of a coarse-grained model for charged amino acid residues

Kazutomo Kawaguchi, Satoshi Nakagawa, Hidemi Nagao (*Inst. Sci. Eng., Kanazawa Univ.*)

Effective interactions between charged amino acid residues play key roles in many protein functions. In our previous study, we have constructed a simple coarse-grained model for hydrophobic amino acid residues in an aqueous solution and reproduced the complex structure of GCN4-pLI tetramer by the coarse grained simulation. In this study, we construct the coarse grained model for charged amino acid residues in an aqueous solution. The coarse grained potential function is constructed to reproduce the effective interaction between two amino acid side chain analogues in an explicit water solvent by all-atom MD simulations. Then, the Langevin dynamics simulation with the coarse grained potential is performed to reproduce the protein complex structure.

2F1525 Dimerization of full-length Aβ peptides by the Hamiltonian replica-permutation method

Satoru Itoh[1,2], Hisashi Okumura[1,2] ([1]*IMS*, [2]*SOKENDAI*)

The amyloid-β peptides (Aβ) form amyloid fibrils which are associated with Alzheimer's disease. It is necessary to clarify the oligomerization process of Aβ in order to understand the amyloid fibril formation process and to find a remedy for Alzheimer's disease. We applied the Hamiltonian replica-permutation method (HRPM) to full-length Aβ peptides, Aβ42 and Aβ40, to study their dimerization process. We will show dimer conformations and discuss difference between Aβ42 and Aβ40 in our presentation.

2F1537 クライオ電子顕微鏡像フィッティングのための新規 MD 法の開発と応用

Development of a new method for efficient cryo-EM fitting simulation

Takaharu Mori[1,2], Osamu Miyashita[3], Marta Kulik[1], Florence Tama[3,4], Yuji Sugita[1,2,3,5] ([1]*RIKEN Theor. Mol. Sci. Lab.*, [2]*RIKEN iTHES*, [3]*RIKEN AICS*, [4]*Nagoya University*, [5]*RIKEN QBiC*)

Single-particle cryo-electron microscopy (cryo-EM) is one of the powerful experimental techniques to determine structures of biomolecules at near atomic resolutions. Molecular dynamics simulations have been often used to construct 3D structures by fitting the all-atom model to low-resolution cryo-EM density map. In this study, we propose a new simulation method for efficient cryo-EM fitting and refinement. We also proposed a new parallel computing algorithm for cryo-EM fitting, where the simulation system is decomposed into several domains according to the number of atoms in the local spaces. We show performance of our method for large systems such as membrane proteins and ribosomes.

2F1549 **MD シミュレーションを用いた構造サンプリングによるドッキングタンパク質ータンパク質複合体結合自由エネルギー評価の精密化**

Refining binding free energies of docked protein-protein complexes by sampling conformations during molecular dynamics simulations

Ai Shinobu, Kazuhiro Takemura, Akio Kitao (*Inst. Mol. Cell. Bio., Univ. Tokyo*)

In this study, we aim to refine relative binding free energies (ΔGC) of protein-protein complex models produced by molecular docking, by subjecting them to molecular dynamics (MD) simulations.
We use a previously developed procedure that estimates ΔGC as the sum of the conformational and solvation free energies.
We show that conformations collected during MD have lower ΔGC values, suggesting that proper hydration achieved by MD is crucial in generating native-like complex structures. Moreover, the calculated ΔGC values are lower for conformations resembling the crystal structure, making this an effective procedure for distinguishing native-like conformations among a set of structures.

2F1601 **Improvement of PaCS-MD based Flexible Docking Methods**

Phuoc Duy Tran[1], Akio Kitao[1,2] ([1]*Graduate School of Frontier Sciences, The University of Tokyo*, [2]*Institute of Molecular and Cellular Biosciences, The University of Tokyo*)

Most of the current rigid-body docking method fails in the case of the extremely flexible protein/peptide docking due to neglect the conformational change of both protein and peptide. In this work, we introduce the docking method based on PaCS-MD [Harada, Kitao, JCC 2013] which allows sampling of the bound conformations without any bias to the system. The obstacle to sample the bound conformation is that the desolvation of the binding interface is slow, and enhanced sampling might neglect those conformations when desolvation of the binding interface is not complete. Here we made an improvement of the method to overcome this problem. The method is applied to MDM2/TAD-p53 system, which is considered as a typical case of flexible protein/peptide docking.

2F1613 **アミロイド核前駆体として機能する前駆中間凝集体のキャラクタリゼーション**

A specific form of prefibrillar aggregates that functions as a precursor of amyloid nucleation

Naoki Yamamoto, Shoko Tsuhara, Atsuo Tamura, Eri Chatani (*Grad. Sch. Sci.*)

Non-fibrillar protein aggregates that appear in the earlier stages of amyloid fibril formation are sometimes considered to play a key role in amyloid nucleation; however, the structural features of these aggregates currently remain unclear. We herein identified a characteristic pathway of fibril formation by the human insulin B chain, in which two major species of prefibrillar aggregates as well as smaller oligomers were identified. Based on the time-resolved tracking of this pathway with far-UV circular dichroism (CD) spectroscopy, dynamic light scattering (DLS), and 1H-NMR spectroscopy, the first prefibrillar aggregate with a hydrodynamic diameter of approximately 70 nm was found to accumulate concomitantly with the formation of a β-sheet structure.

2H1355 **光化学系 I の低温単一分子分光: ブリンキングの起源**

Single-Molecule Spectroscopy of Photosystem I at Low Temperature: the Origin of the Blinking

Sankar Jana[1], Takanori Kobayashi[1], Ting Du[1], Ryo Nagao[2], Takumi Noguchi[3], **Yutaka Shibata**[1] ([1]*Grad. School of Sci. Tohoku Univ.*, [2]*Research Institute for Interdisciplinary Science, Okayama University*, [3]*Graduate School of Science, Nagoya University*)

Our single-molecule fluorescence spectroscopy study on the oxygenic photosystem complex, photosystem I (PSI), at low temperatures has revealed the fluorescence blinking of single PSI molecules, which is intermittent intensity fluctuations of fluorescence. Our analysis on the excitation-power dependence showed that the frequency of the blinking is correlated to the probability of the singlet-annihilation (SA) in the complex, although minority of the complexes suggested existence of a mechanism independent from SA. We interpreted the blinking of PSI based on a hypothesis that it is induced by a modification in the energy-transfer pathway within the complex due to the site-energy change of chlorophyll. The excess energy dissipated by SA may cause the site-energy changes.

2H1407 **光化学系 II 酸素発生中心における酸素分子放出過程についての QM/MM 解析**

QM/MM study on the O2 release mechanism of the oxygen-evolving complex in photosystem II

Mitsuo Shoji[1], Hiroshi Isobe[2], Yasuteru Shigeta[1], Takahito Nakajima[3], Kizashi Yamaguchi[4] ([1]*Univ. Tsukuba*, [2]*Okayama Univ.*, [3]*RIKEN AICS*, [4]*Osaka Univ.*)

The O2 release of the oxygen-evolving complex (OEC) of the photosystem II (PSII) is one of the essential processes responsible for the highly efficient O2 production. Despite its importance, the detailed molecular mechanism is still unsolved. In the present study, we show one potential O2 release process from the Mn cluster based on the quantum mechanics/molecular mechanics (QM/MM) calculations. The present mechanism can explain an efficient removal of the toxic O2 from the catalytic center and implications of the surrounding amino acids near the PSII-OEC.

2H1419 **単一分子分光で明らかになった光合成光保護機構**

Photosynthetic photoprotection mechanism revealed by single-molecule spectroscopy

Toru Kondo[1,2], Alberta Pinnola[3], Wei Jia Chen[1], Luca Dall'Osto[3], Roberto Bassi[3], Gabriela Schlau-Cohen[1,2] ([1]*Mit*, [2]*Mit-Harvard Center for Excitonics*, [3]*Univ. Verona*)

Photoprotective function, known as non-photochemical quenching (NPQ), is crucial for environmental adaptation of photosynthetic organisms. Extensive studies have ever clarified strong associations of the NPQ efficiency with the pH condition and carotenoid composition. However, the quenched states and their conformational and photophysical dynamics have not been identified. The significant but small dynamics are averaged out and obscured in ensemble experiments. Thus, we applied the single-molecule spectroscopy to a light-harvesting complex stress related (LHCSR) protein, identified as a key NPQ factor. We revealed that the pH drop suppressed the dynamics and stabilized the quenched state, and that the carotenoid conversion enhanced the quenching efficiency.

2H1431 **Monitoring of quinone reduction in the thermophilic purple bacterium Thermochromatium tedium by means of isotope-edited FTIR spectroscopy**

Michie Imanishi[1], Rikako Kishi[1], Masayuki Kobayashi[2], Seiu Otomo[3], **Yukihiro Kimura**[1] ([1]*Grad. Sch. Agro., Kobe Univ.*, [2]*Ariake Nat. Col. Tech*, [3]*Fac. Sci., Ibaraki Univ.*)

In purple photosynthetic bacteria, a type-II reaction center (RC) is surrounded by a cylindrical light-harvesting 1 (LH1) complex in a stoichiometric ratio. In Rba. sphaeroides, a C-shaped LH1 ring is composed of 14 ab-subunits with PufX protein, a putative gate keeper of the LH1-ring for the quinone/quinol transport. In contrast, an O-shaped LH1 ring of the thermophilic Tch. tepidum is a 16-mer of ab-subunits with lacking PufX-like protein, indicating significant differences in the mechanism of quinone reduction and following quinol export pathway. In this study, light-induced quinol formation of the LH1-RC from Tch. tepidum was monitored by means of isotope-edited FTIR spectroscopy and discussed the behavior on the basis of the recent structural information.

2H1513 **Crystal structure of biliverdin reductase shows unexpected substrate binding manner; two substrates bind to the one catalytic cleft**

Masakazu Sugishima[1], Haruna Takao[2,3], Yoshinori Hagiwara[4], Ken Yamamoto[1], Keiichi Fukuyama[5], Kei Wada[2] ([1]*Kurume Univ. Sch. Med.*, [2]*Fac. Med., Univ. Miyazaki*, [3]*Grad. Sch. Med. and Vet. Med., Univ. Miyazaki*, [4]*Dept. Biochem. and Appl. Chem., Nat. Inst. Tech., Kurume College*, [5]*Grad. Sch. Eng., Osaka Univ.*)

Biliverdin IXα reductase (BVR-A) is a classical enzyme that is responsible for the last step in heme degradation and produces bilirubin (BR) using NAD(P)H as a cofactor. Here, we determined the crystal structure of the cyanobacterial BVR-A homolog (BvdR) in complex with BV and $NADP^+$ at 2.6 Å resolution. Although the overall folding of BvdR was similar to those of mammalian BVR-As, BV binding manner in BvdR was surprising. Two BV molecules (termed proximal and distal BV relative to the bound $NADP^+$) bind with the stacked geometry in the active site. The location of nicotinamide moiety of $NADP^+$ is ideal for the hydride transfer to the proximal BV. The distal BV would fix the proximal BV at the appropriate position and may function as the proton donor for the catalysis.

2H1443 **時間分解 EPR でとらえる光合成反応中心初期電荷分離の制御機構**

Regulation of Initial Charge Separation in Photosynthetic Reaction Center detected by Transient EPR

Hiroyuki Mino[1], Hiroyuki Tsukuno[1], Risa Mutoh[2,3], Hiroki Nagashima[1,4], Yasuhiro Kobori[4], Genji Kurisu[2], Hirozo Oh-oka[5] ([1]*Grad. School of Sci., Nagoya Univ.*, [2]*Inst. for Protein Res., Osaka Univ.*, [3]*Fac. of Sci., Fukuoka Univ.*, [4]*Mol. Photosci. Res., Kobe Univ*, [5]*Grad. School of Sci., Osaka Univ.*)

There are four kinds of photosynthetic reaction center (RC) on the earth. The initial charge separation is performed between Chl (BChl) and Pheo for type II RC or Chl (BChl) and Chl (BChl) for type I RC. In order to establish high efficient and stable charge separation, the radical pair is bridged with the other Chl (Bchl) molecule. Time resolved EPR gives the interaction between radical pair, expressed by the exchange interaction *J*. The *J*-value obtained in heliobacterial RC (type I) was similar to that in plant photosystem II, but considerably smaller than that found in purple bacterial RC.By the comparison with the reaction centers, we will discuss the evolutionary strategy of the photosynthesis reactions.

2H1525 **カンチレバーを用いた高感度多周波 EPR 測定法の開発とヘミンへの応用**

Development of cantilever-detected high-sensitive multi-frequency EPR method and its application to hemin

Tsubasa Okamoto[1], Hideyuki Takahashi[2], Eiji Ohmichi[1], Hitoshi Ohta[3] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Arg. Adv. Integ. Res., Kobe Univ.*, [3]*Mol. Photosci. Res. Ctr., Kobe Univ.*)

In this presentation, we report novel multi-frequency electron paramagnetic resonance (EPR) technique using a microcantilever. In this technique, EPR signals are detected as a cantilever bending induced by either magnetic torque or field gradient force of a sample mounted on the cantilever. A unique feature of this technique is that sample mass of only micro-gram order is sufficient to detect EPR signals in the terahertz region. In this study, our cantilever-detected EPR method was applied to hemin, which is a model substance of hemoprotein, and EPR signals were successfully observed in the broad frequency range up to 500 GHz at 4.2 K. Further applications to hemoproteins such as myoglobin are also in progress.

2H1455 **溶液中のクロロフィル a とフィオフィチン a の励起状態に関する理論的研究**

Theoretical Study on Excited States of Chlorophyll a and Pheophytin a in Solutions

Ryo Mizutani, Masahiro Higashi (*Grad. Sch. Univ. The Ryukyus*)

We theoretically investigated the excited-state properties of chlorophyll a and pheophytin a pigments in solutions. To examine solvent effects, we used two solvent models. One is a polarizable continuum model (PCM), whereas the QM/MM reweighting free energy self-consistent field (QM/MM-RWFE-SCF) method was adopted in the other case. We found that the absorption energies calculated with the PCM are much different from the experimental ones. On the other hand, the absorption energies calculated with the QM/MM-RWFE-SCF method are close to the experimental one. This result indicates the importance of solvent model to describe the excited-state properties in solutions. We also examined which density functional can reproduce the properties more accurately.

2H1537 **高分解能二次イオン質量分析法による電気細菌代謝の一細胞レベル追跡**

NanoSIMS Analysis of Single Electrogenic Cell Reveals Feedback from Extracellular Electron Transport to Upstream Reactions

Akihiro Okamoto[1], Junki Saito[2], Kazuhito Hashimoto[1] ([1]*National Institute for Material Sciences*, [2]*Dept. Appl. Chem., Univ. of Tokyo*)

Certain microbes are capable of transporting respiratory electrons to electrode surface cell outside, extracellular electron transfer (EET), which make the metabolic reactions electrically controllable. We here analyzed the metabolic activity of the electrogenic bacterial cells respiring on an indium tin-doped oxide electrode with nanoscale secondary ion mass spectrometry (NanoSIMS) for quantification of the anabolism of 15NH4-. Although acceleration of EET did not enhance the average metabolic activity, the distribution of 15N intake among individual cells was bipolarized upon EET rate enhancement, suggesting not only positive but also negative effects on cellular activity. We will discuss about the feedback mechanism from EET to the upstream reactions.

2H1549 **海洋性ビブリオ菌極べん毛の側における形成を抑制する新規因子 SflB の解析**

Characterization of SflB, a novel factor that prevents peritrichous flagellar formation in marine *Vibrio*

Tatsuro Nishikino, Taira Mino, **Seiji Kojima**, Michio Homma (*Div. of Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

Vibrio alginolyticus has a single polar flagellum whose number and position are regulated by FlhF and FlhG. Lack of both FlhF and FlhG mostly abolishes flagellation, but an additional defect in sflA results in peritrichous flagellar formation. SflA is a single transmembrane protein with DnaJ domain in cytoplasm and Tetratricopeptide repeat (TPR) domain in periplasm. In upstream of sflA, there is an open reading frame whose product is predicted to be a membrane protein with a large periplasmic region homologous to outer membrane lipoprotein protein. We named this gene sflB. Deletion of sflB in a ΔflhFG strain conferred flagellation similar to the ΔflhFGΔsflA strain. So SflB may work with SflA to prevent the flagellation. Function of SflB will be examined and discussed.

2H1601 **クライオ電子顕微鏡法で明らかになった、3.8 A 分解能のアクチン-コフィリン複合体構造**

Actin-cofilin complex structure at 3.8 A resolution revealed by cryo-EM

Kotaro Tanaka[1], Shuichi Takeda[1], Kaoru Mitsuka[3], Toshiro Oda[2], Yuichiro Maeda[1], **Akihiro Narita**[1] ([1]*Struct. Biol. Res. Center, Nagoya Univ.*, [2]*Tokai Gakuin Univ.*, [3]*Res. Center for UHV EM, Osaka Univ.*)

Cofilin severs and depolymerizes the actin filaments and accelerates dynamics of the actin filament in the cell. This activity plays a major role in many important cellular functions including cell motility, cell division, muscle maintenance, development, cancer and neural network. We collected cryo-electron micrographs of fully decorated actin filaments by cofilin with Titan Krios at Osaka Univ. We reconstructed structure at 3.8 A resolution from 202,217 particles on 1111 electron micrographs. This newly determined structure combined with our recent crystal analysis enabled us to propose mechanism how cofilin severs the filament, binds to the filament cooperatively and why cofilin prefers ADP-F-actin to ATP-F-actin.

2H1613 **細胞性粘菌のアクチンのカルボキシ末端領域の二型性と Pro109 に導入した変異の関係**

The relationship between the dimorphism of the carboxyl-terminal region and the mutagenesis introduced to Pro109 of *Dictyostelium* actin

Yuki Gomibuchi[1], Taro Q.P. Uyeda[2], Takeyuki Wakabayashi[1] ([1]*Teikyo Univ.*, [2]*Waseda Univ.*)

The *Dictyostelium* actin crystal structures at 1.93-2.03 Å resolution showed that the side chains of the residues 352-356 (FQQMW) changed their configurations in a concerted manner and showed the dimorphism (B-type: the buried Trp356 side chain; E-type: exposed to the solvent). Whereas, the side chain of Glu354 was stabilized by the hydrogen bond between $O_{\varepsilon 1}$ and the amide hydrogen of Glu6 of gelsolin-1, the other side-chains (352-355) changed their configurations in accordance with that of Trp356 side chain. The Pro109Ala mutant tended to show the B-type and the Pro109Ile mutant tended to show the E-type. In comparison with the wild-type actin, the former showed the higher G-actin ATPase and the latter the lower one.

2I1355 **光駆動型ナトリウムイオンポンプロドプシンで見られる弁別的な機能・光化学特性**

Distinctive functional and photochemical properties among light-driven sodium ion pumping rhodopsins

Marie Kurihara[1], Misa Hashimoto[2], Susumu Yoshizawa[3], Keiichi Kozima[1], Takashi Tsukamoto[1,2], Takashi Kikukawa[4,5], Yuki Sudo[1,2] ([1]*Grad. Sch. of Med. Dent. & Pharm. Sci., Univ. Okayama*, [2]*Fac. of Pharm. Sci., Univ. Okayama*, [3]*AORI, The Univ. of Tokyo*, [4]*Fac. Adv. Life Sci., Univ. Hokkaido*, [5]*GSS, GI-CoRE, Univ. Hokkaido*)

On the cell membrane of microorganisms, rhodopsins show various biological functions such as ion pumps, ion channels and sensors. A light-driven outward sodium ion pumping rhodopsin has been firstly identified in 2013 and named KR2. Here we functionally and spectroscopically characterized two KR2-like rhodopsins, Y-NaR and M-NaR, in comparison with KR2. We revealed that ion transport activity, pKa values of the counterion of the retinal and photocyclic reaction were significantly different among them. Based on the results, we discuss the molecular characteristics of sodium ion pumping rhodopsins. Of note, Y-NaR showed both the highest sodium ion pumping activity and thermal stability, suggesting that Y-NaR is a good research model for sodium ion pumping rhodopsins.

2I1407 **ナトリウムポンプ型ロドプシン中間体の過渡共鳴ラマン分光法による研究**

Transient Resonance Raman Spectroscopy of a Light-Driven Sodium-Ion-Pump Rhodopsin from Indibacter alkaliphilus

Kosuke Kajimoto[1] ([1]*Grad. Sch. Sci. Eng. Saga-Univ*, [2]*Fac. Adv. Life Sci., Hokkaido Uni*, [3]*GSS, GI-CoRE, Hokkaido Univ.*)

Sodium-ion-pump rhodopsin (NaR) is a microbial rhodopsin that transports Na+ during its photocycle. Here we explore the photocycle mechanism of NaR from Indibacter alkaliphilus with transient absorption and transient resonance Raman spectroscopy. The transient absorption data indicate that the photocycle of NaR consists of K (545) , L (490)/M (420) , O1 (590) and O2 (560) , where the L and M are formed as equilibrium states. The main component of the transient resonance Raman spectra was due to L which contains a 13-cis retinal protonated Schiff base. The presence of an enhanced hydrogen out-of-plane band as well as its sensitivity to the H/D exchange indicate that the retinal chromophore is distorted near the Schiff base region in L.

2I1419 **海洋性細菌 *Rubricoccus marinus* SG-29^T 株由来の内向き H^+ポンプ型ロドプシン *Rm*XeR の分光学的解析**

Spectroscopic analysis of *Rm*XeR, an inward H^+ pump rhodopsin from the marine bacterium *Rubricoccus marinus* SG-29^T

Saki Inoue[1], Susumu Yoshizawa[2], Keiichi Kojima[1], Takashi Tsukamoto[1], Takashi Kikukawa[3,4], Yuki Sudo[1] ([1]*Grad. Sch. of Med. Dent. & Pharm. Sci., Okayama Univ.*, [2]*AORI, The Univ. of Tokyo*, [3]*Fac. Adv. Life Sci., Hokkaido Univ.*, [4]*GSS, GI-CoRE, Hokkaido Univ.*)

Microbial rhodopsins show a wide variety of biological functions such as ion pumps, ion channels and light sensors. In 2011, a new phylogenetic group named xenorhodopsin (XeR) has been proposed, and one of them (*Po*XeR) has been functionally identified as an inward H^+ pump. Here, we report that *Rm*XeR, an XeR from the marine bacterium *Rubricoccus marinus* SG-29^T, functions as an inward H^+ pump in the cell membrane as same as *Po*XeR. In addition, spectroscopic analysis of the purified *Rm*XeR showed some characteristics including opposite light-dark adaptation and opposite spectral shift by acidification in comparison with outward H^+ pumps such as BR. In the meeting, we will discuss the differences between inward and outward H^+ pumps from a molecular point of view.

2I1431 ラマン光学活性分光を用いた微生物型ロドプシンにおけるレチナール発色団のコンフォメーション解析
Raman optical activity probes the conformation of the retinal chromophore in microbial rhodopsins

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Raman optical activity (ROA) is expected to yield a wealth of stereo-chemical information about conformational details of molecules. We have applied the near-infrared ROA to several photoreceptor proteins. Here, we present the ROA studies on two microbial rhodopsins, Gloeobacter rhodopsin and sodium-ion-pump rhodopsin. These studies demonstrate that the ROA spectrum of the retinal chromophore is sensitive to the out-of-plane distortions near the protonated Schiff base moiety. The use of the ROA combined with quantum chemical calculations is a novel and generally applicable spectroscopic tool to study the chromophore distortions within a protein environment.

2I1443 Towards the structural study of the photocycle of bistable rhodopsin

Midori Murakami (*Dept. Physics, Nagoya Univ.*)

Rhodopsin is a retinal-binding membrane protein. While retinal is hydrolyzes in vertebrate rhodopsin on isomerization, invertebrate rhodopsin can switch between active and inactive states without the release of the chromophore. Newly developed serial femtosecond X-ray crystallography with X-ray free electron lasers is a powerful method to study structural dynamics of proteins. Although this method can provide us a molecular movie of the early steps, it is hard to observe later process with large conformational changes. To study structural dynamics of the photocycle of rhodopsin we are performing crystallization of squid rhodopsin in the dark and photo-activated states for time-resolved studies. We will show some results for micron-sized crystallization in both states.

2I1455 In situ 光照射固体ＮＭＲによるバクテリオロドプシンとその変異体に生成する光反応中間体の定常捕捉
Stationary trapping of photo-intermediates during the photo cycles of bR and its mutants by in situ photoirradiation solid-state NMR

Akira Naito[1], Kyosuke Oshima[1], Yuto Otani[1], Arisu Shigeta[1], Yoshiteru Makino[1], Izuru Kawamura[1], Takashi Okitsu[2], Akimori Wada[2], Satoru Tuzi[3], Tatsuo Iwasa[4] ([1]*Yokohama National University*, [2]*Kobe Phamacutical University*, [3]*University of Hyogo*, [4]*Muroran Institute of Technology*)

The photointermediates that appear in the photoreaction cycle typically have short half-lives. Therefore, it is difficult to detect the photointermediates using solid-state NMR. New in situ photoirradiaton system makes it possible to observe photointermediates using solid-state NMR. Using this in situ photoirradiation solid-state NMR, photo-intermediates of bacteriorhodopsin (bR) and its Y185F and D96N mutants were stationary trapped and characterized. 13C CP-MAS NMR spectra of Y185F mutant were acquired at -40 C in the dark (D1), under irradiation with 520 nm light (L1). The CS (bR548) state changed to a CS* (13-cis, 15-syn)-intermediate. The AT (bR568) state transformed to an N-intermediate, and subsequently transferred to an O-intermediates under dark condition.

2I1513 メラノプシンの 3 平衡状態光反応による光量感知
Melanopsin tristability: a new model of photoresponse for irradiance detection

Takesi Matsuyama Hoyos[1], Masayo Takahashi[1], Yoshinori Shichida[2] ([1]*RIKEN CDB*, [2]*Kyoto University Graduate School of Science*)

Melanopsin is the photosensitive pigment of ipRGCs, which mediate vital irradiance detection functions. We have conducted a comprehensive analyses of the photochemical properties of melanopsin and found that melanopsin exhibits a unique photo-photoreaction consisting of an equilibrium mixture of three photo-labile states. We have also conducted a comprehensive analysis of its G-protein activity, and build a model of melanopsin photoresponse. Our tristable model indicates that different states of melanopsin can form preferentially, depending on the wavelength of light stimulation. Furthermore we show that action spectrum of melanopsin is dependent on the intensity and/or duration of the light stimuli, adding another dimension to the photoresponse of melanopsin.

2I1525 松果体オプシンパラピノプシンの分子特性の細胞応答への寄与
Contribution of a molecular property of a pineal opsin parapinopsin to cellular responses

Seiji Wada[1], Baoguo Shen[1], Emi Kawano-Yamashita[1], Takashi Nagata[1], Satoshi Tamotsu[2], Mitsumasa Koyanagi[1], **Akihisa Terakita**[1] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Fac. Sci., Nara Women's Univ.*)

Parapinopsin (PP) is a pineal UV-sensitive opsin in lower vertebrates. PP possesses a molecular property different from that of vertebrate visual opsins; the inactive dark state (UV-sensitive) and active photoproduct (visible light-sensitive) are interconvertible by light absorption, showing the bistability. Although PP is involved in the discrimination of UV and visible lights in the pineal organs, a contribution of the bistability is still unknown. Here, we successfully measured calcium responses from the PP-expressing photoreceptor cells in zebrafish pineal organ, which suggested that the bistability contributed to generating light-responses involved in the color discrimination. We also discuss a contribution of the bistability to optogenetic application of PP.

2I1537 暗所視を司る錐体視物質の低い熱雑音の進化的獲得
Evolutionary acquisition of low thermal noise of cone pigments for scotopic vision

Keiichi Kojima[1,2], Yuki Matsutani[2], Masataka Yanagawa[3], Takahiro Yamashita[2], Yasushi Imamoto[2], Osamu Hisatomi[4], Yumiko Yamano[5], Akimori Wada[5], Yoshinori Shichida[2,6] ([1]*Grad. Sch. of Med. Dent. Pharm. Sci., Okayama Univ*, [2]*Grad. Sch. Sci., Kyoto Univ.*, [3]*Cell. Info. Lab., RIKEN*, [4]*Grad. Sch. Sci., Osaka Univ.*, [5]*Kobe Pharm. Univ.*, [6]*Ritsumeikan Univ.*)

Most vertebrate eyes have two types of photoreceptor cells, rods and cones for scotopic and photopic vision, respectively. Since scotopic vision requires high sensitivity to detect only a few photons, rhodopsin is optimized for scotopic vision by the acquisition of the low thermal activation rate. Frogs exceptionally have unique rods containing not rhodopsin but blue-sensitive "cone" pigments. However, it remains unknown whether they acquired the rhodopsin-like property. Here, we optimized biophysical and biochemical methods to compare thermal activation rates of visual pigments and their mutants. Our results indicated that frog blue-sensitive cone pigments acquired the low thermal noise by the suppression of protein fluctuation through a single amino acid mutation.

2I1549 光遺伝学に向けた長波長シフト型ナトリウムポンプロドプシンの作製

Red-shifted sodium pump rhodopsin variants for optogenetic application

Keiichi Inoue[1,2], Ryoko Nakamura[1], Hideki Kandori[1] ([1]*Nagoya Inst. Tech.*, [2]*JST PRESTO*)

Sodium pump rhodopsin (NaR) is a member of photoreceptive microbial rhodopsins and it outwardly transports sodium by light. The first identified NaR from *Krokinobacter eikastus* (KR2) was shown to be able to inhibit neuronal activity by light. However, while KR2 absorbs green light (~525 nm), the control by longer-wavelength light which has lower phototoxicity and higher penetration depth is highly demanded. Here, we revealed that a mutation of a proline (Pro219) makes the absorption wavelength 16-nm longer. We applied further mutation for this variant, and finally we achieved >40-nm red-shift. Interestingly, these mutants showed identical sodium transport activity to wildtype. We will discuss the mechanism of red-shift and the potential for optogenetic application.

2I1601 光依存型グアニル酸シクラーゼである微生物型ロドプシン(BeGC1)の機能解析

Functional characterization of rhodopsin-guanylate cyclase, BeGC1

Satoshi Tsunoda[1,2,3], Kazuho Yoshida[2], Hideki Kandori[2,3] ([1]*JST, PRESTO*, [2]*NIT*, [3]*OBTR*)

Microbial-type rhodopsins exhibit diverse functions involving ion transporters, light sensors and light dependent enzymes. Recent studies reveal that a unique microbial-type rhodopsin, BeGC1, from the flagellated swimming zoospores *Blastocladiella emersonii*, fuses a guanylate cyclase domain at the C-terminus region and thus is a directly light-activated guanylate cyclase, serving as a promising optogenetics tool. When BeGC1 is hetelorogously expressed in mammalian cells, intercellular cGMP level can be elevated simply by illumination. To get deeper insights into the light-activation mechanism, we here investigate the spectroscopic property, enzymatic kinetics, and finally evaluate the light-dependent cyclase activity in mammalian cells.

2I1613 ハロロドプシンはヒドロキシイオンを輸送できるか？

Can halorhodopsin pump hydroxyl ions ?

Tsutomu Kouyama, Kenta Suzuki, Keita Naruse, Siu Kit Chan (*Graduate School of Science, Nagoya University*)

Halorhodopsin from Natronomonas pharaonis (pHR) functions as a light-driven chloride ion pump under the physiological conditions. Crystallographic data showed that the removal of chloride ion from pHR at neutral pH, which causes a red shift of the visible absorption band, is accompanied by a shrinkage of the primary anion-binding site. We have recently found that acidification of a halide-ion free form of pHR causes a large blue shift of the visible absorption band. Interestingly, this spectral change is coupled with an enlargement of the primary anion-binding site and insertion of a water molecule or a hydroxyl ion near the retinal Schiff base. We will discuss the charge distribution in the halide-free acidic form of pHR and the capability of pumping hydroxyl ions.

2J1355 細胞の異方的なメカノレスポンスが発生過程の精巣上体細管の径を維持する

Anisotropic Cellular Mechanoresponse Maintains the Radial Size of Developing Epididymal Tubules

Tsuyoshi Hirashima[1], Taiji Adachi[2] ([1]*Grad Sch Med, Kyoto Univ*, [2]*Inst Front Life Med Sci, Kyoto Univ*)

Cellular response to mechanical forces plays important roles in tissue size maintenance during development. However, little is known about mechanisms how the cellular mechanoresponse works to achieve the anisotropic size maintenance in developing tissues. We employed the epididymal tubules of murine embryos to address this issue. By combining experimental and mathematical approaches, we show that the epididymal cells counteract mechanical forces exclusively along the tubule circumferential axis, and propose the anisotropic cellular mechanoresponse at supra-cellular scale would spontaneously maintain the tubule radial size at whole tissue scale. Our results will lead to further understanding of the mechanoresponse system that controls tissue morphogenesis.

2J1407 3 次元的な形態の多様性を説明する細胞の力学の理論的な推定

Theoretical inference of cell mechanics for explaining 3-dimensional morphological diversity

Hiroshi Koyama[1,2], Toshihiko Fujimori[1,2] ([1]*Div. Embryology, NIBB*, [2]*SOKENDAI*)

During morphogenesis of multi-cellular systems, both cell movement and tissue shape transformation are primary determined by mechanical forces. However, the spatio-temporal distributions of the forces exerted by cells are not well understood. Here, on the basis of Bayesian statistic/data assimilation, we constructed a method to infer the forces from in vivo cell movements. We applied this method to cysts of MDCK cells, early embryogenesis in C. elegans and in mice. By analyzing the inferred results, we discovered a geometric rule which can predict the forces. Importantly, subsequent simulations based on the rule reproduced various 3-dimensional morphologies, suggesting that the geometric rule can be a principle for morphological diversity.

2J1419 マウス ES 細胞は、フラッシュラチェット様式をとりながら、集団で分化する

Flashing ratchet-driven collective cell-state transition in mouse embryonic stem cells

Kazuko Okamoto[1], Arno Germond[1], Hideaki Fujita[1,2], Chikara Furusawa[1,3], Yasushi Okada[1,3,4], Tomonobu Watanabe[1,4] ([1]*RIKEN QBiC*, [2]*WPI, IFReC, Osaka Univ.*, [3]*Sch. of Sci, Univ. of Tokyo*, [4]*FBS, Osaka Univ.*)

Collective behaviors can be generated by the action of individual cells in various biological processes such as cell migration. Although the molecular basis of stem cells has been extensively studied, the general driving force guiding the collective dynamics of stem cells at both the individual and group levels remains to be identified from physical aspects. To this end, we monitored the cell-state transition at the single-cell and colony levels during the early differentiation process. Two criteria for the avalanche of the collective-state transition were revealed: spontaneous fluctuation and cell-cell cooperativity. We further demonstrate that this process is similar to a flashing ratchet behavior, suggesting a general mechanism driving the collective differentiation.

2J1431 植物組織では異方的な細胞成長が滑らかな境界形成を促進する。
Anisotropic cell growth promotes smooth boundary formation of stem cell tissue in plant roots

Motohiro Fujiwara, Koichi Fujimoto (*Science Dept. Osaka Univ.*)

Different cell types are sorted out by forming smooth boundaries in tissue. While cell contraction and intercalation are responsible for smooth boundary formation in animal tissue, how plant cells, which are neither intercalated nor contracted, form smooth boundaries is largely unknown. In order to analyze mechanisms of smooth boundary formation in plant tissue, we combined quantifying cell shape dynamics in Arabidopsis root stem cells with tissue mechanical simulations. As a result, we predicted that smooth boundary between two cell types was mainly regulated by the difference of anisotropic cell growth due to differential cell wall extensibility. A cell wall between different cell types was more extensible than a cell wall between same cell type.

2J1443 Bicistronic 2A-peptide-based co-expression reporter revealed the gene expression profiles in developing human photoreceptors

Kohei Homma (*Keio Univ. Sch. of Med. Dpt. of Ophthalmol.*)

Fluorescent reporter genes have been utilized to visualize specific cell lineages, although transgenes are often silenced during cell differentiation in human cells. To overcome the silencing of the reporter gene, we applied the CRISPR/Cas9 genome editing, and the bicistronic 2A-peptide-based co-expression (B2AC) system to the knock-in for the fluorescent cell labeling. By using these technologies, knock-in hPSC lines were established, and the co-expression of target gene, Crx (a photoreceptor marker), and the fluorescent protein was observed during three-dimensional retinal organoid culture. The Crx expression and fluorescent intensity in the cells were positively correlated, suggesting that the B2AC reporter system functioned during human retinal development.

2J1455 Two-dimensional fluorescence lifetime correlation spectroscopy reveals µs-dynamics and distinct folding mechanisms of $preQ_1$ riboswitch

Bidyut Sarkar[1], Kunihiko Ishii[1,2], Tahei Tahara[1,2] ([1]*Molecular Spectroscopy Laboratory, RIKEN*, [2]*RIKEN Center for Advanced Photonics, RIKEN*)

The $preQ_1$ riboswitch regulates the expression of proteins involved in GTP biosynthesis in bacteria. In *B. subtilis*, it is achieved at the transcriptional level by ligand induced conformational change of the riboswitch. We investigate the folding dynamics of a FRET-pair labeled $preQ_1$ riboswitch using two-dimensional fluorescence lifetime correlation spectroscopy (2D FLCS) to reveal (I) µs-conformational dynamics between the folded and open states, (II) distinct binding mechanisms for cofactor Mg^{2+} (conformational selection) and ligand $preQ_1$ (induced fit), and (III) that only a fraction of molecules (~10%) participates in fast µs-dynamics while others may show slower dynamics. We further verify the reaction scheme with synthetic photon data by Monte-Carlo simulation.

2J1513 The reaction mechanism of pH-dependent RecA-mediated DNA strand exchange

Hsiu-Fang Fan (*National Yang-Ming University*)

A single molecule approach (Tethered Particle Motion) was used to investigate the RecA-mediated strand exchang process. D. ficus RecA and E coli dC17 RecA possessing higher DNA binding affinity. The higher DNA strand exchange efficiency under basic condition results from the competition between the formation and the dissociation of three-stranded intermediates in the homologous sequence searching process. Combining multiple sequence alignment and TPM experiments, the loss of partial C-terminal acidic residues makes RecA proteins from bacteria belonging to Deinococcus genera possess a higher DNA binding affinity in order to promote fast DNA stand exchange under server DNA damage process.

2J1525 DNA ナノデバイスの温度応答性能の設計
Engineering thermal response of a DNA nanodevice

Ken Komiya[1], Satoshi Kobayashi[2], John A. Rose[3] ([1]*Sch. Comp., Tokyo Tech.*, [2]*Dept. Comp. Sci., The Univ. Electro-Commun.*, [3]*College APS, Ritsumeikan APU*)

Engineering of stable and sub-stable folds that exist in competitive equilibrium allows us to produce exotic behaviours of DNA nanodevices. Previously, we proposed, modelled, and experimentally validated a temperature-sensitive DNA nanodevice that operates as a thermal band-pass filter. Although its peculiar efficiency profile differs markedly from the common profile of simple isolated folding, no effort was made to reveal the detailed dependencies on the stabilities of device components. In the present work, closed-form expressions for the peak temperature and maximum efficiency are derived and validated. The functional behaviours of these expressions are then examined and harnessed to construct an efficient algorithm for producing designs with desired device response.

2J1537 Nucleosome Repositioning Investigated by Coarse-Grained MD Simulations and Markov State Modeling

Giovanni Brandani, Toru Niina, Cheng Tan, Shoji Takada (*Dept Biophysics, Div Biology, Grad School Science, Kyoto University*)

Nucleosomes are highly stable structures that form the building blocks necessary for chromatin compaction. Yet, they can also spontaneously reposition themselves from low- to high-affinity sequence locations via thermal fluctuations. We performed molecular dynamics simulations to investigate the microscopic details of nucleosome sliding. In our simulations we observed that DNA performs a rotation-coupled motion and reposition via the propagation of a twist defect, in agreement with theoretical modeling. Using our MD trajectories, we constructed a series of Markov state models that clearly illustrate how sequence-dependent DNA flexibility and defect formation control the time scales of repositioning.

2J1549 Osmotic mechanism of loop extrusion process

Tetsuya Yamamoto[1], Helmut Schiessel[2] ([1]*Nagoya Univ., Dep. of Mat. Phys.*, [2]*Leiden U., Inst. Lorentz for Theo. Phys.*)

The loop extrusion theory predicts the locality and stochasticity of chromatin interactions at topologically associated domains in agreement with Hi-C experiments. This theory assumes that cohesin acts as molecular motors that extrude chromatin loops. However, the latter assumption is disproved by recent single molecule experiments. We thus theoretically analyze the dynamics of cohesin rings on a chromatin loop to predict the physical mechanism involved in the loop extrusion process. Cohesin monomers bind to the loader rather frequently and cohesin dimers bind to this site only occasionally. Our theory predicts that cohesin dimers extrude a chromatin loop, where cohesin loader binds to the middle and unloader at the ends due to the osmotic pressure of cohesin monomers.

1Pos001 X 線結晶解析スクリーニングによる BRD4 阻害剤の探索と BRD4ー阻害剤複合体の中性子結晶構造解析

Discovery of BRD4 inhibitors by X-ray crystallographic screening and neutron crystallographic analysis of BRD4-inhibitor complex

Takeshi Yokoyama, Kazunori Matsumoto, Yuko Nabeshima, Mineyuki Mizuguchi (*Fac. of Pharm. Sci., Univ. of Toyama*)

BRD4 (bromodomain-containing protein 4) recognizes acetyl-lysine modified histone tails and regulates gene transcription. BRD4 is an attractive target for anticancer drug due to its important role in regulation of gene transcription. In the present study, we identified isoliquilitigenin, a chalcone compound, as a BRD4 inhibitor using X-ray crystallographic screening and evaluated the binding affinities of 11 isoliquilitigenin derivatives using isothermal titration calorimetry. In addition, to investigate the role of the conserved water molecules in the BRD4-inhibitor complex, large BRD4-inhibitor crystals (1.5 mm3) were prepared for the neutron protein crystallography (NPC). We will show the structure-activity relationship of BRD4-chalcone and the results for NPC.

1Pos002 P-loop を用いた ATP 結合タンパク質のゼロからの設計

Toward design of ATP-binding proteins from scratch using P-loop

Kengo Nakamura[1,2], Takahiro Kosugi[1,2], Nobuyasu Koga[1,2,3] ([1]*SOKENDAI*, [2]*IMS CIMoS*, [3]*JST PRESTO*)

ATP hydrolysis plays important roles in various proteins such as molecular motor. To explore a minimal set for ATP hydrolysis in protein structures, we started to computationally design ATP-binding proteins from scratch. For a phosphate binding site of ATP, the P-loop, a conserved phosphate binding motif, was used. Conducting folding simulations, we found optimal secondary structure lengths and loop types to build structures with the P-loop. Based on these, we designed ATP binding proteins from scratch. One of the designs was found to be monomeric with high thermal stability, however, the binding affinity to ATP was too weak to be detected. We report these results and discuss strategies of how to design strong binders.

1Pos003 gREST 法による Trpcage のフォールディングと自由エネルギー地形

Folding simulation and free energy landscape analysis of Trpcage by gREST

Motoshi Kamiya[1], Yuji Sugita[1,2,3] ([1]*RIKEN AICS*, [2]*RIKEN TMS*, [3]*RIKEN QBiC*)

Conformational search is still one of the important problems in all-atom molecular dynamics (MD) simulations of biomolecules. We developed a new method of the conformational search, which we call gREST (generalized replica-exchange with solute tempering: REST). It generalizes the conventional REST by allowing the flexible separation between solute and solvent and was implemented in GENESIS software package. In this study, we applied gREST to the folding simulation of Trpcage mini protein (TC5b) in explicit water. Multiple folding events were successfully observed in the trajectories of gREST and accurate free-energy landscape was obtained with lower computational cost than the conventional REST. Further details will be discussed in the meeting.

1Pos004 AMED 創薬等ライフサイエンス研究支援基盤事業が提供する最先端クライオ電子顕微鏡システム

State-of-the Art Cryo-EM system provided by AMED Platform Project for Supporting Drug Discovery and Life Science Research

Kenji Iwasaki, Kiyo Tsunezumi, Mika Hirose, Naoyuki Miyazaki (*IPR, Osaka Univ.*)

The Platform Project for Supporting Drug Discovery and Life Science Research (http://pford.jp/) is one of the AMED (Japan Agency for Medical Research and Development) programs started in April 2017. The Titan Krios high-end cryo-electron microscope (cryo-EM) began operating in April 2016 as part of a previous project and has now been handed over to this new one. It currently continuously provides clients with many protein structures at near-atomic resolution. As a special feature, our cryo-EM is equipped with a Cs-corrector and Volta phase plate (VPP). The VPP, in particular, exerts great power to overcome the minimum molecular limit for cryo-EM. Here, we give examples of the results obtained by combining the VPP and automatic data acquisition.

1Pos005 リガンド結合シミュレーションへのタンパク質構造揺らぎの取り込み

Incorporation of protein flexibility into ligand binding simulation

Suyong Re[1], Hiraku Oshima[1], Motoshi Kamiya[2], Yuji Sugita[1,2,3] ([1]*RIKEN QBiC*, [2]*RIKEN AICS*, [3]*RIKEN TMS*)

Accurate prediction of ligand binding structure and energetics remains a challenge. We applied a combined generalized replica exchange with solute tempering (gREST) and replica exchange umbrella sampling (REUS) method to study the ligand binding of Src kinase with focus on the impact of protein flexibility upon the ligand binding. The protein flexibility was incorporated by scaling the temperature of a wide solute region, involving the ligand and the active site residues, using gREST. We show that the native binding structure is correctly predicted and that the sampling efficiency of binding events improves over the long-time simulation, the existing REUS, and REST/REUS simulations.

1Pos006 Cryo-cooling effect on crystalline DHFR studied by replica-exchange molecular dynamics

Tetsuro Nagai[1], Osamu Miyashita[2], Florence Tama[1,2,3] ([1]*Nagoya Univ., Grad. School of Science*, [2]*RIKEN AICS*, [3]*Nagoya Univ., ITbM*)

When X-ray crystallography is performed, a protein crystal is typically cryo-cooled, in order to prevent damage and increase the resolution. Nevertheless, at such a low temperature, the physiological dynamics might not retain. In this study, DHFR was simulated in the crystal environment in a wide range of temperature, from 180 K to 300 K, by replica-exchange molecular dynamics method. We observed a shrink of unit cell and an increase in lattice contact at decreasing temperature. As well, a particularly functionally relevant loop exhibited a decrease in dynamics at the low temperature, revealing the strong effect of cryo-cooling on the biological functioning.

1Pos007 **GPU を用いた加重アンサンブルシミュレーションによるタンパク質の機能性ダイナミクスの探索**
Investigation of protein functional dynamics by GPU-accelerated weighted ensemble simulation

Hironori Kokubo, Atsutoshi Okabe, Etsurou Watanabe (*Research, Takeda Pharmaceutical*)

Predicting and regulating protein functional dynamics is of pivotal importance for drug discovery. However, functional dynamics occurs on a time scale between microsecond and second, which conventional molecular simulations cannot reach. We have worked on the development and application of the simulation method for rational drug design which regulates the functional dynamics. We first applied the weighed-ensemble methods by different criteria/protocols to pharmaceutical target proteins. We found that our method could find conformational changes related to functional dynamics, which could not be sampled by conventional simulation, at practical computational cost.

1Pos008 **The head structure of the Staphylococcus aureus phage S13' at near atomic resolution by cryo-electron microscopy single particle analysis**

Naoyuki Miyazaki[1], Jumpei Uchiyama[2], Shigenobu Matsuzaki[3], Kazuyoshi Murata[4], Kenji Iwasaki[1] ([1]*Institute for Protein Research, Osaka University*, [2]*Azabu University*, [3]*Kochi University*, [4]*National Institute for Physiological Sciences*)

Recently, antibiotics have become less effective because of the emerging infectious diseases caused by drug-resistant bacteria, such as methicillin-resistant Staphylococcus aureus (MRSA). Phage therapy is one of the possible alternative medical treatments, but for the practical use of the phase therapy it is important to understand the detailed mechanism of the phage infection and replication. Here, we investigated the 3D structure of the Staphylococcus aureus phage S13'. The head structure has been determined at 3.2 Å resolution by cryo-electron microscopy single particle reconstruction. The structure of the capsid protein shows the similar protein fold to the bacteriophage HK97 but revealed the unique novel structural features.

1Pos009 **自由エネルギー変分原理に基づく Pim-1 キナーゼ阻害剤系の相対的結合自由エネルギーの予測.リガンド構造の分類**
Relative binding free energy predictions for ligands with Pim-1 kinase based on the free energy variational principle: classify of ligands

Anna Hirai, Takeshi Ashida, Takeshi Kikuchi (*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*)

It is important for drug discovery to calculate values of the binding free energy between a protein and a ligand. In this study, we calculate the relative binding free energy for the Pim-1 kinase system using a method based on the free energy variational principle. It does not need to make samples of the intermediate states and to invoke empirical parameterizations. Pim-1 kinase is the protein found in patients suffering with human hematopoietic malignancies (leukemia and prostatic cancer), and its inhibiter can be medicine for the cancers. In this study, ligands were classified and examined based on structural similarity. The details of the results of the calculated relative binding free energy in several ligands of Pim-1 kinase will be presented in the conference.

1Pos010 **The amino acid sequences analysis of Titin by methods based on the inter-residue average distance statistics**

Panyavut Aumpuchin, Takeshi Kikuchi (*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*)

Proteins consist of the varieties amino acid sequences, then its sequences might stow some folding information. However, it is hard to encode the folding info based on only simple alignment method. In this study, the Average Distance Map (ADM) and the random sampling of 3D structures (F-value) based on inter-residue average distance statistics are used to extract the initial folding segment from Titin's protein sequence (1TIT), compare with the experimental methods. The results show that the highest F-value on the primary ADMs compact area related to the high φ-value and protection factor of NMR results. Moreover, the conserved hydrophobic residues within its Ig-domain are located near the high F-value residues. These conserved residues might be key of protein folding.

1Pos011 **分子動力学法を用いた Hras-GTP/GDP 複合体の構造と溶媒水との水素結合との関連性の研究**
Molecular dynamics study of relationship between the structures of the Hras-GTP/GDP complexes and hydrogen bonds to the solvent water

Takeshi Miyakawa[1], Ryota Morikawa[1], Masako Takasu[1], Kimikazu Sugimori[2], Kazutomo Kawaguchi[2], Hidemi Nagao[2] ([1]*Tokyo University of Pharmacy and Life Sciences*, [2]*Kanazawa University*)

In order to understand the mechanism of hydrolysis of GTP in the Hras-GTP complex, we study the structures of the Hras-GTP/GDP complexes in water solvent by molecular dynamics (MD) simulations.
We evaluated the potential parameters around Mg2+ in Hras-GTP/GDP complexes by quantum chemical calculations. We performed MD simulations of the Hras-GTP/GDP complexes in water solvent using parameters of AMBER03 and our parameters around Mg2+. We found that the positions and orientations of water molecules near GTP are different from those near GDP.
In this study, we analyze the relationship between the structures of the Hras-GTP/GDP complexes and hydrogen bonds to the solvent water.

1Pos012 **親水性/疎水性界面におけるアミロイドβフラグメントの凝集の分子動力学シミュレーション**
All-atom molecular dynamics simulations of amyloid-β fragment aggregation at hydrophilic/hydrophobic interface

Hisashi Okumura[1,2], Satoru G. Itoh[1,2] ([1]*IMS*, [2]*SOKENDAI*)

Amyloids are insoluble and misfolded fibrous protein aggregates and associated with more than 40 serious human diseases. For example, amyloid-β fibrils are known to be associated with the Alzheimer's disease. In this presentation, we will show our molecular dynamics (MD) simulation results of aggregation of Aβ(16-22) peptides. We performed NVT MD simulations of 100 Aβ(16-22) peptides in explicit water solvents. We observed intermolecular β-sheet structures in aggregated conformations of the Aβ(16-22) peptides. We will also discuss the effects of the water solvent.

1Pos013 単一ミオシン結合状態アクトミオシンの高分解能化
F-actin structural changes induced by a single myosin head

Takahiro Namise, Takuo Yasunaga, Kazuaki Yoshida (*Kyushu Institute of Technology*)

It is well-known that muscle contraction is generated by sliding motion between actin filaments and myosin filaments. The molecular mechanism has been proposed as 'lever arm theory', whereas the cooperative and unidirectional conformational changes of actin filaments by binding myosin should also be reported. However, their functions are not understood enough. Here, to understand the functional roles of the cooperative conformational changes, we observed single actin filaments binding a single myosin by cryo-EM. We have detected asymmetrical changes by binding a single myosin to the actin filament. However resolution is not enough, so we try to improvement higher resolution by increase particles and using structural classification like RELION.

1Pos014 XFEL テンプレートマッチング法と粗視化法を用いたクロマチン多重立体配座解析の実現可能性に関する研究
Feasibility study for the multiple conformation analysis of the chromatin structure by using the XFEL template matching and CG simulation

Atsushi Tokuhisa[1,5], Ryo Kanada[1], Yuta Isaka[3,4], Biao Ma[3,4], Shuntaro Chiba[1], Yasushi Okuno[1,2,4,5] ([1]*RIKEN, RC*, [2]*Kyoto University, Graduate School of Medicine*, [3]*FBRI, Pro-Cluster Kobe*, [4]*FBRI, IBRI Laboratory*, [5]*RIKEN, AICS*)

In order to realize the mutational analysis of the gene in cancer cell for the application of medical and drug development, it is important to elucidate multiple conformations of the chromatin. The XFEL template matching method has high capability to elucidate the multiple conformations of the chromatin by using HPC and XFEL. (Tokuhisa,A.,et al. JSB 194, 3, (2016):325-336). However, future issues of the establishment an efficiency sampling for the various candidate modes have been pointed out. We will try to evaluate an efficiency sampling by using coarse-grained model with replica-exchange MD and AI as a feasibility study. Especially, as a coarse-grained model, we will apply AICG model of which the parameters were determined based partly on the atomic interaction.

1Pos015 タンパク質構造の安定化における糖の役割
Role of sugars on the stabilization of protein structure

Satoshi Ajito, Mitsuhiro Hirai (*Grad. Sch. Sci. and Tec., Univ. Gunma*)

Organisms tolerating against extreme environments are known to produce stress proteins and/or accumulate sugars in cells. However, the role of sugar is not clear. By using X-ray and neutron scattering methods, we have studied the stabilizing effect of sugars on myoglobin structure in solutions. The present results suggest that sugars suppress the structural changes of myoglobin induced by acidic conditions, denaturants, and temperature variation. There is no significant difference in the stabilization effect on the protein structure among the sugars, but some superiority of trehalose in it can be recognized. The comparison of the experimental scattering curves with theoretical ones indicates that sugars are excluded from the hydration shell of the protein.

1Pos016 ポリエチレングリコールの存在下でのタンパク質構造安定性の研究
Study of protein structure stability in the presence of polyethylene glycol

Yugo Maezawa, Mitsuhiro Hirai (*Grad. Sch. Sci & Tec., Univ. Gunma*)

The molecular crowding environment is assumed to change the equilibrium states of proteins in solutions. However, the effect of such an environment on protein structures is still ambiguous since many studies of the protein structures have been done under dilute-solutions. Using X-ray and neutron scattering methods complementarily, we have studied the effect of crowding environment on the structure of myoglobin. The co-solute used was polyethylene glycol (PEG). We have found that the protein structure stability against temperature elevation depends on the polymerization degree (DP) of PEG. Namely, the low DP-PEG destabilized the protein structure to lower the tertiary structure transition temperature and the helix-to-sheet transition one, while high-DP PEG vice versa.

1Pos017 分子動力学シミュレーションの緩和モード解析
Relaxation mode analysis of molecular dynamics simulations

Ayori Mitsutake, Hiroshi Takano (*Dept. Phys, Keio Univ.*)

Relaxation mode analysis (RMA) were developed to investigate “dynamic” properties of polymer, homo-polymer, systems. In RMA, slow relaxation modes are extracted from molecular dynamics simulations. Recently, RMA has been applied to proteins, hetero-polymer systems to investigate dynamic properties of structural fluctuations. We also have improved new methods related to RMA. Here, we explain RMA briefly and show the results of some proteins studied by RMA.

1Pos018 NMR-based structural analysis of the locally disordered conformation of outer surface protein A

Takuro Wakamoto[1], Ryo Kitahara[2] ([1]*Graduate School of Life Sciences, Ritsumeikan University*, [2]*College of Pharmaceutical Sciences, Ritsumeikan University*)

The locally disordered conformation of outer surface protein A (OspA) has been investigated by solution NMR spectroscopy combined with pressure and temperature perturbations. However, their structural details remain extremely limited. Here, we report structural analysis of the locally disordered conformation of OspA by paramagnetic relaxation enhancements (PREs) on amide protons. When a paramagnetic probe was covalently attached to cysteine residue in the central part of the protein (e.g. E128C), PREs for amide protons in the N-terminal domain were markedly decreased with increasing temperature. As a consequence of the previous and present studies, the central part was unfolded and left from the folded N-terminal domain in the locally disordered conformation.

1Pos019 **Free energy analysis of cosolvent-induced denaturation through molecular dynamics simulation and energy-representation method**

Yu Yamamori, Nobuyuki Matubayasi (*Osaka Univ. Grad. Sch. Eng. Sci.*)

Energetics of transfer was analyzed for T4-lysozyme from pure water to the series of the mixed solvent of water with urea or its alkylated derivatives to investigate the role of cosolvent on denaturation of protein. The transfer free energy was computed through the combination of molecular dynamics simulation and energy-representation method, and the correlation analysis between transfer free energy and solute-solvent interaction energy components shows that the denaturation caused by the addition of urea or its alkylated derivatives is governed by the direct mechanism through the van der Waals interaction.

1Pos020 **Structure and Dynamics of α-crystellin under crowding condition**

Yusuke Sakamaki[1], Rintaro Inoue[2], Nobuhiro Sato[2], Masaaki Sugiyama[2] ([1]*Grad. Sch. Sci., Kyoto Univ.*, [2]*KURRI*)

Under in-vivo environment, a cell is highly crowded due to the presence of proteins, nuclear acids, and lipids, constituting the condition of so-called “crowding”. One of the typical organs realizing such high protein concentration is eye lens. The protein concentration in eye lens reaches as much as 300~400 mg/ml. Under such a highly concentrated environment, both the structure and function of a-crystallin must be different from those under dilute system, in which osmotic pressure and excluded volume effect are essentially negligible.
In this presentation, we try to reveal the structure and underlying dynamics of a-crystallin under crowding environment attained by highly concentrated glycerol through complementary use of various analytical methods.

1Pos021 **Quantum-chemical analysis of pKa and structural change of amino acid residues in catalytic center of Ser286-mutant firefly luciferases**

Naohisa Wada[1], Kazuya Kato[1], Hironori Sakai[2] ([1]*Food and Nutritional Sciences, Toyo University*, [2]*Institute of Fluid Science, Tohoku University*)

Kato et al. found bathochromic color shift of oxyluciferin binding at the catalytic center of Ser286Ile-mutant luchiferase (mLuc) from Luciola cruciate even at pH 8.0. In this report, the multi-component software DS Ver. 4.5 was applied to generate mLuc in silico basing on the crystal structure of wild-type Luc (wLuc). Moreover, pKa was evaluated by the generalized Born method. As a result, we can attribute the luminescent color change simply to Proto-/Deprotonation in Asp 424 of wLuc depending on pH. On the other hand, the RSMD values of Ser286Gly-mLuc with yellow-green and Ser286Ile-mLuc with red emissions are evaluated relative to wLuc as a reference, the former value was smaller than the latter, so structural homology with wLuc was much higher in the former case.

1Pos022 **結晶中の小さな構造変化からタンパク質のアロステリック機構を読み解く**
Deciphering protein allosteric mechanisms from small structural changes in crystals

Naoya Shibayama[1], Ayana Sato[1], Mio Ohki[2], Sam-Yong Park[2] ([1]*Jichi Med. Univ., Div. of Biophys.*, [2]*Yokohama City Univ., Drug Design Lab.*)

Structural changes are essential for protein functions. X-ray crystallography is the most common technique for the determination of protein structures at the atomic level. However, this method is in general not able to track functionally relevant protein motions, because such motions are often prevented by crystal packing or accompanied by a loss of crystalline order. We present two examples to illustrate the functional motions in crystals, one for CO-bound hemoglobin (Hb) and one for photo-activated adenylate cyclase (PAC). In both cases, small but significant light-induced conformational changes (triggered by photo-dissociation of CO from CO-Hb/photo-activation of flavin chromophore in PAC) were detected in crystals, directing the pathway of allosteric transition.

1Pos023 **3D−RISM 理論を応用した溶液中におけるアスパラギン、Met−enkephalin の構造揺らぎの解析**
Analysis of structural fluctuations of ASN and Met-encephalin in the solution phase by means of 3D-RISM theory

Masatake Sugita[1], Fumio Hirata[2] ([1]*Dept. of Bioinfo., Col. of Life Sci., Ritsumeikan Univ.*, [2]*Toyota Phys. & Chem. Res. Inst.*)

Recently, B. Kim and F. Hirata derived a generalized Langevin equation to describe the structural dynamics of protein in water. In this formulation, variance-covariance matrix is expressed as an inverse matrix of the hessian matrix of the free energy surface that can be defined by the sum of the potential energy and solvation free energy of the protein.
In this study, we analyze structural fluctuation of ASN residue and Met-enkephalin immersed in water by calculating the second order derivative of the solvation free energy in addition with the potential energy, and diagonalizing the hessian matrix. After that comparing the results with those from the Normal Mode analysis and MD simulation.

1Pos024 **アルカン合成関連酵素の機能発現に重要なアミノ酸残基の変異解析**
Mutational analysis of amino acid residues important for the function of an enzyme for alkane biosynthesis

Masashi Nomura, Hisashi Kudo, Yuuki Hayashi, Munehito Arai (*Dept. Life Sci., Univ. Tokyo*)

Cyanobacteria produce alka(e)nes equivalent to diesel fuels from carbon dioxide through photosynthesis using two proteins, an acyl-ACP reductase (AAR) and an aldehyde deformylating oxygenase (ADO). However, little is known about functional mechanism of AAR. Here, to elucidate the amino acid residues important for the function of AAR, we carried out alanine scanning mutagenesis on the AAR residues, including all of the conserved sites. We succeeded in identifying many residues important for the function of AAR. In particular, we found that many functional residues are localized in one of the three domains of AAR. Comprehensive alanine scanning mutagenesis at all positions of AAR is under way.

1Pos025 **Regression method for comparison of multiple protein conformations**

Takashi Amisaki, Shin-ichi Fujiwara (*Fac of Med, Tottori Univ*)

Superposition of protein conformations remains an important problem. In recent years, simultaneous superposition of multiple (more than two) structures are being studied in the context of structural variability and dynamics of proteins. For this problem, we present a method that is build on the basis of statistical regression. In this method, incompleteness of occupancy factors is replaced with missingness, thus allowing comparison of crystal structures involving disordered atoms. To deal with high-dimensionality of working covariance matrices, the following forms are incorporated: diagonal, shrinkage, and correlation modeled. In addition, a norm-based weighting scheme is proposed, which is robust to outlier conformations.

1Pos026 **親水性タンパク質ータンパク質間会合の駆動力に関する MD 及び 3D-RISM 計算**
Driving force of hydrophilic protein-protein associations as studied by MD and 3D-RISM calculations

Honami Sakaizawa, Tadaomi Furuta, **Minoru Sakurai** (*Cent. Biores. Bioinf., Tokyo Tech*)

The vast majority of protein functions in living cells are mediated by protein-protein interactions (PPIs). Thus, in-depth understanding of the PPIs is critical for elucidating the functional mechanism of each protein. Here we investigated the driving force of PPIs using MD and 3D-RISM calculations. We selected the following three PPI systems: barnase-barstar, MJ0796 dimer, UBA-ubiquitin. We decomposed the driving force into three contributions: internal energy, hydration enthalpy and hydration entropy. It was found that i) long-range attraction that works from extremely separated state to encounter complex (EC) comes from the internal energy, and ii) short range attraction from the EC to the stable complex comes from hydration entropy.

1Pos027 **粗視化モデルと全原子モデルを用いた蛋白質複合体シミュレーション**
Simulations of Protein Dimers using a Coarse-Grained Model and All-Atom Models

Takao Yoda, Takuya Yamada, Toshiyuki Tsuji, Tsuyoshi Shirai (*Computer Bioscience, Nagahama Institute of Bio-Science and Technology*)

Solving structures of protein complexes help us to understand physiological functions of those proteins and/or to design drugs. We planned to use molecular dynamics simulations to refine predicted model structures of protein complexes. Since the degrees of freedom can be very large for such a system, to utilize a coarse-grained model should be advantageous. We performed 3-μs molecular dynamics simulations of 13 hetero-dimer systems with Martini model and studied the fragility of those bound conformations. The simulation results suggested a low specificity of natively bound structures with Martini model. We also compare Martini to fine-grained force fields.

1Pos028 **hERG イオンチャネルと薬剤分子の相互作用予測手法の開発**
Prediction of interactions between the hERG potassium ion channel and drug molecules

Tatsuki Negami, Tohru Terada (*Grad. Sch. Agri. and Life Sci., The Univ. of Tokyo*)

All drug candidates are tested for cardiotoxicity. It is well known that binding to the hERG potassium ion channel can cause severe cardiac arrhythmia. Therefore, we are developing a method to predict interactions between cardiac channels and drugs using molecular docking simulations. We constructed structural models of hERG using a combination of homology modeling and targeted MD simulation. The stability of each model was examined by an MD simulation and then drugs were docked to the model. Validity of the docking results was examined by comparing with experimental data. Recently, the structure of hERG has been determined by cryo-electron microscopy. We will present the results of the docking simulation obtained by using the experimental structure.

1Pos029 **ヘモグロビンの酸素親和性制御に関係する大振幅ヘリックス揺らぎの実験的検証：テラヘルツ（THz）分光による研究**
Experimental Investigation of Large Amplitude Fluctuations of Helices Related with Oxygen Affinity of Hemoglobin using THz Spectroscopy

Shigenori Nagatomo[1], Kohji Yamamoto[2], Masako Nagai[3], Teizo Kitagawa[4] ([1]*Dept. Chem., Univ. Tsukuba*, [2]*Res. Center Develop. Far-IR Region, Univ. Fukui*, [3]*Res. Center Micro-Nano Tech., Hosei Univ.*, [4]*Grad. Sch. Life Sci., Univ. Hyogo*)

To investigate experimentally the relationship between oxygen affinity of hemoglobin and large amplitude fluctuations of globin proposed by T. Yonetani (BBA, 1974, 1146-1158, 2008), we have conducted time-domain measurements of terahertz spectra in subterahertz-to-terahertz frequency region for various human hemoglobins with different oxygen affinities. We fixed a sample cell and exchanged hemoglobin solutions by pouring samples from outside of the cell to reduce spectroscopic artifacts arising from cell exchanges. In terahertz difference spectra of absorption and refractive index between deoxy (low affinity) - oxy (high affinity) hemoglobins, no peak was observed in 0.15 - 1.5 THz region. Thus, a positive support for Yonetani's proposal was not obtained in this study.

1Pos030 **Study on the pH-dependent changes in the structure and ligand-binding properties of the perireceptor proteins**

Durige Wen[1], Mituhiro Hirai[2], Mamiko Ozaki[3], Tatsuo Iwasa[4] ([1]*Department of Applied Science and Engineering, Muroran Institute of Technology*, [2]*Graduate School of Science and Technology, Gunma University*, [3]*Department of Biology, Graduate School of Science, Kobe University*, [4]*Center of Environmental Science and Disaster Mitigation for Advanced Research, Muroran Institute of Technology*)

Odorant-binding protein and chemosensory protein are water-soluble proteins that can bind and carry hydrophobic small molecules to the receptors. These two types of proteins are called perireceptor proteins (PRPs). The molecular mechanisms of the process, however, are not well elucidated. We studied effects of the solvent pH on the conformation and ligand-binding capacity of PRPs, Cp-Lip1 and CjapCSP1, by S/WAXS, CD and fluorescent measurements. S/WAXS measurements revealed significant changes in the molecular size of Cp-Lip1 and CjapCSP1 at pH 4.0 and pH 8.0, respectively. The binding capacity of both proteins were also affected by pH. Present results suggest that the environmental pH controls structure and ligand-binding capacity of Cp-Lip1 and CjapCSP1.

1Pos031 pH 一定の分子動力学シミュレーションによって発生させたアミノ酸の様々なプロトン化状態に基づく結合自由エネルギー計算

Binding free energy calculation using various protonation states of amino acids generated by constant pH molecular dynamics simulations

Shin-ichi Fujiwara, Takashi Amisaki (*Fac. Med., Tottori Univ.*)

Binding affinity is important for understanding the function of the protein-ligand binding. Although various computational approaches have been reported to predict the binding free energy, accurate prediction is still difficult. To improve the accuracy, we focused on protonation states of amino acids. Based on the MM/GBSA method, we used for the binding free energy calculation the trajectory data of both coordinates and protonation states generated by the constant pH molecular dynamics simulations. Compared with the conventional method, inclusion of information of protonation states remarkably lowered the calculated binding free energy in the test calculation of MTH1-8OG complex. More detailed results will be discussed in the presentation.

1Pos032 MD シミュレーションを用いた CD44 のヒアルロン酸との結合に関する理論的研究

Theoretical Study on Hyaluronan-Binding to CD44 Using Molecular Dynamics Simulation

Yota Horioka[1], Saki Hongo[1], Yuki Inazuka[1], Yoshifumi Fukunishi[2], Juha M. Lintuluoto[3], Masami Lintuluoto[1] ([1]*Grad. Sch. of Life and Environ. Sci., Kyoto Pref. Univ.*, [2]*Nati. Instit. of Adv. Indust. Sci. and Technol.*, [3]*Grad. Sch. of Eng., Kyoto Univ.*)

CD44 is a protein that is involved in cell adhesion and cell migration and has hyaluronan (HA)-binding domain (HABD). HA binding of CD44 is known to have the role of a cell rolling by repeating adhesion and desorption. CD44 HABD is in the equilibrium between the ordered (O) and partially disordered states (PD). It is also suggested that the human CD44 has two HA binding sites. However, HA binding mechanism and dynamics have not been elucidated completely. In this work, we investigated the conformation of two equilibrium states of CD44 HABD and the HABD-HA complexes by using molecular dynamics simulation. We focused on the effect of the distortion in C-terminal domain and the HA binding to CD44 HABD.

1Pos033 XOR の結合ポケットの中における基質の運動についてー分子動力学による研究ー

The motion of the substrate in the binding pocket of XOR: molecular dynamics study

Hiroto Kikuchi[1], Hiroshi Fujisaki[1], Tadaomi Furuta[2], Ken Okamoto[3], Takeshi Nishino[4] ([1]*Dept. of Phys., Nippon Med. Sch.*, [2]*Sch. of Life Sci. & Tech., Tokyo Tech.*, [3]*Dept. of Biochem., Nippon Med. Sch.*, [4]*Grad. Sch. of Agri. & Life Sci., Univ. Tokyo*)

Xanthine oxidoreductase (XOR) physiologically catalyzes the hydroxylation of hypoxanthine to xanthine, followed by the catalysis of the hydroxylation of xanthine to uric acid. However, no one knows this two-step mechanism with the motion. In this presentation, we show the substrate motion in the binding pocket of XOR using the results of molecular dynamics simulation.

1Pos034 基質結合蛋白質の天然変性領域の網羅的探索および機構解析

Comprehensive search and mechanism analysis of intrinsically disordered region of ligand binding proteins

Satoshi Omori, Hafumi Nishi, Kengo Kinoshita (*Grad. Sch. of Info. Sci., Tohoku Univ.*)

Protein regions that lack the fixed three-dimensional structures are named as intrinsically disordered regions (IDR). It is known that order-disorder transitions occurring in some of IDRs are involved in interactions with other proteins or small ligands. However, their functional relations or molecular mechanisms are still unknown. Meanwhile, recent genome studies yielded the information about single nucleotide polymorphisms (SNPs) that affect molecular functions of proteins. In this study, we tried to identify functional IDRs comprehensively by mapping SNPs to order-disorder transition regions. In addition, the dynamic properties of proteins with functional IDRs were verified by molecular dynamics simulations.

1Pos035 Relating slow-down in diffusion and transient oligomer formation in concentrated villin solutions

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The macromolecular volume fraction inside a cell can be up to 40% and has strongly affected diffusion. Measured relaxation times of chicken villin headpiece in concentrated solutions using NMR revealed that the rotational time scale at dilute condition can be split into fast and slow time scales in crowded media. The slow time scale increases as the concentration increases. Atomistic simulations with an optimized scaling factor tuning protein-water interactions provide insights. At high protein concentrations, villin can form transient oligomers of various sizes, and the diffusion is decreased as the oligomer size increases. Various distributions of different-sized oligomers at different villin concentrations modulate the protein diffusion in the crowed environment.

1Pos036 LEA モデルペプチド及びトレハロースによるリゾチームの熱変性防止

Protective effect of LEA peptides and trehalose on the thermal denaturation of lysozyme

Takao Furuki, Minoru Saukrai (*Tokyo Institute of Technology*)

We tested the protective effect of the following reagents on the thermal denaturation of lysozyme: 1) PvLEA-22, which consists of two tandem repeats of the 11-mer motif characteristic to LEA proteins from an African sleeping chironomide, 2) its scrambled-type peptide, which has the amino acid composition identical with that of PvLEA-22, although its sequence is scrambled, and 3) a disaccharide, trehalose. The results of turbidity, enzyme activity, and circular dichroism (CD) spectrum measurements showed that the LEA model peptide as well as trehalose can inhibit heat-induced denaturation of lysozyme.

1Pos037 カーボンナノチューブによるシステイン残基の酸化
Oxidation of cysteine residues of proteins on carbon nanotubes

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Nanoparticles such as carbon nanotubes (CNTs) are readily coated with plasma proteins when they are taken in biological systems. The protein layers on the nanoparticles are called protein coronas. Investigation of the interactions inducing protein coronas is important for understanding biological impacts of the nanoparticles. In this study, we revealed that CNTs oxidize cysteine, leading to the formation of cystine. Such redox reaction was observed for human serum albumin and reduced hen egg-white lysozyme. The oxidation of cysteine is attributable to the electron transfer from the thiols to the CNTs. The present results suggest that structures of proteins with free cysteine residues can be chemically modified on CNT surfaces even in biological systems.

1Pos038 Structural and thermodynamic analysis for metal-induced three helix-bundle formation

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To analyze structural dynamics, we designed simple model peptides whose structures are changed from random to helix-bundle by forming the stable hydrophobic core in the presence of metal. As the strategy, a de novo designed three helix-bundle protein was destabilized by the substitution of residues in the hydrophobic core to His and small amino acids. The conformational changes of peptides induced upon Zn^{2+} binding to His were analyzed using CD, showing that the peptides, HA and HG, are good candidates for further analyses. The DXT experiments showed that the fluctuation of both peptides are suppressed upon Zn^{2+} binding. The metal binding energy determined from the angular diffusion coefficients was in good agreement with that determined from ITC.

1Pos039 考慮する因子を段階的に増やすモデル解析に基づく蛋白質の折り畳み機構の理論的解明
Unraveling protein folding mechanism by analyzing the hierarchy of models with increasing level of detail

Tomohiko Hayashi[1], Satoshi Yasuda[1,2,3], Skrbic Tatjana[4], Giacometti Achille[4], Masahiro Kinoshita[1] ([1]*Inst. Adv. Energ., Kyoto Univ.*, [2]*Grad. Sch. Sci., Chiba Univ.*, [3]*MCRC, Chiba Univ.*, [4]*Dept. of Molecular Sciences and Nanosystems, Venezia Univ.*)

Structural stabilities of a protein are studied using our free-energy function (FEF) which can account for the water-entropy gain, formation of protein intramolecular H-bonds, and break of protein-water H-bonds and recovery of water-water H-bonds upon folding. We apply the FEF to the native fold of protein G and a number of misfolded decoys with a wide variety of -helix and -sheet contents. Those without side chains are also treated. We test many models differing in the details. In some of them, water is replaced by a hard-sphere solvent. The native fold is identified as the most stable one only when the most detailed model is employed. This special approach enables us to elucidate the role of each physical factor and the result of competition of multiple factors.

1Pos040 アルコール中のメリチンとマストパランのヘリックス構造熱安定性
Thermal stability of helical conformation of melittin and mastoparan in alcohol

Yoshinori Miura (*Center for Advanced Instrumental Analysis, Kyushu University*)

Melittin and mastoparan are short polypeptides composed of 26 and 14 amino acid residues, respectively. It has been known that the peptides form helical conformation in pure methanol solvent. We examined temperature dependence of helical conformation of the peptides in methanol solution using NMR spectroscopy in order to clarify helical conformation stability. We found that their helical conformation are maintained up to at least 54 C. Furthermore, we investigate conformation of those peptides in ethanol and compare them to conformation in methanol.

1Pos041 NtrC の構造転移の経路とその遷移状態のカメレオンモデルによる研究
Characterization of the pathways and transition states of conformational transition of NtrC by the chameleon model

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Nitrogen regulatory protein C (NtrC) exhibits two-state allosteric conformational transition, while the phosphorylation site D54 remains dephosphorylated. This protein is a model system for the single-domain conformational transition, for which there is a controversy on the mechanism between the transient formation of nonnative hydrogen bonds and the local unfolding called cracking. Here we used the chameleon model (Terada et al., J. Phys. Chem. B (2013)) to draw the free energy landscape of the conformational transition of NtrC with different reaction coordinates. Using multicanonical MD, we found that there are two major pathways of the conformational change, and characterized the transition state ensembles by the local conformational change and local unfolding.

1Pos042 定温定圧レプリカ置換分子動力学シミュレーションによって明らかになったシニョリンの準安定状態の温度・圧力依存性
Temperature and pressure dependence of metastable state of a chignolin revealed by an isothermal-isobaric replica-permutation method

Masataka Yamauchi[1,2], Hisashi Okumura[1,2] ([1]*SOKENDAI*, [2]*IMS*)

We developed a replica-permutation molecular dynamics method in the isothermal-isobaric ensemble. The replica-permutation method is a better alternative to the replica exchange method and was originally developed in the canonical ensemble. The replica-permutation method uses the Suwa-Todo algorithm to permute temperatures and pressures instead of the Metropolis algorithm so that the rejection ratio can be minimized.
We applied this method to a β-hairpin mini protein, chignolin. In this simulation, not only the folded state but also the misfolded state are observed. We evaluated some physical quantities and found new phenomenon that misfolded chignolin become more stable under high pressure condition.

1Pos043 **Structural stability of halorhodopsin from Natronomonas pharaonis under acidic condition**

Shinichiro Hayashi, Takanori Sasaki (*Grad. Sch. Adv. Math. Sci., Meiji Univ*)

An extremophile, N.pharaonis lives at high salt concentration (3.5 M) and under alkaline condition (pH 9-11). Hence, it is thought that membrane proteins on N.pharaonis membrane also have a tolerance for extreme environment. A membrane protein halorhodopsin from N.pharaonis (NpHR) is a light driven Cl- pump, and is stable in the presence of Cl-. In this study, we investigated the stability of NpHR under acidic condition which is different from natural habitat of N.pharaonis. In the phosphate buffer at pH 2.1, the maximum absorbance of NpHR at 578 nm was decreased about 51%. Contrary to this, in the hydrochloric acid buffer at pH 2.1, the absorbance was decreased only about 4%. These results suggest that NpHR has the tolerance for acidic condition when binding to Cl-.

1Pos044 **分子回転拡散係数のビリアル展開によるタンパク質間相互作用の解析**

Protein-protein interaction on crystallization revealed by the virial expansion of molecular rotational diffusion coefficient

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The rotational motion and mutual interaction of proteins are decisive for the processes where protein are encountered and rearranged, such as crystallization. We propose the quantitative method of protein-protein interaction by the virial expansion of rotational diffusion coefficient (D_{rot}). D_{rot} of fluorescent-labeled lysozyme under conditions of salting-out using monovalent cation salts are determined by time-resolved fluorescence anisotropy, which can discriminate the entire rotation from the segmental motion. The virial coefficients, estimated from the quadratic dependence of normalized rotational diffusion coefficient (D_{rot}/D^0_{rot}) on lysozyme concentration, showed the attractive and repulsive interaction would be induced responding to the protein crystallization.

1Pos045 **タンパク質構造変化における経路の多様性：マルコフ状態モデルによる解析**

A variety of pathways for a conformational change of a protein analyzed using a Markov state model

Sotaro Fuchigami (*Grad. Sch. of Medical Life Science, Yokohama City Univ.*)

When a conformational change in a protein occurs, its pathway is not always identical but rather shows variability because of the intrinsic flexibility. However, the molecular details remain unclear. In the present study, we characterized pathways for conformational changes of a protein using molecular dynamics (MD) simulations and a Markov state model. As a target protein, we selected lysine-, arginine-, ornithine-binding protein (LAO), which undergoes large-amplitude domain motions. MD simulations of apo-LAO from the closed conformation in explicit water were performed many times. Almost all trajectories showed conformational changes from the closed form to the open form. We will discuss the mechanism underlying the diversity of conformational change pathways.

1Pos046 **何故 4 つのイントロン位置は、タンパク質立体構造上で、平面を形成するか?**

Why four intron positions form a plane in the tertiary structure of protein?

Michiko Nosaka (*Naional Institute of Technology, Sasebo College*)

We have identified planes in the tertiary structures of different proteins. Although we have discussed about the possible reason of this plane since the discovery, the meaning or function of this phenomenon is not clear at this time. Here, we summarize the characteristics of the plane, as follows, and discuss about the hypothesis to explain and the way to verify it.
1, the probability of forming a plane is around 8 percent, which is estimated from the distribution of exon length.
2, substrate analog or ligand of the protein is included partially, sometime almost all, in the plane, whose probability is very low (about 0.2% at most).
3, the plane area is thought to be stable in the structure, however, one of the four positions is known to be movable in the protein dynamics.

1Pos047 **1 分子イメージングによる GPCR の活性推定**

Single-molecule imaging-based estimation of GPCR activity

Masataka Yanagawa[1], Michio Hiroshima[1,2,3], Yuichi Togashi[4], Takahiro Yamashita[5], Yoshinori Shichida[5,6], Masayuki Murata[7], Masahiro Ueda[2,8], Yasushi Sako[1] ([1]*RIKEN*, [2]*QBiC, RIKEN*, [3]*JST, CREST*, [4]*Grad. Sch. Sci., Hiroshima Univ.*, [5]*Grad. Sch. Sci., Kyoto Univ.*, [6]*Research Org. Sci. & Tech., Ritsumeikan Univ.*, [7]*Grad. Arts & Sci., Univ. Tokyo*, [8]*Grad. Frontier Biosci., Osaka Univ.*)

G protein-coupled receptors (GPCRs) are major drug targets. Development of a method for measuring the activity of GPCRs is essential for pharmacology and drug discovery. However, current drug screening assays are not universal because they monitor a downstream signaling event specific to each GPCR. Here, we show that the direct observation of GPCRs by single-molecule imaging provides an alternative method for estimating their activity. First, we demonstrate that the diffusion coefficient of metabotropic glutamate receptor 3 is tightly coupled with its functional states including G protein binding and clathrin-dependent endocytosis. Then, we confirmed the general applicability of the method to many GPCRs regardless of the coupling specificity to G proteins.

1Pos048 **脂質ータンパク協同性による上皮成長因子受容体の膜近傍ドメイン二量体形成機構**

Lipid-protein cooperativity in the regulation of juxtamembrane domain dimer formation in epidermal growth factor receptor

Ryo Maeda[1], Takeshi Sato[2], Kenji Okamoto[1], Yasushi Sako[1] ([1]*Cellular Informatics Lab., RIKEN*, [2]*Kyoto Pharmaceutical Univ.*)

Transmembrane (TM) helix and juxtamembrane (JM) domains (TM-JM) bridge the extracellular and intracellular kinase domains of single-pass membrane proteins including epidermal growth factor receptor (EGFR). It has been proposed that dimerization of TM-JM plays a crucial role for regulation of EGFR kinase activity and phosphorylation of Thr654 on JM conversely leads to desensitization. While interactions of JM with membrane lipids are thought to be important for TM-JM dimerization, conformational mechanisms underlying the dimer formation remain unclear. Here, combining single-molecule FRET imaging and nanodisc techniques, we analyzed how JM conformations are dynamically regulated by membrane lipids molecules, especially PIP2, and a threonine phosphorylation in JM domain.

1Pos049 レプリカ交換 MD シミュレーションによる FGFR3 膜貫通領域の構造サンプリング

Conformation Sampling of FGFR3 TM dimer using replica exchange MD simulation

Daisuke Matsuoka, Motoshi Kamiya, Yuji Sugita (*RIKEN*)

FGFR3 is a signaling protein regulating skeletal growth. It is a single-pass membrane protein and can form a homodimer. The transmembrane (TM) structure has a crucial role in the protein activation and mutations in the TM can cause serious diseases, for instance, G380R mutant for congenital bone disorder. However, experimental information of the FGFR3 transmembrane structure is limited to understand the mechanisms for the mutation effect. In the study, we performed molecular dynamics (MD) simulations of the wild type and G380R mutant and discuss the differences in their dimer structure and their conformational stability. We also examine the efficiency of the enhanced sampling method (REST) on the simulations.

1Pos050 活性型 G タンパク質共役受容体の熱安定化置換の同定

Identification of PtThermostabilizing mMutations for a G-protein coupled receptor in the active state

Simon Hikiri[1,2], Ryosuke Nakano[1], Nanao Suzuki[1], Satoshi Yasuda[1,2,3], Yuta Kajiwara[4], Masahiro Kinoshita[2], Takeshi Murata[1,3,5] ([1]*Graduate School of Science, Chiba University*, [2]*Institute of Advanced Energy, Kyoto University*, [3]*Molecular Chirality Research Center, Chiba University*, [4]*Graduate School of Energy Science, Kyoto University*, [5]*JST, PRESTO*)

Identification of PtThermostabilizing mMutations for a G-protein coupled receptor plays a pivotal role in the structure-guided drug design. We have already made a significant progress along this line for PTMthe inactive state using our free-energy function (FEF) developed on the basis of statistical thermodynamics. As the first step toward achieving an equal success for the active state, we consider the adenosine A_{2a} receptor as an example and apply the same FEF to the prediction of its thermostabilized mutants. Some of them are constructed and experimentally tested, and for those proved to be actually thermostabilized, further experiments are performed for examining if each mutated receptor remains active and an agonist binds to it.

1Pos051 置換により多くの Class A の G タンパク質共役型受容体を安定化するアミノ酸残基の理論的決定

Theoretical Identification of Hot-Spot Residues to be Mutated Common in G Protein-Coupled Receptors of Class A

Satoshi Yasuda[1,2,3], Yuta Kajiwara[4], Yosuke Toyoda[5], Kazushi Morimoto[5], Ryoji Suno[5], So Iwata[5], Yakuya Kobayashi[5], Takeshi Murata[1,2,6], Masahiro Kinoshita[3] ([1]*Grad. Sch. Sci., Chiba Univ.*, [2]*MCRC, Chiba Univ.*, [3]*IAE, Kyoto Univ.*, [4]*Grad. Sch. Ener. Sci., Kyoto Univ.*, [5]*Grad. Sch. Med., Kyoto Univ.*, [6]*JST, PRESTO*)

Structural determination of G protein-coupled receptors (GPCRs) has been hindered by their low stability. Though the stability can be enhanced by amino-acid mutations, a random search with a heavy experimental burden is currently employed to obtain such mutations. We propose a theoretical strategy using our free-energy function for identifying a hot-spot residue whose mutation leads to substantially higher stability for many GPCRs and illustrate the strategy for three GPCRs of Class A in the inactive state. We find that the residue at a position of NBW=3.39 (NBW is the Ballesteros-Weinstein number) is a hot-spot residue. This finding is experimentally corroborated, which is followed by the determination of new three-dimensional structures for two of the GPCRs.

1Pos052 活性型アデノシン A2a 受容体の 4 重置換がもたらす安定化の物理起源

Physical origin of stabilization by a quadruple mutation for the adenosine A2a receptor in the active state

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We elucidate the physical origin of significant stabilization by a recently reported quadruple mutation for the adenosine A2a receptor in the active state. In the crystal structures available, the ligands binding to the receptors without and with the mutation are different. They are removed and the receptor structures are modified using an all-atom molecular dynamics simulation with the characteristics of the active-state structure retained. Our free-energy function is then applied to the two structures for comparing their thermodynamic stabilities. We find that the stabilization is achieved by the mutation in terms of the entropic effect originating from the translational displacement of hydrocarbon groups within the lipid bilayer.

1Pos053 コレステロールを介した上皮成長因子受容体のクラスター形成は EGF シグナル伝達に不可欠である

Cholesterol Mediated Cluster Formation Is Indispensable for the Downstream Signaling of Epidermal Growth Factor Receptor

Michio Hiroshima[1,2], Nario Tomishige[2], Masahiro Ueda[1], Yasushi Sako[2] ([1]*RIKEN QBiC*, [2]*RIKEN*)

Epidermal growth factor (EGF) signaling has been suggested to be concerned with EGF receptor mobility and clustering on the plasma membrane, revealed by our previous single-molecule imaging study. Here, we depleted membrane cholesterol, a primary component of the plasma membrane, and found that the receptor mobility changed from confined to free diffusion. In this condition, although dimerization did not change after the ligand stimulation, the formation of larger clusters dramatically decreased. The ligand-induced phosphorylation of EGFR was increased, on the other hand, that of downstream protein, ERK was reduced significantly. Therefore, the receptor clusters mediated by cholesterol is suggested to relate to the downstream signaling more inextricably than dimers.

1Pos054 赤外分光法による GLIC の pH 依存性チャンネル開閉機構の研究

ATR-FTIR / SEIRAS study on the pH induced gating mechanisms of Gloeobacter violaceus pentameric ligand-gated ion channel (GLIC)

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We present here results of study on the pH induced structural change of Gloeobacter violaceus pentameric ligand-gated ion channel (GLIC) by means of FTIR and Surface Enhanced Infrared Absorption (SEIRA) spectroscopy. GLIC is a bacterial homologue of eukaryotic pentameric ligand-gated ion channels (pLGICs). It has been known that the gating of GLIC is activated by proton binding at pH range between 4 and 7. It is natural to speculate a titratable amino acid residue that has a pKa value in this pH range relates to the gating mechanism. In this work, we employed FTIR spectroscopy to monitor the protonation state of Asp/Glu groups in GLIC for wild-type and various mutants in order to identify pKa values of single amino acid residues.

1Pos055 バクテリオロドプシンの DC-DFTB-MD シミュレーション：光反応サイクル上でのプロトンダイナミクス
DC-DFTB-MD simulations of bacteriorhodopsin: Proton dynamics along the photocycle

Minori Imai[1], Junichi Ono[1], Yoshifumi Nishimura[2], Hiromi Nakai[1,2,3,4] ([1]*Grad. Sch. of Adv. Sci. & Eng., Waseda Univ.*, [2]*RISE, Waseda Univ.*, [3]*JST-CREST*, [4]*ESICB, Kyoto Univ.*)

Theoretical research on the divide-and-conquer based density-functional tight-binding molecular dynamics (DC-DFTB-MD) method for the light-driven proton pump, bacteriorhodopsin (BR), which actively translocates a proton across cell membranes, is carried out to reveal the proton dynamics. Starting from the latest crystal structures captured by X-ray free electron laser, along the photocycle of BR, the full DC-DFTB-MD simulations of BR with membrane and solvent water (50,000 atoms) were performed using K-computer. Thus, the entire biological system including all the ubiquitous protons are treated quantum mechanically. In this presentation, the structural and dynamical differences among the intermediate states on the photocycle of BR will be discussed.

1Pos056 生細胞での膜タンパク質の拡散運動の網羅的解析
Comprehensive Diffusion Analysis of Membrane Proteins in Living Cells

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Protein diffusion in cell membranes plays a key role in many signaling processes. To clarify a relation between diffusion and membrane protein's structure in living cells, we measured diffusion coefficients of 30 kinds of the proteins in cell membrane by using single molecule imaging. The results showed that most of membrane proteins have 3 different diffusion states and each state obeys the Saffman-Delbruck model which is a famous theoretical model of diffusion in artificial membrane and predicts a logarithmic dependence of a protein's diffusion coefficient on its inverse hydrodynamic radius. These results suggest that mobility of various membrane proteins is similar to each other in the regions with similar viscosity regardless of the molecular size.

1Pos057 膜貫通タンパク質の細胞内局在要因の同定
Identification of the subcellular localization factors of transmembrane proteins

Tatsuki Kikegawa, Yuri Mukai (*Dept. Electronics, Grad. Sch. Sci. Tech., Meiji Univ.*)

The amino acid propensity around signal-anchors (SAs) in plasma, ER and the Golgi membrane proteins was calculated to elucidate the transport mechanisms of transmembrane (TM) proteins. The discrimination accuracy of each group was estimated by the scores calculated by the position-specific scoring matrix of TM domains. Each group members could be discriminated with high accuracy based on the 5-fold cross-validation test, and the result suggested that the amino acid propensity around TM domain was related to the localization mechanisms. To verify this presumption by experimental methods, the GFP-SA proteins were designed and expressed in HeLa cells. The subcellular localization of GFP-SAs was evaluated by confocal laser fluorescence microscope.

1Pos058 Membrane binding structure of Bombinin H2 and H4 peptides in leishmania mimetic membrane as studied by solid-state NMR and MD simulation

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Bombinin H4 containing D-allo-Ile is one of antimicrobial peptides isolated from the frog skin secretion of Bombina species. The peptide H4 was found the significant lower LC50 value than H2 against *leishmania*. In our paper, the carpet-like activity of bombinin H2 and H4 for *leishmania*-mimetic membrane was revealed by ^{31}P solid-state NMR. We performed a number of MD simulations on H2 and H4 to reveal atomic-level information about their interactions of *leishmania* membrane. D-allo-Ile was rapidly attached to the hydrophobic part of the membrane in presence of H4 on the surface. This attachment gives an ability to rapidly penetrate into surface of the membrane. The structure of H4 was stablized by the interactions between D-allo-Ile and the mimic membrane.

1Pos059 Novel microsystem for high throughput production of small liposome with size uniformity

Naoki Soga[1], Rikiya Watanabe[1,2], Hiroyuki Noji[1] ([1]*Dept. of App. Chem., The Univ. of Tokyo*, [2]*AMED-PRIME*)

Transport proteins play crucial roles in cell physiology by transporting molecules across bio-membrane. Liposomes are used as general platform to analyze the transport activity in vitro, however, it is hard to produce small liposomes with size-uniformity, preventing highly sensitive and quantitative analysis of transporters. To address this issue, we developed a novel microsystem to produce >10,000 uniform liposomes at a time. Liposomal volume can be modulated down to 100 aL with ~10% deviations, allowing highly sensitive and quantitative analysis of transport proteins, e.g. α-hemolysin. Our microsystem thus expands the versatility of liposome to highly quantitative analysis of transport proteins, and will offer a platform to understand their working principles.

1Pos060 バクテリオロドプシンの DC-DFTB-MD シミュレーション：プロトン放出基における余剰プロトンの非局在化ダイナミクス
DC-DFTB-MD simulations of bacteriorhodopsin: Delocalization dynamics of an excess proton in proton releasing group

Junichi Ono[1], Minori Imai[1], Yoshifumi Nishimura[2], Hiromi Nakai[1,2,3,4] ([1]*Grad. Sch. of Adv. Sci. & Eng., Waseda Univ.*, [2]*RISE, Waseda Univ.*, [3]*JST-CREST*, [4]*ESICB, Kyoto Univ.*)

In bacteriorhodopsin (BR), five proton transfers arising from photoisomerization of retinal successively occur, resulting in the conversion of light into chemical energy through membranes. In particular, an excess proton related to the second proton transfer is stored in proton releasing group (PRG) of BR, and is considered to be the origin of the specific IR continuum band of BR. However, the microscopic storage mechanism of the excess proton has been unclear. In the present study, divide-and-conquer density-functional tight-binding molecular dynamics (DC-DFTB-MD) simulations, where chemical reaction dynamics are unambiguously described, are performed to clarify the proton dynamics in PRG of BR. The dynamical behavior of the delocalized excess proton will be discussed.

1Pos061 ナノポアと DNA を用いたナノ空間内におけるホフマイスター効果の検証

Investigation of Hofmeister effect in nanospace using nanopore and DNA as a probe

Masaki Matsushita, Ryuji Kawano (*Grad. Sch. Biotech. and Life Sci., TUAT*)

Several studies have reported the behavior of materials on the nanoscale is different from that in the macroscale. We have developed a nanopore probe, which is an α-hemolysin (αHL) nanopore containing a short hairpin-DNA (hpDNA), to clarify the nanoscale behavior of the solution and molecules. The hpDNA moves in the nanospace under applying voltages, and the movement reflects the nano-environment. In this study, we have attempted to study the Hofmeister effect in the nanospace. Hofmeister effect is one of the modern mystery in physical chemistry in terms of molecular mechanism. As the results, we found that hpDNA movement became slow with increasing salting-out effect of ion in the nanospace. In addition, the stable state of the hpDNA was also changed with ions.

1Pos062 ホタルルシフェリン酸化反応経路の pH 依存性

pH dependence of oxidation reaction pathway of firefly luciferin

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In these days, the molecular structures of substrate and emitter of firefly bioluminescence, which changes depending on the solvent pH value, were elucidated by assignments of these spectra using quantum chemical calculations. We have theoretically investigated the emission process by comparing potential and free energy profiles for the formation of emitters from the substrates, including the intermediate molecules. Actually, our results show that the oxidation pathway of firefly luciferin changes when pH value goes beyond pH 8.

1Pos063 光電子放出を用いたサーモフィリックロドプシン膜の電子構造の観測

Electronic structure of a thermophilic rhodopsin film observed by techniques using photoelectron emission

Daisuke Sano[1], Astushi Matsuzaki[1], Yuki Takeda[1], Takuya Miyauchi[1], Takeshi Murata[2,3], Yuki Sudo[4], Hisao Ishii[1,3,5] ([1]*Graduate School Science and Engineering Chiba University*, [2]*Graduate School of Science Chiba University*, [3]*Molecular Chirality Research Center Chiba University*, [4]*Graduate School of Medicine Dentistry and Pharmaceutical Science Okayama University*, [5]*Center for Frontier Science*)

The electronic structures of bio molecules are indispensable for understanding bio-related processes. For non-biological materials, techniques using photoelectron emission such as UV photoelectron spectroscopy (UPS) have been applied to examine their electronic structures. In this study, we have tried to evaluate the electronic structure of a protein having photoreceptor called thermophilic rhodopsin (TR) by using UPS and photoelectron yield spectroscopy (PYS). The UPS spectra of a TR film prepared by using spray deposition were measured with synchrotron light source to investigate the whole valence region. High-sensitivity UPS was also performed to probe the photoelectron from retinal in TR. The details will be discussed with results of PYS for retinal solution.

1Pos064 アミロイドβ凝集における亜鉛イオンの役割の計算解析

Computational analysis of the role of a zinc ion in the amyloid-β aggregation

Hiroaki Nishizawa[1], Hisashi Okumura[1,2] ([1]*IMS*, [2]*SOKENDAI*)

An amyloid fibril of amyloid-β (Aβ) peptides is well known as the cause of the Alzheimer's disease. A part of the Aβ, i.e. Aβ(1-16) fragments, is considered to be important of initial formation of the amyloid fibrils. Furthermore, some experimental research indicate that the Aβ aggregation is accelerated under existence of metal ions. Based on the experimental results, computational approaches have been also carried out. However, in these approaches, the numerical models that is designed to reproduce experimental data is used. In this presentation, we investigate the aggregation of Aβ under existence of a metal ion using more general model using the molecular mechanical theory and density-functional tight-binding method, which is one of the electronic structure theory.

1Pos065 部分波展開法と 3D-RISM 法の結合による新たな溶媒和自由エネルギー計算式の提案

New solvation free energy expression for the 3D-RISM combined with the distributed partial wave expansion

Shoichi Tanimoto, Norio Yoshida, Haruyuki Nakano (*Grad. Sch. Sci., Kyushu Univ.*)

The solvation free energy (SFE) is an important thermodynamic quantity in dealing with biological processes in solution. The RISM theory, an integral equation theory of molecular liquids, is one of the most powerful tools to evaluate the SFE. The RISM theory produces the accurate relative free energy change. However, the absolute SFE itself sometimes shows large error. To improve the accuracy of the SFE, a correction method based on the distributed partial wave (PW) expansion has been proposed by Ten-no et al. The method greatly improves the accuracy of the SFE. In this study, we aimed to develop a method that improves the accuracy of the SFE and is applicable to the solvation of huge biomolecules by applying the PW correction to the 3D-RISM theory.

1Pos066 Size-consistent multipartitioning QM/MM 法により量子化学効果を取り込んだ陽イオンの溶媒和

Cation solvation with quantum chemical effect incorporated by size-consistent multi-partitioning QM/MM method

Hiroshi Watanabe[1,2], Maximilian Kubillus[3], Tomas Kubar[3], Robert Stach[4], Boris Mizaikoff[4], Hiroshi Ishikita[1] ([1]*UTokyo, RCAST*, [2]*UTokyo, ACHEM*, [3]*Karlsruhe Institute of Technology*, [4]*University of Ulm*)

In condensed phase, quantum chemical properties are critical determinants for solvation structure and dynamics. To incorporate the properties, quantum mechanical (QM) molecular description is required for both solute and solvent. However, it has been a challenging issue to conduct molecular dynamics (MD) simulations for condensed system based on QM potential with sufficient size-scale. To overcome the problem, we recently developed the size-consistent multi-partitioning (SCMP) quantum mechanics/molecular mechanics method and realized stable and accurate MD simulations adapting QM potential. In the present study, as the first application of the SCMP method, we investigated structures and dynamics of several cations in solution based on nanosecond scale sampling.

1Pos067 蛋白質構造の安定性と熱変性に関する相互作用成分解析
Interaction-component analysis of protein stability with regard to heat denaturation

Yoshihiko Tokunaga, Yu Yamamori, Ryosuke Ishizuka, Nobuyuki Matubayasi (*Grad. Eng. Sci., Univ. Osaka*)

Controlling protein stability against heat is crucial for controlling the function such as enzyme. Protein structure couples strongly with the solvation and the stability is determined by the intramolecular energy and the solvation free energy. Therefore, quantitative analysis of solvation free energy is important to identify which of the electrostatic interactions, van der Waals interactions, and excluded volume effects controls temperature effects. Also, we need to analyze at an atomic level in order to take account of the influence of microscopic interaction such as hydrogen bond. From the correlation analysis of total energy and each interaction-component, we identified which interaction-component is the factor of heat denaturation.

1Pos068 機械学習による水和水の研究
Machine-learning approach for behavior of hydration water

Taku Mizukami[1], Viet Cuong Nguyen[3], Tien Lam Pham[2], Heiu Chi Dam[2] ([1]*JAIST, Materials Science*, [2]*JAIST, Knowledge Science*, [3]*HPC Systems*)

Water plays an important role in biological systems. Numerous biomolecules function in a hydrated environment, via mechanisms that are strongly influenced by interactions with water. Protein function depends on the dynamics and the (dynamic or static) structure of the surrounding water.
In this study, we present a machine-learning approach to quantitatively analyze the structure of water surrounding solute. We modeled the “motion behavior” and dynamic structure of all water molecules present in classical molecular dynamic simulations of solute-solvent system. The behavior of water molecules was then categorized by using learning and/or classification techniques. Analysis of the resulting classes leads a prediction for physicochemical features i.e. free energy.

1Pos069 筋原線維懸濁液の ATP 分解素過程中のプロトン NMR 緩和経過
Spin-spin relaxation of 1H NMR signals from myofibril suspension during cross-bridge cycling

Tetsuo Ohno (*Dept. Physiol., The Jikei Univ. Sch. Med.*)

The spin-spin relaxation process of 1H-NMR signals from suspension of myofibril prepared from rabbit could be well represented by the summation of several exponentials indicating that water molecules in the suspension could be conveniently grouped into several components based on the relaxation time constant (T2). In the absence of MgATP, myofibril affects water molecules within 500 nm from its surface differently from water molecules in the bulk solution, and releases many water molecules in the presence of MgATP, and the almost the same change was caused by MgADP. This may suggest that the potential of the water molecules that surround myofibrils are dynamically changed during cross-bridge cycling.

1Pos070 水溶液からアルキルアミン含有有機溶媒へのリン酸化合物分配の熱力学的解析
Thermodynamic analysis for partitioning of phosphoric compounds between water and organic solvent containig alkyl amine

Hideyuki Komatsu (*Biosci. & Bioinfo. Kyushu Inst. Tech.*)

To evaluate hydration of phosphoric (P_i-) compounds in aqueous solution, partitioning of phosphoric compounds from aqueous solution into organic solvent (octanol) containing alkyl amine was thermodynamically characterized under constant pH conditions. The partition coefficient (K_p) increased with increasing number of charge of P_i-compounds under all condition used. The vant’Hoff enthalpy changes (ΔH) of the partitioning were dependent on deprotonation heat of buffer used. These results suggest that the partitioning is associated with the protonation of P_i-compounds. Recently, the partitioning ΔH values have been directly measured by using isothermal titration calorimetry, and the obtained values will be discussed together other data in this presentation.

1Pos071 蛋白質の二次構造と水和ダイナミクスの相関に関する分子動力学的研究
Molecular dynamics study on the relationship between the protein secondary structure and its hydration dynamics

Takafumi Fujiyoshi[1], Kota Kasahara[2], Takuya Takahashi[2] ([1]*Graduate School of Life Science, Ritsumeikan University*, [2]*College of Life Science, Ritsumeikan University*)

Hydration water plays important roles in determining the structure and function of proteins. However, relationship between the dynamic feature of the hydration water and the protein structure is not fully understood yet. Here, we examined differences in hydration dynamics among several different conformations (helix, coil, extended, and energy-minimized structures) with model peptides (polyglutamic acid, FS12, and p-53 C-terminal domain) by using molecular dynamics simulations. In addition, we also tested differences between the two water models (SPC/E and TIP4P-D). As a result, in the first hydration layer, the hydration dynamics around the helix was the fastest in the tested structures. Moreover, we also found the helix structure showed the largest fluctuation.

1Pos072 イオン周囲の水分子の運動性を再現する新規 Lennard-Jones パラメータの検討
Reproduction of the water mobility around an ion by introducing a new Lennard-Jones parameter

Yuki Takimoto[1], Kota Kasahara[2], Takuya Takahashi[2] ([1]*Grad. Life. Sci., Ritsumeikan Univ.*, [2]*Col. Life. Sci., Ritsumeikan Univ.*)

Molecular dynamics (MD) simulation is an effective method for analyzing the dynamics of water molecules. However, it is difficult to reproduce “fast water dynamics” around ions with the conventional water models. Here, we modified the conventional TIP5P water model to improve the reproducibility of water dynamics such as rotational relaxation time and translational diffusion coefficient. We introduced a new Lennard-Jones (LJ) potential between ion and water, i.e., ion-hydrogen pair and ion-pseudo atom pair, and examined a wide range of parameter values. As a result, the new model improved the water dynamics compared with the conventional water models. We also analyzed relationship between LJ parameter change and water dynamics to gain knowledge to further development.

1Pos073 疎水表面による静電相互作用の強化

Enhancement of electrostatic interaction by hydrophobic surface

Takato Sato[1], Tohru Sasaki[1], Jun Ohnuki[1], Koji Umezawa[2,3], Mitsunori Takano[1] ([1]*Dept. of Pure & Appl. Phys., Waseda Univ.*, [2]*Grad. Sch. of Sci. & Tech., Shinshu Univ.*, [3]*IBS, Shinshu Univ.*)

Protein-protein interaction is generally considered to be composed of two independent factors: electrostatic and hydrophobic interactions. However, they are not independent: hydrophobic surfaces may strengthen the intermolecular electrostatic interaction by lowering the dielectric constant around the surface. By using molecular dynamics simulation, we explored this possibility. We found that the transient ordering of water molecules near the hydrophobic surface lowers the dielectric constant so that the electrostatic attraction between oppositely-charged particles is enhanced. Since charged residues are often found on a hydrophobic surface in proteins, it is considered that proteins use their hydrophobic surfaces to enhance the electrostatic attraction.

1Pos074 小角散乱、中性子準弾性散乱、及び中性子結晶学による蛋白質水和水の統一的解析

Coordinated analysis of protein hydration water by small-angle scattering, quasielastic neutron scattering, and neutron crystallography

Satoru Fujiwara[1], Tatsuhito Matsuo[1], Fumiaki Kono[1], Shin-ichi Takata[2], Yasunobu Sugimoto[3], Tatsuya Kikuchi[2], Kenji Nakajima[2], Toshiyuki Chatake[4] ([1]*QuBS, QST*, [2]*J-PARC Center*, [3]*Nagoya Univ.*, [4]*RRI, Kyoto Univ.*)

Proteins constantly interact with surrounding water molecules. This hydration water is a necessary constituent of proteins, which plays an important role in functions. Characterization of hydration water is thus important for understanding the mechanisms of the protein functions. Here we employ small-angle X-ray and neutron scattering (SAS), quasielastic neutron scattering (QENS), and neutron crystallography to characterize the structure and dynamics of hydration water around a protein. We systematically apply these methods to RNase A, one of the typical globular proteins. The average density and dynamics of hydration water are characterized by SAS and QENS. This information is compared with the high-resolution hydration structure obtained by neutron crystallography.

1Pos075 リゾチームの動的ストークスシフト測定と分子動力学計算によるその解釈

Measurement of dynamic Stokes shift of lysozyme and its interpretation by molecular dynamics simulation

Asahi Fukuda[1,2], **Tomotaka Oroguchi**[1,2], Masayoshi Nakasako[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*)

Dynamic Stokes shift of hen-egg-white lysozyme between 320-370 nm was measured in 1-500 ps after excitation using laser pulses of 290 nm by a custom-made ps-resolved fluorescence measurement system. The time-course of dynamic Stokes shift was approximated by two exponential curves of fast and slow decays (1.2 and 29.6 ps, respectively). To interpret the cause of the slow decay and discuss the influence of hydration network, a solvent response function reconstructed from the dynamic Stokes shift data was compared with time-correlation functions of protein-water interactions calculated from a molecular dynamics simulation of lysozyme in an explicit water system. The results indicated that the rigidity of hydration network around the protein contributed to the slow decay.

1Pos076 演題取り消し

1Pos077 細胞質ダイニンの歩行運動の異方性に関する理論的研究

Theoretical study on the anisotropy of Cytoplasmic dynein locomotion

Shintaoh Kubo, Shoji Takada (*Grad. Sci., Univ. Kyoto*)

Cytoplasmic dynein is a molecular motor which transports various vesicles to the minus-end of microtubules (MT) by bipedal walking mechanisms. While much knowledge has been gained on the walking mechanism of kinesin which transport to the plus-end of MT, dynein's motility has been poorly understood. In this study, we analyzed the movement of the microtubule binding domain (MTBD) of dynein on MT using molecular dynamics simulation of a coarse-grained model which represents one amino acid as one particle. We propose a new bipedal walking model by analyzing how the MTBD with high- and low- affinity to MT moves differently upon being pulled from the plus and minus-ends of MT.

1Pos078 確率的モデリングによるミオシン V の化学ー力学ネットワーク

Chemomechanical network modeling of myosin V

Tomonari Sumi (*Res. Inst. Interdisciplinary Sci., Okayama Univ.*)

We present a systematic chemomechanical-network modelling of myosin V based on both the nucleotide-dependent binding affinity of the head to actin filament (AF) and the asymmetry and similarity relations among the chemical transitions due to intramolecular strain between the two heads. The network model shows as follows: (1) the main forward cycle strongly depends on ATP concentration as observed in kinesin; (2) the high ratio of forward-step to ATP hydrolysis can be achieved even at low ATP concentrations by dual force-generating mechanical transitions; (3) the forward stepping at high ATP concentrations is explained by the front head-gating mechanism wherein the power stroke is triggered by ATP hydrolysis on the leading head.

1Pos079 **Two antagonistic regulatory domains of DCTN1 modulate the microtubule-binding affinities of both dynein and dynactin**

Takuya Kobayashi[1], Kei Saito[1], Takuya Miyashita[1], Takashi Murayama[2], Yoko Y Toyoshima[1] ([1]*Department of Life Sciences, Graduate School of Arts and Sciences, The University of Tokyo*, [2]*Department of Pharmacology, Juntendo University School of Medicine*)

Dynactin is a dynein modulator and has been considered for long time to promote dynein motility. However, recent studies revealed that single molecules of dynein-dynactin complex did not exhibit processive movement. To elucidate the regulatory mechanism of dynactin, we focused on DCTN1 subunit of dynactin. While the full-length DCTN1 induced processive movement of dynein, a DCTN1 splicing isoform lacking the K-rich domain severely reduced the microtubule-binding affinity of dynein and suppressed dynein motility. This inhibitory effect was attributed to the CC1 domain and the K-rich domain antagonized the inhibitory effect of CC1, and thus, DCTN1 has two antagonistic domains to promote or suppress dynein motility.

1Pos080 **Development of a nano-patterning of kinesins to control the number and arrangement of motors by combining Au nano-pillars and SAM**

Taikopaul Kaneko[1], Shotaro Ohba[1], Ken'ya Furuta[2], Kazuhiro Oiwa[2], Hirofumi Shintaku[1], Hidetoshi Kotera[1], Ryuji Yokokawa[1] ([1]*Kyoto Univ. Eng. Micro.*, [2]*NICT*)

Many cellular processes such as mitosis and flagellar motility are achieved by a team of motor proteins. However, the coordination of motors remains poorly understood due to the experimental difficulty in controlling the number and arrangement of motors, which are considered to affect the coordination. Here, we proposed a nano-patterning method of kinesins that enables to define the number and arrangement of motors propelling a microtubule. Au nano-pillars were fabricated on a silicon oxide (SiO_2) substrate. To immobilize kinesin only on Au pillars, SiO_2 surface was selectively coated by PEG self-assembled monolayer for the blocking kinesin. By using this method, we revealed kinesin-1 and Ncd have the different dependency of microtubule velocity on motor number.

1Pos081 **微小管結合タンパク質アルファシヌクレインの微小管および微小管依存細胞内輸送における機能解析**

Alpha-synuclein binds unconventional microtubules that have a unique function

Shiori Toba[1], Mingyue Jin[1], Masami Yamada[1], Sakiko Matsumoto[1], Takuo Yasunaga[2,3,4], Yuko Fukunaga[5,6], Atsuo Miyazawa[5,6], Hiroaki Kojima[7], Yoshiyuki Arai[8], Takeharu Nagai[8], Shinji Hirotsune[1] ([1]*Osaka City Univ. Grad. Sch. of Medicine*, [2]*Faculty of Computer Science and Systems Engineering, Kyushu Inst. of Technology*, [3]*JST-SENTAN*, [4]*JST-CREST*, [5]*Grad. Sch. of Life Science, Univ. of Hyogo*, [6]*RIKEN SPring-8 Center*, [7]*Advanced ICT Research Inst., National Inst. of Information and Communications Technology*, [8]*Inst. of Scientific and Industrial Research, Osaka Univ.*)

The neuronal protein α-synuclein has been linked to Parkinson's disease; however, the mechanism through which synucleins play a causative role is not clear. Here, we show that α-synuclein is required for the creation of unconventional microtubules named transportable MTs (tMTs), which function as carriers that enable anterograde cytoplasmic dynein transport. Live-cell imaging demonstrated the co-transport of synuclein with cytoplasmic dynein to the plus ends of tMTs. PALM revealed fibrous co-localization of α-synuclein, tubulin, and dynein. Electron microscopy observations showed that α-synuclein surrounded MTs *in vitro*. Through our work, we have uncovered the distinctive structure of tMTs and a potential mechanism for the pathogenesis of Parkinson's disease.

1Pos082 **アーキアべん毛の回転を駆動するモーターは速度一定型である**

The Archaellar Motor Produces Variable Torques to Maintain Constant Rotation Speed

Seiji Iwata, Yoshiaki Kinosita, Daisuke Nakane, Takayuki Nishizaka (*Dept. of Phys., Gakushuin Univ., Japan*)

Archaea swim by rotating archaeal flagellum termed as 'archaellum'. Here, to grasp the torque-generation mechanism of archaellar motor under various loads, we applied a bead assay, with different sizes in the presence of a viscous agent ficoll, to *Halobacterium salinarum*. In conventional 2-D tracking, the trajectory of the bead attaching to the archaellum were ellipse because each archaellum obliquely protruded from the cell body. To estimate the precise radius of rotation, the bead position was localized by 3-D tracking microscopy. Notably, rotation speed of archaeal motor were ～20 Hz under the torque of 0-4000 pN·nm, indicating the motor has a propensity to maintain constant speed in this range. The speed appeared to drop under the torque more than ～4000 pN·nm.

1Pos083 **真核生物鞭毛軸糸の Ca^{2+}濃度による構造変化の X 線繊維回折による解析**

Structural responses of *Chlamydomonas* flagellar axonemes to Ca^{2+} studied with X-ray fiber diffraction

Kazuhiro Oiwa[1,2,3], Junya Kirima[2], Misaki Shiraga[2], Hiroyuki Iwamoto[4] ([1]*Adv. ICT Res. Inst. NICT*, [2]*Grad. Sch. Life Sci. Univ. Hyogo*, [3]*CREST Biodynamics*, [4]*Japan Sync. Rad. Res. Inst. SPring-8*)

The mechanism of waveform changes coupled with intracellular Ca^{2+} concentrations found in *Chlamydomonas* flagella has remained a long-standing unresolved issue. We investigate this mechanism using continuous shear-flow for alignment of flagellar axonemes and X-ray fiber diffraction in the synchrotron radiation facility SPring-8, BL40XU. We explored the spatial arrangement and dynamics of axonemal components under various concentrations of Ca^{2+}. In the high Ca^{2+} concentrations, the radial-spoke-originating 1/48-nm^{-1} and 1/24-nm^{-1} meridional reflections split each into the layer lines, suggesting changes in helical nature of nine doublet microtubules in the axoneme.

1Pos084 **Cell-like locomotion of self-organized motor-filament complex**

Takayuki Torisawa[1,2], Masahiro Sawada[2,3], Daisuke Taniguchi[4], Shuji Ishihara[2,3], Kazuhiro Oiwa[1,2] ([1]*Advanced ICT Inst., NICT*, [2]*CREST, JST*, [3]*Grad. Sch. Arts and Sciences, Univ. Tokyo*, [4]*Dept. of Pharm., Grad. Sch. Med, Kyoto Univ.*)

The self-organization in motor-filament system plays critical roles in various biological processes including cell migration. We recently observed novel dynamics of the radial microtubule array (aster) in 2D space. The asters formed in the mixture of homotetrameric kinesin and microtubule displayed diverse spatiotemporal patterns including cell-like crawling when they attached to the glass surface. The movement of asters is a consequence of the dynamical balance between the contractile forces by motors in an asters and the traction forces by motors attached to the glass surface. Together with the temporal analysis of aster morphology, our results suggest that the simple feedback between the morphology and the movements alone can cause a cell-like locomotion.

1Pos085 *de novo* 設計した人工コイルドコイルは回転子として機能する。
The *de novo* designed artificial coiled-coil functions as a rotor of rotary motor

Jun-ichi Kishikawa, Mihori Baba, Atsuko Nakanishi, Ken Yokoyama (*Dept. Mol. Biosci., Kyoto Sangyo Univ.*)

V_1-ATPase is a marvelous molecular machine which converts the energy of ATP hydrolysis into the rotation of rotor. The mechanism of torque generation of V_1 is still controversial. To understand this mechanism, we *de novo* designed parallel coiled-coil composed of repeating sequence and examined whether it functions as a rotor. Single particle analysis revealed that the designed rotor penetrates through the center of V_1 stator. The ATPase activity of the complex was enhanced by insertion of the designed rotor. The rotation of the designed rotor was observed by single molecule observation. These results demonstrate that parallel coiled-coil also functions as a rotor. Our result is the first report that *de novo* designed protein functions as a part of molecular motor.

1Pos086 Structural and mechanistic insights into the ε subunit from bacterial ATP synthases

Alexander Krah[1,2], Shoji Takada[2], Changbong Hyeon[1] ([1]*School of Computational Sciences, Korea Institute for Advanced Study (KIAS)*, [2]*Department of Biophysics, Graduate School of Science, Kyoto University*)

The ε subunit from bacterial ATP synthases undergoes a large conformational change from the ATPase inhibitory up- to the non-inhibitory down state upon ATP binding. However, the ATP binding affinity of ε subunits from different organisms is dramatically different, from 4 μM to 20 mM, while others may not bind ATP at all. We use MD simulations to clarify reasons for the different ligand binding affinities of the ε subunit from different organisms. In this work, we obtain the ATP binding site structure of the ε subunit from *E. coli*, deriving molecular reasons for the decreased binding affinity compared to ε subunits from other organisms. Furthermore, we observe that the protonation state of one carboxylate group is essential to allow ATP binding.

1Pos087 DNA ペイント法を用いた RNA ポリメラーゼの超解像イメージングと細胞個性の分子メカニズムの解明
Super-resolution imaging of RNA polymerases with DNA-PAINT for understanding the molecular mechanism of cell individuality

Keisuke Fujita[1,2], Toshio Yanagida[1,2], Mitsuhiro Iwaki[1,2] ([1]*QBiC, RIKEN*, [2]*Grad. Sch. of Front. Bioscience., Osaka Univ.*)

Cell individuality plays a significant role in many biological processes such as decision making in bacterial cells and differentiation of mammalian cells and transcriptional bursting is a potential source of it. We have analyzed the kinetics of reconstituted E. coli transcription and proposed that transcriptional bursting can be spontaneously caused by RNA polymerases (RNAP) during transcription. However, it is critical to directly visualize the flow of RNAP in a cell for a comprehensive understanding of the molecular mechanism of transcriptional bursting. In this meeting, we will introduce an application of DNA-PAINT imaging technique for this purpose. The technique is capable of discrete molecular imaging with sub-5-nm spatial resolution.

1Pos088 F_1-ATPase のシリンダー部分の 1 分子立体構造変化観察
Single-molecule observation of conformational dynamics in the cylinder part of F_1-ATPase

Ryuichi Yokota[1], Mitsuhiro Sugawa[2], Yuta Nomura[1], Junichiro Yajima[2], Tomoko Masaike[1,3] ([1]*Dept. Appl. Biol., Sch. Sci. and Tech., Tokyo Univ. of Sci.*, [2]*Grad. Sch. Arts and Sci., Univ. of Tokyo*, [3]*Imaging Frontier Center, Tokyo Univ. of Sci.*)

Rotation of the central shaft γ in F_1-ATPase is driven by cooperative conformational dynamics of the surrounding cylinder $\alpha_3\beta_3$. First, we identified local conformational changes in β for the purpose of revealing the sequential structural dynamics which were triggered at the catalytic site and then propagated to the C-terminal domain. These identified conformational changes in β should be related to interactions with α. We then performed single-molecule FRET measurement in which fluorescent probes were attached to α-helices of both α and β. We observed two-state transitions of FRET efficiency in the presence of ATP and ATPγS, which may reflect loose/tight motions of the αβ interface.

1Pos089 キネシン-微小管の運動性を利用したデフォーカス角度イメージングの単一蛍光色素のテンプレートの獲得
Acquisition of raw sequential templates of a single fluorophore under defocused orientation imaging using kinesin-MT motility assay

Shoko Fujimura[1], Kazuki Goto[2], Kengo Adachi[3], Takayuki Nishizaka[2] ([1]*Sch. of Med, Keio Univ.*, [2]*Dept. Phys., Gakushuin Univ.*, [3]*Engin., Waseda Univ.*)

Measuring single-molecule orientation, such as defocused orientation imaging, reveals a wealth of information on the dynamic motions of motor proteins. However, it is not understood the level of accuracy in the polar angle of the single molecule transition dipole moments. Here we propose a new method to acquire sequential images of a single fluorophore, which form templates for defocused orientation imaging. The distance between the sample and objective were precisely adjusted by the commercial 'perfect focus system' under the advanced isotropic TIRF illumination (Fujimura et al., *BBRC* 2017). Our method was applied to monitor the angle of βs labeled by Cy3-maleimide in single molecular motor F_1-ATPase.

1Pos090 Novel photochromic inhibitor of kinesin composed of dronpa tandem dimer

Kohei Uchida, Shinsaku Maruta (*Grad. Sch. Eng., Univ. Soka*)

Previously we have demonstrated that incorporation of photochromic molecules into the microtubules binding site of kinesin enabled photo-reversible regulation of kinesin ATPase activity. In this study, we prepared the photo-switching protein “Dronpa derivative 145K-145N” fused with “Loop11” and “Loop12” which are the microtubule binding site, in order to control kinesin motor activity photo reversibly. The photochromic fusion protein showed photo reversible absorption spectral change accompanied by photo-isomerization. Microtubule stimulated ATPase activity and microtubules gliding of the conventional kinesin were significantly inhibited by 145K-L11-145N. We also examined the photo-reversible interaction of Dronpa 145K-L11-145N with microtubules.

1Pos091　細胞内シグナル伝達における膜電位の役割

Role of membrane potential in intracellular signal transduction

Yusuke V. Morimoto[1,2,3], Masahiro Ueda[2,3] ([1]*Dept. of Biosci. Bioinfo., Kyushu Inst. Tech.*, [2]*RIKEN, QBiC*, [3]*Grad. Sch. Frontier Biosci., Osaka Univ.*)

Plasma membrane potential is required for various cellular functions. The social amoebae *Dictyostelium discoideum* is a model organism to study chemotaxis, directed cell migration and differentiation. Chemotactic stimulation by cAMP is known to elicit cationic fluxes, involving H^+ and Ca^{2+}, across the plasma membrane. This suggests that the membrane potential is changed by cAMP stimulation. However it remains unknown how the membrane potential works in the cell motility and signal transduction. To investigate the role of membrane potential, we measured periodic membrane potential changes depending on the cAMP signal relay and controlled the membrane potential using optogenetic tools in *Dictyostelium* cells.

1Pos092　原始真核生物の細胞分裂過程を細胞内小器官の 3D 構造モデルから読み解く

Reading out the cell division process of primitive eukaryotes from 3D structural model of intracellular organelles

Takako M. Ichinose[1,2], Rina Nagai[1,2], Hikari Mori[1], **Atsuko H. Iwane**[1,2] ([1]*RIKEN, QBiC, Cell Struct.*, [2]*Osaka Univ., Grad. Front. Biosci.*)

Sequential 2D-EM images and 3D reconstruction will provide us several information not only to the 3D-structural shape and connection. However, to overcome some weak point of EM, we think that an approach to correlate well with fluorescent microscope observation is necessary to identify molecules and to be dynamics.
Last annual meeting we selected *C. merolae* , a primitive eukaryote, as a model organism for mitosis and presented the interaction between individual several organelles during mitosis cycle using FIB-SEM and 3D-reconstruction technique. In this meeting we will reveal individual morphology details inside of each organelle by reference to time laps observation. We will discuss you a new view about the role of its organelles.

1Pos093　角化細胞においてアクトミオシン活性が増殖の接触阻害に必須である

Actomyosin activity is required for contact inhibition of keratinocyte proliferation

Hiroaki Hirata[1,2], Mikhail Samsonov[3], Masahiro Sokabe[1] ([1]*Nagoya Univ Grad Sch Med*, [2]*R-Pharm Japan*, [3]*R-Pharm*)

Confluence-dependent inhibition of keratinocyte proliferation is crucial for epidermal homeostasis. We observed that under actomyosin inhibition E-cadherin-mediated cell-cell adhesions per se promoted proliferation of keratinocytes. Actomyosin activity in confluent keratinocytes inhibited β-catenin- and YAP-driven cell proliferation. Confluent keratinocytes developed actomyosin cables connected to E-cadherin adhesions. Elimination of the actin-to-E-cadherin linkage by depleting α-catenin increased proliferation of confluent keratinocytes. By contrast, application of pulling force to E-cadherin adhesions using magnetic beads attenuated their proliferation. Our results suggest that tensile force at cell-cell adhesions inhibits proliferation of confluent keratinocytes.

1Pos094　エンドセリン B 受容体のシグナル伝達における GRP78 の役割

Roles of GRP78 in endothelin B receptor signaling

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Endothelin (ET) is known as vasoconstricting peptide. Recently, ET-1 is reported to be involved in tumour growth, invasion and survival. ET-1 receptor consists of two receptors, ET type A receptor (ET_AR) and ET type B receptor (ET_BR). ET_AR is present on vascular smooth muscle cells, and upon agonist stimulation, it induces vasoconstriction. On the other hand, ET_BR is present on vascular endothelial cells, upon agonist stimulation, it induces vascular relaxation. Here, we attempted to identify ET_AR or ET_BR specific binding proteins to elucidate molecular mechanisms of their different. We found that GRP78 specifically binds to ET_BR. In addition, GRP78 is partially colocalized with ET_BR in plasma membrane. We will discuss roles of GRP78 in ET_BR signaling.

1Pos095　細胞形状が誘発するアメーバ細胞の集団運動

Cell shape driving collective migration of amoeba cells

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Cells exhibit collective migrations in various biological phenomena. Even for amoeba cell like as Dictyostelium discoideum, the shape of cells affects the motion. We theoretically investigated how the time averaged shape of cells affects collective behavior of cells based on cellular Potts model. We found a transition from collective to individual movement of cells. When the shape of cell elongates in the direction of movement, cells show a collective migration. In contrast to this, when the shape of cell elongates in the perpendicular direction of motion, cell motion occurs individually.

1Pos096　γ-tubulin は中心子のトリプレット微小管形成に関与する

Evidence for involvement of γ-tubulin in assembly of centriolar triplet microtubules

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γ-tubulin ring complex plays a pivotal role in nucleation of the cytoplasmic microtubule. However, it has been unknown whether it also nucleates the centriolar triplet microtubule, which serves as the base for the flagellar doublet microtubule. We isolated novel Chlamydomonas mutants, named bld13-1 and bld13-2, that show partial defects in producing flagella. Interestingly, genetic analyses showed that this phenotype is caused by a single dominant-negative mutation in conserved amino acid residues of γ-tubulin (T292I or E89D). Observation by electron microscopy revealed that the mutant centrioles frequently lack a part of the protofilaments of the triplet microtubules. This is the first evidence for the involvement of γ-tubulin in centriolar microtubule assembly.

1Pos097 単一心筋細胞に対する赤外レーザ照射の影響
Influence of focused infrared laser irradiation on beating rate in single cardiomyocytes

Kento Nozawa, Yukino Motohashi, Maki Ishii, **Tomoyuki Kaneko** (*LaRC, FB, Hosei Univ.*)

The beating rate of cardiomyocytes is regulated by several factors, e.g. temperature, ion concentration and physical stimulation. To control the beating rate of cardiomyocytes, we tried to irradiate the focused infrared laser to the single cardiomyocytes. The single cardiomyocytes were beating spontaneously and infrared laser was focused on cytosol near the nucleus in a cardiomyocyte. The beating rate of cardiomyocytes with irradiation of focused infrared laser was faster depending on the laser power than before irradiation. These results were suggested that cardiomyocytes could be focally heated by the irradiation of infrared laser. Therefore we were succeeded to control the beating rate of the single cardiomyocytes by focal heating with infrared laser irradiation.

1Pos098 Protein with tau-like repeats (PTL-1)と細胞骨格線維の相互作用
Interaction between cytoskeletal filaments and a protein with tau-like repeats, PTL-1

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A protein with tau-like repeats (PTL-1) found in C. elegans is a microtubule-associated protein (MAP) containing a repeat of assembly promoting sequences similar to the mammalian MAPs. In this study, we analyzed the interaction of PTL-1 to microtubule and F-actin, and compared the activities to those of mammalian MAPs. To evaluate microtubule-assembly promoting activity and F-actin binding activity of PTL-1, we performed co-sedimentation assay and fluorescence microscopic observation. The results revealed that PTL-1 showed microtubule-assembly promoting activity and F-actin binding activity as mammalian MAPs. We also found that the PTL-1-induced microtubules were shorter than that of mammalian MAPs-induced microtubules.

1Pos099 ゾウリムシ繊毛メタクロナールウェーブの発振源
Sources of Metachronal Wave in *Paramecium* Cilia

Naohiko Himata, Chika Okimura, Manabu Hori, **Yoshiaki Iwadate** (*Fac. Sci., Yamaguchi Univ.*)

Ciliary movements in protozoa show metachronal coordination so as to maintain a constant phase difference between adjacent cilia. This coordination is called as “metachronal wave”. We can see the ciliary beat only at the side of live *Paramecium* cells under optical microscopy, because of the thickness of the cell.
We observed ciliary metachronal wave propagations in ciliary cortical sheets, which is one of the most appropriate techniques developed by Noguchi in Toyama Univ. to observe the two-dimensional ciliary metachronal waves. The waves seemed to be propagated from two areas, the top of the cell and the periphery of oral groove. Cutting of both areas from the sheet prevented the wave propagations. We will discuss the sources of metachronal wave propagation.

1Pos100 魚類表皮ケラトサイトの遊走のための車輪
A Wheel for Migration in Fish Keratocyte

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In general, the energy efficiency of the movement of organisms is greater than that of man-made machines. Although the energy efficiency of wheel rotation is very high, no organisms that move by the use of wheels have been discovered.
Fish epidermal keratocytes maintain a nearly constant fan shape during their migration. Each cell is composed of a frontal crescent-shaped lamellipodium and a rear spindle-shaped cell body. In keratocytes, stress fibers composed of actomyosin are positioned to connect the rear left and right focal adhesions. We found that the autonomous rotation of a wheel composed of stress fibers in keratocytes is required for their directional crawling migration.

1Pos101 マイコプラズマの滑走速度を示す分子速度計
Molecular speedometer indicating gliding speed in *Mycoplasma pneumoniae*

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Mycoplasma pneumoniae, a human pathogenic bacterium, glides on host-cell surfaces by unknown mechanism. It forms an attachment organelle: a membrane protrusion at a cell pole composed of a highly organized rod-like cytoskeleton. Here, we constructed several mutants by a genetic manipulation to increase or decrease coiled-coil regions of HMW2, a 200-kDa protein aligned in parallel along the cytoskeleton. Notably, these mutants showed different gliding speed under a phase-contrast microscope. We compared the speed with the length of rod quantified by TEM image, and found simple correlation that the speed was increased as the length became longer. It suggests that the size of cytoskeleton could be a molecular speedometer indicating the gliding speed in this species.

1Pos102 単一細胞内グルココルチコイド受容体のホモ二量体形成と転写活性の関連解析
Quantitative analysis of glucocorticoid receptor dimerization and transcriptional activity in single cell using advanced imaging technique

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The aim is to reveal a dimerization of glucocorticoid receptor (GR) and its relationship with a transcriptional activity in the living cells. It is well-known that the GR dimer binds to glucocorticoid response element (GRE) in a promoter region of target genes and regulates their gene expression upon ligand binding. However, the GR dimerization in the living cells and relationship between GR dimer and transcriptional activity are unclear, yet. In this study, we applied fluorescence cross-correlation spectroscopy (FCCS) to determine the dissociation constant of GR dimerization in the living cells, and a combination method with microwell chip to determine the relationship between GR dimerization and transcriptional activity in single cell.

1Pos103 **Actin-like MamK cytoskeleton tethers bacterial magnetosome organelles in a static chain**

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Magnetotactic bacteria are a unique group of bacteria that synthesize a magnetic organelle termed the magnetosome, which they use to assist with their magnetic navigation. The cytoskeletal filaments consisting of the actin-like protein MamK are associated with the magnetosome chain. Here, we conducted live-cell time-lapse fluorescence imaging analyses employing highly inclined and laminated optical sheet microscopy. The distance that magnetosomes travelled in mamK deletion mutant cells suggests that magnetosomes moved through simple diffusion. We found that the MamK cytoskeleton anchors magnetosomes through a mechanism that required MamK-ATPase activity throughout the entire cell cycle to prevent simple diffusion of magnetosomes within the cell.

1Pos104 **ロクロクビムシのプロボーシスの伸縮機構**
Extension and Contraction Mechanism of the Proboscis of a Ciliate, *Lacrymaria olor*

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The free-living ciliate, *Lacrymaria olor* has a proboscis, which rapidly extends up to 10 times longer than its original length. To reveal the extension–contraction mechanism, we conducted detailed analyses of the extension–contraction of the proboscis using several microscopic observation techniques. The results indicate that (1) ciliary movement of an oral part on the distal end of the proboscis mainly contributes to the extension, (2) the proboscis has a property like a nonlinear spring, and (3) some contractile factor which works only during contracting period exists in the proboscis. Our study confirmed contribution of the oral ciliary movement for the extension of the proboscis and revealed characteristic physical properties of the proboscis of *L. olor*.

1Pos105 **バクテリアべん毛輸送ゲート複合体構成蛋白質間の相互作用**
Interactions between flagellar type III export gate proteins

Miki Kinoshita[1], Akihiro Kawamoto[1], Keiichi Namba[1,2], Tohru Minamino[1] ([1]*Graduate School of Frontier Biosciences, Osaka Univ.*, [2]*QBiC, RIKEN*)

The bacterial flagellar type III export apparatus, which is required for flagellar assembly beyond the cell membranes, consists of a transmembrane export gate complex and a cytoplasmic ATPase complex. The assembly of the export gate complex begins with FliP ring formation with the help of the FliO scaffold, followed by FliQ, FliR and FlhB and finally FlhA during MS ring formation. But it remains unknown how they interact with each other in the gate complex. Here, we analyzed direct protein-protein interactions between export gate proteins by co-purification assay. We show that FliQ and FliR directly bind to the FliP ring. We will discuss interaction networks in the export gate complex.

1Pos106 **べん毛蛋白質輸送装置の基質認識モード切り替えにおける FlhA リンカー領域の役割**
The role of a flexible linker of FlhA in substrate specificity switching of the bacterial flagellar type III export apparatus

Yumi Inoue[1], Mamoru Kida[2], Miki Kinoshita[1], Katsumi Imada[2], Keiichi Namba[1,3], **Tohru Minamino**[1] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [2]*Grad. Sch. Sci., Osaka Univ.*, [3]*QBiC, RIKEN*)

The flagellar type III export apparatus switches its export specificity upon completion of the hook structure, thereby terminating hook assembly and initiating filament assembly. A transmembrane export gate protein, FlhA, forms a nonameric ring structure, and acts as a sorting platform to coordinate flagellar protein export with assembly. Intermolecular interactions of a linker region of FlhA with its neighboring subunit are critical for the export function of FlhA. Here, we carried out genetic and structural analyses of FlhA(E351A/W354A/D356A). We show that the E351A/W354A/D356A mutation allows FlhA to adopt a semi-closed conformation, thereby inhibiting flagellar filament assembly. We will discuss the substrate specificity switching mechanism of the export apparatus.

1Pos107 **細菌べん毛モーター固定子付随蛋白質 FliL のペリプラズム領域の構造**
Structure of a periplasmic fragment of FliL, a bacterial flagellar stator associated protein from *Vibrio alginolyticus*

Norihiro Takekawa[1], Miyu Isumi[1], Mayuko Sakuma[2,3], Seiji Kojima[2], Michio Homma[2], Katsumi Imada[1] ([1]*Dept. of Macromol. Sci., Grad. Sch. of Sci., Osaka Univ.*, [2]*Div. of Biol. Sci., Grad. Sch. of Sci., Nagoya Univ.*, [3]*Radioisotope Res. Cent., Nagoya Univ.*)

For the efficient rotation of the bacterial flagellar motor, a single transmembrane protein, FliL, is crucially important because deletion of *fliL* affects the stator assembly and reduces the motor performance under highly viscous condition. Here we report the crystal structure of a periplasmic fragment of FliL ($FliL_P$) from *V. alginolyticus* at 2.1 Å resolution. $FliL_P$ forms a helical tube structure in the crystal. $FliL_P$ shows structural similarity with the extracellular domain of stomatin, a mammalian protein involved in mechanosensing and regulatation of ion channels, suggesting the periplasmic region of FliL may interact with the stator and control the stator in response to the mechanical stimuli.

1Pos108 **多電極電位計測システムを用いたライン状心筋細胞の伝導速度測定**
Measuring Conduction Velocity of Line-Networked Cardiomyocyte

Tetsuro Yoshida, Yui Okabe, Tomoyuki Kaneko (*LaRC, FB, Hosei Uni.*)

Development of a system precisely to examine side effects of drugs is necessary. To develop the novel examination of drug's effects, we used chick embryo cardiomyocytes and measured the conduction velocity of line-networked cardiomyocytes by using a multi electrode array system. The coefficient of variation of conduction velocity between the electrodes was smaller in a CO2 incubator than temperature-controlled box. Then, we measured the responses to the terfenadine, an anti-allergic drug, in the CO2 incubator. As a result, the direction of conduction was changed in 10 μM terfenadine. It was suggested that the risk of false negative drugs such as terfenadine could be predicted by measuring the conduction velocity of the line-networked cardiomyocyte.

1Pos109 1細胞レベルで再構成した心筋細胞ネットワークによる外部電気刺激への応答解析

Analysis of response to external electric stimulations by cardiomyocytes-network arranged at single-cell-level

Koki Fujii[1], Fumimasa Nomura[2], Tomoyuki Kaneko[1] ([1]*Laboratory for Reconstructive Cell Biology, Frontier Bioscience, Hosei University*, [2]*Department of Biomedical Information, Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University*)

Myocardial infarction (MI) disturbs blood circulation. After MI, ventricular remodeling like cardiomyocytes extension and fibroblasts proliferation occurs. To understand the electrophysiology of remodeling site, we lined up cardiomyocytes at single-cell-level by using cell handling micro pipette and agarose microchambers, reconstructed the structure suffering from remodeling, and examined their response to electrical stimulation. We found that the length of cell-network was a key factor in the parallel electric field, while orthogonal one required constant voltage. Moreover cell-network which was longer or consisting more cells expanded the responsible range of the stimulation frequency. These results could contribute to the development of novel therapeutic methods.

1Pos110 新規マイクロ流体システムで解明する赤血球の非線形非平衡変形能

Non-linear and non-equilibrium deformability of a red blood cell unraveled with a novel microfluidic platform

Hiroaki Ito[1], Ryo Murakami[1], C.-H. Dylan Tsai[1], Motomu Tanaka[2,3], Makoto Kaneko[1] ([1]*Grad. Sch. Eng., Osaka Univ.*, [2]*iCeMS, Kyoto Univ.*, [3]*Phys. Chem. Inst., Univ. Heidelberg*)

We propose a new method for quantifying red blood cell (RBC) deformability based on the combination of a microfluidic constriction channel and a “robotic pump”, which enables real-time high speed, precise manipulation of a RBC inside the channel. Using this system, we applied precisely controlled large deformation to the whole cell. After the constriction, the cell shape recovers depending on various loading patterns and internal amount of adenosine triphosphate (ATP). The analysis unraveled non-linear viscoelasticity and non-equilibrium mechanics in the timescale of 100 s, which could be involved in global cytoskeletal remodeling in response to the applied stress. A potential application of this method for a novel diagnostic test of diseased RBCs is also discussed.

1Pos111 Dynamics of Actin Cytoskeleton Remodeling Induced by Femtosecond Laser Ablation

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A number of studies proved that dynamic remodeling of cytoskeleton greatly influences cell functions, e.g. migration, adhesion, etc. In this work, we have studied the dynamics of cytoskeleton remodeling of myoblast cells expressing Lifeact-mRFP induced by a local disruption of actin fibers with femtosecond laser ablation. We found that the lamellipodia spreading retrograded immediately after the local disruption in the micrometer-sized area of actin fibers. Then the disrupted area showed the recovery of actin fiber networks within 1 hour, and which seemed to activate anisotropic spreading and migration. In the presentation, we look forward to discussing the detailed results and potential applications for the spatiotemporal control of cell functions by laser ablation.

1Pos112 ベシクル可溶化法によるリン脂質ーリン脂質間相互作用熱力学量の測定

Phospholipid-Phospholipid Interactions in Bilayers Determined by Vesicle Solubilization

Keisuke Ikeda, Minoru Nakano (*Grad. Sch. Med. Pharm. Sci., Univ. Toyama*)

We report an experimental method for determining the change in the free energy and the enthalpy that accompanies the mixing of two phospholipids in lipid bilayers. The enthalpy change originated in the thermal changes of disrupting lipid bilayer vesicles titrated into a surfactant micelle solution and is monitored using isothermal titration calorimetry. The Gibbs free energy changes were estimated by determining the thermodynamic equilibrium constants of forming a molecular complex between phospholipids and methyl-beta-cyclodextrin. We show that mixing of anionic phosphatidylglycerol and zwitterionic phosphatidylcholine is explained well by the entropic term of the electrostatic free energy of a charged surface in the Gouy-Chapman model.

1Pos113 コレステロール含有ホスファチジルエタノールアミン膜とシトクロム P450 基質薬剤クロルゾキサゾンの相互作用

Interaction between cholesterol-containing phosphatidylethanolamine bilayers and cytochrome P450 substrate drug chlorzoxazone

Hiroshi Takahashi (*Grad. Sch. Sci. & Tech., Gunma Univ.*)

Many drugs are oxidized by cytochrome P450 (CYP) located in endoplasmic reticulum (ER). One of the features of ER is its lower content of cholesterol (CHOL). Previously, we studied CHOL-concentration dependence of the interaction of chlorzoxazone (CZX), a CYP substrate drug, with 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) bilayers. We found that high CHOL concentration (30-50 mol%) tends to prevent CZX from binding to POPC bilayers (*Biochemistry* **55** (2016) 3888). In this study, the above findings were reexamined using another phospholipid, 1-palmitoyl-2-oleoyl-phosphatidylethanolamine (POPE), in consideration of the diversity of membrane lipids of real biological membranes. As a result, a slightly different tendency was observed in the POPE/CHOL/CZX systems.

1Pos114 ガラス基板に固定した細胞膜中の脂質と膜タンパク質の電気泳動

Electrophoresis of lipids and membrane proteins in the cell membrane fixed on a glass substrate

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Supported lipid bilayer electrophoresis is useful method for measuring physical properties of lipids and membrane proteins. Electrophoretic properties of the cell membrane have not well understood. To measure electrophoretic properties of the cell membrane, the cell membrane preparing from HeLa cells was fixed on a glass surface. We attempted electrophoresis of the fluorescently labeled lipid (NBD-PE), dye (DiI), peripheral membrane protein (palmitoylated-GFP) and transmembrane protein (TFR-GFP) in the membrane. NBD-PE, DiI and palmitoylated-GFP were observed to migrate at the electric fields. Migration of TFR-GFP was not observed at any electric fields. We will discuss about electrophoretic properties of lipids and membrane proteins in the cell membrane.

1Pos115 分子動力学シミュレーションを用いたメリチンによる膜細孔形成の自由エネルギー解析

Free energy analysis of membrane pore formation by melittin using molecular dynamics simulations

Yusuke Miyazaki, Wataru Shinoda, Susumu Okazaki (*Grad. Sch. Eng., Univ. Nagoya*)

Membrane pore formation is included in many pivotal biological processes such as membrane fusion, gene therapy and drug delivery. Therefore, understanding of the molecular mechanism is of key importance for shedding a light into a wide range of biophysical processes. Melittin, an antimicrobial peptide, can form a transmembrane pore by self-assembly on membranes. Its pore formation process has been extensively studied by experiments and simulations. However, the relation between membrane structure and free energy of pore formation is still poorly understood. In this study, we elucidate the mechanism of membrane pore formation in the presence of melittin peptides by means of molecular dynamics simulations and free energy analysis.

1Pos116 界面通過法 GUV-膜タンパク質発現バキュロウイルス間膜融合の可視化解析

Analysis of membrane fusion between membrane protein-expressing baculovirus virions and GUVs prepared with a droplet transfer method

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We present a novel technique for preparing proteo-GUVs by membrane fusion between recombinant protein-expressing budded viruses (BVs) of baculovirus and GUVs prepared using a droplet transfer method [1].
Using CLSM, we analyzed the BV-GUV membrane fusion, and described a fusion curve to elucidate the pH dependence related to the function of the viral protein GP64. We further investigated how the retention of entrapped calcein was affected by the fusion. The results indicated that this method could provide proteo-GUVs with a moderate leakage of the inner compounds. We will discuss the distribution of lipophilic fluorescent dyes and membrane proteins on the GUVs, comparing it with the case of the gentle hydration.
[1] Nishigami M et al. Colloids Surf B 155 (2017) 248.

1Pos117 Change of binding ability of halorhodopsin for bacterioruberin accompanied by retinal binding / dissociation on archaeal membrane

Shun Yano, Takanori Sasaki (*Graduate School of Advanced Mathematical Sciences, Meiji University*)

Halorhodopsin (NpHR) from N.pharaonis acts as a light driven anion pump and forms a trimer on the archaeal membrane. NpHR also binds tightly with a carotenoid of bacterioruberin (BR) at the crevice between the NpHRs in the trimer. In this study, we investigated the changes of binding affinity of NpHR for the BR accompanied by the retinal binding / dissociation. The BR bound to the NpHR was removed from the membrane by Tween 20 treatment only when the retinal has been dissociated from the NpHR by hydroxylamine. Moreover, apoprotein on the membrane without the BR bound the retinal and formed trimer again. These results suggest that binding affinity of the NpHR to the BR corresponds the protein structure dependent on the retinal binding / dissociation.

1Pos118 Role of cholesterol in membrane phase separation observed via coarse-grained simulations of ternary mixtures

George A. Pantelopulos, John E. Straub (*Chem. Dept., Boston U., USA*)

Formation of micro- and macroscale lipid domains is of great interest to understanding membrane protein structure and function. Cholesterol (CHOL) is understood to play an essential role in the formation of micro- and macroscale lipid domains. We present a study of the micro- and macroscopic domain structures observed in the phase-separating mixture of DPPC:DIPC:CHOL at equimolar lipid and various CHOL concentrations. We find CHOL to modulate the domain formation mechanism and cause formation of anti-registered domains at high concentration. Additionally, the formation of CHOL “threads” at high concentration cause for loss of membrane mobility and undulation of the membrane surface while forming a ordered liquid co-crystal with DPPC.

1Pos119 Reconstitution amount of membrane proteins was controlled by components of asymmetric lipid vesicles

Koki Kamiya[1], Toshihisa Osaki[1,2], Ryuji Kawano[1], Shoji Takeuchi[1,2] ([1]*Kanagawa Institute of Industrial Science and Technology*, [2]*IIS, University of Tokyo*)

Cell membranes are composed of asymmetric lipid membranes. In the plasma membranes of eukaryotic cells, phosphatidylcholine (PC) and sphingomyelin (SM) are located on the extracellular leaflet, while phosphatidylserine (PS) and phosphatidylethanolamine (PE) are located on the intracellular leaflet. The asymmetry of the cell membrane plays a role in the biological reactions of the living cells. In this study, to investigate lipid-membrane protein interactions in the asymmetric membranes, the membrane proteins conjugated with GFP, which were expressed by cell-free synthesis systems, were integrated into asymmetric lipid vesicles containing PS lipids. We found the efficient reconstitution of this protein into asymmetric lipid vesicles containing PS on the outer leaflet.

1Pos120 リガンド添加による脂質二分子膜相転移温度変化の熱力学的解釈

Thermodynamic interpretation for variation in phase-transition temperatures of lipid bilayer membranes by adding a ligand

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The variation in phase-transition temperatures of dipalmitoylphosphatidylcholine (DPPC) bilayer membrane by adding two membrane-active ligands, a long-chain fatty acid (palmitic acid (PA)) and an inhalation anesthetic (halothane (HAL)), was investigated. The results were so contrastive for both ligands, PA showed a strong affinity with the gel phase in a micro-molal concentration range, about 20% smaller transfer volume of the lamellar gel phase than the liquid crystal phase and the suppression of the bilayer interdigitation, whereas HAL showed a strong affinity with the liquid crystal phase in a milli-molal concentration range, about twice larger transfer volume of the liquid crystal phase than the ripple gel phase and the promotion of the interdigitation.

1Pos121 ポア形成ベータシートペプチドのデザイン
Design of pore-forming β-sheet peptides in lipid bilayer

Keisuke Shimizu[1], Naoki Saigo[1], Yusuke Sekiya[1], Kenji Usui[2], Ryuji Kawano[1] ([1]*Kawano Lab. Tokyo University of Agriculture and Technology*, [2]*Usui Lab. Konan University*)

Several β-sheet peptides, such as amyloid β, are known to assemble the several monomers and to form pores in bilayer lipid membranes. Although the pore-forming phenomenon are related to the pathology of Alzheimer's, Parkinson diseases, and so on, the mechanism of pore-formation is still unclear. In order to elucidate the features of pore-formation with β-sheet, we have attempted to observe the pore-formation behavior of simple model peptides. As a model structure, we designed β-sheet peptides, which have once or twice transmembrane region(s). We have measured the channel current of these peptides using artificial lipid bilayers and show pore-forming activities and characteristics of them.

1Pos122 コレステロールによるジアルキルホスファチジルコリンの指組構造化の抑制
Suppression of bilayer interdigitation of dialkyl-phosphatidylcholine by cholesterol

Nobutake Tamai[1], Takuya Izumikawa[2], Maiko Uemura[2], Masaki Goto[1], Hitoshi Matsuki[1] ([1]*Grad. Sch. Technol. Indus. Soc. Sci., Tokushima Univ.*, [2]*Grad. Sch. Adv. Technol. Sci., Tokushima Univ.*)

We investigated the phase behavior of cholesterol (Chol)-containing binary membrane of dihexadecylphosphatidylcholine (DHPC), one of dialkyl-PCs, by DSC and Prodan fluorescence spectroscopy as a function of the mole fraction of Chol (Xch). The DSC data showed that the chain-melting transition was abolished at Xch = ca. 0.50. The Prodan fluorescence spectra successfully detected the coexistence of the interdigitated and non-interdigitated gel phase, allowing us to explain the Xch-dependent non-linear behavior of the induction of the non-interdigitated gel phase by the incorporation of Chol. We will also discuss the differences in the phase behavior of the Chol-containing binary membranes of DHPC and its diacyl counterpart, dipalmitoylphosphatidylcholine.

1Pos123 Quantitative analysis of water permeation into model lipid membranes for the stratum corneum intercellular lipids by FTIR-ATR

Kohei Oka, Hiromitsu Nakazawa, Satoru Kato (*Grad. Sch. Sci & Tech., Univ. Kwansei Gakuin*)

We have been developing a new method to analyze the substance permeation into a model lipid membrane of stratum corneum. A model membrane containing one kind of ceramide, cholesterol and free fatty acid is formed directly onto the FTIR-ATR prism. The substances mounted onto the model membrane are detected when they approach close to the ATR prism surface. In this study we tried to theoretically analyze the diffusion process and quantitatively determine the physical properties such as diffusion constant and partition coefficient. Growth of the IR signal after drop of water onto the membrane was traced and analyzed on the basis of simple diffusion theory. The analysis suggested that the diffusion process involves at least two diffusion constants.

1Pos124 マイクロ流路デバイスを用いた細胞サイズ液滴の充填パターン
Hexagonal packing of cell-sized lipid droplets using microfluidic device

Shougo Fujiwara, Kan Shouji, Ryuji Kawano, **Miho Yanagisawa** (*Tokyo Univ. Agri. Technol.*)

Hexagonal packing of cells is one of the popular packing geometries of cells. To understand mechanism to regulate the geometry, here we propose a model system of adhesive microdroplets coated with lipid layers [1]. By using microfluidic device, we prepared monodisperse lipid droplets. After the droplets were gathered in the U-shaped part in the device, the droplets adhered to each other and generated hexagonal packing pattern via self assembly. This geometry was strongly affected by structure of polymers confined inside the droplets. We will discuss the relationship between the droplet geometry and the intracellular structure.
[1] M. Yanagisawa, et al., 2013 Soft Matter 25:5891

1Pos125 粗視化モデルによる混合脂質ベシクルの構造安定性に関する理論的研究
Theoretical study on the structural stability of vesicle consisting of mixed lipids by coarse-grained model

Tetsu Matsuura, Shohei Takagi, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Sch. Nat. Sci. Tech., Kanazawa. Univ*)

Self-assemble dynamics and structure changes of lipid vesicle induced by binary mixture of lipids has been studied using coarse-grained molecular simulations. The purpose of this study is to investigate formation and distribution change of molecules in vesicle induced by the changing kinds of the lipid molecules. An amphiphilic molecule is modeled as the rigid rod which consists of three spherical particles. The hydrophobic interaction is mimicked by the local density potential of the hydrophobic particles(H.Noguchi, et at. *Phys.Rev.E.* (2001)). We change potential parameters and size of the molecules to present the two kinds of amphiphilic molecules. By the change of the parameters, we found random distribution of molecules, phase separation and vesicle devision.

1Pos126 親水性アミノ酸残基の位置に依存した膜貫通ペプチドのリン脂質 flip-flop 促進能の評価
Effect of hydrophilic amino acid residues and their relative position in transmembrane peptides on phospholipid flip-flop promotion

Yuta Sugimoto[1], Hiroyuki Nakao[2], Keisuke Ikeda[2], Minoru Nakano[2] ([1]*Fac. of Pharm. and Pharm. Sci., Univ. of Toyama*, [2]*Grad. Sch. of Med. and Pharm. Sci., Univ. of Toyama*)

The mechanism of rapid phospholipid flip-flop in the endoplasmic reticulum (ER) is still unknown. We have previously revealed that a membrane-spanning sequence of a human ER protein, EDEM1, promotes the flip-flop. In the EDEM1 peptide sequence, two hydrophilic residues are located at the same side of an α-helix structure. Therefore, we hypothesized that relative position of two hydrophilic residues in the helix may be important for flip-promotion ability of peptides. In this study, we synthesized model transmembrane peptides containing two hydrophilic residues at various positions in the sequences and evaluated their activity. We found that the peptides with two hydrophilic residues at the same side of the helix significantly increased the flip rate.

1Pos127 **脂質膜の熱的揺らぎは細胞透過ペプチド・トランスポータン10(TP10)の単一ベシクルへの侵入に影響を与える**
Thermal Fluctuation of Lipid Bilayers Affect the Entry of Cell-Penetrating Peptide Transportan 10 (TP10) into Single Vesicles

Md. Zahidul Islam[1], **Sabrina Sharmin**[1], Victor Levadnyy[1,2], Sayed Ul Alam Shibly[1], Masahito Yamazaki[1,3,4] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Rus. Acad. Sci.*, [3]*Res. Inst. Ele., Shizuoka Univ.*, [4]*Grad. Sch. Sci., Shizuoka Univ.*)

To reveal the mechanism underlying the entry of a cell-penetrating peptide, TP10, into cells, we examined the effects of the mechanical properties on the entry of CF-TP10 into single DOPG/DOPC (2/8)-GUVs (1). Lateral tension increased the rate of entry of CF-TP10 into the GUV lumen before leakage of AF647, i.e., pore formation. A high concentration of cholesterol inhibited the entry of CF-TP10 into single GUVs by suppressing the translocation of CF-TP10 from the outer to the inner monolayer. We discussed the role of thermal fluctuation of lipid bilayers on the entry of CF-TP10 into the GUV lumen and proposed a hypothesis on the mechanism that CF-TP10 translocates across a bilayer through transient hydrophilic prepores in the membrane.
(1)Langmuir, 33, 2433, 2017

1Pos128 **混合脂質二重膜中における孔側壁の線張力係数の孔径依存性：分子動力学シミュレーション**
Pore Radius Dependence of Nano-Pore Edge Tension in Mixed Lipid Bilayers: Molecular Dynamics Simulation

Taiki Shigematsu[1], Kenichiro Koshiyama[2], Shigeo Wada[2] ([1]*Global Center for Medical Engineering and Informatics, Osaka University*, [2]*Graduate School of Engineering Science, Osaka University*)

Edge tension of a transmembrane pore in lipid bilayers is one of the important factors that govern the dynamics of the pore. Theoretically, the edge tension is considered to depend on the pore radius R when R is less than several nanometers, i.e., nano-pore. However, to estimate the nano-pore edge tension is challenging in experiments. We performed molecular dynamics simulations of pure DPPC and DPPC/cholesterol (CHOL) bilayers with a nano-pore and estimated the edge tensions of nano-pores with various R. We found that the edge tension for the DPPC/CHOL bilayer increases with the increase of R while that for the pure DPPC bilayer is insensitive to R. This shows the pore radius dependence of the edge tension varies on the bilayer composition.

1Pos129 **A New Coarse-Grained Lipid Model for the Study of Lipid-Membrane Protein Systems**

Diego Ugarte, Shoji Takada (*Dept. Biophysics, Div. Biology, Grad. Sch. Sci., Kyoto University*)

This works aims to develop a new coarse-grained (CG) lipid model that permits to simulate, within the appropriate time and length scale, various large-scale biomolecular processes in which membrane and membrane proteins are involved. In this model, the dipalmitoylphosphatidylcholine (DPPC) phospholipid is mapped into five linearly-connected beads. For the parameterization, we take a hybrid approach, in which the intramolecular interactions are bottom-up coarse-grained through the Iterative Boltzmann Inversion (IBI) method while the intermolecular interactions are top-down coarse-grained using tunable functions.

1Pos130 **脂質膜の張力は水の膜透過係数を増加させる**
Lateral Tension increases membrane permeability of water in lipid membranes

Rajib Ahmed[1], Sayed Ul Alam Shibly[1], Md. Zahidul Islam[1], Masahito Yamazaki[1,2,3] ([1]*Grad. Sch. Sci., Shizuoka Univ.*, [2]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [3]*Res. Inst. Ele., Shizuoka Univ*)

Application of tension to biomembranes induces their stretching, which plays various important roles (1,2). Here we examined the effect of tension on membrane permeability of water across lipid bilayers (i.e., water permeability) of GUVs. To measure water permeability, we analyzed the time course of the volume change of a GUV when it was transferred to a hypotonic solution under application of a constant tension. Water permeability greatly increased with tension without leakage of water-soluble fluorescent probes, i.e., without pore formation. The present theories on water permeability cannot explain this enhanced water permeability. We proposed a new theory (i.e., prepore model) for the water permeability.
(1)PCCP, 18, 13487, 2016, (2) Biophys. J. 111, 2190, 2016

1Pos131 **細胞透過ペプチド・トランスポータン 10 の脂質膜透過に与える膜電位の効果**
Effect of Membrane Potential on the Translocation of Cell-Penetrating Peptide Transportan 10 (TP10) across Lipid Bilayers

Md Mizanur Moghal[1], Md. Zahidul Islam[1], Sharmin Sabrina[1], Masahito Yamazaki[1,2,3] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Res. Inst. Ele., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

To elucidate the mechanism of the translocation of cell-penetrating peptide, TP10 across lipid bilayers, we investigated the effect of the membrane potential on the entry of fluorescent probe-labeled TP10 (CF-TP10) into single DOPG/DOPC-GUVs using the method developed by us (1,2). Various membrane potential were applied to GUV membranes using the K+ concentration gradient, which was confirmed by the potential sensitive-fluorescence probe. The rate of entry of CF-TP10 into the GUV lumen before leakage of AF647, i.e., pore formation, increased with an increase in membrane potential. We discuss the effects of membrane potential on the elementary processes of the entry of CF-TP10 into single GUVs.
(1)Biochemistry, 53, 586, 2014, (2) Langmuir, 33, 2433, 2017

1Pos132 **コリネ型バクテリアの機械受容チャネル MscCG の C 末端構造による開閉機構の制御**
Modulation of gating MscCG, the mechanosensitive channel of Corynebacterium glutamicum, by the C-terminal domain

Yoshitaka Nakayama[1], Michael Becker[2], Haleh Ebrahimian[3], Tomoyuki Konishi[4], Hisashi Kawasaki[4], Reinhard Kramer[2], Boris Martinac[1,5] ([1]*Victor Chang Cardiac Research Institute*, [2]*University of Cologne*, [3]*Wollongong University*, [4]*Tokyo Denki University*, [5]*University of New South Wales*)

The mechanosensitive channel MscCG from Corynebacterium glutamicum exports glutamate when membrane tension is increased. To understand the function of MscCG, we investigated functional properties of the chimeric channel MscS-CtMscCG, a fusion protein between the E. coli mechanosensitive channel MscS and the C-terminal domain of MscCG, using a patch-clamp recording from E. coli giant spheroplasts and proteoliposomes. We found that the C-terminal domain of MscCG altered the activation threshold and gating kinetics of MscS. Moreover, the chimeric channel showed strong gating hysteresis at physiological membrane potentials. These results suggest that the role of the C-terminal domain of MscCG consists in adjusting the gating of MscCG for continuous release of glutamate.

1Pos133 N 末端変異リアノジン受容体における分子動力学計算法とカルシウムシグナルの相関解析

Correlation of molecular dynamics analysis and Calcium dynamics in mutant type 1 ryanodine receptors

Toshiko Yamazawa[1], Takashi Murayama[2], Maki Yamaguchi[1], Hideto Oyamada[3], Nagomi Kurebayashi[2], Junji Suzuki[4], Kazunori Kanemaru[4], Takashi Sakurai[2], Masamitsu Iino[4,5] ([1]*Dept Mol. Physiol., Jikei Univ. Sch. Med.*, [2]*Dept. Pharmacol., Juntendo Univ. Sch. Med.*, [3]*Dept. Pharmacol., Sch. Med., Showa Univ.*, [4]*Dept. Pharmacol., Grad. Sch. Med., The Univ. Tokyo*, [5]*Dept. Cell. Mol. Pharmacol., Nihon Univ. Sch. Med.*)

We investigated properties of the type 1 ryanodine receptor (RyR1) channels carrying disease-associated mutations at the N-terminal region. HEK293 cells expressing the mutant RyR1 channels exhibited alterations in Ca^{2+} homeostasis, i.e., enhanced caffeine sensitivity, Malignant hyperthermia (MH) decrease of ER Ca^{2+} contents, increases in resting cytoplasmic Ca^{2+} concentration. Molecular dynamics analysis revealed that changes in pattern of electrostatic interaction were correlated with the alteration in Ca^{2+} homeostasis. This result suggests that exploration of the functional mutations of RyR1 is effective in preventive diagnosis of patients associated with MH disease.

1Pos134 哺乳類 2 ポアドメインカリウムチャネル TWIK-1 の機能特性と機能制御メカニズムの解析

Functional properties and the regulating mechanisms of a mammalian two-pore domain potassium channel TWIK-1

Hisao Tsukamoto[1], Koichi Nakajo[2,3], Yoshihiro Kubo[3], Yuji Furutani[1] ([1]*Institute for Molecular Science*, [2]*Osaka Medical College*, [3]*National Institute for Physiological Sciences*)

Unlike other K^+ channels, a mammalian two-pore domain K^+ channel TWIK-1 can conduct Na^+. Whereas previous electrophysiological analyses showed that Thr-118 in the selectivity filter is responsible for the unique ion selectivity, TWIK-1 possesses an almost identical filter shape to other K^+ channels in their crystal structures. In this study, we assessed the functional properties of TWIK1 using purified proteins. Purified TWIK-1 also showed lower ion selectivity than the Thr-118 mutant. Furthermore, we applied ATR-FTIR spectroscopy to TWIK-1 and found that the Thr-118 lowers affinity of the filter for K^+ relative to Na^+. Based on the biochemical and spectroscopic data, we will discuss how ion selectivity is regulated in TWIK-1.

1Pos135 イオンチャネル電流測定の自動化

Automated system for channel current measuremen

Minako Hirano[1], Nobuyuki Kawashima[2], Masahisa Tomita[2], Toru Ide[3] ([1]*GPI*, [2]*SYSTEC Corporation*, [3]*Grad. Schl Sci. Tech. Okayama Univ.*)

We have developed an automated system to form a lipid bilayer membrane containing ion channels, which is based on a simple technique we previously developed. This system consists of a driving device for forming the bilayer membrane and ionic current-detecting system, and ion channels are automatically inserted the membrane. By using the system, we easily made the bilayer membrane with channels and automatically measured currents from several types of ion channels such as K^+ channels. This system makes it possible to increase the measurement efficiency of channel's activities.

1Pos136 電位依存性ホスファターゼ VSP の疎水的な膜相互作用部位の重要性

The critical role of the hydrophobic membrane interacting region in voltage-sensing phosphatase (VSP)

Akira Kawanabe[1], Masaki Hashimoto[1], Tomoko Yonezawa[1], Yuka Jinno[1], Souhei Sakata[2], Yasushi Okamura[1] ([1]*Grad. Sch. Med., Osaka Univ.*, [2]*Fac. Med., Osaka Med. Col.*)

Voltage-sensing phosphatase (VSP) consists of a transmembrane voltage sensor domain and a phosphatase domain, which dephospholyrates $PI(4,5)P_2$ regulated by membrane potential (Murata et al. 2005). Previous our studies showed the mutations of the hydrophobic membrane interacting region in the phosphatase domain (L284 and F285) affected the phosphatase activity of Ci-VSP.
In this study, we attempted to detect voltage dependent conformational changes in phosphatase domain by the genetic incorporation of a fluorescent unnatural amino acid, Anap. Results suggest that VSP has two or more enzyme active states, which are regulated by hydrophobic nature of the side chain of the membrane interacting region. COI:No

1Pos137 KcsA チャネルからのイオンの自発的流出

Spontaneous exits of ions from the KcsA channel

Takashi Sumikama, Shigetoshi Oiki (*Univ of Fukui*)

The ratio of water flux over ion flux through the KcsA channel was experimentally measured. The ratio was one at the physiological concentration and increased when the concentration decreases. Here, we investigated the molecular mechanism that determines this concentration dependence using the molecular dynamics simulation. It was found that the ratio was one, when the ions in the channel start moving when the next ion enters the channel. On the other hand, when the concentration decreases, in contrary to the well-known knock-on mechanism, the ions in the channel spontaneously exit from the channel before knocking of the next ion, leaving a space for water molecules to fill in. Thus, this spontaneous exit was found to be necessary to explain the increase in the ratio.

1Pos138 Single channel recordings of ion channels immobilized on a solid substrate

Toru Ide[1,2], Masahiro Yamakami[1], Minako Hirano[2], Hiroaki Yokota[2], Junya Ichinose[1] ([1]*Grad Schl Nat Sci Tech, Okayama Univ*, [2]*GPI*)

The artificial bilayer single channel recording technique is commonly used to observe detailed biophysical properties of ion channel proteins. It permits easy control of the experimental conditions such as the solution and membrane lipid composition. However, its use is limited due to a low measurement efficiency. We reported a novel artificial bilayer technique in which bilayers are made and channels are reconstituted into the membranes by contacting a gold electrode to a lipid-solution interface. Here we improve this technique and measure the single channel currents of several types of channel including P2X4 and BK, which were immobilized on the tip of the gold electrode. This technique requires only one simple action, increasing measurement efficiency very much.

1Pos139　A simple method for promoting liposome-bilayer fusion

Kohei Miyatani[1], Minako Hirano[2], Toru Ide[1] ([1]*Okayama Univ*, [2]*GPI*)

The artificial bilayer single channel recording technique is a powerful tool to study biophysical and pharmacological properties of ion channel proteins. However, the measurement efficiency of this technique is low because an incorporation of channel proteins into the bilayer requires commonly a certain amount of time. The popular method for incorporation, liposome fusion, is one of the rate-limiting steps for a successful experiment. Here we develop a method to promote vesicle fusion by encapsulating a magnetic bead in liposomes. A magnet on the other side of the membrane attracts the liposomes to promote the liposome-bilayer fusion. Using this method, we successfully promoted the fusion, measuring ionic current of several types of channel protein.

1Pos140　Characterization of the channel pore formed by Cry46Ab toxin from soil bacterium Bacillus thuringiensis

Akira Sakakibara[1], Tohru Hayakawa[1], So Takebe[2], Toru Ide[1] ([1]*Univ. Okayama*, [2]*Kindai Univ.*)

Cry46Ab derived from Bacillus thuringiensis TK-E6 is a new member of mosquitocidal toxin, and is not homologous to previously reported mosquitocidal toxins (Cry or Cyt toxins). Based on its structural similarity, Cry46Ab is classified as an aerolysin-type pore-forming toxin. In this study, we examined the ability of Cry46Ab to permeabilize an artificial lipid bilayer. Single-channel analysis revealed current transitions between open and closed states similar to typical ion channels, and the single-channel conductance in 150 mM KCl, NaCl and CaCl2 were 103, 32 and 24 pS, respectively. Here, we discuss about characteristics of the channel-like pore formed by Cry46Ab. Our study can be a milestone to evaluate the usability of Cry46Ab as novel bio-insecticide.

1Pos141　ミトコンドリア凝集に伴う表面ｐ H の変化の計算
Calculation of surface pH change of mitochondria due to aggregation

Takuya Takahashi[1], Kota Kasahara[1], Yoshihiro Ohta[2] ([1]*Dept. of Biosci. and Bioinformatics, Ritsumeikan Univ.*, [2]*Div. of Biotech. and Life Sci., Inst. of Eng., Tokyo Univ. of Agr. and Tech.*)

Distribution of mitochondria, which produce ATP and reactive oxygen species, are not uniform in cells. Previous studies revealed the effect of close location of mitochondria on their activities. That is, when the isolated mitochondria from porcine heart were adsorbed on dishes, the ATP production rate significantly increased with the density of mitochondria adsorbed on a dish. In this study, we calculated the change of the electrostatic potential and pH distribution around mitochondria due to aggregation and found the correlation between surface electrostatic potential and the density of mitochondria. To reproduce the function of mitochondria more quantitatively, detailed calculation conditions are investigated.

1Pos142　反転膜を用いたべん毛 III 型蛋白質輸送の定量測定
Quantitative analysis of the flagellar type III protein export using the inverted membrane vesicles

Tsuyoshi Tono[1], Hiroyuki Terashima[1,2], Kazuhito Tabata[3], Hiroshi Ueno[3], Hiroyuki Noji[3], Katsumi Imada[1] ([1]*Grad. Sch. of Sci., Osaka Univ.*, [2]*Grad. Sch. of Sci., Nagoya Univ.*, [3]*Sch of Eng., Univ. of Tokyo*)

The flagellar protein export apparatus is a protein transporter used for the bacterial flagellar construction. The protein transport is driven by proton motive force, but ATP hydrolysis energy is further needed for efficient transport. To understand the molecular mechanism of protein transport, we are developing an in vitro transport assay system using inverted membrane vesicles (IMVs) for quantitative analysis. Transport of fluorescent-labeled substrate proteins has detected using TIRF or confocal microscopy. Using this technique, we found ATP-dependent increase of fluorescence even for the IMVs prepared from a transport-defective mutant cells, suggesting a part of ATP hydrolysis energy may be utilized to accumulate the substrates near the export apparatus.

1Pos143　シグナルペプチド配列のバリエーションと細胞内局在に関する考察
Sequence variation of signal-peptides and protein subcellular localization

Tomonao Iibuchi, Tatsuki Kikegawa, Keiya Inoue, Naoyuki Takachio, Kenji Etchuya, Yuri Mukai (*Dept. Electronics, Grad. Sch. Sci. & Tech., Meiji Univ.*)

Proteins are localized to particular organelles in order to carry out their biological functions. Signal-peptide is known as a localization signal which transport biosynthesized proteins to the endoplasmic reticulum. However, the reason why there is the diversity in the sequence length, hydropathy and amino acid propensity in signal-peptide is unclear.
In this study, the subcellular localization of GFP and mCherry chimeric proteins expressed in HeLa cells which have different signal-peptides respectively, was observed by confocal laser microscopy.

1Pos144　浸透圧がミトコンドリアの活性に及ぼす影響
Effects of osmolality on mitochondrial activities

Sawako Kimura, Yoshihiro Ohta (*Tokyo University of Agriculture and Technology*)

Reactive oxygen species (ROS) are mainly generated in mitochondria and act as signal molecules. Once excessively generated, ROS are known to induce cellular damages. Therefore, adequate control of ROS generation is necessary for cells. So far, we have observed that mitochondria produce more ROS in the buffer with higher osmolality. The aim of this study is to examine the mechanism by which higher osmolality of the buffer leads to more ROS generation in mitochondria. For this purpose, we isolated mitochondria from porcine hearts and changed the osmolality of the buffer surrounding mitochondria. The effects of osmolality on mitochondrial activities and ROS generation were examined. The detailed conditions and results of the measurements will be discussed.

1Pos145 基質存在下・非存在下での多剤排出輸送体 AcrAB-TolC の細胞内動態解析

Analysis of the in cell dynamics of a multi-drug exporter AcrB in the absenc e and presence of substrates

Tomoki Matsuda, Seiji Yamasaki, Kunihiko Nishino, Takeharu Nagai, Akihito Yamaguchi (*ISIR, Osaka Univ*)

We analyzed diffusion of AcrB on the plasma membrane of living *E. coli* cells by FDAP (fluorescence decay after photoconversion) analysis. In the case where small size substrates that are bound at the distal pocket in the crystal structures were added, the diffusion speed was similar to that in the absence of substrate. On the other hand, diffusion is decelerated when large size substrates that bound at the proximal pocket is added. Introduction of mutations into AcrB to disturb transport of proximal binding substrates eliminated this substratedepended deceleration. These results suggest that some fraction of AcrB formed AcrAB-TolC complex without substrates and the complex formation is more stabilized when proximal binding larger substrates are added.

1Pos146 ERK 情報処理過程の共焦点局所画像を用いた定量解析

Quantitative measurement for information processing of ERK using localized confocal image analyses

Kazunari Mouri[1], Yasushi Okada[1,2] ([1]*RIKEN, QBiC*, [2]*Univ. Tokyo, Grad. Sch. Sci., Dept. Phys*)

The accuracy and basic principles of cellular information processing are still unknown, but important for understanding computation techniques of molecules. The quantitative measurements of input-output relations for ERK phosphorylation and translocation are difficult, because the in/output signals can be a function of concentration, on/off rates, and diffusion coefficients of ERK. To derive this, we developed a new FCS, where we can calculate the auto/cross-correlation functions using line images of confocal microscopy aided with hybrid detector, resonant scanner, and wavelet analyses. We found that ERK translocation was not diffusion-limited but transport-limited. These are essential for revealing systems level architecture of information processing.

1Pos147 In vitro 1 分子イメージングによる PTEN-PI(4,5)P2 相互作用の解析

In vitro single molecule-imaging analysis of interactions between PTEN and phosphatidylinositol 4, 5-bisphosphate

Daisuke Yoshioka[1,3], Seiya Fukushima[1,3], Daichi Okuno[3], Satomi Matsuoka[3], Toru Ide[4], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. of Sci., Osaka Univ.*, [2]*Grad. Sch. of Front. Biosci., Osaka Univ.*, [3]*RIKEN QBiC*, [4]*Grad. Sch. of Nat. Sci. and Tech., Okayama Univ.*)

PTEN, a 3-phosphatase of PI(3,4,5)P3, is a peripheral membrane protein undergoing the shuttling between cytoplasm and cell membrane. PTEN is localized on posterior membrane in a polarized cell, which is essential factor for cellular polarization. To clarify the mechanisms of the interaction between PTEN and membrane, we have developed in vitro assay system for single-molecule analysis on artificial lipid bilayers. Both membrane recruitment and binding stability of PTEN increased with PI(4,5)P2. The results suggest a positive feedback mechanism for PTEN membrane binding, in which its enzymatic product PI(4,5)P2 enhances the membrane localization of PTEN. We will discuss the possible contribution of PTEN-PI(4,5)P2 interaction to cell polarity and efficient cell migration.

1Pos148 MCF7 細胞内における p52shc の細胞膜移行ダイナミクス計測

p52SHC translocation to the plasma membrane of MCF7 cells

Ryo Yoshizawa[1,2], Nobuhisa Umeki[2], Masataka Yanagawa[2], Masayuki Murata[1], Yasushi Sako[2] ([1]*Grad. Sch. Arts and Shi., Univ. Tokyo*, [2]*Wako Inst., RIKEN*)

SHC proteins are downstream targets of the ErbB receptors (ErbB1-B4). Here, to understand the mechanism of ErbB signaling to p52SHC, a subtype of SHC, we measured translocation dynamics of p52SHC tagged with fluorescent protein (SHC) in living MCF7 cells. Stimulation of wild type MCF7 cells with heregulin (HRG) induced a sustained translocation of SHC from the cytoplasm to the plasma membrane for at least 60 min. In contrast, in ErbB1 overexpressed cells, SHC translocation was transient, suggesting that ErbB1 acts as a negative regulator of the sustained localization of SHC on the plasma membrane. Since HRG is the ligand of ErbB3/ErbB4 but not ErbB1, we assume that hetero-oligomerization between ErbB1 and ErbB3/ErbB4 is involved in this negative regulation.

1Pos149 A single EGF molecule is sufficient to activate a preformed EGFR dimer

Ei-ichiro Saita, Dingze Mang, Ichiro N. Maruyama (*OIST*)

Despite of extensive studies for decades, the molecular mechanism of EGFR activation induced by ligand (e.g. EGF) binding is still controversial. To address this question, we directory visualized interaction among EGFR, EGF labeled with two different fluorescent compounds, and GFP-tagged Shc1, by using a multi-color TIRF microscope. Within 30 sec of application of the dye-conjugated EGF to cultured cells, three-color fluorescent spots of EGF and Shc1 appeared on the cell surface. Unexpectedly, two different fluorescent colors derived from EGF do not co-localize, and instead, single-colored EGF binding induces Shc1 recruitment to EGFR. These results suggest that binding of single EGF molecule can activate preformed EGFR dimer.

1Pos150 コレラ菌タウリン走性受容体 Mlp37 遺伝子の温度による発現制御

Temperature-regulated expression of the gene encoding the taurine chemoreceptor Mlp37 of *Vibrio cholerae*

Shiori Onogi[1], Noriaki Sagoshi[1], So-ichiro Nishiyama[1,2], Yoshiyuki Sowa[1,2], **Ikuro Kawagishi**[1,2] ([1]*Dept. Frontier Biosci., Hosei Univ.*, [2]*Res. Cen. Micro-Nano. Tech., Hosei Univ.*)

Vibrio cholerae, the etiological agent of cholera, shows chemotaxis, which has been implicated in pathogenicity. We recently reported that the bacterium is attracted strongly by taurine at 37C but not at lower temperature. In this study, we found that the gene encoding the taurine chemoreceptor Mlp37 is regulated in response to culture temperature at the level of transcriptional initiation. Forced expression of the *mlp37* gene from the foreign promoter abolished the temperature dependence of taurine taxis. Furthermore, the *mlp37* expression was negatively regulated by the transcription factor ToxR, which is required for the expression of genes encoding cholera toxin and other virulence factors, suggesting the inverse correlation between taurine taxis and pathogenicity.

1Pos151 サルモネラ属細菌クエン酸走性受容体 Tcp のリガンド認識における 2 価金属イオンの役割

Role of divalent metal cations in ligand recognition by the citrate chemoreceptor Tcp of *Salmonella enterica*

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The chemoreceptor Tcp of *Salmonella enterica* is unique in that it mediates attractant responses not only to citrate but also to divalent metal cations in the presence of citrate but not in its absence. Tcp is therefore supposed to sense citrate and metal-citrate complexes as distinct attractants. In this study, we first determined the crystal structure of a periplasmic fragment of Tcp. In each ligand-binding pocket of the Tcp homodimer, a Zn^{2+} ion was accommodated with a citrate molecule. We then carried out ligand-binding assay. ITC measurements demonstrated that the Tcp fragment binds citrate in the presence of Mg^{2+}, but not in its absence. Based on these results, we propose a new model of ligand recognition by Tcp with the emphasis in the role of a metal ion.

1Pos152 ヒト人工多能性幹細胞由来の内胚葉及び中胚葉細胞により模倣されるヒト原腸形成期の細胞運動

Cell Migration in the Human Gastrulation Stage Mimicked by Endoderm and Mesoderm Derived from Human Induced Pluripotent Stem Cells

Kenshiro Maruyama, Shota Miyazaki, Kiyoshi Ohnuma (*Grad. Sch. Eng., Univ. Nagaoka Tech.*)

Gastrulation is the initial systematic deformation of embryo, hence is a critical stage for forming human body. Although the morphology of human gastrulation is known to follow the pattern observed in birds, the dynamics are unknown because of ethical and technical limitations. Here we utilized human induced pluripotent stem cells (hiPSCs) to study cell dynamics during human gastrulation stage in vitro. We induced differentiation to mesoderm and endoderm cells from hiPSCs to analyze cell movement by single-cell monolayer time-lapse imaging. At the early stage of differentiation, cell movement in mesendoderm was fast and random. We will report the difference of movement in mesoderm and endoderm specification.

1Pos153 形態形成における集団運動を制御する細胞間シグナル伝達の動態の変遷

Transition of the dynamics of cell-cell communication controlling collective cell migration during morphogenesis of Dictyostelium cells

Hidenori Hashimura[1,2], Masato Yasui[1], Yusuke Morimoto[1,3], Masahiro Ueda[1,2,4] ([1]*RIKEN QBiC*, [2]*Dep. Biol. Sci., Grad. Sch. of Sci., Osaka Univ.*, [3]*Dept. of Biosci. Bioinfo., Kyushu Inst. Tech.*, [4]*Grad. Sch. of Front. Biosci., Osaka Univ.*)

Cell-cell communication plays essential roles in coordinating collective cell movement. The social amoebae Dictyostelium discoideum cells aggregate and form migrating multicellular bodies on starvation. The collective cell motion during aggregation is controlled by intercellular signaling called cAMP relay, but its roles in the morphogenesis of multicellular bodies is still unclear. To investigate the relationship between cAMP relay and collective cell migration in the multicellular stage, we monitored the cell velocity and intracellular signal changes depending on cAMP relay simultaneously during the formation of multicellular bodies. We will report the transition of cAMP relay among cell populations during morphogenesis.

1Pos154 Mechanics of the Nucleus and Cell Body during Early Mouse Development with Implications for Reproductive Medicine

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Mammalian development is an intriguing process starting from a single fertilized egg to a complete embryo. Experimental data regarding the micromechanical principles governing morphogenesis during early mammalian development remain largely unknown. A newly developed 'feedback-controlled microrheology' method makes it feasible to measure the mechanics of the cells' interior. The aim of this study is to characterize the mechanics of the nucleus and cell body of undifferentiated embryonic stem cells, and differentiated trophectoderm and primitive endoderm cells derived from them in vitro by using feedback-controlled microrheology. This study will give a better understanding of processes such as assisted reproductive strategies including in vitro fertilization.

1Pos155 高時間分解・長時間撮影による、線虫 *C.elegans* の原腸貫入運動の解析

Particle tracking analysis of gastrulation in C. elegans embryos

Yukinobu Arata[1], Yuki Shindo[1], Hiroaki Takagi[2], Yashushi Sako[1] ([1]*Cell. Info., RIKEN*, [2]*Dept. of Phys. Nara Med. Univ.*)

Gastrulation is a process to generate the digestive tract in animal development. In 26-cell stage of *C. elegans* embryos, two primordial endodermal cells ingress into the center of embryo, and eventually the two cells form the intestinal tube. Ingression is thought to be achieved by constricting the apical surface of the endodermal cells via act-myosin system. However, it remains unknown how the other cells in the embryo cooperate for the gastrulation movement. Here, we analyzed the movement of cell cortex by particle tracking analysis on the movies recorded at high spatio-temporal resolution. Interestingly, cell cortex rotated around the center of cortex of each cell. We propose a new model, in which endodermal cells ingress by coordinating rotation and adhesion.

1Pos156 高速三次元光シート顕微鏡によるマウス胚ノード流の三次元解析

Three-dimensional analysis of the nodal flow in the mouse embryo by the rapid 3-D light-sheet microscopy

Atsushi Taniguchi, Shigenori Nonaka (*Spatiotemp. Reg., Natl. Inst. Basic Biol.*)

In mammalian development, cilia-driven fluid flow at the node toward the left (nodal flow) is critical for the establishment of left-right asymmetry, leaving the flow-sensing mechanism in question. One of the major hypotheses proposes that the cilia work as mechanosensor in addition to as flow generator, and detect difference of the flow velocity that is claimed to be faster at the left side of the node than the right. To test this hypothesis, measurement of 3D flow distribution at the node is inevitable. We constructed an ultrafast light-sheet microscope that enables data acquisition at ~10 volume/sec, and visualized the nodal flow of mouse embryos by 0.2 μm microbeads added into the medium. Preliminary data analysis will be presented in the meeting.

1Pos157 上皮組織変形の連続体モデル
Continuum model of epithelial mechanics

Shuji Ishihara[1], Marcq Philippe[2], Kaoru Sugimura[3] ([1]*Grad. Sch. Arts. Sci., Univ. Tokyo*, [2]*Inst. Curie, Univesite Paris 6*, [3]*iCeMS, Kyoto Univ.*)

During tissue morphogenesis, cells proliferate, die, deform, and move to shape a tissue. We previously developed experimental methods to quantify deformation, velocity, and stress fields in a developing tissue. Here, we present a new continuum model of epithelial mechanics, which includes internal variables representing cell shape and cell rearrangement. The model can describe the link between tissue-level mechanics and deformation and cellular-level morphogenetic processes and mechanical determinants, such as cell-junction tension and cell area elasticity. Further, the model can incorporate cellular activities, by which we found a novel mechanism of contraction-elongation whereby tissue flow occurs perpendicularly to the direction of cell elongation.

1Pos158 in vitro でのヒト原腸形成期における細胞運動に対する細胞間相互作用の影響
The effects of cell-cell interaction on the cell dynamics during human gastrulation in vitro

Shota Miyazaki, Kenshiro Maruyama, Gen Kato, Tohru Sasaki, Kiyoshi Ohnuma (*Grad. Sch. Eng., Univ. Nagaoka Tech.*)

The dynamics of human embryogenesis are unknown because of ethical and technical limitations. Human pluripotent stem (iPS) cells are useful model cells to study human embryogenesis, because iPS cells can differentiate into all types of cells, are easy to control, and are easy to observe (monolayer culture). We focused on the dynamics of gastrulation, which is the initial systematic deformation of embryo to form germ layers. A random walk analysis of time-lapse images of dispersed single cells showed that the migration modes of mesendodermal cells (future gut) are random, which might be suitable for forming a homogeneous cell layer of future gut of human. This year, we will present cell dynamics in the colony, where the cell-cell interaction are strong as in vivo.

1Pos159 カエルの神経筋伝達の短期間シナプス可塑性におけるドッキングタンパク質の新たな役割
Novel Distinctive Roles of Docking Proteins in Short-term Synaptic Plasticity of Frog Neuromuscular Transmission

Yasuhiro Imafuku[1], Koh-ichi Enomoto[2], Hiroko Kataoka[2], Isao Ito[1], Takashi Maeno[3] ([1]*Dept Biol., Kyushu Univ.*, [2]*Shimane Univ.*, [3]*Prof. Emeritus, Shimane Med. Univ.*)

Short-term synaptic plasticity (SSP) is a basic mechanism for temporal processing of neural information in synaptic transmission. Using Botulinum neurotoxins A and C (BoNT-A and -C), we investigated roles of SNAP-25 and syntaxin, docking proteins exclusively participating in the vesicular events composed of docking, priming and exocytosis. We found that truncations of SNAP-25 and syntaxin by BoNT-A and -C respectively suppressed potentiation and augmentation, slow and intermediate components of the synaptic plasticity, and that double poisoning with BoNT-A and -C gave rise to unprecedented biphasic postsynaptic response. We conclude that SNAP-25 and syntaxin not only play passive roles as the cooperative exocytotic machinery, but also have active roles in the SSP.

1Pos160 海馬神経シナプスを制御する神経ステロイドの non-genomic 信号系
Non-genomic signaling of neurosreroids, regulating synapses in the hippocampus

Suguru Kawato[1,2] ([1]*Dep. Cognitive Neuroscience, Pharma-Science, Teikyo Univ.*, [2]*Dep. Urology, Grad Sch Medicine, Juntendo Univ.*)

Rapid action of neurosteroids (sex steroids) has been extensively studied in the brain over more than decades, and a significant progress has been achieved in clarification of essential molecular mechanisms.
We here describe synaptic (classic) sex steroid receptors which trigger rapid modulation of dendritic spinogenesis in rat hippocampal slices, including estradiol (E2), progesterone (PROG), dihydrotestosterone (DHT) and testosterone (T). We then describe the role of kinase-dependent signaling mechanisms which can well explain non-genomic modulation of dendritic spinogenesis by sex-steroids.

1Pos161 微小管の物理的特性に与える MAPs の影響
Influence of microtubule-associated proteins on the physical properties of microtubules

Miki Tamura[1], Kazufumi Matsui[1], Miyuki Siga[1], Kabir Arif Md. Rashedul[2], Akira Kakugo[2], Susumu Kotani[3], Kiyotaka Tokuraku[1] ([1]*Div. Sust. Env. Eng., Muroran Inst. Tech.*, [2]*Fac. Sci., Hokkaido Univ.*, [3]*Fac. Sci, Kanagawa Univ.*)

Structural microtubule-associated proteins (MAPs) bind to the surface of microtubules (MT), stimulate MT assembly, and stabilize formed MT. In this study, we examined the effects of microtubule-binding domain (MBD) of the structural MAPs on physical properties of microtubules. Fluorescence microscopic observation showed that the MBD fragments of MAP2 and MAP4 induced wavy MT bundles. In contrast, the MBD fragment of tau induces straight MT bundles. These different properties of MT may be involved in the development of cell processes such as dendrites and axons of neurons. In this study, we further analyzed the mechanical properties of MT bound MBD fragments of MAPs by mechanical deformation test. The results suggested that MAPs affected mechanical strength of MT.

1Pos162 神経細胞における細胞骨格アクチンの修復の分子メカニズム
Molecular Mechanism of Cytoskeletal Actin Repairing in Nerve Cells

Tomoya Higo[1], Takuo Yasunaga[2], Shinji Aramaki[3] ([1]*Kyushu Institute of Technology*, [2]*Kyushu Institute of Technology*, [3]*Tvips GmbH*)

Recent researches in neuroscience have shown that broken nerve cell has potentials to repair. Also, electron microscopy has been developed to observe cell structure under the physiological conditions.
We photographed the tips of the filopodia by cryo-electron microscopy. We found out that the tips have two types of shapes. One is round, the other is sharp. In the former, there was no actin filament to be seen, and, in the latter, actin filament could be seen. Thus, we supposed that the shape of the tip should depend on actin filaments, or the presence of actin filaments should rely on the tip shape, i.e., the elongation and shrinkage of filopodia might be related to the tip structure. We will observe filopodial structure by correlative light and 3D electron microscopy.

1Pos163　演題取り消し

1Pos164　チャコウラナメクジの匂い味覚条件付け学習における記憶形成に対するエピカテキンの影響

Epicatechin enhances the long-term memory of odor aversive learning in the land slug

Yoshimasa Komatsuzaki[1,2], Taiyou Nakamura[1], Ken Lukowiak[2], Minoru Saito[3] ([1]*Dept. of Phys., CST, Nihon Univ.*, [2]*Hotchkiss Brain Inst, Cumming Sch of Med, Univ of Calgary, Canada*, [3]*Dept. of Biosci., CHS, Nihon Univ.*)

Epicatechin (epi), a food-derived flavonoid, has been known as an enhancing factor of memory formation in molluscs. Here we investigated the effect of epi on long-term memory formation of an odor aversive learning in the land slug, Limax valentianus. When slugs were preexposed to 15 μg/g of epi 1 h prior to the odor aversive training, which typically results in memory lasting ~3 days, they formed LTM lasting at least 1 week. The procerebrum (PC) of the land slug is a central nervous system for odor processing and learning. The PC shows an oscillatory local field potential at about 0.7 Hz, which is modulated by conditioned odor stimuli. We studied at the level of neural activities in the PC how epi lead to the enhancing effects of the memory formation.

1Pos165　Structure of the Neuron-to-Neuron Network of Drosophila Connectome

Chi-Tin Shih (*Tunghai University*)

We constructed the neuron-to-neuron network of the Drosophila brain from 28,573 single neuron images. By performing the complex network analysis on this network, key neurons in information exchange and structural stability were identified from several types of centrality measurements. Eight communities were detected and identified as right/left olfaction, olfactory core, auditory, motor, pre-motor, and right/left vision. We found overall small-worldness for the Drosophila brain network but with some degree of inter-community diversity. Olfaction and the motor communities are not small world, whereas the rest five are. Abundant loops with length smaller than seven neurons were detected, suggesting unique characteristics in the information processing inside the brain.

1Pos166　神経細胞ネットワークの 1 細胞レベル自発発火を解析する拡張型コンパクトオンチップ細胞外電位計測技術の開発

Extracellular electrophysiological measurement of spontaneous firing of single neurons in neuronal circuit using expandable on-chip assay

Shota Aoki[1], Takahito Kikuchi[2], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Masao Odaka[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., WASEDA Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*)

We have developed a new four-channel module-type single cell external field potential measurement system for analyzing of long-term neuronal network functioning. The advantages of the system are; (1) compactness, the measurement and A/D conversion unit is small enough to set on the stage of microscopes, (2) flexible expansion, measurement channels can be expanded flexibly by adding the A/D module blocks as many as needed, (3) simultaneous measurement/stimulation ability of each channel, and (4) flexible design of neuronal network patterns by combining with the agarose microfabrication technology. Using this system, we have examined the reaction of stimulation of neurons and succeeded in the measurement of firing of single neurons.

1Pos167　オンチップ 1 細胞培養系を用いた神経細胞から伸長する神経突起の特性の解析

Neurite elongation characteristics in the width-controlled channels using an in situ on-chip photothermal microfabrication assay

Takahito Kikuchi[1], Shota Aoki[2], Hideyuki Terazono[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Masao Odaka[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*Waseda Biosci. Res. Ins. in Singapore (WABIOS)*)

For understanding the relationship between the neurite elongation and its differentiation, we examined the neurite elongation characteristics in the width-controlled channels using an in situ photothermal microfabrication assay. First, we fabricated width-controlled microchannels in an agarose thin layer on a cultivation dish with a focused 1064/1480-nm dual infrared laser; then, the single neuron was cultivated in each microchannel; and, neurite elongation was measured by a phase-contrast microscope with image analyzer. In 3 μm in width, 19% of neurites were elongated longer than 100 μm, whereas in 12 μm in width, 71% were elongated. The results indicate the existence of minimum microchannel width for steady neurite extension.

1Pos168　カエル神経筋接合部シナプスにおける促通 2 成分間の数学的関係性の解明：加算的なのか積算的なのか和のベキ的関係なのか

What mathematical relationship of two components of facilitation at the frog NMJ: Additive, multiplicative, or power of summation ?

Naoya Suzuki, Junpei Yamaguchi (*Dept. Phys., Grad. Sch. Sci., Nagoya Univ.*)

To investigate the mechanism of stimulation induced enhancement of transmitter release, we analyzed a type of short-term synaptic plasticity, facilitation, quantitatively using several mathematical relationships of fast and slow component of facilitation. Facilitation was induced by single or double (with an interval of 200 msec) train of 8 stimuli at 100 Hz. According to the mathematical model described by Zengel and Magleby, facilitation during train of stimuli was reconstructed using parameters obtained by the fitting of its decay process. Additive model failed to reproduce the observed data. Multiplicative model and 2nd power model reproduced the observed data almost well. Higher power model, 3rd and 4th power, gradually reproduced the observed data less well.

1Pos169 線虫の whole-brain イメージングデータに関する因果性解析
Causality analysis on whole-brain imaging data of C. elegans

Yuishi Iwasaki[1,7], Takayuki Teramoto[2,7], Suzu Oe[2,7], Terumasa Tokunaga[3,7], Osamu Hirose[4,7], Stephen Wu[5,7], Yu Toyoshima[6,7], Moon Sun Jang[6,7], Ryo Yoshida[5,7], Yuichi Iino[6,7], Takeshi Ishihara[2,7] ([1]*Fac. Eng., Ibaraki Univ.*, [2]*Grad. Sch. Sci., Kyushu Univ.*, [3]*Grad. Sch. Comp. Sci. and Sys. Eng., Kyushu Institute Tech.*, [4]*Institute. Sci. and Eng., Kanazawa Univ.*, [5]*Institute Stat. Math.*, [6]*Grad. Sch. Sci., Univ. Tokyo*, [7]*JST, CREST*)

We study causality between each pair of time series in the whole-brain imaging data of C. elegans. Neuronal activities in the whole central nervous system were measured by our 4D calcium imaging system. Causality is determined by two well-known methods; the Granger causality test and the transfer entropy. The Granger causality test quantifies "predictability" between two processes on the basis of statistical hypothesis test using the auto-regression model. On the other hand, the transfer entropy quantifies "information flow" on the basis of information theory. Both methods find directional influence between two processes; whether influence, if it exists, is one-way or bi-directional. The results are compared with the identified synaptic pathway in C. elegans.

1Pos170 ニワトリ胚由来の神経細胞から伸長する軸索の制御
Control of axon elongation of neuron derived from chicken embryos

Hayato Toriumi, Tomoyuki Kaneko (*LaRC, FB, Hosei Univ.*)

Recently, axon guidance is focused on the various field such as artificial neural network. To investigate possibilities of controling the axon in vitro, we measured the velocity of axon elongation from arranged neuron cell and tried to control axon with agarose microchamber by infrared laser system. As a result, agarose microchamber enabled us to arrange the axon linearly and found slight dynamics of the axon like a dynamic instability of microtubule. Howeve, It was difficult to change the direction of axon elongation in progress of the elongation in the conditions. Since neural network composed of the axon connection was communicated with membrane potential, we expected that electric stimulation might be effective to control it more closely.

1Pos171 集光フェムト秒レーザーによる単一神経細胞の光刺激メカニズム
Stimulation Mechanisms in Living Neuronal Cells with a Focused Femtosecond Laser

Yuji Fujioka[1,2], Suguru N. Kudoh[2], Takahisa Taguchi[3], Chie Hosokawa[1,2,4] ([1]*Biomed. Res. Inst., AIST*, [2]*Grad. Sci. &Tech., Kwansei Gakuin Univ.*, [3]*CiNet, NICT*, [4]*PhotoBIO-OIL, AIST*)

Neurons in the brain form highly complex networks and operate via spatio-temporal activity patterns of neuronal spikes. In order to identify functional connections in neuronal networks, we demonstrate femtosecond laser-induced stimulation into neuronal cells and discuss the stimulation mechanisms. When a femtosecond laser focused into target neuron, intracellular Ca^{2+} immediately increased. Under extracellular Ca^{2+} free condition and blocking conditions in Ca^{2+} pumps or channels in endoplasmic reticulum (ER), intracellular Ca^{2+} elevation was not observed after laser irradiation. These results suggest that laser irradiation should trigger Ca^{2+} influx via extracellular due to multiphoton absorption and the extracellular Ca^{2+} influx lead to release Ca^{2+} from ER.

1Pos172 脳における発火頻度依存性シナプス可塑性の数理的解析
Numerical simulations and mathematical analysis of synaptic plasticity based on the rates of presynaptic firing

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In the brain, many neurons transmit signals to each other via synaptic connections. The change in this connection strength is called “synaptic plasticity”, which is essentially involved in memory and learning. Synaptic plasticity is generally classified into long-term potentiation (LTP) and long-term depression (LTD). LTP/LTD is a long-lasting strengthening/ weakening in synaptic signal transmission. In the hippocampus of the brain, stimulation of synaptic input fibers with a frequency of 10-100 Hz triggers LTP. LTD, on the other hand, is induced by low frequency stimulation of 1-5 Hz. In this study, we investigate numerically and analytically the synaptic plasticity dependent on the frequency of stimulation.

1Pos173 経頭蓋磁気刺激法における細胞外媒質まで考慮したケーブル理論
Cable theory considering extracellular medium in transcranial magnetic stimulation method

Toshiaki Kaminaka[1,2], Osamu Yokoi[1,2], Katsuhiko Hata[2,3,4] ([1]*DPEMS, Kokushikan Univ*, [2]*Res Cent for Math Med*, [3]*Sch. Emerg. Med. Sys. Kokushikan Univ*, [4]*Sakurai Hosp*)

There is a method called transcranial magnetic stimulation method (TMS) that externally applies a variable magnetic field to the cranium using a coil and stimulates neurons in the brain using electromagnetic induction.
By using this method, long-term potentiation and long-term depression can be caused.
By applying this stimulus continuously, it is possible to give long-term changes to the brain and it is said to be an effective treatment for neurologic symptoms such as Parkinson's syndrome.
The effect of the induced electric field on the nerve is determined by the cable model.
Normally, analysis is carried out assuming that the extracellular space around the membrane is perfect resistance.
We are studying how cable theory considering extracellular media is described.

1Pos174 反復リップルノイズを使った聴性脳幹反応の聴覚レベル判定
Auditory level determination of auditory brainstem response using iterated ripple noise

Osamu Yokoi[1,2], Toshiaki Kaminaka[1,2], Katuhiko Hata[1,2,3] ([1]*DPEMS Kokushikan Univ*, [2]*Res Cent for Math Med*, [3]*Dept of Emerg. Med. Sys., Kokushikan Univ*)

Using functional magnetic resonance imaging (fMRI), the region of Heschl's gyrus (HG) was identified as the pitch treatment region (Patterson et al. 2002). In their experiments, iterated ripple noise (IRN) was used as an acoustic stimulus generated by taking a sample of wideband noise and adding this noise with delay. The area of the auditory cortex that responds to the pitch of the sound can be identified. When melody was generated and pitch was changed, there was activation in the region beyond HG and planum temporale (PT), especially in superior temporal gyrus (STG) and planum polare (PP) region. The auditory level is measured using the electroencephalograph, fMRI for the iterated ripple noise (IRN).

1Pos175 人工ニューラルネットワークによる運動想起脳波信号の多クラス特徴抽出

Artificial neural network for multiclass feature extraction from motor imagery EEG

Ippei Yabe[1], Takuya Inoue[1], Hideo Mukai[1,2] ([1]*Dept. Comp. Sci., Grad. Sch. Sci. & Tech., Meiji Univ.*, [2]*Dept. Comp. Sci., Sch. Sci. & Tech., Meiji Univ.*)

Prosthetic arm is an important brain computer interface (BCI) device to support the daily needs of people lacking forelimb as well as amyotrophic lateral sclerosis patients.
In the context with BCI, we successfully classified left/right hand motion signals from desynchronization/synchronization (ERD/ERS) in EEG data collected in experiments with healthy subjects. However the degrees of freedom in arm/hand movement are still insufficient to enable multiple naturalistic movements.
To circumvent these problems, we introduced artificial neural networks such as variational autoencoder (VAE), to extract multiclass patterns in ERD/ERS within EEG to move the hand or arm. Currently we are trying to improve the network by supplying EEG data in each electrode channel.

1Pos176 Specific Nucleotide Distributions and Nucleosome Positioning around Simple Sequence Repeats in the Human Genome

Takeru Kameda, Atsushi Ikegaya, Naoaki Sakamoto, Akinori Awazu (*Dept. of Mathematical and Life Sciences, Hiroshima University*)

Human genome contains various types of simple sequence repeats. In this study, we analyzed the frequency of G/C nucleotides around these repeat sequences, and found that A/T-rich repeats were classified into two groups; the repeats with the upstream sequences that show high similarity to Alu elements and those that do not show. The analysis of publicly available experimental datasets for human lymphoblastoid cell line showed that A/T-rich repeats tend to exhibit specific nucleosome positioning in their vicinity but such positioning specificities were much different between former and latter groups. These results indicate that simple sequence repeats together with the neighboring site-specific G/C frequency and nucleosome-positioning may play roles in the human genome.

1Pos177 MNase, as a probe to study the sequence-dependent site exposure in the +1 nucleosomes of yeast

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The first nucleosome in the downstream of transcription start site is called as +1 nucleosome, which is expected to be readily unwrapped for DNA transcription. To investigate the DNA accessibility of +1 nucleosome, MNase-seq assays were carried out using 20 reconstituted +1 nucleosomes of yeast. We find that MNase cleaves not only the relatively more accessible terminal regions, but also the further inward sites where AA/TT dinucleotide is abundant. Since AA/TT is known as a rigid dinucleotide resistant to DNA bending, this internal cleavage reflects the local site exposure in nucleosomes encoded by DNA sequence. As the 5' end of +1 nucleosomes in yeast is AA/TT-rich, we suggest this sequence pattern may play a role in facilitating DNA unwrapping for transcription.

1Pos178 相互作用プロファイルによる細菌走化性タンパク質間相互作用ネットワーク解析

Protein interaction surfaces of protein-protein interaction networks in bacterial chemotaxis networks using profile methods

Nobuyuki Uchikoga[1], Yuri Matsuzaki[1], Masahito Ohue[2], Yutaka Akiyama[1,2] ([1]*Tokyo Tech. ACLS*, [2]*Tokyo Tech, Sch. of Computing, Dept. of Computer Sci.*)

A profile method was proposed for analysis of protein-protein interactions using rigid-body docking process. Many candidate protein complex structures (decoys) are generated and their interaction surfaces can be treated by profiles, composed of frequencies of interacting amino acid pairs. We could use profiles of each decoys for improving accuracy of protein-protein interaction predictions [Uchikoga & Hirokawa 2010 BMC Bioinfo. 11:236]. On the other hand, the profile method could be useful for investigating protein-protein interaction networks. In this work, bacterial chemotaxis were investigated and discussed by a profile generated by assembling whole docking decoy interaction surfaces, called Broad Interaction Surfaces (BIPs) [Uchikoga et al. 2016 BPPB. 13:105].

1Pos179 生体内低分子化合物三次元構造データベースのアップデートと構造精度向上のための取り組み

Recent development of 3DMET database: New release and efforts to improve data accuracy

Miki Maeda, Tomomi Komaba, Tomoki Yonezawa (*NARO AAC*)

We have been developed a three-dimensional structure database of natural metabolites (3DMET). This database was automatically developed from the data of the other compound databases in the early stage. Since 2009, we started manual input referred from books and articles to obtain new entries. As a number of 3D-structure data could be developed, the 3DMET was renewal as a new release. This release is completely renewed to manually curated data from automatically converted and confirmed by correspondence of SMILES or InChI because confirmation by line notations had some errors. Because many new entries are added to the database, the data ID was also reorganized. Some database links are also increased to utilize the other information related to compounds of the entries.

1Pos180 Revisiting a classical threading method with novel scoring function of sequence-structure compatibility

Kyosuke Tomoda, Yota Masuyama, George Chikenji (*Grad. Sch. Eng., Nagoya Univ.*)

Threading is one of most reliable protein structure prediction methods for protein pairs which have high structural similarity while having weakly or not related sequences. Traditionary, the concept of threading is considering mainly the compatibility of target sequence-template structure. It is highly required to develop the scoring function, which can discriminate between native structure and decoys. Here, we revisit a classical threading method with newly developed scoring function based on the physical characteristics of sequence-structure compatibility. The scoring function is novel in that well represents the environment of residues in the structure;buried or exposed. This presentation will describe the detail of our method and show the results of benchmark tests.

1Pos181 ホモダイマー構造変化の網羅的解析
Structural changes of homodimers in PDB

Ryotaro Koike, Takayuki Amemiya, Tatsuya Horii, Motonori Ota (*Grad. Sch. Info., Nagoya U.*)

Protein complexes are involved in various biological phenomena. These complexes are intrinsically flexible, and structural changes are essential to their functions. To perform a large-scale analysis of the structural changes of complexes, we used two original methods: SCPC and Motion Tree. This approach was applied to all available homodimers in the Protein Data Bank (PDB). We defined two complex-specific motions, interface motion and over-subunits motion, and all structural changes were classified and examined. The dimeric interfaces of interface motion were determined to be small and flat, while those of over-subunits motion were large and rugged. The interface properties of homodimers correlated with the type of complex-specific motion.

1Pos182 SLC 輸送体の構造および変異特性の統合解析のための情報基盤構築
Platform for integrated computational analyses of structural property and mutation effect on SLC transporters

Akiko Higuchi[1], Kei Yura[2,3] ([1]*Grad. Sch. Fornt. Sci. , Univ. Tokyo*, [2]*Cent. Info. Bio., Ochanomizu Univ.*, [3]*Sch. Adv. Sci. Engr., Waseda Univ.*)

The solute carrier (SLC) transporter superfamily plays a key role in mass transport system at a cell membrane. It consists of 52 families, and at least 386 human transporter genes have been identified. Despite their functional importance, many of their three-dimensional structures, evolutionary history and relationship to diseases are still unknown. We, therefore, built a new database to assist the search for the relationship amongst structural properties and pathogenic mutations on human SLC transporters. We found that the mutations at several conserved arginine, particularly to tryptophan and glutamine, were frequently involved in diseases. They are located at the highly conserved residue-cluster in three dimension on the cytoplasmic side of the protein.

1Pos183 Towards predicting functional consequences of genetic variants in humans through supramolecular complex structures

Atsushi Hijikata[1], Toshiyuki Tsuji[1,2], Masafumi Shionyu[1], Tsuyoshi Shirai[1] ([1]*Nagahama Inst. Bio-Sci. Tech.*, [2]*Mita Intl. Sch.*)

Recent advances in high-throughput sequencing technologies enable us to identify pathogenic mutations associated with particular genetic diseases in humans. However, the molecular mechanisms and functional consequences of the mutations are not fully understood. In the present study, functional effects of missense mutations on three-dimensional supramolecular complex (SC) structures were explored. The results showed that the types of molecular interactions in SC affected by mutations were significantly associated with the major types of mechanisms of dominant inheritance diseases. According to the results, we attempted to develop a method for predicting the functional consequences of the missense mutations. The performance of the method will be discussed.

1Pos184 マルチカノニカル分子動力学法を用いた転写因子天然変性領域による DNA 結合制御メカニズムの検討
Multicanonical molecular dynamics study of transcription factor-DNA binding regulation via the intrinsically disordered region

Kota Kasahara[1], Masaaki Shiina[2], Junichi Higo[3], Kazuhiro Ogata[2], Takuya Takahashi[1], Haruki Nakamura[3] ([1]*Col. Life Sci., Ritsumeikan Univ.*, [2]*Grad. Sch. Med., Yokohama City Univ.*, [3]*IPR, Osaka Univ.*)

Ets1 is an essential transcription factor in metazoan. Its DNA binding is regulated via the intrinsically disordered region (IDR), however the molecular mechanisms remain unclear especially at the atomic level. Here, we analyzed the free energy landscape of the 45-residue IDR in the molecular complex consisting of ETS domain and DNA, by using all-atom multicanonical molecular dynamics (McMD) method. As a result, several sub-stable conformations were observed at 300 K. In the most stable state, Lys301 side-chain in the IDR approached to a phosphoric acid of DNA near the interface with Leu337, which has been identified as a key residue to the DNA recognition. We hypothesize that this IDR-DNA interaction modulates the DNA conformation and affects on Leu337-DNA interaction.

1Pos185 生物表面に見られる曲面の機能：曲面による進行波の分裂
Functions of living matter surfaces: Curvature-driven splitting of a traveling wave

Kazuya Horibe[1], Ken-ichi Hironaka[2], Katsuyoshi Matsushita[2], Koichi Fujimoto[2] ([1]*Grad. Sch. of Info Sci and Tech., Osaka U.*, [2]*Grad. Sch. of Sci., Osaka U.*)

Surfaces of living matter or its constituents, cells, tissues, organs, individuals, are geometrically curved. These surfaces biologically function in the propagation of traveling waves of biochemical or electrical activities. The geometries of these surfaces determine the propagation direction of traveling waves thereby inducing split of wave. To understand this propagation process, we constructed a mathematical model of traveling waves on curved surfaces. We applied this model to a bell-shape surface. We showed that the bell-shape induced split of traveling waves transmitted by the surface for certain conditions. On the basis of this condition, we can predict split of wave from surface geometry and thereby understand the function of the surface of living matter.

1Pos186 細胞外領域への伝導不均一性の導入による致死性不整脈の抑制
Suppression of life-threatening cardiac arrhythmia by introducing inhomogeneity of electric conductivity in extracellular region

Kojiro Inoue (*Future Univ Hakodate*)

During ventricular fibrillation, that accounts for about 90% of the sudden cardiac death, many rotating spiral waves occur in the heart. The only cure for ventricular fibrillation is to apply large damaging electric shocks to the chest. On the other hand, even in the plasmodium of true slime mold which oscillates like a heart, many spirals occur, but they spontaneously disappear. In this study, we propose a treatment method for the fibrillation by constructing a numerical model which takes into account a nature of the true slim mold into the myocardium, and investigated spiral wave dynamics. By introducing high conductance fiber or mesh type regions into the extracellular region, it is possible to inhibit the transition from tachycardia to fibrillation.

1Pos187 多様な環境で生育するシアノバクテリア由来 KaiC ATPase の生化学的解析

Biochemical characterization of KaiC ATPases from cyanobcateria living in various habitants

Atsushi Mukaiyama[1,2], Yoshihiko Furuike[1,2], Shuji Akiyama[1,2] ([1]*IMS*, [2]*SOKENDAI*)

Circadian clock from *Synechococcus elongatus* PCC7942 is composed of three kinds of proteins, KaiA, KaiB and KaiC, and can be reconstructed *in vitro* by co-incubating the three kinds of proteins with ATP. Since discovery of *in vitro* reconstruction, Kai-protein clock has been extensively studied as the model system to elucidate the molecular mechanism behind circadian clock.
KaiC is a core oscillator of circadian clock, and we recently revealed that periodicity of the clock is implemented in KaiC ATPase. This finding led us further question: Does KaiC ATPase universally functions as a circadian pacemaker in whole cyanobacterial species?
To address this question, we characterized ATPase of KaiCs from various species. In this poster session, the detail will be presented.

1Pos188 人工自走粒子から見る、集団運動の普遍性

Universality of Collective Motion investigated in Artificial Systems

Junichiro Iwasawa[1], Daiki Nishiguchi[1,2], Masaki Sano[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*CEA, Saclay*)

Collective motion is a fascinating feature of nature which we can observe in systems such as flocks of birds and schools of fish. Since the proposal of the Vicsek model, which was a statistical physical approach to such kinds of flocks, both theoretical and experimental work has been conducted concerning the ordered phase of the model. Here, we conducted an experimental approach using asymmetric spherical colloidal particles so-called Janus particles. By applying an AC electric field to Janus particles dispersed in water, we have succeeded in realizing a fluctuating but highly ordered phase of polar collective motion. As a confirmation of its collective dynamics, we observed anomalous density changes in the system which is consistent with the standard Vicsek model.

1Pos189 温度補償能を欠損した時計タンパク質 KaiC 変異体の同定

Identification of Clock Protein KaiC Mutants Losing Temperature Compensation Ability

Yoshihiko Furuike[1,2], Atsushi Mukaiyama[1,2], Eiki Yamashita[3], Takao Kondo[4], Shuji Akiyama[1,2] ([1]*Research Center of Integrative Molecular Systems (CIMoS), Institute for Molecular Science (IMS)*, [2]*Department of Functional Molecular Science, SOKENDAI (The Graduate University for Advanced Studies)*, [3]*Institute for Protein Research, Osaka University*, [4]*Graduate School of Science, Nagoya University*)

The 24 hours period of the biological clock has the robustness against the temperature changes which is called as temperature compensation ability. In cyanobacteria, three clock proteins, KaiA, KaiB, and KaiC, compose the temperature compensated central oscillator, which can be reconstituted even in vitro. The phosphorylation states of KaiC work as time stamps, and its time information propagate to other related proteins. Based on the in vitro experiment, we have found several kinds of single amino acid mutations on KaiC result in the loss of temperature compensation ability. The biochemical properties of these mutants such as phosphorylation patterns and ATP hydrolysis activities will be discussed in the presentation.

1Pos190 概日反応における時計蛋白質 KaiA のプロトマーの役割

Functional roles of each protomer of homodimeric clock protein KaiA in circadian rhythm

Risa Imada[1], Shun Terauchi[1], Takahiro Iida[2], Hiroyuki Noji[3], Masahiro Ishiura[4], Kosuke Maki[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Faculty Sci., Fukuoka Univ.*, [3]*Grad. Sch. Eng., Univ of Tokyo*, [4]*Nagoya Univ*)

Circadian clocks of cyanobacterium Synechococcus elongatus PCC7942 are composed of three clock proteins, KaiA, KaiB and KaiC. A mixture of the three proteins in the presence of ATP exhibits a circadian rhythm in a test tube. It has been indicated that change in the multimeric state is important on circadian reaction for KaiB from Thermosynechococcus elongatus. Although KaiA is also multimeric, forming homologous dimer, it is unclear whether the homodimeric structure plays some roles in circadian reaction. Here, we investigated functional roles of each protomer of homodimeric KaiA on circadian reaction by a mutant KaiA with a single inactive protomer, and found circadian rhythm was qualitatively detected with the mutation.

1Pos191 C. elegans 集団が形作る動的ネットワーク構造

Dynamical network structure in C. elegans group

Ken Nagai[1], Hiroshi Ito[2], Takuma Sugi[3] ([1]*JAIST*, [2]*Kyushu Univ.*, [3]*Shiga Univ. Med. Sci.*)

Microtubules driven by axonemal dynein c grafted to glass plate form the lattice of vortices. This phenomenon is caused by long-time memory of rotation rate of microtubules and short range nematic alignment interaction. Indeed, the vortex lattice can be reproduced by the simple multi-agent model where these two rules are considered.
It is known that various animals including C. elegans show circular trajectories. The group of C. elegans formed many vortices in the whole experimental cell. The dependence of the collective motion of C. elegans on external environment was well reproduced by the almost same model as microtubules' collective motion, which indicates that collective motion comprising vortices is formed by groups of various other self-propelled particles.

1Pos192 走査型イオンコンダクタンス顕微鏡を用いた神経細胞のナノスケールイメージング

Nanoscale Neuron Topography Imaging using Scanning Ion Conductance Microscopy

Yasufumi Takahashi[1,2], Takafumi Miyamoto[1], Yuanshu Zhou[1], Takeshi Fukuma[1] ([1]*Kanazawa Univ.*, [2]*JST PREST*)

A dendritic spine is a small membranous protrusion from a neuron's dendrite that typically receives input from a single axon and changes its volume. To understand the function of the synapse, nanoscale imaging and stimulation technique is required.
Scanning ion conductance microscopy (SICM) is able to visualize the nanoscale cell surface topography with non-invasive manner. However, , imaging time of conventional SICM is about 20 min/image.
To reduce the scanning time, we selected next scanning area at the specific region by using previous obtained topography information and improved temporal resolution (3 min/image). By using this scanning mode, we visualized the volume change of neurites, transport of cargo molecule transport, and the structure change of growth cone.

1Pos193 アルギン酸細胞封入技術を使った細胞塊分取技術の検討
A simple method for encapsulating single cells in alginate microspheres

Masao Odaka[1,2], Akihiro Hattori[1,2], Kenji Matsuura[1,2], Moe Iwamura[3], Yuki Yamanaka[3], Kento Iida[4], W.Davis Ronald[5], D.Crosby Laurel[5], Kenji Yasuda[1,2,3,4] ([1]*Org. Univ. Res. Initiatives, Waseda Univ.*, [2]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*, [3]*Dept. Pure & Appl. Phys., Grad. Schl. Adv. Sci. & Eng., Waseda Univ.*, [4]*Dept. Pure & Appl. Phys., Schl. Adv. Sci. & Eng., Waseda Univ.*, [5]*Stanford Genome Tech. Ctr., Stanford Univ.*)

Microdroplets are an effective platform for identification and separation of individual cells for single cell-based analysis. However, a key challenge is to maintain and to release the captured cells in the microdropets without any destruction or invasion. We offer a method for embedding cells in alginate microspheres and performing multiple serial operations on the isolated cells. Cells were diluted in alginate polymer and enraptured into microdroplets using hydrodynamic focused microfluidic pathways. The encapsulated cells were monitored with the digital microscope camera attached to the microfluidic pathway, and identified the cells encapsulated in a microdroplets. The captured cells were released from the microdroplets in chelate buffered.

1Pos194 集束光による局所直接加熱技術を用いたゼラチン微細加工技術の開発
Development of real time microfabrication technology of gelatin with focused photo-thermal etching

Kento Iida[1], Yuki Yamanaka[2], Moe Iwamura[2], Masao Odaka[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[3,4] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*WASEDA Biosci. Res. Ins. in Singapore(WABIOS)*)

Flexible microfabrication technology of gelatin has been developed for single cell analysis of new-born vein formation in cancer diagnostics. To form the microstructures, the thin gelatin layer coated on the glass slide was spot heated and melted by the focused 1480-nm infrared laser, which has an absorbance to water. The advantages of gelatin microfabrication are (1) flexible change of their shapes even during cultivation, (2) inner surface of gelatin microstructures such as tunnels has affinity to cells for their movement, and (3) simple set-up of the method and fabrication technology. Moreover, this is complementary to the agarose microstructure technology. We examined and confirmed laser power dependence of microfabrication size was linearly correlated.

1Pos195 集束光による局所直接加熱技術を用いたナノ粒子埋包アガロース微細加工技術の開発
Development of real time microfabrication technology of nano-particle suspended agarose microstructures with focused photo-thermal etching

Yuki Yamanaka[1], Kento Iida[2], Moe Iwamura[1], Masao Odaka[3,4], Kenji Matuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*)

For single cell analysis of new-born vein formation, we need microfabrication of biochemical functionalization of micro structures. We have developed the indirect grafting method using functionalized carboxylic nanospheres suspended in agarose-gel. This method has three advantages: (1) flexible change of their shapes even during cultivation, (2) versatile applicability to various types of hydrogels and proteins with common principle, and (3) applicability to the quantitative spatial control of distribution and density of different kinds of proteins on nanospheres. The HUVEC cells are successfully cultured on the surface of the nanoparticle doped surface of agarose. The results indicate that the nanoparticle in agarose can work for functional surface of cell cultivation.

1Pos196 軟 X 線ライブセルイメージングによるシアノバクテリアの細胞内元素濃度の可視化
Visualization of Intracellular Element Concentration in cyanobacteria with soft x-ray live cell imaging

Takahiro Teramoto[1], Chihiro Azai[2], Masashi Yoshimura[3], Kazuki Terauchi[2], Toshiaki Ohta[3] ([1]*Col. Sci & Eng, Ritsumeikan Univ.*, [2]*Col. Life Sci, Ritsumeikan Univ.*, [3]*SR Center, Ritsumeikan Univ.*)

A cellular filament of the nitrogen-fixing cyanobacterium Anabaena sp. PCC 7120 consists of two different-form cells: photosynthetic “vegetative cell” and nitrogen-fixing “heterocyst”. The heterocyst lacks the O2-evolving photosynthesis activity because nitrogenase is easily inactivated by O2. The heterocyst differentiates from a vegetative cell, which requires increase of a cellular carbon-to-nitrogen (C/N) ratio. However, the critical value of C/N ratio have been unclear and even O2 concentration have never been observed in individual cells. In this study, we observed the Anabaena cells by soft X-ray microscopy; the soft X-rays around N1s and O1s absorption thresholds visualized subcellular distributions of C/N ratio and O2, respectively.

1Pos197 Visualization of microvilli dynamics on living cell surface using high speed scanning ion-conductance microscopy

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Nanoscale dynamics on living cell surface topography is essential to understanding cell functions. The scanning ion-conductance microscopy (SICM) is one of scanning probe microscopy and has been used to visualize the nanoscale morphology on living cell surfaces without invasive. However, conventional SICM does not have enough temporal resolution to observe rapid cell dynamics. Therefore, we developed high-speed SICM with new scanning algorithm. As a result, a topographic image is taken within 18 s with a 64 × 64 pixels, at 10 × 10 mm. The high speed SICM is enable to visualize cell surface dynamics without invasion and characterize microvilli dynamics on living cell surfaces after treatment of epidermal growth factor.

1Pos198 線虫 *C. elegans* 胚発生における細胞形状の自動抽出
An automated cell shape extraction in *C. elegans* embryogenesis

Yusuke Azuma, Shuichi Onami (*QBiC, RIKEN*)

The development of *C. elegans* proceeds through an invariant cell lineage. However, it is unclear to what extent the cellular dynamics is invariant. To address this question, we developed a method to evaluate the variability of cellular dynamics quantitatively. The method first detects positions of nuclei from 3D time-lapse images of embryos by a local maxima based image processing. The detected nuclei are subsequently used as markers for seeded-watershed segmentation of cellular regions. By applying the method, we extracted cell shape dynamics in five embryos and found variability in cell volume, cell division timing and cell-cell contacts. Currently we plan to extract the dynamics in dozens of embryos to analyze the variability exhaustively.

1Pos199 新規誘電率顕微鏡(SE-ADM)による生きた培養細胞と CD44 膜タンパク質結合ビーズのナノスケール観察

Nanoscale imaging of living cells bound by nanobeads-connected anti-CD44 antibody in medium using newly developed dielectric microscopy

Tomoko Okada, **Toshihiko Ogura** (*National Institute of Advanced Industrial Science and Technology, Biomedical Research Institute*)

Scanning electron microscopy (SEM) has widely been used to analyzing of the biological specimen's structures. However, SEM observations of these specimens under high vacuum conditions require specific sample preparation protocols involving glutaraldehyde fixation and negative staining. Here, we show that our developed scanning electron-assisted dielectric microscopy (SE-ADM)(1,2) system is clearly observing antibody-binding nanoparticles in liquid-phase(3). Moreover, we successfully observe nanobeads directly binding to living cancer cells via anti-CD44 antibody in a medium and their intracellular structure at the same time(3).

(1)T.Ogura, BBRC, 459, pp. 521-528 (2015); (2)T.Okada & T.Ogura, Sci.Rep., 6, 29169 (2016); (3)T.Okada & T.Ogura, Sci.Rep., 7, 43025 (2017).

1Pos200 Two-dimensional crystals of tamavidin 2 for a quick and easy method of immobilization of biotinylated biomolecules

Daisuke Noshiro[1], Noriyuki Kodera[1], Toshio Ando[1,2] ([1]*Bio-AFM FRC, Inst. of Sci. & Eng., Kanazawa Univ.*, [2]*CREST, JST*)

High-speed AFM has become a powerful tool for visualization of dynamic behaviors of biological molecules in physiological solutions. Development of the methods of modifying substrate surface for immobilization of the target molecules is particularly important for successful imaging. One of the widely available substrates is streptavidin 2D crystals on lipid bilayers for selective immobilization of biotinylated samples. In this study, we developed a simple method for preparing 2D crystals of tamavidin 2, a fungal protein with biotin-binding activity similar to that of streptavidin. The 2D crystals of tamavidin 2 were prepared on mica surface directly with no need for lipid bilayer, providing a quick and easy method of immobilization of biotinylated biological molecules.

1Pos201 高速 AFM 及び光ピンセット複合システム開発による一分子操作された分子の直接観察

Developing a Combined System of High-Speed AFM and Optical Tweezers for Direct Visualization of Single-Molecules under Manipulation

Motonori Imamura[1], Shin'nosuke Yamanaka[2], Toshio Ando[1] ([1]*Bio-AFM FRC, Kanazawa Univ.*, [2]*Grad. Sch. Sci., Kanazawa Univ.*)

High-speed AFM (HS-AFM) allows us to directly visualize the dynamics of biomolecules in sub-molecular resolution. Optical tweezers (OT) have been widely used to manipulate single molecules. In this study, we combined both techniques to observe the dynamic behavior of biomolecules while the molecules are being pulled with the OT. In order to easily find a target molecule, we also added fluorescent microscopy to this system. Besides this total system, we also prepared substrate surfaces and long λ DNA (~11 μm) strands that are used to link a target molecule and a microbead to be pulled by the OT. Since the experiment of observing HS-AFM images of the target molecule under an OT force is complicated, we are now trying to establish a procedure for this experiment.

1Pos202 ソフトウェア「闇魔」を用いた XFEL-CXDI 実験データの分類

Classification of XFEL-CXDI Imaging Experimental Data using the Software "EMMA"

Takashi Yoshidome[1], Yuki Sekiguchi[2,3], Yamamoto Takahiro[2,3], Oroguchi2 Tomotaka[2,3], Nakasako Masayoshi[2,3], Ikeguchi Mitsunori[4] ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*Fac. of Sci. and Tech., Keio Univ.*, [3]*RIKEN SPring-8 Center*, [4]*Grad. Sch. of Med. Life Sci. Yokohama City Univ.*)

Coherent X-ray diffraction imaging (CXDI) experiments with the X-ray free-electron laser (XFEL) enable us to visualize the structures of non-crystalline particles with micrometer to sub-micrometer dimensions. To analyze experimental data, classification of the data is inevitable. Recently, we have implemented the software "EMMA" to classify data without prior knowledge of the number of classes [1], and its usefulness has been demonstrated through simulation studies for XFEL-CXDI experiments. Here we present results of the classification of electron density maps of copper oxide nano particles from XFEL-CXDI experiments. We show that the maps are classified in terms of their sizes and internal structures.

[1] T. Yoshidome et al., PRE, 92, 032710(2015).

1Pos203 低温コヒーレント X 線回折イメージング・トモグラフィー実験による分裂期原始紅藻シゾンの三次元構造解析

Three-dimensional structure of Cyanidioschyzon merolae by using coherent X-ray diffraction imaging tomography at cryogenic temperature

Amane Kobayashi[1,2], Yuki Takayama[3], Yuki Sekiguchi[1,2], Mao Oide[1,2], Asahi Fukuda[1,2], Takahiro Yamamoto[1,2], Koji Okajima[1,2], Tomotaka Oroguchi[1,2], Sachihiro Matsunaga[4], Yoshiki Kohmura[2], Masaki Yamamoto[2], **Masayoshi Nakasako**[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*, [3]*Schl. Sci. Univ. Hyogo*, [4]*Faclt. Sci. Tech. Tokyo Univ. Sci.*)

Tomography version of coherent X-ray diffraction imaging was applied to visualize the 3D structure of a single Cyanidioschyzon merolae cell at the cell division state. Diffraction patterns beyond a resolution of 30 nm were collected by rotating the frozen-hydrated cell at an angular interval of 1.5 or 3.0 degrees by using a custom-made diffractometer at BL29XUL of SPring-8. The projection map at each rotation angle was retrieved from the diffraction pattern. Then, the three-dimensional electron density map at an effective resolution of approximately 130 nm was reconstructed from the maps by applying the back-projection method. In the session, the feasibility and problems of the tomography experiment and problems in the structure analysis will be discussed.

1Pos204 サイズ分画機能を備えた画像認識型セルソーターによる血中循環腫瘍細胞の測定

Monitoring of circulating tumor cell clusters in blood using size classifying imaging cell sorter

Moe Iwamura[1], Masao Odaka[3,4], Yuki Yamanaka[1], Kento Iida[2], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ*, [4]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*)

Circulating tumor cells (CTCs) in blood is important biomarker for metastasis. We have developed an on-chip imaging cell sorting assay for identifying CTCs only with their morphological characteristics. In the assay fabrication of poly-dimethylpolysiloxane size separation microstructure, we succeeded in stably producing precise designed structure to overcome the 80% structure shrank in the microfabrication process. We examined the obtained blood of rats implanted prostate cancer cell line, and found that the frequency of clustered cells increased exponentially over time after implantation. The similar results were acquired in human patient blood. These results suggest that the imaging biomarker of CTC clusters has a potential to be one of the indicator of metastasis.

1Pos205 Direct observation and analysis of bacteria within giant liposomes

Masamune Morita, Naohiro Noda (*Biomed. Res. Inst., Natl. Inst. Adv. Ind. Sci. Tech. (AIST)*)

Direct observation of bacteria in a small confined space has been adapted for applications in bio production, and so on. Although direct observation of bacterial growth system by using water-in-oil microdroplets have been increasingly reported, the application of this system is limited because it contains oil. Giant liposomes are a well-studied microreactor system, due to the unique ability of their biological resemblance to cell membranes. However, there is a lack of straightforward methodology to encapsulate and observe bacteria inside liposomes. Here, we demonstrate the encapsulation and observation method of bacteria inside giant liposomes by using DSSF (Morita, et al. ChemBioChem 2015) for forming liposomes.

1Pos206 人工細胞での DNA 論理回路を用いた最小限の意識を生み出すオートマトン
Automata that generates minimum consciousness using DNA logic circuits in artificial cells

Hiroki Watanabe[1], Ryuji Kawano[2], Masahiro Takinoue[1] ([1]*Dept. Compt. Sci., Tokyo Tech*, [2]*Dept. Bio. Life Sci., Tokyo Univ. Agri. Tech.*)

Integrated information theory (IIT) has recently received attention in terms of the evaluation and construction of 'consciousness'. However, it remains to be elucidated whether consciousness can be constructed based on biomolecular systems. In this study, we propose to construct a method to create minimum consciousness based on automata that meet the IIT using DNA logic circuits in artificial cells. The DNA logic circuits are constructed using DNA molecules for input/output information and droplet interface bilayer with protein nanopores for logic operation and electrical detection of output. We believe that this system would show the possibility to create micrometer-sized molecular robots with consciousness and could be applied to biomedical technologies.

1Pos207 カップ形状 AFM チップを用いた様々な基板に対する細胞接着強度の評価
Adhesion strengths of living cells for various substrates measured by using cup-shaped AFM chip

Hyonchol Kim[1,2], Kenta Ishibashi[2], Kosuke Matsuo[3], Atsushi Kira[3], Yui Onomura[1], Tomoko Okada[1], Chikashi Nakamura[1,2] ([1]*Biomed. Res. Inst., AIST*, [2]*Grad. Sch. Eng., Tokyo Univ. Agric. Technol.*, [3]*Japan Aviation Electronics Ind., Ltd.*)

In our previous study, a cup-shaped metal hemisphere was attached to an apex of cantilever of the atomic force microscope (AFM), a cell was trapped to the inner concave of the cup and picked up from a substrate, and intercellular adhesion strengths were quantitatively measured. In this study, the method was applied to measure adhesion strength of a cell against various substrates to control cell adhesion patterns on a chip. Force measurements were performed using three types of substrates; one is metal-deposited, another is highly adhesive, and the other is less adhesive. In notable results, substrates modified with perfluoroalkyl groups extremely inhibited cell adhesions. These results contribute smooth fabrication of desired cell patterning on a substrate.

1Pos208 Photo-regulation of Small GTPase Ras Using Photochromic Peptide

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Small G protein Ras is guanine nucleotide binding protein which are related to important cellular signaling and serve as a molecular switch. Their activity is regulated by two factors, GEF and GAP. The molecular mechanism of Ras was well studied and it is already known that αH Helix region on SOS (RasGEF) interact with Ras. Previously we have demonstrated that SOS αH helix mimicking peptide which is intramolecularly cross-linked with bifunctional azobenzne derivative ABDM competitively inhibited guanine nucleotide exchange activity of SOS. In this study, the inhibition of MAPK/ERK pathway with the ABDM-peptide in HeLa cell was examined by western blot analysis. Phosphorylation of ERK was reduced in the presence of ABDM-peptide.

1Pos209 DNA 分子ロボットのためのマイクロドロップレットの機械的安定性評価
Evaluation of mechanical stability of microdroplet-based DNA molecular robots

Misato Tsuchiya[1], Daisuke Ishikawa[1], Yuki Suzuki[2], Masayuki Endo[3], Masahiro Takinoue[1] ([1]*Dept. Comput. Sci., Tokyo Tech.*, [2]*Fronti. Res. Inst. Interdiscip. Sci., Tohoku Univ.*, [3]*WPI-iCeMS., Kyoto Univ.*)

Recently, construction of molecular robots mimicking environmental responsibility of living cells has attracted attention. We have been constructing a molecular robot using water-in-oil microdroplets and amphiphilic DNA-origami nanoplate. To add the environmental responsibility to the molecular robot, it is required to evaluate and increase the mechanical stability of the droplet-based molecular robot. However, its stability has not been well evaluated yet because of the measurement difficulty. Here, we constructed an evaluation system of the molecular robot stability based on microscope observation and image processing of the droplet fusion time course. We believe this system will contribute to the construction of environmentally responsive molecular robots.

1Pos210 バーコード様 DNA と生体ナノポアによる胆管癌特異的マイクロ RNA 発現パターンの認識
MicroRNA pattern recognition for cholangiocarcinoma using barcode-like DNA and biological nanopore

Moe Hiratani, Ryuji Kawano (*The Dep. of Biotech. and Life Sci., Tokyo Univ. of Agr. and Tech.*)

MicroRNA (miRNA) has been receiving an attention as a next-generation of an early diagnostic marker for every cancers. In the case of cholangiocarcinoma, it has been reported that five types of miRNAs are overexpressed. Identifying those expression patterns is significant to diagnose cholangiocarcinoma. For the simple detection of those patterns, we proposed the programmable DNA system using DNA computing and nanopore techniques. In this study, we constructed the barcode-like DNA which codes the information of overexpressed miRNAs from cholangiocarcinoma. Additionally, that information is decoded electrically by nanopore. Our system enabled us to recognize miRNA expression pattern of cholangiocarcinoma with real-time and label-free.

1Pos211 Construction of steric cardiac tissue by three dimensional printer using gelatin-agarose mixed scaffold

Naoki Tadokro, Ami Takasaki, Tomoyuki Kaneko (*Hosei Univ. FB LaRK*)

To use therapeutic cells in regenerative medicine, cells are required to culture in a three dimensional (3D) environment instead of two-dimensional general cell culture method. To establish 3D culture methods, we studied the scaffold material and molding technology to hold the cells in a steric structure arrangement and precisely control the structure. As a result, the mixture containing 7% gelatin and 0.6% agarose is suitable as the scaffolding material for 3D culture using 3D printers from three points of gelling temperature condition, lamination and molding. Moreover, a tubular steric structure containing myocardial cells were able to formed.

1Pos212 バクテリア走化性応答の解析に基づく水溶液識別法の構築
Construction of aqueous solution discrimination method based on analysis of bacterial chemotactic response

Hiroto Tanaka[1], Yasuaki Kazuta[1], Ikuro Kawagishi[2], Yoshiyuki Sowa[2], Yasushi Naruse[3], Yukihiro Tominari[1], Masato Okada[4], Kazuhiro Oiwa[1], Hiroaki Kojima[1] ([1]*Adv ICT Res Inst, NICT*, [2]*Housei Univ*, [3]*CiNet, NICT*, [4]*Tokyo Univ*)

Detection and recognition of chemicals are primitive but vital for living organisms to survive. We have focused on the organisms' ability of recognition of chemicals, and developed engineering use of the ability. As a proof of concept, by using cells' behaviors to chemical stimuli, we have constructed a simple chemical sensor equipped with Escherichia coli (E. coli). This prototype cell-based sensor (CBS) distinguished more than three chemicals (amino acid attractants) by using only one E. coli strain. Here, as an application of the CBS, we show discrimination of aqueous solutions. We have succeeded to distinguish chemical mixtures, beverages, etc., by only one E. coli strain. Our results provide a basis for novel bio-inspired sensors.

1Pos213 固体試料における紫膜の積層ならびにバクテリオロドプシンの機能に対する固体化媒体の影響
Comparative study on purple membrane stacking and bacteriorhodopsin functionality in immobilized samples with various hydrogels

Shunsuke Yano[1], Hiakru Tanaka[1], Yasunori Yokoyama[1], Hiroshi Takahashi[2], Masashi Sonoyama[2], Takashi Kikukawa[3,4], Koshi Takenaka[1] ([1]*Grad. Sch. Eng., Nagoya Univ.*, [2]*Grad. Sch. Sci. & Tech., Gunma Univ.*, [3]*Grad. Sch. Life Sci., Hokkaido Univ.*, [4]*Gl-CoRE, Hokkaido Univ.*)

Bacteriorhodopsin (bR), a photochromic membrane protein, is one of candidate for industrial applications of biomaterials. We have recently reported that photocycle behavior of bR immobilized with poly(vinyl alcohol) (PVA) gel was almost identical to that in suspension system, and that purple membranes (PMs) became stacked in the PVA gel. To reveal effects of immobilization medium on PM stacking and bR function, immobilization PM samples with various gel media were examined. Interestingly, the PM stacking was not observed in the PM immobilized with agarose gel. This suggests that the PM stacking is strongly correlated with gelling mechanisms of the immobilization media. We will discuss the effects of immobilization media, from comparison among various hydrogels.

1Pos214 演題取り消し

1Pos215 シッフ塩基形成反応を利用したゴシポール配糖体の合成とその分子特性
Synthesis and properties of gossypol schiff-bases having two-glycoside appendages

Masaki Nakamura[1], Yoshitsugu Amano[1], Teruaki Hasegawa[2] ([1]*Grad. Sch. of Life Sci., Toyo Univ.*, [2]*Dept. of Life Sci., Toyo Univ.*, [3]*Bio-Nano Electronics Research Centre, Toyo Univ.*)

Gossypol (Gos), a terpenoid contained in cottonseed in large amounts, has unique bioactivities including anticancer activities and antiviral activities. In this respect, chemical modifications on Gos to develop various Gos derivatives with improved/modified bioactivities are of quite interest in medicinal chemistry. Introduction of carbohydrate modules onto Gos scaffold is also of quite interest because of potential site/cell-specificities. Recently, we developed new Gos derivatives through couplings between native Gos and *p*-aminophenyl-glycosides. Detailed synthetic procedures and spectroscopic properties of the resultant glycoGos would be discussed in Symposium.

1Pos216 Self-assembly of two-dimensional DNA origami lattices with designed geometries on lipid membranes

Yuki Suzuki[1,2], Ibuki Kawamata[2], Satoshi Murata[2] ([1]*Fronti. Res. Inst. Interdiscrip. Sci., Tohoku Univ.*, [2]*Grad. Sch. Eng., Tohoku Univ.*)

Hierarchical self-assembly has attracted great attention as a method to design and construct multifunctional supramolecular architectures that can mimic biological systems. In this study, we have designed a three dimensional (3D) DNA origami block whose sides have shape-complementary patterns. The weak adsorption of DNA origami blocks onto the fluidic lipid bilayer membrane allows their lateral diffusion on the surface and promotes self-assembly into a lattice with designed geometry through homomultimerization based on self-complementary shape-fit. Our study will provide a general approach to the construction of custom DNA origami lattices that serve as a scaffold for organization of various biological molecules on a lipid-bilayer membrane.

1Pos217 Development of a cell-sized molecular robot controlled by an external molecular signal

Yusuke Sato[1], Yuki Suzuki[2], Ibuki Kawamata[1], Satoshi Murata[1], Yuichi Hiratsuka[3], Ken Komiya[4], Masayuki Endo[5], Shin-ichiro M. Nomura[1] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*FRIS, Tohoku Univ.*, [3]*Sch. Mat. Sci., JAIST*, [4]*Sch. Comp., Tokyo Tech.*, [5]*iCeMS*)

Development of cell-sized molecular robots having external stimulus-responsivity is one of the attractive challenges in bioinspired robotics field. We previously demonstrated a liposome-based molecular robot that can express shape-changing behavior in response to signal DNAs produced inside the robot by photo-irradiation. In order to control the robot by external molecular signals, we newly designed and used a DNA origami device that could penetrate liposomal membrane and trigger a signal amplification system implemented in the liposome. The amplification system consists of sequence-designed DNAs and enzymes. We believe that the mechanism developed in this study would be useful tool for not only molecular robots but also artificial cell models.

1Pos218 フォトクロミック分子の光刺激による二酸化硫黄発生の反応機構

Reaction mechanism on sulfur dioxide generation by photoexcitation of a photochromic molecule

Satoshi Yokojima[1], Ryuhei Kodama[2], Kimio Sumaru[3], Shinichiro Nakamura[4], Kingo Uchida[2] ([1]*Tokyo University of Pharmacy and Life Sciences*, [2]*Ryukoku University*, [3]*AIST*, [4]*RIKEN*)

Sulfur dioxide at elevated concentrations is known to induce oxidative damage to biomacromolecules such as proteins, lipids, and DNA. We have developed a reagent for sulfur dioxide gas generation by photochromic reaction with thermal stability. We investigated the mechanism on sulfur dioxide generation by photoexcitation. By using the reagent, we successfully induced the cell death upon irradiation with UV light locally.

2Pos001 **自由エネルギー変分原理に基づく check point kinase1 阻害剤系における相対的結合自由エネルギー予測**
Prediction of relative binding free energy based on a free energy variational principal for the Check point kinase1-inhibitor system

Daichi Kondo, Takeshi Ashida, Takeshi Kikuchi (*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*)

It is important to predict accurate binding free energy of a ligand to a target protein in drug discovery process. There are many methods to predict it. However, conventional methods include some problems. For example, some methods require much computational cost and some needs to tune parameters. Therefore, we use a new method without above flows. This study's purpose is to calculate more accurate relative binding free energies by a free energy variational principal method and to check correlation with the experimental values. In this time, we apply this method for check point kinase1-inhibitor system. There are 44 ligands with known experimental values and we use 11 ligands among them. We will present the details in this meeting.

2Pos002 **Property of sequences analysis of beta-Trefoil protins with irregular structures on their folding**

Risako Kimura, Takeshi Kikuchi (*Depat. of Bioinf Col. Life Sci Ritsumeikan Univ*)

The β-Trefoil Fold protein has a similar trifoliate structure despite its low amino acid sequence identity between proteins from different superfamilies. In this study, we analyze the folding mechanism from the amino acid sequence of a β-Trefoil Fold protein including partially irregular structure. Based on the statistical information on the inter-residue distance, we used the Average Distance Map (ADM) analysis for predicting the compact area and F value analysis for predicting highly interacting residues by calculating the contact frequency. In addition, we predict folding cores by analyses of conserved hydrophobic residues. As a result, our research shows that after formation of units at each of the both ends, the central unit interacts with them to cause folding.

2Pos003 **Estimation of relative binding free energy for the CDK2 protein-ligand system**

Takayuki Kawano, Takeshi Ashida, Takeshi Kikuchi (*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*)

In a drug discovery process, estimation of binding free energy between a protein and a ligand is often performed with a computational technique. In this study, we apply the free energy variational principle (FEVP) method for this purpose. The feature of this method does not require intermediate state sampling and entropy calculation.
We apply this technique to the protein Cyclin Dependent Kinase 2 ligand inhibitor system to be reported their IC50. We try to predict the relative binding free energies for this system and compare them with the experimental values. We will report the detail at this conference.

2Pos004 **P53 タンパク質四量体化ドメインへの残基間平均距離統計に基づくコンタクトマップによる天然変性領域の予測法の応用**
Application of the prediction technique of IDRs to tetramerization domain of p53 protein

Takumi Shimomura, Takeshi Kikuchi (*Dept. of Bioinf., Col. of Life Sci., Ritsumeikan Univ.*)

It is difficult that the 3D-structure determination of IDP(intrinsically disordered protein) which does not have specific 3D-structure on physiological conditions analyses by X-ray crystallography and NMR analysis. Therefore, a research for the 3D-structure prediction method from only amino acid sequence is very useful. We use a contact map based on inter residue average distance statistics, and find that predicted long-distance contact density appeared in the relatively short-range is useful for discrimination between order and disorder regions. In this study, we apply this method to the tetramerization domain of p53 protein which is involved in DNA repair, cell cycle and apoptosis, and investigate the difference between p53 monomer and dimer in our prediction.

2Pos005 **紅色光合成細菌由来の電子伝達複合体の共結晶化**
Co-crystallization of a bacterial photosynthetic electron-transfer complex

T. Kawakami[1], T. Liang[1], K. Okazaki[1], Y. Kimura[2], S. Otomo[1] ([1]*Ibaraki Univ.*, [2]*Grad. Sch. Agri. Sci., Kobe Univ.*)

In photosynthetic bacteria, the oxidized reaction center (RC) generated by charge-separation is reduced by small soluble electron-carrying proteins. It is well known that the electron donor is a cytochrome *c* in the purple bacteria of α-subgroup, while a high-potential iron-sulfur protein (HiPIP) usually serves as the electron donor in the β- and γ-subgroup bacteria. In this work, we focus on the pair of HiPIP and light-harvesting reaction center (LH1-RC) complex from a thermophilic purple sulfur bacterium *Tch. tepidum* (γ-subgroup), which was reported to form a electron-transfer complex in vivo and in vitro but the identity has not been determined. We will present here the preliminary results on the co-crystallization and structural analysis of the HiPIP and LH1-RC.

2Pos006 **新規抗体断片 Fv-clasp を用いたラミニン受容体インテグリン α6β1 の結晶化と構造決定**
Crystallization and structure determination of laminin-binding integrin α6β1 aided by the use of Fv-clasp technology

Takao Arimori, Junichi Takagi (*IPR, Osaka Univ.*)

Integrin α6β1 is a major cell adhesion receptor that plays important roles during tissue development. Although several crystal structures of integrins belonging to RGD-dependent or leukocyte-specific subfamilies have been reported, no structural information is available for the third class, i.e., laminin receptors including α6β1. Recently, we have developed a novel antibody fragment format termed "Fv-clasp", which outperforms conventional antibody fragments such as Fab and single-chain Fv in an application called as "crystallization chaperone". By using an anti-integrin antibody with the Fv-clasp design, we have succeeded in the determination of the crystal structure of integrin α6β1 ectodomain at 2.9 Å resolution for the first time.

2Pos007 MM/3D ー RISM 法を用いた水・エタノール混合溶液中での HP-β-シクロデキストリンによるフルアステロン包摂反応の結合自由エネルギー予測

Binding free energy calculation of fluasterone and HPβCD in cosolvent by MM / 3D-RISM method

Kazuma Kondo[1], Masatake Sugita[1], Takeshi Kikuchi[1], Humio Hirata[2] ([1]*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*, [2]*Toyota Phys. & Chem. Res. Inst.*)

To predict the binding affinity between molecules in a biological condition, it is necessary to consider the effect of cosolvent. However, sampling of the configuration using only the MD simulation is sometimes problematic for the sampling of the cosolvent in a complicated surface in an active site of protein. To this issue, the 3D-RISM theory, or an analytical theory of the molecular liquid can make a significant contribution.
In this study, we estimate the binding free energy of a host-guest system in a water/ethanol solution using MM/3D-RISM method, which is a combination of MD simulations and 3D-RISM theory. We apply the method to an inclusion process of fluasterone by HPbCD and examine whether the binding free energy can be accurately estimated or not.

2Pos008 Barrier-to-autointegration factor の変異による構造変化解析

Structural change analysis by mutation of Barrier-to-autointegration factor

Chiaki Yamaguchi[1], Masatake Sugita[1], Toshiya Hayano[2], Takeshi Kikuchi[1] ([1]*Dept. of Bioinf., Col. Life Sci., Ritsumeikan Univ.*, [2]*Dept. of Biomed., Col. Life Sci., Ritsumeikan Univ.*)

Barrier-to-autointegration factor (BAF) is a 10 kDa conserved protein. It localizes to nuclear lamina via LEM-domain proteins and binds dsDNA as a homodimer. A coding mutation (c. 34G>A[p. A12T]) in BANF1 gene was reported as the genetic basis of Nestor-Guillermo progeria syndrome (NGPS), however the mechanism underlying NGPS remains unclear and no effective treatment has been found.
Therefore, in this study, MD simulations are performed on BAF monomers, dimers, and DNA-BAF complexes and its mutant. As a result, it is predicted that the fluctuation of the structure, particularly the α1 helix, in the mutant became larger. For further investigation, we perform structural analysis of other mutants. We also try to calculate binding free energy between each state.

2Pos009 自由エネルギー変分原理を用いたタンパク - リガンド間相対的結合自由エネルギー計算の DHFR-TMP 系への応用

Calculation of relative binding free energy between DHFR-TMP system on the basis of free energy variational principle

Naoto Nishimura, Takeshi Kikuchi (*Dept. of Bioinf. Col. of Life Sci. , Ritsumeikan Univ*)

In drug development process, an accurate prediction of the binding affinity of a drug candidate molecule to its target protein is essential for efficient chemical structure optimization to identify promising lead compounds.
Although recently some computational methods are improved, these methods still require further improvement.
An aim of our study is to establish a new in silico method with low cost and no parameter tuning.
Our target protein is dihydrofolate reductase with inhibitors which is derivatives from Trimethoprim.
Here, we calculate relative binding free energies on the basis of the free energy variational principle and MD simulations.
It is demonstrated that correlation coefficient between experimental and calculated values is improved by clustering of ligands.

2Pos010 ビタミンD受容体リガンド結合ドメインのアポ体及びアンタゴニスト複合体の溶液構造解析

Apo- and antagonist-binding structures of vitamin D receptor ligand-binding domain elucidated by SAXS experiments and MD simulations

Yasuaki Anami[1], Nobutaka Shimizu[2], **Toru Ekimoto**[3], Daichi Egawa[1], Toshimasa Itoh[1], Mitsunori Ikeguchi[3], Keiko Yamamoto[1] ([1]*Showa Pharmaceutical Univ.*, [2]*KEK PF*, [3]*Yokohama City Univ.*)

Vitamin D receptor (VDR) regulates the expression of genes related to calcium homeostasis etc. Crystal structures of agonist/antagonist-binding VDR ligand-binding domain (LBD) have been solved so far, however, all the crystal structures are almost identical, regardless of agonist/antagonist binding. In addition, no crystal structures of apo form has been reported. To understand an exact conformation of the apo form and the antagonist activity, we analyze them by a combination approach of small-angle x-ray scattering (SAXS) experiments and molecular dynamics (MD) simulation, and report a reliable solution structure for each form in atomic resolution. In both forms, helix 12 does not adopt the active form unlike the previously reported crystal structures.

2Pos011 Crystallization of Hepatitis B virus Core Protein in genotype C

Katsumi Omagari, Yasuhito Tanaka (*Dept. of Virology, Medical School, Nagoya City University*)

Hepatitis B virus (HBV) is a major human pathogen that causes serious liver disease. HBV has been classified into 8 geographically, genetically, and clinically diverse genotypes A to H. Genotype C, which is associated with more serious liver disease, is prevalent in Japan.. HBV replicates through reverse transcription of an RNA intermediate, the pregenomic RNA (pgRNA). The replication occurs inside core protein (Cp). Although knowledge of the structure of Cp would be valuable for understanding the molecular basis, no empirical structural data exist for genotype C. The analysis with electron microscope reveal that the purified recombinant Cp assembled into spherical shells of 30nm in diameter. We try to crystallize the Cp to obtain implications for drug developments.

2Pos012 MM/3D-RISM 法を用いた HP-b-CD と HP-g-CD によるコレステロールの結合様式と結合自由エネルギーの予測

Estimation of the binding free energy for inclusion processes of cholesterol by HP-b-CD and HP-g-CD using MM/3D-RISM method

Yuji Hayashino[1], Masatake Sugita[1], Tetsumi Irie[2], Fumio Hirata[3], Takeshi Kikuchi[1] ([1]*Dept. of Bioinfo., Col. Life Sci., Ritsumeikan Univ*, [2]*Dept. of Clin. Chem. Inf., Kumamoto Univ*, [3]*Toyota Phys. Chem. Res. Inst.*)

Niemann-Pick Disease Type C (NPC) is a lysosomal storage disease which is characterized by abnormal accumulation of free cholesterol. HP-b-CD have been used as a drug for the NPC to remove cholesterol molecules accumulated in cells. Recently, it was found that HP-g-CD also inhibits the accumulation of the free cholesterol in different manner from HP-b-CD. Moreover, HP-g-CD has a less side-effect compared to HP-b-CD. However details of the molecular mechanism of HP-b-CD and HP-g-CD inhibiting the accumulation of the cholesterol is unclear. In this research, we estimate the binding mode and binding free energy of target molecules by using MM/3D-RISM method to get a hint for the functional mechanism of HP-b-CD and HP-g-CD.

2Pos013 バクテリオロドプシンの高分解能X線結晶構造解析
Crystallographic analysis of bacteriorhodopsin at high resolution

Nagayuki Hasegawa, Hideyuki Jonotsuka, Kazuki Takeda, Kunio Miki (*Grad. Sch. Sci., Kyoto Univ.*)

Bacteriorhodopsin (bR) from Halobacterium salinarum has the retinal chromophore and acts as a light-driven proton pump. A previously reported structure of bR at 1.55 Å resolution (1C3W) is insufficient in resolution to discuss spectroscopic properties and the mechanism of proton pumping. We optimized the crystallization and measurement conditions of X-ray diffraction experiments, and succeeded in collecting undamaged high-resolution X-ray data. By the refinement with anisotropic temperature factors, we identified the hydrogen bonding network of multi-conformational residues and water molecules in the proton channel. Non-hydrogen atoms are observed separately, then the distortion of the retinal polyene chain is determined more accurately.

2Pos014 常磁性効果を用いた溶液NMR法による蛋白質の立体構造解析
Protein structural refinement using paramagnetic effects in solution NMR

Mayu Okada[1], Teppei Ikeya[1], Rajesh Sundaresan[1], Eri Nojiri[1], Tsutomu Mikawa[2], Yutaka Ito[1] ([1]*Grad. Sch. of Sci. & Eng., Tokyo Met. Univ.*, [2]*RIKEN, QBiC*)

Paramagnetic effects such as paramagnetic relaxation enhancement (PRE) and pseudo-contact shift (PCS) have become an indispensable technique for protein structural analysis by solution NMR. These provide substantially long-range distance and orientation information (~40 Å). However, the process to extract a maximum amount of structural information from the data and lead to 3D conformations has not been sufficiently established yet. We recently developed a refinement method that iteratively optimizes explanatory variables of those effects, signal assignment, and protein structure. Here we discuss its performance and future perspective, and also show a protein structure refinement of yeast ubiquitin hydrolase 1 (YUH 1) as a practical application of the paramagnetic NMR.

2Pos015 小さな膜タンパク質KcsAのクライオ電子顕微鏡法による構造解析の取り組み
An Approach to Structural Analysis of a Small Membrane Protein KcsA by Cryo-electron Microscopy

Hiroko Takazaki[1,2], Hirofumi Shimizu[3], Naoko Kajimura[4], Kaoru Mitsuoka[2,4], Takuo Yasunaga[1,2] ([1]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*, [2]*Abis*, [3]*Fac. Med. Sci., Univ. Fukui*, [4]*Research Center for Uhvem, Univ. Osaka*)

In recent years, near atomic resolution structures of membrane proteins, which are difficult to crystallise, have been solved using cryo-electron microscopy and single particle analysis in succession. Meanwhile, analyses of small proteins, whose Mw is less than 100K, are challenging and are little reported.
We here are trying to analyse the structure of small membrane protein KcsA. KcsA is a potassium channel with a total Mw of 70K. It has open and closed conformations under acidic and neutral conditions, respectively. We prepared cryo samples under each of conditions, observed them by EM with a direct detector, and then reconstructed their 3D structures with low resolutions. We aim to get fine structure and discuss differences between open and closed conformations.

2Pos016 X線結晶構造解析を目指した精製二量体VSOPの特性に関する研究
Studies of characteristics the purified dimeric VSOP for X-ray crystallography

Satoko Mochida[1], Yusuke Goto[1], Akima Yamamoto[1], Satomi Shibumura[1], Yasushi Okamura[4,5], Atsushi Nakagawa[1,5], Kohei Takeshita[1,2,3] ([1]*IPR, Osaka Univ.*, [2]*JST, PRESTO*, [3]*IAI, Osaka Univ.*, [4]*Grad. Sch. of Med., Osaka Univ.*, [5]*JST, CREST*)

Voltage gated proton channel (VSOP) exists as a dimer in a plasma membrane. It has the unique property that the protons permeate through the voltage sensor (VSD). In the previous studies, we proposed that VSOP prevents leakage of protons by the hydrophobic barrier in the VSD in the resting state based on the crystal structure. However, the structural knowledge is limited because of the artificial trimeric structure, that is caused by the chimeric construct, in the crystal. The dimeric structural information of VSOP must be necessary for understanding of the proton channel mechanism, but there are many difficulties for preparation of a dimeric VSOP. In this presentation, we will discuss the preparation of dimeric VSOP protein and its properties as a dimeric channel.

2Pos017 β-シート中の隣接したstrand上のCys-Cysペアは好まれる
Cys-Cys pairs on the strands arranged adjacently are preferred in β-sheets

Hiromi Suzuki (*Sch. Agri., Meiji Univ.*)

We selected 21,312 protein chains showing less than 30% sequence identity from PDB and analyzed patterns of 164,878 amino acid triplets (combination of three amino acid residues each located on each of strands arranged adjacently) in anti-parallel β-sheets taking hydrogen bonding pattern into account. Among 8000 possible triplet patterns, 982 patterns were not observed and 200 of them did not include any Pro. Cys-Cys-Cys showed the highest preference score (46 times more than expected). Triplets including an adjacent Cys-Cys pair (9 X-Cys-Cys and Cys-Cys-Trp) also ranked within top 30. Alternatively charged patterns (Lys-Glu-Lys, Glu-Lys-Glu, Glu-Arg-Glu, Arg-Glu-Arg) were other preferred cases. These results suggest high propensity for amino acid triplets.

2Pos018 クライオ電子顕微鏡によるグルタミン酸脱水素酵素ドメイン運動の研究
Cryo-electron microscopy study toward detecting domain motion of glutamate dehydrogenase

Mao Oide[1,2], Takayuki Kato[3], Tomotaka Oroguchi[1,2], Keiichi Namba[3,4], Masayoshi Nakasako[1,2] ([1]*Grad. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*, [3]*Grad. Sch. of Front. Biosci., Osaka Univ.*, [4]*RIKEN, QBiC*)

Hexameric glutamate dehydrogenase (GDH) is a large enzyme (Mw 280k). Each subunit comprises two functional domains forming a large active-site cleft between them. X-ray crystal structure analysis and molecular dynamics simulation of unliganded GDH have revealed several metastable conformations in the domain motion to open/close the cleft. More importantly, the hydration structure changes suggest a cooperative variation of hydration in coupling with the domain motion. In this study, we investigated the structures of GDH by using cryo-electron microscopy toward visualizing domain motion and concerted hydration structure changes. We will report the progress of this study, especially, focus on the classification of metastable states of domain motion.

2Pos019 **Implementation of Fragment Molecular Orbital Replica-Exchange method (FMO-REM) in GAMESS-US simulation package**

Shingo Ito[1], Stephan Irle[2], Yuko Okamoto[1] ([1]*Grad. Sch. Sci., Univ. Nagoya*, [2]*Oak Ridge National Laboratory*)

The Replica-Exchange Method (REM) and Replica-Exchange Umbrella Sampling (REUS) method, which are one of generalized ensemble algorithm, has been used in Molecular Dynamics (MD) and Monte Carlo (MC) simulation with not only classical, but also Quantum Mechanics (QM) / Molecular Mechanics (MM), which combines QM and classical force filed calculation, to study biomolecules. However, it is difficult to use these methods with full QM-MD or MC simulation, which treat whole system as a QM region, because of its high computational cost. To overcome this problem, we combined Fragment Molecular Orbital Method (FMO) with REM (and REUS) and implemented FMO-REM (and FMO-REUS) in GAMESS-US simulation package. We will show the results of test simulation using these method in poster.

2Pos020 **分子動力学シミュレーションによる抗 HIV 中和抗体 PG16 の CDR-H3 の変異における中和能への影響の解析**
Molecular dynamics study of mutation effects on the neutralizing ability in CDR-H3 of an anti-HIV antibody PG16

Ryo Kiribayashi[1], Hiroko X. Kondo[1], Daisuke Kuroda[2,3], Toru Saito[1], Jiro Kohda[1], Akimitsu Kugimiya[1], Yasuhisa Nakano[1], Kouhei Tsumoto[2,3], Yu Takano[1] ([1]*Grad. Sch. Info. Sci., Hiroshima City Univ.*, [2]*Grad. Sch. Eng., Univ. Tokyo*, [3]*Ins. Med., Univ. Tokyo*)

PG16 is a broadly neutralizing antibody to HIV-1. The antigen-binding fragment of PG16 has a characteristic long 28-residue complementarity determining region (CDR) H3. Experiments have shown that a mutation from Tyr^{H100Q} to Ala reduces the neutralizing ability. In this study, using molecular dynamics simulations, we have examined effects of the mutation on the CDR-H3 of PG16. Although the CDR-H3 slightly fluctuated around the equilibrium structure in the simulations of the wild-type PG16, a large structural change occurred in the simulation of the mutant. Therefore, the significant structural change in the CDR-H3 caused by the mutation from Tyr^{H100Q} to Ala might be responsible for the reduction of the neutralizing ability.

2Pos021 **The Free Energy Profile for Dissociation of Ligand from Zn2+ Ion of CA I Activesite**

Arwansyah Muhammad Saleh, Isman Kurniawan, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Sch. of Nat. Sci. and Tech. Kanazawa University*)

Carbonic anhydraseas (CAs) family have an essential role mechanism to catalyze the reversible hydration of carbondioxide to bicarbonate thus, it becomes a potential area to inhibit its activesite with promoting drugs. The structure of CA I activesite contains Zn2+ ion therefore, the forcefield parameter of Zn metal binds three histidin residues was calculated with potential energy surface (PES). We performed MD simulation and potential mean force (PMF) to obtain the free energy profile as function of distance between an atom of ligand and Zn2+ ion of CA I activesite. The WHAM method was used to obtain the accurate free energies from biased molecular simulation. Our result predicted that the free energy reaches a minimum reaction coordinate at 2.05 A.

2Pos022 **タンパク質の基準振動モードのネットワーク解析：中心性指標 betweenness とアロステリック機構**
Network analysis of normal modes of proteins: betweenness centrality and allosteric behavior

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Normal mode analysis provides dynamic aspects of a protein molecule from static-structure information of PDB. We applied a network analysis method to the low-frequency normal modes by considering a network made by connecting a pair of spatially neighboring residues that move in a coherent manner. We focused our attention to one of the centrality measures, betweenness. A residue with higher betweenness would have more control over the network, because more residues communicate each other passing through that residue. We analyzed a DNA-binding allosteric protein as an example. Interestingly, residues with higher betweenness constructed a pathway from cAMP binding site to DNA binding site. The network analysis is useful to characterize allosteric behavior of proteins.

2Pos023 **ガス圧 NMR 法を用いた酸素結合部位の解析：Outer Surface protein A**
Analysis of O2-binding sites in proteins using gas-pressure NMR spectroscopy: outer surface protein A

Takahiro Kawamura[2], Takuro Wakamoto[2], Soichiro Kitazawa[1], Shun Sakuraba[3], Tomoshi Kameda[4], **Ryo Kitahara**[1] ([1]*Coll. Pharm. Sci., Ritsumeikan Univ.*, [2]*Grad. Sch. Life. Sci.*, [3]*Grad. Sch. Frontier Sci., Univ. Tokyo*, [4]*AIST*)

Internal cavities in proteins produce conformational fluctuations and enable the binding of small ligands. Here, we report a NMR analysis of O2-binding sites in Outer surface protein A (OspA) by O2-induced paramagnetic relaxation enhancements (PREs) (Kawamura et al. Biophys. J. 112, 1820-1828, 2017). We observed significant O2-induced PREs for amide protons located around the largest cavity and at the central β-sheet of the protein. We suggested three potential O2-accessible sites in the protein based on the 1/r6 distance dependence of the PRE. MD simulations permitted the visualization of the translational motions of O2 within the largest cavity, egress of O2 from the cavity, and ingress of O2 in the surface crevice of the β-sheet.

2Pos024 **Conformational dynamics of Human Protein Kinase CK2α and its effect on function and inhibition**

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Protein Kinase CK2 is ubiquitously expressed and highly conserved enzyme. Its catalytic subunit (CK2α) shows remarkable flexibility as evidenced in numerous crystal structures. Here, using multiple crystal structures and molecular dynamics simulations, we explore the conformational flexibility of CK2α. We found that among multiple conformations of the hinge region, observed during the dynamics, most populated conformation was inadequately represented in the crystal structure ensemble. The comparison of dynamics in apo and inhibitor bound state exhibits inhibitor induced suppression in dynamics of the enzyme. Together, this work gives novel insights into the function, dynamics and inhibition of CK2α, and paves way for development of better inhibitors.

2Pos025 生体系の結合標準自由エネルギー計算の新しい手続き
A new calculation workflow for the standard free energy of binding in biomolecular system

Yoshiaki Tanida, Azuma Matsuura (*Fujitsu Laboratories Ltd.*)

Accurate estimates for the binding free energy are of great interest in structure-based drug discovery and biosensor development. We propose a new workflow for the quantitative prediction of the binding affinity using the combination of metadynamics, reweighting and alchemical free energy calculation.

2Pos026 差分距離行列によるタンパク質構造変化の研究
Difference Distance Matrix enhanced molecular dynamics study on protein

Yasushige Yonezawa (*IAT, Kindai*)

Conformational change of proteins is of importance for understanding the function and mechanism. A modern standard molecular dynamics simulations using advanced computer cannot reach the working time range of proteins. To address the problem, we developed a difference distance guided molecular dynamics simulation to enhance the dynamical conformational change. In this method, a difference of distance matrix of two conformational states of proteins is used to push the dynamics of the protein. The method applied to open and close forms of Adenylate kinase. As a result, our method effectively produced the transition states between the two states.

2Pos027 B 細胞抑制性因子 CD72 の分子表面電荷分布によるリガンド結合制御機構
Charge distribution regulates the ligand-binding affinity of B cell inhibitory receptor CD72

Nobutaka Numoto[1], Chizuru Akatsu[2], Kenro Shinagawa[1], Takeshi Tsubata[2], Nobutoshi Ito[1] ([1]*Dept. Struct. Biol., Med. Res. Inst., Tokyo Med. & Dent. Univ.*, [2]*Dept. Immunol., Med. Res. Inst., Tokyo Med. Dent. Univ.*)

CD72 is an inhibitory cofactor expressed on B cells and suppresses autoimmune diseases such as systemic lupus erythematosus. We have determined the crystal structure of the ligand-binding domain of mouse CD72 at 1.2 Å resolution, and demonstrated that CD72 binds to the nuclear autoantigen Sm/RNP composed of proteins and nucleic acids (1). Electrostatic potential analysis of the molecular surface of the ligand-binding domain of CD72 and a homology model analysis of that of CD72c, which is the allelic form of CD72 in a model mouse of autoimmune disease, suggest that charge distribution at the putative ligand-binding site appears to affect the binding affinity between CD72 and Sm/RNP.
(1) Akatsu et al., J. Exp. Med., 213, 2691-2706, 2016.

2Pos028 EGF 受容体 C-末端天然変性ドメインの１分子 FRET 計測
Single-molecule FRET measurement of the intrinsically disordered C-tail domain of the epidermal growth factor receptor

Kenji Okamoto, Yasushi Sako (*RIKEN*)

The epidermal growth factor receptor (EGFR) possesses binding sites for various adaptor proteins, including Grb2, on its intracellular C-tail (CT) domain. As Morimatsu et al. suggested the existence of multiple binding states[PNAS, 104, 2007], structural flexibility of intrinsically disordered CT domain may contribute to regulation of Grb2 binding kinetics. We used single-molecule Förster resonance energy transfer (smFRET) measurement to investigate the structure and its dynamics of EGFR-CT. CT fragment molecules are labeled with ATTO532/647N, immobilized on polyethylene-glycol (PEG)-coated glass surface and imaged by a sCMOS camera with a W-view system. The results indicate that phosphorylation of Grb2 binding sites opens structure and enhance its flexibility.

2Pos029 ヘテロ３量体 G 蛋白質相互作用因子 Gip1 の網羅的アラニンスキャン変異解析
Comprehensive alanine scanning analysis of heterotrimeric G protein interacting partner Gip1

Hiroyasu Koteishi[1], Takero Miyagawa[2], Yoichiro Kamimura[1], Yukihiro Miyanaga[2], Masahiro Ueda[1,2] ([1]*RIKEN, QBiC*, [2]*Fron. Biosci., Osaka Univ.*)

Gip1 has been recently discovered as an interaction partner with heterotrimeric G protein (Gαβγ) from Dictyostelium discoideum, known as a model organism for chemotaxis. The interaction between the proteins sequesters Gαβγ into the cytosol and releases it toward the membrane in chemoattractant (cAMP) concentration dependent manner. To investigate the essential residues for the Gip1 function, Ala scanning analysis was performed for all residues of Gip1. Activity of Gip1 mutants was evaluated by observing translocation of Gαβγ upon cAMP stimulation and key residues for binding or releasing Gαβγ were identified. Furthermore, compared the Ala scanning results with the crystal structure of the Gip1 C-terminal domain, important regions for Gip1 function have been revealed.

2Pos030 クモ糸タンパク質ナノファイバーの自己集合
Self-assembly of nanofibers from spider silk fibroin

Yugo Hayashi[1], Tomoaki Murakami[1], Mai Arakawa[1], Keito Yoshida[1], Yoichi Yamazaki[1], Takehiro K. Sato[2], Hironari Kamikubo[1] ([1]*Grad. Sch. Mat. Sci. Nara Inst. Sci. Tech.*, [2]*Spiber Inc.*)

Spider silk is one of the toughest material we know. To achieve the exceptional mechanical properties, fibroin is required to assemble into ordered structures on the nanoscale. Recent studies reported that the repetitive region (RR) containing poly-Ala repeats are responsible to form β-sheet nanocrystal, which plays a key role in the mechanical properties of spider silk. Here, we investigated self-assembling of the RR fragments from *Araneus diadematus* fibroin 3 (RR-ADF3). RR-ADF3 was dissolved and allowed to stand under specific conditions. We eventually observed increase in fluorescence intensity of Thioflavin-T coexisting in the solution. IR and TEM measurements revealed formation of nanorod particles involving aligned β-sheets.

2Pos031 抗体 G2 は異なる 3 つの配列を強く特異的に認識する
A three-in-one monoclonal antibody G2 recognizes completely different epitope sequences with high affinity

Md. Nuruddin Mahmud[1], Masayuki Oda[2], Daiki Usui[2], Yasuo Inoshima[1,3], Naotaka Ishiguro[1,3], **Yuji O. Kamatari**[4] ([1]*United Grad. Sch. of Vet. Sci., Gifu Univ.*, [2]*Grad. Sch. of Life and Environ. Sci., Kyoto Pref. Univ.*, [3]*Fac. of Appl. Bio. Sci., Gifu Univ.*, [4]*Life Sci. Res. Ctr., Gifu Univ.*)

A monoclonal antibody G2 reacts with at least three proteins (ATP6V1C1, SEPT3, and C6H10orf76) other than its original antigen, chicken prion protein (ChPrP). The epitopes on ChPrP and ATP6V1C1 have been identified previously. In this study, we identified the epitope in the third protein, SEPT3. Interestingly, there was no amino acid sequence similarity among the epitopes on the three proteins. SPR indicated that these epitopes had high binding affinities to G2. Additionally, competitive ELISA indicated that the binding sites on G2 overlapped, suggesting that the antigen-binding site may be flexible in the free form and adapt at least three different conformations to enable interactions with three different antigens.

2Pos032 二次構造に基づいた蛋白・蛋白相互作用面の階層的分類
Hierarchical classification of protein-protein interfaces based on their secondary structures

Takashi Fujii, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. of Bioinformatics. Soka Univ.*)

Protein-protein interactions play crucial roles in many biological functions. There are various databases that classify complexes based on similarity of domain structures. However, it has been known that there are structurally unrelated complexes with similar interfaces. In this study, we hierarchically classified complexes based on their secondary structures of interface residues. First level of the hierarchy is defined using the composition of secondary structures of interface residues. Second level of the hierarchy is represented by the composition of the secondary structure in the partner subunit and the total number of interface residues. This result will be released shortly on our website: OLIGAMI (http://protein.t.soka.ac.jp/oligami).

2Pos033 Gip1 は Gγ の脂質修飾部位を疎水性空隙で覆うことで三量体 G 蛋白質を細胞基質に隔離する
Gip1 sequesters heterotrimeric G proteins in the cytosol by masking their lipid-modification site with the hydrophobic cavity

Takero Miyagawa[1], Yoichiro Kamimura[2], Hiroyasu Koteishi[2], Kohei Takeshita[3], Atsushi Nakagawa[3], Masahiro Ueda[1,2] ([1]*Grad. Sch. Front. Biosci., Osaka Univ.*, [2]*QBiC, RIKEN*, [3]*IPR, Osaka Univ.*)

G protein shuttling is a novel spatial regulation of heterotrimeric G proteins (Gαβγ) between the plasma membrane and the cytosol. This mechanism plays an essential role in the extension of the chemotactic dynamic range and requires Gip1, which binds to Gβγ subunit in the cytosol. To reveal the structural basis of G protein shuttling, we determined the crystal structure of the Gβγ binding region of Gip1. It has a hydrophobic cavity composed of six α-helices. Further biochemical analyses showed that the binding ability of Gip1 with G proteins depended on the hydrophobic cavity of Gip1 and the lipid modification of the Gβγ subunit. Taken together, Gip1 facilitates the sequestration of Gαβγ in the cytosol by masking their lipid-modified site with the hydrophobic cavity.

2Pos034 Framework for computational protein science written in functional language Scala

Itaru Onishi, **Masayuki Irisa** (*Comp. Sci. and Sys. Eng., Kyushu Inst. of Tech.*)

A protein-science application framework written in functional language Scala for execution environment of molecular modeling and simulation allows non-technical users: 1) to extract desired contents from hierarchical data in a PDBML/XML format file by giving regular expressions; 2) to use GUI manipulation made with widget toolkit SWT, and molecular graphics representation including stereoscopic representation for checking results of regularization and solvation of a X-ray structure; 3) to write rule sets in simple and natural manner, “case”-statements, for performing molecular simulations, 3D-RISM and MD; 4) to create a “monad” data-structure, which is powerful for a set of data lacking values in some elements and suitable for parallel computation of enormous data.

2Pos035 ファミリー 4 ウラシル DNA グリコシラーゼ–DNA 複合体の結晶構造解析
Crystal structure of family 4 uracil-DNA glycosylase in complex with DNA

Akito Kawai[1], Teruya Nakamura[2], Kazumi Shimono[1], Yuriko Yamagata[3], Shuichi Miyamoto[1] ([1]*Fac. of Pharmaceut. Sci., Sojo Univ.*, [2]*Priority Organization for Innovation and Excellence, Kumamoto Univ.*, [3]*Grad. Sch. of Pharm. Sci., Kumamoto Univ.*)

Deamination is a common base modification in DNA. Cytosine, adenine and guanine deaminations produce uracil, hypoxanthine and xanthine or oxanine, respectively. These deaminated bases cause the transition mutations if the errors are not repaired. Enzymes of uracil-DNA glycosylase (UDG) family remove these deaminated bases from DNA by catalyzing the N-glycosidic bond hydrolysis, thereby initiating the repairing pathway. We are particularly interested in family 4 UDGs, which are found in the thermophiles and excise uracil from both double- and single-stranded DNA. Recently, we succeeded to determine a crystal structure of its complex form with DNA at 2.1 Å resolution. Here we report the structural features and propose the catalytic mechanism of family 4 UDG.

2Pos036 細胞内アクチンの分子構造に対するミオシン阻害剤の効果
Effect of myosin inhibitor on the atomic structure of actin in cells

Shiori Nishinaka[1], Q.P. Taro Uyeda[2], Q.P. Taro Noguchi[1] ([1]*National Institute of Technology, Miyakonojo College*, [2]*Waseda University*)

To study atomic structure of actin, we previously developed FRET actin, of which the large and small domains were labeled with donor and acceptor dyes (Noguchi et al., 2015). In the 2014 meeting, we reported that FRET actin introduced into PtK2 cells revealed the distributions of different actin structures depending on higher order architectures such as stress fibers and meshwork structure of actin.
Here, we introduced FRET actin into fish keratocytes with a large lamellipodia, and found that the atomic structure of actin within lamellipodia differed locally. Furthermore, the myosin inhibitor (Y27632) decreased FRET index of FRET actin in both PtK2 and keratocytes, suggesting that the activity of myosin modulates the atomic structure of actin in cells.

2Pos037 ヒトフェリチン L 鎖の解離と変性に関する研究

A study on dissociation and unfolding of recombinant human ferritin L chain

Tomoki Yamamoto[1], Daisuke Sato[2], Kazuo Fujiwara[2], Masamichi Ikeguchi[1,2] ([1]*Grad. Sch. Bioinfo., Univ. Soka*, [2]*Fac. Sci. and Eng., Univ. Soka*)

Ferritin is a spherical shell-shaped protein consisting of 24 subunits. Each subunit has a structure that is composed of a four helix bundle (helices A-D), a long loop between B and C helices, and a short E helix at the C-terminus. Human ferritin is a hetero-polymer of H and L chains, which have different amino acid sequences and functions. The composition of H and L chains is tissue-dependent, and both H and L chains can form a homo-polymer. In this study, the dissociation/unfolding and refolding/reassembly of recombinant human L ferritin (HFL) was investigated by circular dichroism, ultracentrifugation, and gel permeation chromatography as functions of pH and denaturant concentration. The results showed that the dissociation/unfolding of HFL was partially reversible.

2Pos038 新規 NMR 法を用いた ALS 関連タンパク質 SOD1 の線維形成メカニズムの解明

Elucidation of fibrillization mechanism of ALS-related protein SOD1 using novel NMR spectroscopy

Naoto Iwakawa[1], Daichi Morimoto[1], Erik Walinda[2], Kenji Sugase[1], Masahiro Shirakawa[1] ([1]*Grad. Sch. Eng., Kyoto Univ.*, [2]*Grad. Sch. Med., Kyoto Univ.*)

Amyloid fibril formation of superoxide dismutase 1 (SOD1) in motor neurons causes amyotrophic lateral sclerosis (ALS). To date, the following two questions on the fibril formation have remained unclear. The first question is why SOD1 forms fibrils inside cells even though it is stable *in vitro*. Our NMR relaxation dispersion experiments revealed that the cell-mimicking crowded environment destabilized SOD1 thermodynamically, suggesting that the intracellular macromolecular crowding induces fibril formation. The second question is how SOD1 forms fibrils. We have developed a high-sensitivity Rheo-NMR instrument and detected atomic-level structural changes of SOD1 during fibrillization. We will determine the intermediate structure during fibrillization using Rheo-NMR.

2Pos039 Measurement of microtubule persistence length with sub-pixel resolution revealed its dependency on the growth rate

Naoto Isozaki[1], Kazuki Ukita[1], Hirofumi Shintaku[1], Hidetoshi Kotera[1], Taviare L. Hawkins[2], Jennifer L. Ross[3], Ryuji Yokokawa[1] ([1]*Dept. Micro Eng., Grad. Sch. Eng., Kyoto Univ.*, [2]*Dept. Phys., UW-La Crosse*, [3]*Dept. Phys., UMass Amherst*)

Microtubules regulate their mechanical stiffness depending on their intracellular roles. Although a number of groups measured their persistence length to find out the regulation mechanism, measured values and stiffening/softening factors varied significantly. To elucidate reasons of the discrepancy, we investigated effects of localization precision of microtubule shape and microtubule growth rate on persistence length determination. As a result, we found the nanometer-level localization precision was required to minimize the measurement error. Simultaneous measurement of growth rate and persistence length by using the measurement method revealed that the persistence length is constant below a threshold of growth rate, ~1.0 um/min, and decreases above the threshold.

2Pos040 アルカリ条件下におけるカロテノイドと古細菌脂質の結合に伴うハロロドプシンの熱安定化

Thermal stabilization of Halorhodopsin by binding carotenoid and archaeal lipids under alkaline condition

Kenichi Takeda[1], Takashi Kikukawa[2], Makoto Demura[2], Takanori Sasaki[1] ([1]*Grad. Sch. Adv. Math. Sci., Meiji Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*)

Halorhodopsin from N. pharaonis (NpHR) binds archaeal lipids and a carotenoid of bacterioruberin (BR) on the membrane. In this study, we researched the effect of binding BR and archaeal lipids to the thermal stability of NpHR. In particular, thermal bleaching ratios for NpHR obtained by E.coli expression system (eNpHR), artificial eNpHR-BR complex, and NpHR-BR-lipid complex from N.pharaonis membrane were compared in the anion-free, pH 8.5 condition. Although eNpHR and eNpHR-BR showed about 52% and 20% of bleaching at 40 °C for 1h, NpHR-BR-lipid did not show bleaching until 45 °C. In addition, about 50% of bleached NpHR-BR-lipid at 45 °C recovered the active state rapidly by addition of NaCl. These results suggest that BR and archaeal lipids contribute to stabilize NpHR.

2Pos041 酵素処理が LDL の物性に与える影響

Effect of enzymes treatment on physical properties of low-density lipoprotein

Seiji Takeda[1], Agus Subagyo[2], Shu-Ping Hui[1], Hirotoshi Fuda[1], Kazuhisa Sueoka[2], Hitoshi Chiba[1] ([1]*Faculty of Health Sci, Hokkaido Univ.*, [2]*Grad Sch of Inf Sci and Tech, Hokkaido Univ.*)

Oxidation of the low-density lipoproteins (LDLs) induce development of cardiovascular disease. Recently, we reported that elastic modulus of LDL is decreased by its metal oxidation by atomic force microscopy (AFM). However, the mechanism of the decreasing of the elastic modulus is not well investigated. We postulated that the disorder of the structure of the LDL might contribute the decreasing of the elastic modulus. In this study, to clarify the mechanism, we measured the elastic modulus of LDL before and after incubation with V8 protease, alpha-chymotrypsin and phospholipase A2 by AFM. We would like to discuss the effect of enzyme treatment on the physical properties of LDL.

2Pos042 一価陽イオン溶液におけるリゾチームの回転及び並進拡散運動に基づくビリアル係数

The virial coefficients based on the rotational and translational diffusions of lysozyme in the monovalent cation solutions

Yudai Katsuki[1], Akane Kato[1], Etsuko Nishimoto[2] ([1]*Grad. Sch. Bioresour. Bioenviron. Sci., Kyushu Univ.* , [2]*Fac. Agr., Kyushu Univ.*)

Osmotic second virial coefficient (B_{22}) originally indicates the solute-solute interaction is now applied to the important criterion for the protein crystallization. In the last session, we introduced second and third virial coefficients based on the rotational diffusion analysis of lysozyme to describe the protein-protein interaction and to establish the criterion for the protein crystallization. In the present studies, we obtained B_{22} due to the lysozyme-lysozyme interaction in the buffer solution including various monovalent cations by precise measurements of static light scattering. The results were examined and compared with B_{22} estimated by the fluorescence depolarization studies keeping the protein interaction potential determines the radial distribution in view.

2Pos043 時間分割スペクトルによるヒト血清アルブミンの Trp214 残基周辺の水和状態に対する１価陽イオンの影響の解析

Effect of monovalent cation on the hydration state near Trp214 of human serum albumin revealed by the time-resolved fluorescence spectrum

Shoutaro Kubo[1], Etsuko Nishimoto[2] ([1]*Grad. Sch. Bioresour. Bioenviron. Sci., Kyushu Univ.* , [2]*Fac. Agr., Kyushu Univ.*)

Protein stability and interactions with small molecules would be influenced by the hydration of proteins surface. However, the detail has not been cleared because analyzing methods is limited. Trp residue is a powerful probe for studying the protein hydration because it shifts the fluorescence maximum according to the interaction with surrounding water molecule(s). The time required for the spectral shift can reveal well the hydration state around Trp. Here, we studied the hydration dynamics around Trp214 of HSA in the presence of various concentration of monovalent cation by measuring the time-resolved fluorescence spectrum based on global analysis of TCSPC over the full spectral region. Furthermore, the correlations with the ligand binding were investigated.

2Pos044 *Archaeoglobus fulgidus* ferritin assembly studied by time-resolved small-angle X-ray scattering

Daisuke Sato[1], Yuta Okada[2], Boyce Hong Ping Law[3], Ambrish Kumar[3], Sierin Lim[3], Masamichi Ikeguchi[1,2] ([1]*Fac. Sci. and Eng., Soka Univ.*, [2]*Dept. Bioinfo., Gra. Sch. Eng., Soka Univ.*, [3]*Sch. Chem. and Biomed. Eng., Nanyang Tech. Univ., Singapore*)

Ferritins are iron storage proteins present in most organisms. They share a hollow spherical structure consisting of 24 subunits with 4/3/2 symmetry. Unlike other ferritins, *Archaeoglobus fulgidus* ferritin (AfFtn) has a unique structure with large triangular holes. Interestingly, K150A/R151A mutant (AfFtnAA) has a closed shell structure like other ferritins. Both apo wild-type AfFtn and apo AfFtnAA dissociated to dimers under low ionic concentration, while they form the 24-mer under high ionic concentration. We investigated the salt-induced assembly of the two proteins using small-angle X-ray scattering (SAXS). The structural difference between AfFtn and AfFtnAA was confirmed by SAXS. Kinetic experiments showed that the assembly of AfFtnAA was faster than that of AfFtn.

2Pos045 キチン結合タンパク質(CBP21)の構造安定性に対する銅イオンの効果

Effects of copper ions on the structural stability of chitin-binding protein 21

Hayuki Sugimoto[1], Erina Katagiri[1], Akiyoshi Tanaka[2], Takeshi Watanabe[1], Kazushi Suzuki[1] ([1]*Fac. Agri., Niigata Univ.*, [2]*Grad. Sch. Bioresources, Mie Univ.*)

Chitin-binding protein 21 (CBP21), a lytic polysaccharide monooxygenase, is a promising resource for efficient processing of chitin biomass. CBP21 contains a copper ion binding site. The copper ion is essential for catalysis. Effects of copper ions (Cu^{2+}) on the structural stability of CBP21 were elucidated by measuring the thermal unfolding of CBP21. The unfolding temperature $t_{1/2}$ of apoCBP21 was 65.3°C (pH 5). Addition of Cu^{2+} to apoCBP21 solution increased $t_{1/2}$ by 9°C. The value of $t_{1/2}$ did not increase with increasing Cu^{2+} concentration. Similar results were obtained in the case of urea-induced unfolding. These results suggested that CBP21 was substantially stabilized by binding of Cu^{2+} and that the dissociation of Cu^{2+} was not involved in the unfolding process.

2Pos046 競争的凝集形成機構に基づいた蛋白質異常凝集の理解

Understanding of aberrant protein aggregation based on the competitive aggregation mechanism

Masayuki Adachi, Masatomo So, Yuji Goto (*Inst. Protein Res., Osaka Univ.*)

Although many diseases are associated with protein aggregation, the mechanism is far from clear. With β2-microglobulin, we focused on the effects of heating on amyloid fibrillation. At pH 2.0 under low salt concentrations, heating-induced fibrillation occurred at a certain temperature. Then, fibrils were degraded at higher temperature. Upon heating under high salt concentrations, preformed amorphous aggregates were transformed to fibrils and then degraded. These results suggest that fibrils formed coupled with dissolution of amorphous aggregates and that further increase in temperature degraded fibrils. Finally, we discuss that relationship between the effects of salt and temperature on the basis of a salt concentration- and temperature-dependent phase diagram.

2Pos047 時間分割蛍光測定による生体防御タンパク質 momorcharin のアンフォールディング/リフォールディング中間体に関する研究

The time-resolved fluorescence studies on the unfolding and refolding intermediate state of defense-related protein, momorcharins

Chie Matsunaga[1], Etsuko Nishimoto[2] ([1]*Grad. Sch. Bioresour. Bioenviron. Sci., Kyushu Univ.* , [2]*Fac. Agr., Kyushu Univ.*)

In many trials to elucidating the protein folding/unfolding mechanism, it is most essential to characterize the conformation of the intermediate because it connects structural features of the folding/unfolding states. The fluorescence of Trp-residure in protein has provided valuable information on the protein folding/unfolding intermediate through reflecting the subtle changes in interactions and dynamics of Trp. In addition, we lately proposed the change in protein hydration state as characteristics of the refolding /unfolding intermediate of protein which is revealed in the time-resolved emission spectrum (TRES) of Trp. TRES of momorcharins were reconstituted using the experimental date in the fluorescence decay kinetics in TCSPC over the full-spectrum region.

2Pos048 ストップトフロー過渡回折格子法のタンパク質変性反応への適用

Application of stopped-flow TG method to denaturation dynamics of a photosensory protein

Shunki Takaramoto, Yusuke Nakasone, Masahide Terazima (*Dep. Chem., Sch. Sci., Kyoto Univ.*)

By combining the transient grating (TG) method with a stopped-flow system (stopped-flow TG (SF-TG)), we constructed a new system to detect protein reactions which are not triggered by photoexcitation. As an example, we will present a result of denaturation dynamics of a photosensory protein (photo1LOV2-linker) triggered by a pH jump using the SF-TG method. We measured the kinetic trace of the pH induced denaturation of the protein as a decrease of number of photoreactive molecule. The data showed that the unfolding underwent at least two steps. We suggested that a local structure of the LOV domain denatured to decrease the reactivity in the early event, whereas the helical structure of linker region unfolded in the latter event.

2Pos049 **テトラヒメナ外腕ダイニンにおける変異導入システムの確立とα重鎖Pループの機能**

Establishment of a mutation system in *Tetrahymena* outer arm dynein and P-loop functions of the alpha heavy chain (Dyh3p)

Masaki Edamatsu (*Dept. Life Sci., Grad. Sch. Arts Sci., Univ. Tokyo*)

Axonemal dyneins are large AAA+ type motor proteins that exhibit unique motor properties during ciliary beating. This study established a mutation system for *Tetrahymena* outer arm dynein and characterized four nucleotide-binding loops (P1-P4) in the alpha heavy chain (Dyh3p). Transformation experiments showed that nucleotide-binding at the P1 and P2 sites but not the P3 or P4 sites was required for intracellular function of Dyh3p. In addition, an *in vitro* motility assay showed that the P3 mutation but not the P4 mutation abolished motor activity of Dyh3p. This mutation system will be useful for further molecular studies of diverse axonemal dyneins and ciliary motility.

2Pos050 **Identification of residues in SecM that are responsible for stabilizing the translation arrest**

Mikihisa Muta, Ryo Iizuka, Takashi Funatu (*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*)

SecM, a bacterial secretion monitor protein, contains a specific amino acid sequence at its C-terminus called arrest sequence, which interacts with the ribosomal tunnel and arrests its own translation. It has been widely believed that the sequence is sufficient and necessary for translation arrest. However, we have found that the nascent SecM chain outside the ribosome stabilizes the translation arrest. In this study, we performed alanine-scanning mutagenesis to identify residues responsible for the stabilization. Of these residues, positively-charged residues (His84, Arg87 and Arg91) significantly contribute to the stability of the translation arrest, suggesting that these residues associate with negatively-charged ribosomal surface.

2Pos051 **TnaC翻訳アレスト中のリボソームにおける解離因子の作用**

Action of release factors on the stalled ribosome during translation of TnaC

Tomoki Shinozawa, Ryo Iizuka, Zhuohao Yang, Takashi Funatsu (*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*)

The *Escherichia coli* TnaC is a leader peptide of the tryptophanase (*tna*) operon and regulates expression of the downstream genes in response to the cellular concentration of tryptophan. Under low concentration of tryptophan, translation of TnaC is terminated at the stop codon (UGA) by release factor 2 (RF2). In contrast, when the concentration is high, the translating ribosome is stalled at the stop codon and peptide release by RF2 is inhibited, enabling the downstream gene expression. Interestingly, we found that release factor 1 (RF1) efficiently recognizes the non-cognate stop codon to release TnaC peptide from the stalled ribosome. In the meeting, we will discuss the action of RF1 and RF2 on the stalled ribosome during translation of TnaC.

2Pos052 **A single-molecule kinetic analysis of ATP hydrolysis and substrate degradation by the 26S proteasome**

Akira Sato, Takahiro Saito, Takashi Okuno (*Grad. Sch. Sci., Univ. Yamagata*)

The 26S proteasome (26S) is a huge protease that degrades polyubiquitinated proteins. To degrade a substrate protein, ATP hydrolysis reaction must be coupled at AAA subunits located in regulatory particle of 26S. The relationship between substrate degradation and ATP hydrolysis has not been cleared. The binding of fluorescence labeled ATP (FL-ATP) to the 26S was monitored by TIRFM. Cumulative dwell time distribution could be fitted satisfactorily with a double exponential decay function. Interestingly, the ATPγS inhibits only the long-lived dwell time (694 ms), but not short one. This result suggested that releasing of FL-ATP is directly dependent of hydrolysis of ATP binding other subunit. We will discuss about binding property of modeled substrate protein to the 26S.

2Pos053 **大腸菌で生産される *Pyrovaculum islandicum* 由来グルタミン酸脱水素酵素の活性に対するFK506結合タンパク質の影響**

Effect of FK506 binding protein in the activity of glutamate dehydrogenase from *Pyrovaculum islandicum* produced in *Escherichia coli*

Shuichiro Goda, Junpei Yagi, Hideaki Unno, Tomomitsu Hatakeyama (*Grad. Sch. of Eng., Nagasaki Univ.*)

Glutamate dehydrogenase from *Pyrovaculum islandicum* (Pis-GDH) produced in *Escherichia coli* showed almost no activity and the enzymatic activity was fully activated by heating at 90°C for 15 min. To analyze the effect of the temperature for the folding of Pis-GDH, heat activated Pis-GDH was denatured in 6 M GuHCl and refolded in 4°C. Refolded Pis-GDH showed enzymatic activity same as active enzyme. Then, to analyze the effect of chaperone, Pis-GDH was co-expressed with FK506 binding protein from *Thermococcus* sp. KS-1 (TcFKBP). Co-produced Pis-GDH showed relatively high activity than without TcFKBP. TcFKBP has peptidyl-prolyl cis-trans isomerase activity. This result suggests that the isomerization of proline affects the enzyme activity of Pis-GDH produced in *E. coli*.

2Pos054 **[NiFe]ヒドロゲナーゼの活性準備状態 Ni-SI_r と活性状態 Ni-SI_a 間の酸塩基平衡機構の解明**

Elucidation of the acid-base equilibrium mechanism between the ready Ni-SI_r and active Ni-SI_a states of [NiFe] hydrogenase

Hulin Tai[1,2], Liyang Xu[1], Koji Nishikawa[3], Yoshiki Higuchi[2,3], Shun Hirota[1,2] ([1]*Grad. Sch. Mater. Sci., NAIST*, [2]*CREST, JST*, [3]*Grad. Sch. Life Sci., Univ. Hyogo*)

[NiFe] hydrogenase is a metalloenzyme which catalyzes the interconversion of H_2 and $2H^+ + 2e^-$. The acid-base equilibrium between the ready Ni-SI_r and active Ni-SI_a states is a common feature among [NiFe] hydrogenases, but its mechanism remains unrevealed. We have shown that the Ni-SI_r state is photo-activated to its Ni-SI_a state by light irradiation with a laser at 514.5 nm (H. Tai *et al*. *PCCP* 2016). The light-induced Ni-SI_a state converted back to the Ni-SI_r state when light irradiation was stopped at 173-203 K. The reconversion rate was ~10 times faster at pH 8.5 compared to that at pH 8.0, where the increase was caused by the increase in the activation entropy. These results provide new insights into the acid-base equilibrium of [NiFe] hydrogenase.

2Pos055 Zymoseptoria tritici 真菌チューブリンは異常な特性を有する
Zymoseptoria tritici fungal tubulin has unusual properties

Douglas Drummond[1], Naomi Sheppard[2], Robert Cross[2] ([1]*Kyushu Univ.*, [2]*Univ. of Warwick, UK*)

We have purified tubulin from the filamentous fungus *Zymoseptoria tritici* that causes Septoria leaf blotch, an economically important disease of wheat crops. Preliminary observations suggest that purified *Z. tritici* tubulin assembles at high concentrations into microtubule like structures that are more resistant to disassembly at cold temperatures and in calcium ion solutions than microtubules assembled from yeast or mammalian tubulins. Thus, despite high levels of protein sequence similarity to other tubulins, *Z. tritici* tubulin appears to have distinct functional properties.

2Pos056 Spectroscopic studies of hydrogen sensing [FeFe] hydrogenase from *Thermotoga maritima*

Nipa Chongdar[1], Krzysztof Pawlak[1], James A. Birrell[1], Wolfgang Lubitz[1], **Hideaki Ogata**[1,2] ([1]*MPI CEC*, [2]*ILTS Hokkaido Univ.*)

Hydrogenases catalyze the reversible oxidation of hydrogen.They have been classified into three groups, [NiFe], [FeFe] and [Fe]-only hydrogenases based on the metal content at the active sites. Among them the prototypical [FeFe] hydrogenases are well-known for their high turnover frequencies for H_2 production.
Distinct feature of the sensory [FeFe] hydrogenases is the presence of a PAS (Per-Arnt-Sim) signalling domain, at the C-terminus. Also, in contrast to prototypical and electron-bifurcating [FeFe] hydrogenases, identities of amino acids residues at the active site H-cluster binding pocket in sensory type [FeFe] hydrogenase vary at some positions. We will present FT-IR spectroscopic characterization of the putative sensory [FeFe] hydrogenase from *Thermotoga maritima*.

2Pos057 線虫 Cytochrome b_{561} ホモログ・Cecytb-2 の分子機能解明
Elucidation of the molecular function of *Caenorhabditis elegans* Cecytb-2, a cytochrome b_{561} homologue

Mika Fujimura, Masahiro Miura, Tetsunari Kimura, Motonari Tsubaki (*Dept. of Chem., Grad. Sch. Sci., Kobe Univ.*)

Cytochrome b_{561} is a heme protein residing in neuroendocrine vesicles and regenerates ascorbate. In higher animals, there are 6 homologues belonging to the b_{561} family. One of them, Dcytb is a ferric reductase localized in the duodenum. Among 7 b_{561} homologues in *C. elegans*, Cecytb-2 is most similar to Dcytb and is specifically expressed in digestive organs. In this study, we attempted to clarify the iron-binding site of Cecytb-2 for functioning as a ferric reductase. We have introduced several mutations around the putative iron-binding site and expressed the mutants using *Pichia pastoris* system. We attempted to measure the ferric reductase activity of the purified protein in a solubilized micellar condition.

2Pos058 Theoretical study on light-activation mechanism of LOV photoreceptor protein

Masahiko Taguchi, Cheng Cheng, Chika Higashimura, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

It is important to receive light for plants and bacteria which is responsible for photosynthesis. LOV domain which exists in light-receptor site is a protein complex with FMN as a chromophore. Light absorption of FMN leads to an adduct formation between FMN and a cysteine, followed by dissociation of an α-helix, which initiates the signal transduction. As a result, a variety of light-receiving activation movements of plants -changes in the chloroplast, control of the pore movement, and phototropism- occur. In addition, recently, this LOV domain is expected for application of optogenetics, i.e., control of biomolecular and cellular activities by light. We carried out free energy geometry optimizations with QM/MM RWFE-SCF method and found the detailed molecular structure.

2Pos059 複数のアミロイド性ペプチドの混在する複雑な系におけるアミロイド線維形成機構
Amyloid Fibrillation in Promiscuous Systems Containing Various Amyloidgenic Peptides

Hiroya Muta[1], Masatomo So[1], Kazumasa Sakurai[2], Yuji Goto[1] ([1]*IPR, Osaka Univ.*, [2]*Inst. of Advan. Tech., Kindai Univ.*)

Amyloid fibrils form in supersaturated solutions through a nucleation and growth mechanism. While there are many studies addressing amyloid fibrillation of a single peptide, fibrillation in promiscuous systems containing various peptides has been obscure. As a model under a promiscuous system, we studied fibrillation of a mixture of proteolytic fragments (K1 to K9) of β2-microglobulin, a protein associated with dialysis-related amyloidosis. Among the nine fragments, K3 formed fibrils easily with a short lag time. Solution NMR combined with kinetic measurements revealed that the peptide-peptide interactions among the fragments retarded the fibrillation of K3. This is a typical example that intermolecular interactions inhibit fibrillation in a promiscuous system.

2Pos060 機械学習を用いたシミュレーションと実験の統合によるタンパク質ダイナミクス解析
Linking single-molecule experiment and simulation of protein dynamics by machine learning

Yasuhiro Matsunaga[1,2], Yuji Sugita[1,3,4] ([1]*RIKEN AICS*, [2]*JST PRESTO*, [3]*RIKEN TMS*, [4]*RIKEN QBiC*)

Single-molecule experiment and molecular dynamics (MD) simulation are indispensable tools for investigating protein conformational dynamics. Here we devise a machine learning algorithm to link the two approaches and construct an atomically detailed and experimentally consistent model of protein dynamics. It is applied to the folding dynamics of a dye-labeled WW domain of the formin-binding protein. MD simulations over 400 microseconds led to an initial Markov state model, which was then refined using single-molecule FRET time-series data through hidden Markov modeling. The refined model reproduces experimental FRET efficiency and features hairpin 1 in the transition-state ensemble, consistent with mutation experiments.

2Pos061 ヒドロゲナーゼ/シトクローム c_3 間電子移動における静電相互作用の役割

Role of the electrostatic interactions in the electron transfer from [NiFe] hydrogenase to cytochrome c_3

Yu Sugimoto[1], Yoshitaka Moriwaki[1], Thoru Terada[1], Kenji Kano[2], Kentaro Shimizu[1] ([1]*Grad. Sch. of Agri. and Life Sci. Univ. of Tokyo*, [2]*Grad. Sch. of Agri. Kyoto Univ*)

Electrostatic interactions between proteins are key factors of protein-protein association and its reaction rate. We determine the second-order reaction rate constant (k) of electron transfer from [NiFe] hydrogenase (H_2ase) to cytochrome (cyt) c_3 at various ionic strengths (I). The k value decrease with I. The crystal structures of the proteins indicate that almost the entire surfaces of the proteins have positive potentials, which may cause increase of the k value with I. However, there exists a small region with negative potential on the surface of H_2ase at which the electron transfer from H_2ase to cyt c_3 may occur. Therefore, the local electrostatic interactions between H_2ase and cyt c_3 determine the reaction rate of the electron transfer between them.

2Pos062 X 線 1 分子追跡法による TRPV1 チャネルの分子運動解析

3D MOTION MAPS OF TRPV1 CATION CHANNEL DEPICTED BY DIFFRACTED X-RAY TRACKING METHOD

Kazuhiro Mio[1], Keigo Ikezaki[2], Masahiro Kuramochi[2], Hiroshi Sekiguchi[3], Tai Kubo[1], Yuji C. Sasaki[2] ([1]*OPERANDO-OIL, AIST*, [2]*Frontier Science, Univ. of Tokyo*, [3]*JASRI*)

TRPV1 is a nonselective cation channel that responds to various signals. To understand the gating mechanisms of TRPV1, we adopted the Diffracted X-ray Tracking (DXT) technique, in which individual protein was labeled with gold nanocrystals and the motion of X-ray diffraction spots from the gold crystal were investigated as intramolecular movement in real time. Purified TRPV1 was immobilized on the Ni-NTA coated polyimide substrates and the motion was three dimensionally (tilting, rotation, and time) analyzed. Brownian motion of outer helices was enhanced by capsaicin in dose dependent manner, detected as anisotropic rotation movement around the particle reflecting channel gating process. This was further compared to the high temperature evoked TRPV1 activation.

2Pos063 高次構造に特異的な人工タンパク質を用いた抗体医薬品の品質評価モニタリング

Quality control monitoring of therapeutic antibodies based on an artificial protein specific for higher order structures of IgG

Hideki Watanabe[1], Seiki Yageta[1,2], Hiroshi Imamura[1], Shinya Honda[1,2] ([1]*BMRI, AIST*, [2]*Grad. Sch. of Frontier Sci., The Univ. of Tokyo*)

Ideal quality control of therapeutic antibodies involves analytical techniques with high-sensitivity, high-resolution, and high-throughput performance. Few technologies, however, meet all the required demands. We developed a biosensing method for the quality control of therapeutic antibodies based on an artificial protein, AF.2A1, which discriminates between the native and non-native three-dimensional structures of immunoglobulin G (IgG). AF.2A1 was applicable to quantification of non-native IgG formed under various pH conditions and accelerated tests of the long-term stability of IgG. AF.2A1, capable of being combined with established methods, provides the potential for quality control monitoring with high-sensitivity, high-resolution, and high-throughput performance.

2Pos064 チオフラビン T とアミロイド β 凝集体の結合：蛍光寿命測定による解析

Thioflavin T binding to amyloid-beta peptide aggregates: Analyses with fluorescence lifetime measurements

Akinori Oda, Hiroshi Satozono, Tomomi Shinke (*Hamamatsu Photonics K. K.*)

Thioflavin T (ThT) is widely used for detecting amyloid-beta peptide (Aβ) aggregates. Nevertheless, the detail of binding mode of ThT to Aβ aggregates is not fully understood. We have demonstrated that the fluorescence decay of ThT binding to $A\beta_{1\text{-}42}$ aggregates can be decomposed into three exponential components with different fluorescence lifetimes. In this study, we found that the longest lifetime component was quenched in ThT high concentration condition. Time-resolved fluorescence spectroscopy in this condition showed ThT excimer fluorescence which has its emission peak at about 550 nm in long lifetime region. These results suggest that, in high concentration condition, two ThT molecules can simultaneously bind to the same binding site of $A\beta_{1\text{-}42}$ aggregates.

2Pos065 タンパク質間相互作用観測を目指した蛍光相関分光装置の開発

Development of Fluorescence Correlation Spectrometer for the Elucidation of Protein Interactions

Asami Izaki[1,2], Hiroyuki Oikawa[1,2], Takeshi Tomita[3], Satoshi Takahashi[1,2] ([1]*IMRAM, Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*, [3]*Dept. Pharmacol., Tokyo Women's Medical Univ.*)

We constructed a device for fluorescence correlation spectroscopy (FCS) to investigate the interaction between chaperonin and substrate proteins and that between serum amyloid A3 (SAA3) and toll like receptor. FCS is a powerful method to obtain diffusional properties of samples by observing fluorescence intensity fluctuations in the micro detection volume. We utilized a simple confocal optics combined with single hybrid photodetector, which enables us to detect correlation data without the afterpulse effect up to sub-microsecond range. We confirmed that the FCS data obtained by the system could be used to analyze a sample with two components having different hydrodynamic radii. Currently, labeled-SAA3 preparation for the FCS analysis is ongoing.

2Pos066 Influence of the PYP domain on Photoreaction of the phytochrome domain in Ppr

Jia Siang Sum, Yoichi Yamazaki, Yugo Hayashi, Hironari Kamikubo (*Grad. Sch. of Mater. Sci., NAIST*)

PYP-phytochrome-related (Ppr) is a member of a bacteriophytochrome (Bph) superfamily. Ppr contains *p*-coumaric acid and biliverdin as chromophores, which are located in PYP-like domain and phytochrome (Phy) domain, respectively. Well-known Bphs undergo structural changes during photoconversion between Pr and Pfr but no obvious structural difference is observed between Pr and Pfr of Ppr. We expect the extra domain of PYP plays a role to mediate the structural changes, but it remains unclear. To investigate the role of PYP in Ppr, we prepared mutants lacking the PYP domain. Spectroscopic measurements revealed that the decay rate from Pfr to Pr are different between WT and mutants, indicating that PYP domain influences the Phy domain to perturb the chromophore environment.

2Pos067 分子動力学シミュレーションによるβシート凝集の自由エネルギー解析

Free energy analysis of β-sheet aggregation by molecular dynamics simulation

Keiichi Masutani, Kang Kim, Nobuyuki Matubayasi (*Graduate School of Engineering Science, Osaka University*)

Amyloid aggregation has β-sheet conformation and is considered to be a cause of amyloidosis diseases. In the field of protein engineering, the aggregation of the expressed protein often results in the inclusion bodies, which is not suitable for a large-scale protein expression. We focused on NACore, which corresponds to the 68th to 78th residue of α-synuclein. This is considered as a causal substance of Parkinson's disease and is the key region of aggregation. Molecular dynamics simulations of its aggregate in water are carried out to study the structures and relative stabilities of the aggregates. The effect of added urea was further addressed, and it is shown that urea suppresses the tendency of aggregation by orders of magnitude in terms of the protein concentration.

2Pos068 赤色蛍光タンパク質, Akane families (*Scleronephthya gracillima*) の緑と赤の蛍光は海域によらない共通特性

Common properties of red fluorescent protein Akane families having green and red emissions irrespective of ocean areas

Yuko Kato[1,2], Ikki Fujimoto[2], Yukimitsu Imahara[3], Mitsuru Jimbo[4], Kei Amada[2], Toshio Yamaguchi[1], Shu Nakachi[3] ([1]*Univ. Fukuoka*, [2]*Fukuoka Inst. Tech.*, [3]*Kuroshio Bio Research*, [4]*Univ. Kitasato*)

Akane families are RFP (red fluorescent protein) separated from octocoral, *Scleronephthya gracillima*. They have HYG chromophore like Kaede and *Dendronephthya* to emit green and red fluorescence. In this study, we have studied 4 types based on the slight differences in color in life which are capable of dual fluorescent emissions in different ocean areas. As a result, the following common properties have been observed for the octocorals.
(1) Akane families first emit green fluorescence, followed by emission of red fluorescence. In another ocean area, the octocoral also shows two emissions of green (490~510 nm) and red (590~638 nm) fluorescence.
(2) pH dependence of the octocorals on the emission property is discussed.

2Pos069 PF-AR NW12A における顕微分光装置の開発

The development of spectroscopic system for UV-visible absorption at PF-AR NW12A

Masahide Hikita[1], Yusuke Yamada[1], Masahiko Hiraki[2], Naohiro Matsugaki[1], Toshiya Senda[1] ([1]*PF/SBRC, IMSS, KEK*, [2]*Mechanical Engineering Center, Applied Research Laboratory, KEK*)

In the functional analysis of proteins, it is essential to know the crystal structure at the atomic level and its electronic and chemical changes. Spectroscopy is the effective technique for detecting the structural states of proteins, even within crystals. Therefore, spectroscopic analysis has been complementarily combined with X-ray diffraction studies to evaluate the protein status. In the spectroscopy, UV-visible absorption spectroscopy is more readily available and effective for detecting structural states of proteins. In order to measure the UV-visible absorption spectrum of protein crystals, the spectroscopic system is currently developing at the macromolecular crystallography beamline, PF-AR NW12A. Here, the progress of the spectroscopic system will be reported.

2Pos070 理想タンパク質の安定性のオリジンを探る

Stability for de novo designed ideal proteins revisited

Mami Yamamoto[1,2], Rie Koga[1], Takahiro Kosugi[1,2], Nobuyasu Koga[1,2,3] ([1]*IMS, CIMoS*, [2]*SOKENDAI*, [3]*JST, PRESTO*)

We designed ideal protein structures completely from scratch, in which secondary structure and loop lengths are optimized for folding. Most of the designs are very stable: their melting temperatures(Tm) > 100C. To elucidate the factors for such high stability, multiple mutations of the designs are conducted. Hypothesizing the number of carbon atoms in the core is a key to the stability, large hydrophobic amino acids were mutated to small hydrophobic ones, which were investigated for how the stability changes. These mutations certainly impaired the stability. However, the mutant in which all Leu and Ile are changed to Val was found to be monomer and form tertiary structure in solution, and the Tm was above 100C, implying the optimized backbones hold the high stability.

2Pos071 エングレイルドホメオドメインを用いた新たな転写因子の設計

Designing a new artificial transcription factor based on engrailed homeodomain

Tomoko Sunami, Hidetoshi Kono (*QST*)

Widely used genome editing enzymes such as TALEN and CRISPR have a relatively high molecular weight. To develop a novel genome editing enzyme with smaller molecular weight, we have focused on engralied homeodomain protein. The wild type of engrailed homeodomain recognizes AT-rich six bps. To create a protein that can recognize longer DNA sequences, we connected two homeodomains with a linker of different lengths. The activities and binding-sequence profiles of them were assessed by bacterial-one hybrid assay and EMSA assay. They showed a good activity for the target sequence, however, they also bound to undesired sequences. We designed some mutants to avoid undesired binding and characterized them. We present how such mutations changes binding-profiles.

2Pos072 タンパク質へのワンポット飽和変異導入におけるヌクレオチドとアミノ酸のバイアス

Bias in nucleotides and amino acids in one-pot saturation mutagenesis of protein

Akasit Visootsat[1], Fumihiro Kawai[2], Akihiko Nakamura[2,3], **Ryota Iino**[1,2,3] ([1]*IMS, NINS*, [2]*OIIB, NINS*, [3]*SOKENDAI*)

Here we developed a method of one-pot saturation mutagenesis of protein. Our method consists of PCR with mixed primers of NNN codons, DpnI treatment, SLiCE reaction and transformation. As proof of principle, we applied our method to a non-fluorescent GFP mutant, GFPmut3(Y66H). After transformation, 2.2% of colonies showed fluorescence, indicating gain-of-function mutation (H66Y). Then, to measure fractions of 4 nucleotides (ATGC) incorporated quantitatively, all colonies were collected and analyzed by deep sequencing. As results, we found that fractions of T and G were much higher than those of A and C, and this bias resulted in high fractions of Val (15%), Leu (12%), Phe (12%) and Gly (11%) among 20 amino acids. Now, we are investigating the cause to improve the bias.

2Pos073 天然に存在しないフォールドを持つタンパク質の合理的デザイン

Rational design of new fold proteins yet-unexploited in nature

Shintaro Minami[1], Rie Koga[1], George Chikenji[2], Nobuyasu Koga[1,3] ([1]*CIMoS, IMS*, [2]*Grad. Sch. of Eng., Nagoya Univ.*, [3]*PRESTO, JST*)

Recently, we have succeeded in designing proteins with various shapes based on our discovered design rules. However, the designed proteins are only those with naturally observed folds, and it is still unclear whether it is possible to create new fold proteins that do not exist in nature. Here, we attempted rational design of new fold proteins. Based on the knowledge gained by analysis of the known protein structures, we found several target folds which are not present in nature but are expected to be able to design. For these targets, we designed amino acid sequences from scratch. In the presentation, we will present the computational designs together with experimental results.

2Pos074 多様な all-α タンパク質のデザイン

Design of diverse all-α proteins

Koya Sakuma[1,2], Rie Koga[2], Takahiro Kosugi[1,2], Nobuyasu Koga[1,2,3] ([1]*SOKENDAI*, [2]*CIMoS, IMS*, [3]*JST, PRESTO*)

Naturally occurring protein structures like Globin tell us that structural diversity of all-α proteins remains to be explored by protein designers. To reach more complex de-novo all-α structures, we identified 18 helix-loop-helix motifs and computationally generated myriad all-α backbone conformations with 5, 6 or 7 α-helices connected by these typical loop motifs. Selecting backbones with new topologies, we designed amino-acid sequences that show funnel-like energy landscape in-silico. As for a topology named fold-0, we found that 6 out of 10 design sequences have α-rich secondary structures by CD and fold into specific tertiary structures as monomers by ^{15}N HSQC-NMR and SEC-MALS.

2Pos075 水酸化酵素 PHBH の没食子酸産生変異体の構築とその理論的考察

Modification of *p*-Hydroxybenzoate to produce gallic acid and its theoretical insight

Yoshitaka Moriwaki[1], Tohru Terada[2], Kentaro Shimizu[1] ([1]*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [2]*Agri. Bioinfo. Res. Unit, Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

p-Hydroxybenzoate hydroxylase (PHBH) catalyzes the hydroxylation of *p*-hydroxybenzoate (*p*-OHB) to 3,4-dihydroxybenzoate (3,4-DOHB). It does not catalyzes the reaction for 3,4-DOHB despite that it can bind 3,4-DOHB. Previously, we created a mutant, L199V/Y385F, that can convert 3,4-DOHB into 3,4,5-trihydroxybenzonate (gallic acid). To get insight into the mechanism underlying the substrate specificity, we performed MD simulations and QM/MM calculations for the wild-type and mutant proteins. We found that the H-bond network between the reaction site and the solvent was altered by the mutations, and that the peroxide group attached to flavin came close to the substrate in the mutant. Thus, indirect interactions contribute to determining the substrate specificity of PHBH.

2Pos076 可逆的光架橋プローブを用いた翻訳の制御

Photo-control of the ribosome movement along mRNA using a reversible photo-crosslinking probe

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Here, we present a method to control the movement of ribosome along mRNA. This method requires only a DNA oligonucleotide containing a 3-cyanovinylcarbazole nucleoside, which serves as a reversible photo-crosslinker. The oligonucleotide is covalently crosslinked to mRNA with its complementary sequence by irradiation at around 366 nm, stopping ribosomal movement. The ribosome would restart to move when the crosslinking is cleaved upon irradiation at around 312 nm. We performed a proof-of-concept experiment to demonstrate the feasibility of our method. Using this method, we are now trying to investigate the dynamic movement of ribosome during translation at a single-molecule level.

2Pos077 カルモジュリン融合・共発現系を用いた抗菌ペプチド fowlicidin 大量生産法

Mass production of fowlicidin, a cathelicidin antimicrobial peptide by a calmodulin-peptide fusion and coexpression system

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Antimicrobial peptides (AMPs) are essential in innate immunity. AMPs have the potential to be the candidate of new drugs. Recombinant AMPs are rarely expressed in E. coli because of their toxicity to the host or digestion by protease. In previous works, it was succeeded that peptide is expressed a lot with calmodulin as a fusion protein (Ishida et al., J. Am. Chem. Soc. 2016). This overexpression system is suitable for various AMPs. However, fowlicidin, a chicken cathelicidin was also expressed but moderately. In this research, another calmodulin was added to the plasmid as coexpression partner. The result showed the total amount of fowlicidin was increased. Because it is estimated that the toxicity was reduced, we are investigating the mechanisms.

2Pos078 Some factors that make a structure of a beta-sheet protein more designable

Hayao Imakawa[1], Nobuyasu Koga[2], George Chikenji[1] ([1]*Dept. of App. Phys., Nagoya Univ.*, [2]*CIMoS, IMS*)

Recently, de novo protein design (i.e. identifying the amino acid sequences that fold into a given target structure guided by physics) has remarkable progress. One of the most important problems for success is absence of procedure to select a designable target structure rationally. Therefore, it is selected intuitively by human hands, and there is no guarantee that it is always designable. Thus, a criterion to select a designable target structure correctly is needed. In this study, we take statistics on features of beta-sheet (e.g. strand length), and developed the criterion from it to select designable target structure. This procedure should improve success rate drastically of de novo protein design.

2Pos079 転写因子 NF-kB の核内クラスター形成の観察
Analysis of NF-kB clusters formation in the cell nucleus

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The transcription factor NF-kB is a hub of signaling networks and is responsible for various gene expressions. The translocation of NF-kB into the nucleus is one of the critical steps in their functions. We have observed the GFP fusion of NF-kB in chick DT40 cells to study its behavior in response to B-cell maturation signals. Single-cell observation showed formation of NF-kB clusters in the nucleus in addition to a concentration increase in the nucleoplasm. The amount of NF-kB in a nucleus mean the intensity of signaling response and the cluster sites might indicate the regulation sites of gene transcription. We will analyze the clusters formation process and discuss the role of clusters of NF-kB in the regulation of gene expressions.

2Pos080 ヌクレオソーム動態解析を指向した化学合成ヒストンタンパク質
Chemically synthesized histone proteins for analysis of nucleosome dynamics

Gosuke Hayashi[1], Takuma Sueoka[1], Akimitsu Okamoto[1,2] ([1]*Dept. Chem. and Biotech., Univ. of Tokyo*, [2]*RCAST, Univ. of Tokyo*)

Posttranslational modifications (PTMs) of histone proteins are an essential factor for epigenetic gene regulation. To reveal the functions of PTMs, it is necessary to prepare site-specifically modified histone proteins. To date, we have achieved chemical synthesis of core histone H2A, H2B, and linker histone H1. We also designed and synthesized intramolecular FRET histone H2B and fluorescence-turn on histones. In this presentation, we show the recent progress of biological application using synthetic histone proteins.

2Pos081 大腸菌非六量体型 DNA ヘリカーゼ UvrD 変異体の多量体形成の 1 分子イメージング
Single-molecule imaging of the oligomeric form of the non-hexameric *Escherichia coli* helicase UvrD mutants

Hiroaki Yokota (*Grad. Sch. Creation Photon Indust.*)

Escherichia coli UvrD protein is a non-hexameric superfamily I DNA helicase which plays a crucial role in nucleotide excision repair and methyl-directed mismatch repair. We performed direct single-molecule fluorescence visualization of the helicase and reported that the helicase unwinds DNA in the form of an oligomer (dimer or trimer) (*Biophys. J.* 2013). Although the oligomeric form is responsible for the unwinding of DNA, only monomeric structures of the helicase are available (*Cell* 2006). Here, to address the relationship between the oligomer dynamics and helicase activity, we applied the visualization to several helicase mutants that exhibit non-wildtype helicase activity.

2Pos082 Structural change of ALS-liked mutant of TDP-43

Akira Kitamura, Sachiko Yuno, Ai Shibasaki, Fusako Gan, Makoto Oura, Johtaro Yamamoto, Masataka Kinjo (*Laboratory of Molecular Cell Dynamics, Faculty of Advanced Life Science, Hokkaido University*)

TAR RNA/DNA-binding protein 43 kDa (TDP-43) is an amyotrophic lateral sclerosis (ALS)-causative protein. ALS-associated mutation is conserved in the carboxyl terminal glycine-rich region (GRR), which is intrinsically disordered region (IDR), of TDP-43. However, structure of TDP-43 in living cells is still unclear. We performed that structural investigation of TDP-43 using fluorescence energy transfer (FRET) in living cells and Fluorescence cross-correlation spectroscopy (FCCS) in cell lysate containing TDP-43-GFP and RFP-hnRNPA1. It is suggested that ALS-linked mutant in the IDR of TDP-43 can change the orientation of IDR structure, and the change may lead to affect the function of TDP-43 (e.g., RNA splicing).

2Pos083 Sequence Dependent Spontaneous Nucleosome Slidings Revealed by Molecular Dynamics Simulation

Toru Niina, Giovanni Brandani, Cheng Tan, Shoji Takada (*Grad. Sch. Sci., Kyoto Univ.*)

Nucleosomes are basic units of chromatin folding. While their locations on the genomic DNA play important roles for gene regulation, the detailed mechanism how nucleosome moves along DNA is not well understood. Here we investigated mechanisms of spontaneous nucleosome sliding employing coarse-grained molecular dynamics simulations. To account for specific histone-DNA interactions we developed a novel orientation-dependent interaction approximaing hydrogen bonds. Analyzing DNA rotation upon sliding, we found two distinct sliding modes, rotation-coupled and uncoupled ones. Relative population of the two modes strongly depends on the DNA sequence.

2Pos084 Real-time observation of flexible domain movements in Cas9

Saki Osuka, **Kazushi Isomura**, Shohei Kajimoto, Tomotaka Komori, Hiroshi Nishimasu, Tomohiro Shima, Osamu Nureki, Sotaro Uemura (*Grad. Sch. Sci, Univ. Tokyo*)

Cas9 is a widely used genome editing tool that cleaves target DNA through the assistance of a single-guide RNA (sgRNA). Structural studies have demonstrated sequential domain movements in Cas9 molecules upon binding to sgRNA and the target DNA. However, dynamics of the domain movement remains obscure. Here, we directly observed dynamic fluctuations of Cas9 domains using single-molecule FRET. A Cas9 nuclease domain accessed to the DNA cleavage position only during such flexible movement, suggesting the importance of this flexibility in the DNA cleavage process. We will discuss the potential roles of the domain fluctuations in driving Cas9 catalytic processes.

2Pos085 **2 つのヌクレオソームの配向多様性は H4 tail により生成しうる。**

The diversity in the orientation of two nucleosomes is potentially produced by H4 tails

Hisashi Ishida, Hidetoshi Kono (*QST, Molecular Modeling and Simulation*)

Histone tails play an important role in internuclesomal interaction and chromatin compaction. To understand how the H4 tails are involved in the interaction, an adaptively biased molecular dynamics simulation of 63 models of stacked two NCPs was carried out. For the models which showed distinctive orientations of the two NCPs, the free-energies of the separation of the NCPs were further investigated using umbrella sampling simulations. The force between the NCPs was estimated to be 15-18 pN per one H4 tail. Additional simulations on the NCPs with H4 tail truncated showed that the force became repulsive from -3 to -7 pN. Taken together, we concluded that the H4 tails potentially produce the diversity in the orientation of the two NCPs.

2Pos086 **Model building of overlapping dinucleosome from SAXS and SANS data**

Atsushi Matsumoto[1], Hidetoshi Kono[1], Rintaro Inoue[2], Masaaki Sugiyama[2], Daiki Kato[3], Yasuhiro Arimura[3], Hitoshi Kurumizaka[3] ([1]*QST*, [2]*Kyoto Univ.*, [3]*Waseda Univ.*)

In this study, we built the atomic models of the overlapping dinucleosome in solution by the computational approach based on the experimental data of the small-angle X-ray scattering (SAXS) and the small-angle neutron scattering (SANS). In this computational approach, first, the initial atomic model is deformed by the simulation techniques to generate a lot of deformed atomic models with different conformations. Then, the SAXS and SANS profiles are computed from each deformed atomic model. Finally, these computed profiles are compared with the experimental ones to find the best-fitting atomic models. For the accurate reproduction of the experimental data, it was important to model correctly the histone tails, which are not observed in the X-ray crystal structure.

2Pos087 **マイクロ液滴界面上での相分離による人工細胞核の形成の DNA ユニット依存性の解析**

Analyses of DNA unit dependence of artificial cell nuclei formed by phase separation on microdroplet interface

Yu Kasahara, Risa Watanabe, Masahiro Takinoue (*Tokyo Institute of Technology/School of Computing/Computer Science*)

DNA nanotechnology allows us to construct self-assembled DNA nano/microstructures such as DNA origami and DNA hydrogels. They are expected to be applied to artificial cells, autonomous molecular robots, etc. To date, we found that the viscoelastic phase separation of the DNA sol was involved in the formation of hydrogel microstructures on the interface of water-in-oil microdroplets. To elucidate the relationship between DNA viscoelasticity and the microstructures, we have investigated the dependence of Y-shaped DNA unit on the resultant DNA microstructures and found that the structural patterns depended on the unit. We believe that the knowledge will be applied to the construction of the artificial cells and their artificial cell nuclei.

2Pos088 **マイクロ液滴界面を利用した RNA 転写可能な人工細胞核の構築**

Construction of artificial cell nuclei with RNA transcription capability using a microdroplet interface

Risa Watanabe[1], Masamune Morita[1,2], Miho Yanagisawa[3], Masahiro Takinoue[1] ([1]*Dept. Comput. Sci., Tokyo Tech.*, [2]*Biomedical Res. Inst., AIST*, [3]*Dept. Appl. Phys., Tokyo Univ. Agri. Tech.*)

In cell nuclei, gene expression is dynamically controlled by various factors including gel-like physical DNA condensation in chromatin structures. However, such physical control of gene expression based on the condensation of gel-like DNA has never been well revealed and achieved yet. Here, we report the construction of DNA hydrogel microstructures with RNA transcription sequences by DNA self-assembly on interface of water-in-oil microdroplets covered with cationic lipids. We confirmed that RNA was transcribed from this structure. We expect that RNA transcription efficiency can be controlled depending on the density of hydrogels. We believe that this structure can be used as a model of cell nuclei.

2Pos089 **TIRF 顕微鏡を用いた良溶媒中の直鎖／環状 DNA の形状揺らぎの長時間観察と相関時間の計測**

Long-time observations of linear/circular DNA in a good solvent by TIRF to measure a correlation time of configuration fluctuations

Takafumi Iwaki, Masato Tanigawa (*Fac. Med., Oita Univ.*)

Relaxation time of the end-to-end distance of micrometer-size linear DNA has been measured to be from milliseconds to seconds. This characteristic time is related to others, e.g., a correlation time of long-axis length. We measured this quantity for linear/circular architectures, and found the magnitude of fluctuations for a circular DNA was abnormally inhibited. However, the past experiments had limitation in observation time, and long-time sequential data was shortened for linear DNA. In this presentation, we developed a long-time observation of linear/circular DNA, to supplement the previous experiments. In addition, we investigate the effect of viscosity to the correlation time to elucidate whether a molecule-solvent interfacial interaction is continuously modeled.

2Pos090 **クラスター凝集モデルに基づく球面上の DNA マイクロ構造体形成の数値シミュレーション**

Numerical simulations of DNA fractal microstructure formation on spherical surface based on cluster-cluster aggregation

Tetsuro Sakamoto, Risa Watanabe, Masamune Morita, Takinoue Masahiro (*Department of Computer Science, Tokyo Institute of Technology*)

Many kinds of microstructures have been reported because of their availability in many areas. Recently, we reported a DNA fractal microstructure formed on a water-in-oil microdroplet interface, and experimental data suggests that the formation mechanism is cluster-cluster aggregation (CCA) of small DNA microparticle on the interface. However, the mechanism has never been completely revealed yet. In this study, we performed numerical simulations based on the CCA, and fractal structures similar to the experimentally observed structures were produced. We believe that comparison between simulation results and experimental results enable us to evaluate the validity of the model and also we can apply the model to control the shapes and functions of microstructures.

2Pos091 二次構造予測から三次構造予測へ：検証と分子動力学シミュレーションを用いた応用

From secondary structure prediction to three dimensional structure prediction: the validation and application using MD simulation

Tomoshi Kameda (*AIRC, AIST*)

To understand the function of RNA, it is essential to know the structure of RNA. However, it is often difficult to determine RNA structure by experimental methods such as X-ray or NMR. So, theoretical prediction of RNA structure is used, especially secondary structure prediction is used. Recently, we can predict not only secondary structure but also three dimensional(3D) structure of RNA easily. For example, RNA composer server(http://rnacomposer.cs.put.poznan.pl) can predict 3D structure using information for 2D structure within one minute. In this presentation, we discuss the validity of 3D structure prediction server. Next, we talk about the MD simulation study using predicted 3D structure.

2Pos092 シスプラチンとトランスプラチンによる DNA の高次構造と機能への影響の比較研究

The effect of cisplatin and transplatin on the higher order structure and function of DNA

Toshifumi Kishimoto[1], Yuko Yoshikawa[2], Kenichi Yoshikawa[1] ([1]*Fac. Life Med. Sci., Univ. Doshisha*, [2]*Nano. Bio., Univ. Doshisha*)

Cisplatin, a platinum-based compound, is widely used as a chemotherapeutic drug for cancer treatment, where nuclear DNA is the primary target of the drug. On the other hand, transplatin, the trans-isomer of cisplatin, is regarded as clinically ineffective. In this study, we compared the effects of these compounds on the higher order structure of a large DNA molecule in aqueous solution through a single molecule observation by fluorescence microscopy to gain insight into the mechanism of their anticancer effects. It has become clear that transplatin has more effective on DNA compaction than cisplatin. We will discuss such conformational characteristics of DNA in relation to their effects on gene expression activity.

2Pos093 Structure and function of DNA in the presence of linear-chain polyamines with a valency from 2+ to 5+

Hiroko Tanaka[1], Ai Kanemura[1], Yuko Yoshikawa[2], Naoki Umezawa[3], Takahiro Kenmotsu[1], Kenichi Yoshikawa[1] ([1]*Fac. Life Med. Sci., Univ. Doshisha.*, [2]*Nano. Bio., Univ. Doshisha.*, [3]*Grad. Sch. Phar Sci., Univ. Nagoya City.*)

Polyamines exist in almost all living cells and play important roles in the cell division and protein synthesis. We examined the effect of linear-chain polyamines, cadaverine [2+], spermidine [3+], spermine [4+] and homocardopentamine [5+], on the higher-order structure of DNA through a single molecule observation. The efficiency of gene expression was evaluated by adapting an in vitro luciferase assay. It was found that homocardopentamine [5+] is much more potent at promoting DNA compaction than others. Interestingly, maximum acceleration of gene expression is observed at certain concentration of each polyamine, being critically dependent on its valency. We will discuss the relationship between DNA structure and gene activity in the presence of polyamines.

2Pos094 金属イオンがグロビュール状 DNA-ヒストン凝集体の大きさに与える影響

Effects of metal ions on the size of globular DNA-histone aggregates

Kyoji Natsume, Yoshifumi Amamoto, Yuichi Masubuchi, Tetsuya Yamamoto (*Grad. Sch. Eng., Univ. Nagoya*)

Nucleosome is a structure in which an anionic DNA is wound around cationic histone octamers. As a primitive model of nucleosomes, DNA-histone aggregates have been studied. We investigated the structural changes of DNA-histone aggregates for various metal ions, which exist in eukaryotic cells. In our experiments, we observed the aggregates with a fluorescence microscope and measured the long-axis length of DNA. Irrespective of ionic species and their charges, with increasing the concentration, the aggregates shrink up to a certain critical concentration, and then, it swell in the higher concentration regime. For the observed non-monotonic behavior, internal degrees of freedom of histone molecules seem effective.

2Pos095 直鎖・分岐ポリアミン存在下での DNA 高次構造の特異性と温度依存的な変化

Temperature-dependent structural changes of large DNA in the presence of linear- and blanched-chain polyamines

Takashi Nishio[1], Kenichi Yoshikawa[1], Yuko Yoshikawa[1], Naoki Umezawa[2] ([1]*Lab. Biol. Phys., Facul. Life Med. Sci., Doshisha Univ.*, [2]*Pharmaceutical. Sci., Nagoya City Univ.*)

Linear-chain polyamines such as spermidine and spermine are found in many organisms and are known to play important roles in various biological functions including gene expression. On the other hand, a branched-chain polyamine, N4-bis(aminopropyl)spermidine [3(3)(3)4], is only found in thermophilic microorganisms living at higher temperatures environments. Here, we report the effect of linear- and branched-chain polyamines on the higher-order structure of genome-sized DNA molecules by the use of single-molecule observation with fluorescence microcopy and atomic force microscopy, especially by focusing our attention on the conformational change at higher temperatures.

2Pos096 How a small change in ligand functional groups affects the dynamics of an aminoglycoside riboswitch?

Marta Kulik[1,2], Takaharu Mori[1], Yuji Sugita[1], Joanna Trylska[2] ([1]*RIKEN*, [2]*Univ. of Warsaw, Poland*)

Riboswitches are regulatory elements in non-coding regions of mRNAs. Binding of different aminoglycosides evokes a varying response of the N1 synthetic riboswitch: neomycin inhibits the expression of genes in yeast and paromomycin is inactive, yet they differ by only one chemical group. To explain the ligand recognition mode of this riboswitch, we performed all-atom molecular dynamics simulations with replica exchange. We also proposed the equilibrium conformations of the aminoglycoside-free riboswitch. We found that ligands active in yeast stabilize the nucleobase A17, whereas in paromomycin complex the A17 base is only partially stabilized and creates a frequent, but unstable hydrogen bonding with paromomycin. This hydrogen bond was not captured in NMR experiments.

2Pos097 トリヌクレオソーム構造のリンカー DNA の長さ依存性
Tri-nucleosome folding dependent on the linker DNA length

Hiroo Kenzaki[1], Shoji Takada[2] ([1]*ACCC, RIKEN*, [2]*Grad. Sch. Sci., Univ. Kyoto*)

Nucleosomes are connected by linker DNAs, where nucleotide pairs are rotated about 35 degrees per base step around the helical axis. Thus, the structural arrangement of neighboring nucleosomes should be subject to this rotary angle. Previously, we simulated di-nucleosomes by coarse-grained model with various lengths of linker DNAs. In this study, we examined how the structure of tri-nucleosome changes depending on the linker DNA length. We found that the tri-nucleosome structure is highly restricted, and take various arrangements of three nucleosomes by the linker DNA. Interaction between nucleosome is mainly stabilized by histone tails, and each structure is contributed by different histone tails.

2Pos098 Protective effect of PEG against DNA double-strand breaks caused by photo irradiation

Moe Usui, Yuko Yoshikawa, Kenichi Yoshikawa (*Grad. Sch. Life and Medical Sciences, Doshisha Univ*)

Direct attack to genomic DNA by reactive oxygen species (ROS) causes various types of lesions, including base modifications and strand breaks. The most significant lesion is considered to be unrepaired double-strand breaks (DSBs) that can lead to fatal cell damage. We have directly observed DSBs of DNA stained by a fluorescent cyanine dye, YOYO-1, in solution, where YOYO-1 is known to have the ability to photo-cleave DNAs by generating ROS. We have investigated the protective effect of PEG (polyethylene glycol) against DSBs in a quantitative manner. It was found that PEG decreases the probability of DSBs. We will discuss the protective mechanism in relation to the consumption of ROS by PEG.

2Pos099 塩基配列非特異的に誘起された長鎖 DNA の折り畳みにおよぼす共存イオンの効果
The Effects of Ions on the Folding of Giant ds DNA Chains Induced by Nonspecific Interaction with Poly-cations and Proteins

Tatsuo Akitaya[1], Toshio Kanbe[2], Anatoly Zinchenko[3], Shizuaki Murata[3], Makoto Demura[4], Kenichi Yoshikawa[5] ([1]*Asahikawa Medical Univ.*, [2]*Nagoya Univ.*, [3]*Nagoya Univ.*, [4]*Hokkaido Univ.*, [5]*Doshisha Univ.*)

Large-scale conformational change of genomic DNA is the most essential feature of gene activation. Although many efforts have been made for revealing those mechanisms in terms of key-lock interaction, i.e. sequence-specific binding between DNA and proteins, those have not reached to the higher-order structure of long ds DNA chains. We found that nonspecific weak interaction with short poly-cation can induce ON/OFF discrete transition of higher-order structure of long ds DNA in contrast to long multiply charged poly-cation inducing continuous gradual change, and analyzed the effect of co-existing ions in the solution. We also examined the manner of folding of giant DNA chains with nonspecific binding proteins. Physicochemical mechanisms of DNA folding will be discussed.

2Pos100 Pt(II)化合物の DNA 高次構造に対する影響のその場計測：レーザー・マニピュレーション
Evaluation of the effect of dinuclear Pt(II) complexes on DNA conformation through laser manipulation

Yusuke Kashiwagi[1], Masatoshi Ichikawa[2], Seiji Komeda[3], Koichiro Sadakane[1], Yuko Yoshikawa[1], Kenichi Yoshikawa[1] ([1]*Grad. Sch. Life and Medical Sciences, Doshisha Univ.*, [2]*Grad. Sch. Physics, Kyoto Univ.*, [3]*Fac. Pharm. Sch. Suzuka Univ Med Sci*)

It is getting clear that cationic dinuclear Pt(II) complexes are potent next generation of anticancer drug candidates. Here, we have examined the effect of a cationic tetrazolato-bridged dinuclear Pt(II) complex, 5-H-Y, on the higher order structure of DNA by single molecular observation with fluorescence microscopy. It is shown that 5-H-Y induces the shrinking of DNA into a compact state. Interestingly, individual compact DNA molecules are stably trapped by focused laser without any modification such as attachment of micro plastic beads. We have performed the optical transportation of the compact DNA to a region of high salt concentration. It is noted that the compact globule structures are stable even at high salt concentration.

2Pos101 Reverse mapping to reconstruct atomistic structures from coarse-grained models for DNA-protein complexes

Masahiro Shimizu, Shoji Takada (*Grad. Sch. Sci., Kyoto Univ.*)

Coarse-grained (CG) molecular simulations enable us to investigate dynamical behavior of large DNA-protein complexes. From the obtained CG models, reconstructing atomistic detail can be useful. Here we propose a method to reverse map a CG DNA-protein complex structure into atomistic model with accurate interaction interfaces. First, we developed a method to back-map CG DNA models to atomistic ones: In a DNA fragment library made from the protein-data-bank, we looked for the locally best-fit atomistic structure to the query. Then, for proteins, combining known structure information and existing tools, we re-constructed their structures with conserved sidechain orientations at the DNA interface. Benchmark tests showed promising results.

2Pos102 Reconstitution system of Siwi- and Vasa-coupled piRNA biogenesis

Tomotaka Komori, Ryo Murakami, Tomohiro Shima, Mikiko Siomi, Sotaro Uemura (*Univ. of Tokyo*)

Piwi-interacting RNA (piRNA) is germ cell-specific small RNA relating to the defense of the genome against transposons. In germ cells, piRNA biogenesis follows a specific amplification scheme known as a “ping-pong cycle”. Biochemical assays using cell lysate have shown that DEAD box helicase Vasa is required for the efficient release of cleaved RNA from Bombyx mori Piwi, Siwi in the ping-pong cycle. However, the molecular mechanism that regulates this Vasa-dependent RNA release remains to be explained. To tackle this issue, we have constructed a reconstitution system using purified Siwi and Vasa. At this meeting, we will discuss our recent progress using the reconstitution system.

2Pos103 人工細胞デバイスを用いたT7プロモーター配列の進化分子工学手法の開発

Directed evolution of T7 promoter sequence with artificial cell reactor device

Tomoya Nishimura[1], Yi Zhang[1,2], Hiroshi Ueno[1], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*JAMSTEC*)

This study aims to establish a method for directed evolution of T7 promoter sequence by use of femtoliter chamber array device. The principle strategy is as follows. First, we prepare a saturation mutagenesis library of T7 promoter sequence that is followed by a reporter gene, Venus. The library DNA molecules are enclosed in femtoliter chambers at single molecule level with cell-free transcription-translation mixture. The promoter activity is measured from the fluorescence intensity of Venus produced in each reactor. Then, DNA molecules are recovered from the chambers displaying the highest fluorescence intensities for subsequence DNA sequence analysis. We will report technical challenges found during the development of this method and preliminary results.

2Pos104 人工細胞デバイス内における無細胞タンパク質発現ノイズの解析

Gene expression noise of cell-free system in artificial cell reactors

Shiori Fujimoto[1], Yi Zhang[1,2], Hiroshi Ueno[1], Kazuhito Tabata[1], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*JAMSTEC*)

Gene expression noise can be categorized into extrinsic and intrinsic noise. The fluctuations in the amount of components involved in gene expression are the primary factor of extrinsic noise, resulting in a positively correlated fluctuation. The intrinsic noise results from the inherent stochastic biochemical process, resulting in an uncorrelated fluctuation. In this work, we investigate gene expression noise of cell-free protein synthesis system entrapped in the femtoliter chamber array system. The present system allows us to quantify the gene expression noise in a well-defined volume with defined components. We confirmed the correlation in expression between two genes and this preliminary data suggests that extrinsic noise is predominant in this system.

2Pos105 Protein-peptide dissociation at high pressure studied by parallel cascade selection molecular dynamics simulations

Hiroaki Hata[1], Yasutaka Nishihara[1], Masayoshi Nishiyama[2], Ikuro Kawagishi[3], Akio Kitao[1] ([1]*IMCB, UTokyo*, [2]*The Hakubi Center, Kyoto Univ.*, [3]*Dept. of Frontier Biosci., Hosei Univ.*)

Protein-peptide association/dissociation plays important roles in functional regulation of biomolecules. However, it currently needs a very long time to simulate such conformational changes of large-scale systems using conventional molecular dynamics (MD) simulation. Here we simulated a dissociation of a protein-peptide complex, $CheY^{P}$-$FliM_{N}$, at different pressure conditions using a recently developed MD method, parallel cascade selection molecular dynamics. Subsequently, the binding free energy was calculated using the Markov state model. We found that the binding energy decreased at high pressure. Our results support the previously proposed mechanism that high pressure suppresses the $CheY^{P}$-$FliM_{N}$ binding and fixes the rotational direction of flagella motor.

2Pos106 Rng2がアクチンフィラメントとミオシン間の協同的結合に与える影響の解析

Analysis of influence of Rng2 on cooperative binding between myosin and F-actin

Taiga Imai[1], Masak Takaine[2], Kentaro Nakano[2], Osamu Numata[2], Taro Uyeda[3], Kiyotaka Tokuraku[1] ([1]*Muroran Institute of Technology*, [2]*University of Tsukuba*, [3]*Waseda University*)

Rng2 is an IQGAP protein localizing in the contractile ring (CR) of fission yeast, and plays a role in the regulation of the CR. Recently, we found that a substoichiometric amount of Rng2CHD, which is an actin-binding site of Rng2, strongly inhibited gliding of F-actin on an HMM-coated surface in in vitro motility assay. To examine the inhibition mechanism of myosin motility by Rng2CHD, in this study, we analyze the effect of Rng2CHD for actin-HMM interaction by co-sedimentation assay and fluorescence microscopic observation. The results showed that the binding between HMM and F-actin was inhibited by Rng2CHD in the presence of ATP. Quantitative analysis suggested that the binding of Rng2CHD affects the conformations of a few to 10 of neighboring actin protomers.

2Pos107 Minicell tethered assay that enables simultaneous observation of a flagellar motor rotation and the incorporation of stators to the motor

Takao Nakajima, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Biosci., Osaka Univ.*)

Bead assay is a useful method to accurately measure rotation of a flagellar motor, and tethered cell assay is also useful to observe the components in a rotating motor under the TIRF system. Here, we constructed the minicell tethered assay by combining the advantage of both methods (the diameter of a minicell is about 1 μm). In tethered minicell assay using wild-chimeric stators, the motor showed almost the same performance (~80 Hz, ~2500 pN nm) compared to bead assay (φ = 1 μm). After the Na^{+} concentration around cells was increased 0 to 5 μM, stepwise increments of rotational speed (resurrection) were observed. We are now trying to simultaneously measure motor's rotational speed and the incorporation of GFP-fused stators into the motor using minicell tethered assay.

2Pos108 Repetitive buckling of microtubules driven by dynein arms reconstituted on singlet microtubules

Misaki Shiraga[2], Jyunya Kirima[2], Kazuhiro Ooiwa[1,2] ([1]*NICT*, [2]*Grad. Sch. Sci., Univ. Hyogo*)

The coordination among dynein arms makes flagella beat in an organized manner. To reveal this mechanism, we reconstituted axonemal structures in vitro in a bottom-up manner. High-salt extract of dynein arms from Chlamydomonas axonemes were added to the microtubules immobilized on the glass surface via biotin-avidin interaction. Dynein arms were self-organized into regular arrays on the microtubules. Microtubules freshly added to these dynein arm-microtubule complexes formed bundles with them. Addition of ATP elicited sliding of microtubules and occasionally showed repetitive buckling at the frequency of 1-3 Hz. These results suggest that repetitive bending of the axoneme is derived simply from self-regulated dynein-microtubule interactions.

2Pos109 係留されたキネシン頭部の微小管への結合解離の直接観察
Direct observation of the binding and unbinding motions of the tethered kinesin head to microtubule

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Kinesin-1 is a motor protein that moves along microtubule by alternately moving two motor domains (heads). The kinetic analysis using stopped flow revealed how the detachment and attachment of the head from/to the microtubule are coupled with ATP turnover cycle, however, it was difficult to determine using this method how fast the detached head rebinds to the microtubule. In this study, we anchored a monomer head to microtubule via a long flexible linker and observed the binding and unbinding motions of the head using single-molecule fluorescent and dark-field microscopy. We found that the rebinding occurs 3 ms on average after the detachment, suggesting that some conformational change of the unbound head is required to become compatible with ADP release.

2Pos110 温度適性に着目した、糸状菌由来のキネシンの特性
Properties of kinesins from filamentous fungi focused on the thermal aptitude

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A filamentous fungus Aspergillus nidulans (optimal growth temperature, 37 degrees C) possesses AnKinA as a kinesin-1 subfamily member. Another filamentous fungus Sclerotinia borealis, living under snow, possesses a kinesin-1 subfamily member, named SbKin1. Head domains of the two kinesins showed high amino acid sequence similarity (83% identities). Therefore, it is suggested that only a modest difference would change the optimal temperature of the enzymatic activity. We obtained recombinant AnKinA and two mutants intended to be adapted to low temperature. We will present the properties of the kinesins, especially focused on the thermal aptitude.

2Pos111 Conformational change in azimuth and tilting angles of F_1-ATPase revealed with defocused orientation imaging

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To drive rotation of the central γ shaft in molecular rotary motor F_1-ATPase, a series of cooperative motions of three β subunits are assumed to be highly orchestrated, but the coupling of each reaction and the shaft angle is still enigmatic. To detect the angle of a single fluorophore in great detail, we developed a technique “defocused imaging” with the appropriate calibration using kinesin-MT motility assay (Fujimura et al., *BBRC* 2017). We here applied the method to monitor the angle of one of three βs labeled by Cy3 in single F_1 molecule, and successfully monitor the change in both azimuth and tilting angles simultaneously, 40-50° and ～20°, respectively. We will extend the analysis system to F414E/F420E mutant, which has extremely slow k_{on} of ATP binding.

2Pos112 Morelloflavone による有糸分裂キネシン Eg5 の阻害効果の生化学的解析
Biochemical analysis on the effect of morelloflavone as a novel inhibitor of mitotic kinesin Eg5

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Previously, employing in silico tool, we found morelloflavone (a natural biflavonoid) as a potential ATP-noncompetitive inhibitor of mitotic kinesin Eg5 which binds to Eg5 in a manner similar to well-known potent inhibitors. The results indicated the high affinity and inhibitory potential of this compound on Eg5. As a part of verification of this result, we evaluated morelloflavone (MF) as anticancer agent targeting Eg5 in vitro using biochemical analysis for its inhibitory effect against Eg5. In agreement with the in silico prediction, MF inhibited microtubule-stimulated Eg5 ATPase activity with IC50 of 63uM and also decreased the velocity of microtubule gliding. However, the inhibitory effect was more moderate than that we estimated from the data of in silico study.

2Pos113 Modification of V_1 rotary molecular motor of *Thermus thermophilus*

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V_1-moiety of bacterial V-ATPase is an ATP driven rotary molecular motor consisting of central rotor of DF and stator hexamer A_3B_3. Conformation of stator was continuously changed by ATP hydrolysis in three catalytic sites of V_1. The stator motion is somehow transmitted to the rotor protein, resulting in the stepwise rotation. In this study, we tried to create faster and stronger molecular rotary motor based on the V_1 motor. First, we attempt to enhance the rotation speed of V_1 motor by insertion of a modified rotor into the stator hexamer. Second, we inquire whether homo AAA hexamer containing six ATP catalysis sites functions as a stator of rotary motor. The complex is expected to rotate the rotor using six ATP per revolution.

2Pos114 DNA オリガミ-ミオシン II モーター混合システムの高速原子間力顕微鏡観察
High-speed AFM imaging of DNA origami-myosin II motor hybrid system

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Muscle contraction is generated by a coordinated motion of myosin II motors in thick filaments. While mechanical motions of isolated single myosins are well characterized, how individual myosins in an assembly are coordinated is unclear. To resolve the internal dynamics in the filament at the single molecule resolution, we have developed a programmable artificial myosin filament using DNA origami to which oligonucleotide-labeled skeletal myosin II could be attached, providing precise control of motor number, type, spacing and orientation. Here, we apply high-speed atomic force microscopy to our programmed myosin filaments to directly monitor the behaviors of individual myosins, which will reveal the mechanism of cooperative actions of myosin motors in the filament.

2Pos115 新規フォトクロミック阻害剤であるスピロピラン誘導体を利用した有糸分裂キネシン Eg5 の光制御

Photoregulation of mitotic kinesin Eg5 using a novel photochromic inhibitor composed of spiropyran

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Recently, mitotic kinesin Eg5 draws attention as a target of anti-cancer therapy. A number of small-molecule inhibitors of Eg5 have been discovered. Interestingly, the inhibitors bind to the common pocket in Eg5 motor domain. Photochromic molecules such as spiropyran which change their structures and properties reversibly by light irradiation are expected to be applicable to photo-regulation of Eg5 inhibitors. In this study, we synthesized novel photochromic Eg5 inhibitors (SP-APA) composed of spiropyran. SP-APA inhibited significantly ATPase activity and motor activity photoreversibly. We also analyzed that which step in ATPase cycle is influenced by SP-APA using stopped-flow method. Furthermore, we examined the effect of SP-APA against cell proliferation.

2Pos116 High speed AFM imaging of structural changes in actin filaments bound tropomyosin-troponin in presence of myosin S1 and ATP

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Based on high speed AFM real time observations, we previously reported that repetitive transient binding of S1 to actin filaments in the presence of ATP increases the helical pitch by 8% and strongly inhibits cofilin binding. Here, we found that decoration of the filaments by Tm-Tn in the presence of ATP and Ca2+ suppresses the lengthening of the helical pitch by S1. This explains why previous x-ray diffraction studies on contracting muscle fibers did not detect changes in helical pitch. Nonetheless, cofilin binding to Tm-Tn actin filaments was strongly inhibited by S1 with ATP and Ca2+. This suggests that the essential feature of structural changes in actin filaments induced by cycling S1 to modify affinities for cofilin does not depend on untwisting of the helix.

2Pos117 Development of simultaneous observation system for flagellar components and motor rotation with external load by electrorotation

Kenta Morishima, Akihiko Ishijima, **Hajime Fukuoka** (*Grad. Sch. Frontier Biosci., Osaka Univ.*)

E. coli regulates the rotational direction of its flagella motor by CheYp-binding to a motor. To investigate whether the external biased torque to a motor affect to chemotactic response, such as binding affinity to CheYp, we developed the microscopic system combined the simultaneous observing system of motor rotation and CheYp-binding and generating system of electrorotation utilizing 4 microelectrodes. We confirmed the rotational torque of tethered cell is proportional to the square of applied voltage as shown in previous report (Washizu *et al.* 1993). Now, we are trying to measure the change in the rotational speed both CCW and CW states by applying the biased torque, and to investigate the effect for the applied biased torque for the CheYp-binding to a motor.

2Pos118 Can we make KIF5 faster?

Taketoshi Kambara[1], Yasushi Okada[1,2] ([1]*RIKEN, QBiC*, [2]*Univ. of Tokyo, Grad. Sch. of Sci.*)

Axonal transport is essential for various neuronal functions including neurite formation and extension, synaptic functions and survival. Many neurodegenerative diseases are known to be caused by impaired axonal transport due to decreased velocity of kinesin. For example, various point mutations in the motor domain of KIF5A, or kinesin-1 in vertebrate, is known to be causative for hereditary spastic paraplegia (HSP). The HSP mutations impair the motor activity of KIF5a and decrease its velocity by 25-75%. Here, we ask a simple question which amino acid is responsible for governing the velocity of kinesin. To address this question, we searched for the amino acids to influence the velocity of KIF5.

2Pos119 生体分子モーターと光応答性 DNA を用いた分子輸送技術の構築

Construction of a nano-transportation system by using a biomolecular motor and photoresponsive DNA

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Biomolecular motor systems, such as microtubule-kinesin, are the smallest natural machines which perform mechanical works by consuming chemical energy. Nowadays reconstructed microtubule-kinesin system has been drawing much attention for different nanotechnological applications, for example nano-transportation. However, regulation of nano-transportation through controlled loading and unloading of cargos at a desired place and time has not been realized yet. In this study, by employing photoresponsive DNA, we aim to spatiotemporally regulate the microtubule-kinesin based transportation by controlling the loading and unloading of cargo materials. This work will widen the applicationsb of biomolecular motor systems for targeted transportation of nanomaterials.

2Pos120 細菌べん毛 III 型分泌装置の精製と再構成

Purification and reconstitution of the flagellar type III protein export apparatus

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The flagellar type III export apparatus is a molecular machine used to construct the bacterial flagellum. It consists of a transmembrane export gate and a cytoplasmic ATPase complex enclosed by the basal body MS-ring and C-ring. The export gate is composed of six types of membrane proteins, FlhA, FlhB, FliO, FliP, FliQ and FliR. Purification of the type III secretion apparatus is a challenging task because it's a huge complex with the molecular mass of ca. 7 MDa. We have purified the functional export gate complex with the MS- and C- rings from inverted membrane vesicles. We are trying to incorporate the purified export gate into lipid membrane vesicles to reconstitute the active type III secretion apparatus for in vitro protein transport assay.

2Pos121 LAT 小胞はマスト細胞の中で自己完結型信号伝達場として働く：1 分子観察による解明

The LAT vesicle works as a self-contained signaling platform in mast cells; discovery by single molecule tracking

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Linker for activation of T cells (LAT) is a transmembrane adaptor molecule in mast cells, which mediates the signal from the antigen-activated receptor to cellular responses. Using single-molecule imaging in live mast cells, we found that 10% LAT existed in vesicles that were temporarily (on the order of 10 s) recruited from the cytoplasm and tethered to the plasma membrane (PM) via exocyst complexes. Upon stimulation, LAT vesicles, but not LAT in the PM triggered the PLCγ2-IP_3-Ca^{2+} pathway. Furthermore, PLCγ2 substrate PI(4,5)P_2 and other PI metabolites existed in LAT vesicle, whereas PI-kinases and phosphatases, including PIP5K and PTEN, were recruited or existed in LAT vesicles. These results suggest that LAT vesicles serve as a self-contained signaling platform.

2Pos122 Detection of the activity in receptor cluster by single cell FRET and motor rotation in Escherichia coli cell

Yu Mitoro (*Grad. Sch. Biosci., Univ. Osaka*)

Rotational switching of two motors on a same cell is highly coordinated, suggesting the high cooperative activation of receptor cluster. To validate our suggestion, we are trying to detect the activity of receptor cluster by performing a single cell FRET. For FRET measurements, functional CheA-fluorescent protein(FP) fusion is required, though it has not been considered at previous reports. By carefully choosing the inserting position of FPs, we succeeded in constructing functional CheA-FPs. Furthermore, by adopting mTurquoise2 and mVenus, we also succeeded in measuring motor rotation without critical cell-damage by laser and observing fluorescence for a long time. We are now trying to simultaneously measure FRET from receptor cluster and switching of motors.

2Pos123 β-arrestin independent mechanism is involved in the temporal trapping of diffusing GPCR on cell surface

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To maintain the functions of G-protein coupled receptor or GPCR, upon the stimulation, GPCR is captured by β-arrestin, a cytosolic protein, leading to the internalization. However, it is not well understood how GPCR is organized for the internalization. To answer this, we simultaneously observed dopamine D2 receptor (DRD2) and β-arrestin at the single molecule level in β-arrestin-1/2 knock out cell. As a result, we found that the stimulation induced mostly irreversible binding of DRD2 to β-arrestin, while some DRD2 molecules were transiently immobilized without β-arrestin. This means that unknown mechanism like a scaffolding is involved in this temporal trapping, which would be important for the arrestin independent internalization and/or fine tuning of GPCR signals.

2Pos124 Rotation assay of the proton-driven bacterial flagellar motor under near zero load

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The bacterial flagellar motor is a nanomachine fueled by proton motive force. Torque generated by the basal body is transmitted to the filament via the hook. Most research on the torque generation mechanism of the motor has been analyzed by labeling microbead to the filament but further reduction of load may uncover a hidden mechanism. Here we directly labeled nanogold to a genetically solidified and straightened hook without filament. Previous studies showed that the motor speed is dependent on internal pH but not on external pH; however, our assays showed that the motor speed is increased by lowering external pH. This result suggests that protonation of the stator from outside is also a late-limiting step in the mechanochemical reaction cycle under near zero load.

2Pos125 原子間力顕微鏡によるマウス顎下腺上皮組織のレオロジー測定

Rheological properties of epithelium in mouse submandibular gland measured by atomic force microscopy

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The submandibular gland (SMG) of mouse undergoes a branching morphogenesis, in the early stage of development, which is the process of extending the surface area by forming many tufts called “bud” with clefts. The understanding of the cell mechanical behaviors during the branching morphogenesis is crucial for regenerative medicine such as the development of artificial organs. We have previously reported the elastic property of SMG measured by atomic force microscopy (AFM) (1). Here, we developed an AFM that enables mapping the stress relaxation behaviors of SMG in a large region and found the epithelium in SMG followed a power-law rheology. We will present the AFM system and the spatial rheological properties of epithelium in SMG.

(1)Y. Nakajima et al. The 53rd BSJ

2Pos126 Flagella-associated protein in Chlamydomonas flagella, FAP85 is one of the microtubule inner proteins (MIPs)

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We focused on FAP85, a 25kDa flagella-associated protein of unknown function from *Chlamydomonas* axonemes and determined its localization in the axoneme. Western blotting of axonemes prepared from the wild-type and several mutants missing some of major-axonemal components suggested that FAP85 binds to the doublet microtubules (DMTs). EDC-crosslinking of DMTs produced a 75kD complex, which was recognized by anti-FAP85 antibody and identified as beta-tubulin-FAP85 complex using MALDI-TOF-MASS. Immuno-gold electron microscopy on Sarkosyl-treated axonemes showed many gold-particles on the A-tubules of DMTs exposing their inner walls but none on intact DMTs. These results suggest that FAP85 is one of the microtubule inner proteins binding on the inner wall of A-tubules.

2Pos127 細菌べん毛モーターの固定子組み込みとトルク発生におけるプロトン透過の関わり

Implication of proton translocation for stator assembly and torque generation in the bacterial flagellar motor

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The bacterial flagellar motor is composed of a rotor and a dozen stators, which converts proton influx through the stators into torque. The stator consists of MotA and MotB. We previously found that MotA-Met206 plays a key role for protonation of the stator. By labeling stators with fluorescent protein, we here show that the MotA(M206I) mutation reduces subcellular localization of stators. Furthermore, based on results of resurrection experiments we show that motor speed produced by a single M206I stator is slower than that of WT one. We also show that the stator assembly in the M206I motor is recovered by lowering external pH, but motor speed produced by a single M206I stator is not the case. We discuss the relationship between protonation and stator dynamics.

2Pos128 アクチン繊維の集団運動により形成される構造は繊維の物理的性質によって決まる

The characterization of size and filament distances of band patterns of moving actin filaments

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HMM molecules on the hydrophobic glass surface moves actin filaments in the presence of Mg-ATP. Unlabeled filament was reported to bring about some collective motions of the filaments. We have reported the collective motion is not simple oriented but also accompanied by mutual association of filament to form unique patterns with association of circular patterns of about 20 μm band width to form about 100 μm circle in diameter. Here we report that the formation of this band-like pattern mainly depends not on the localization HMM on the glass but on the physical properties of actin filaments.

2Pos129 *Bacillus alcalophilus* 由来べん毛固定子蛋白質の MotS のペリプラズムフラグメントの構造

Structural of a periplasmic fragment of MotS, a flagellar stator protein of *Bacillus alcalophilus*

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The flagellar motor consists of the rotor and the stator, and the torque is produced by the rotor-stator interaction coupled with specific ion flow through the channel in the stator. The stator of Gram-negative bacteria is anchored to the peptidoglycan layer to generate torque by changing the conformation of the periplasmic region of the B subunit of the stator, and the structural change is coupled with the opening of the ion channel. MotS is a stator protein of Bacillus alcalophilus, a Gram-positive bacterium, and the counter part of the B subunit. To elucidate the stator anchoring mechanism of Gram-positive bacteria, we purified and characterized a periplasmic fragment of MotS and obtained crystals diffracted to 1.4 Å resolution. The structure analysis is underway.

2Pos130 細胞内温度への微小管の寄与の検討

Investigating the contribution of microtubules on intracellular temperature variation

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Recent studies have shown that thermal dynamics in cells is different from that in solutions, which might significantly influence on cell functions. However, the mechanism of this phenomenon is unclear. In this study, we measured the temperature by using fluorescence thermometer and analyzed the thermal reduction in microtubule disrupted cells. First, we revealed that disruption of microtubules interfered with cellular temperature increase under mitochondria stimulation by FCCP. Next, we found that stress granules, which can be provoked by local thermogenesis by FCCP, did not form in microtubule disrupted cells. These results indicated that microtubules are essential for intracellular thermal dynamics.

2Pos131 Polarized ArfA activation directs PTEN to posterior plasma membrane for eukaryotic cell migration

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Although cellular polarity formation is a crucial process for various biological phenomena, the detail architecture of molecular network associated with polarity formation remains elusive. Here, we report that polarized ArfGTPase activation dictated PTEN localization in motile D. discoidium cells. Fluorescent imaging enlightened that active ArfA recruited PTEN to the posterior plasma membrane. Furthermore, we identified Arf-GEF, SEC7, involved in polarized ArfA activation and PTEN recruitment to plasma membrane. PTEN degrades phosphatidylinositol trisphosphate (PIP3) and inhibits protrusion at the posterior side. Thus, we concluded that polarized ArfA activation suppressed PIP3 accumulation through PTEN recruitment and led to a spatially coordinated protrusion.

2Pos132 ネスチンと緑茶カテキン(-)エピガロカテキンガレートの細胞弾性への効果

Effect of nestin and (-)-epigallocatechin gallate on cell elasticity

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Nestin, an intermediate filament protein, is considered to increase metastatic ability of cancer cells. We focus on nestin as a target for suppressing cancer metastasis. Previously, we found that knockout of nestin gene in highly metastatic mouse breast cancer cell FP10SC2 caused an increase in elastic modulus of the cell. Nestin might enable cells to passage through narrow space in the connective tissue. Additionally, treatment with (-)-epigallocatechin gallate (EGCG) has been reported to increase elastic modulus of the cancer cells. In this study, we found that the elastic moduli of both FP10SC2 and nestin knockout cells treated with EGCG were increased. This result indicates that nestin and EGCG are involved in different mechanisms controlling cell stiffness.

2Pos133 ビブリオ菌極べん毛数と位置へ影響する FlhF の精製とその GTPase 活性検出

Purification of FlhF to detect the GTPase activity effecting on the number and location of the polar flagellum of *Vibrio alginolyticus*

Shota Kondo, Michio Homma, Seiji Kojima (*Grad. Sch. of Sci., Nagoya Univ.*)

Vibrio alginolyticus has a single polar flagellum whose number and placement are regulated positively by FlhF. FlhF is a GTPase and homolog of signal recognition particle (SRP) protein Ffh and SRP receptor FtsY. FlhF is localized at cell pole and directs the formation of flagellum. We have found that the mutations of the GTPase motif reduce the polar localization of FlhF. We want to detect the GTPase activity from the purified FlhF. FlhF was easy to precipitate and difficult to purify the protein. Now, we found that the amount of soluble FlhF increased if $MgCl_2$ and GTP were added in solution. The GTPase activity of purified FlhF will be measured and its effect on the number and location of the polar flagellum will be discussed.

2Pos134 ERK, Akt の多重可視化よる細胞周期制御機構の定量的な解析

Quantitative analysis of cell-cycle control mechanisms by multiplexed imaging of ERK and Akt activity

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The Ras-ERK pathway and the PI3K-Akt pathway are the chief mechanisms for many cell functions such as cell proliferation and cell survival in response to extracellular stimuli. These pathways coordinately regulate each other through cross-talk, feedforward and feedback regulations. The open question remains how Ras-ERK and PI3K-Akt pathways are integrated to control cell cycle progression. To address this issue, we developed a multiplexed live-imaging system for monitoring ERK and Akt activity at the single cell level. With ERK-KTR and Akt-FoxO3a-KTR, we have quantified dynamics of ERK and Akt activity in single cells under a basal or EGF-stimulated condition, demonstrating that ERK and Akt were cooperatively regulated in cell-cycle-dependent manner.

2Pos135 運動性シアノバクテリアの双方向性運動の解析

Analysis of bidirectional motion of motile cyanobacteria

Takashi Kosaki, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

Motile cyanobacteria, Pseudanabaena sp., exhibit various colonial morphology, which could have an advantage to adapt to environment. The motion mechanism is, however, unclear. In this study, the relation between size and motion was analyzed. The bacteria showed periodic bidirectional movement and the period increased according to the size. This result suggested the possible mechanism of Pseudanabaena's movement is similar to that of soil bacteria, F. johnsoniae, whose movement mechanism was recently revealed. In addition to this, it was observed Pseudanabaena secreted the slime material, forming the bound, whose boundary would initiate the turning movement. Detailed investigation of the effect of slime is ongoing.

2Pos136 繊維状インフルエンザウイルスの運動様式

Motility of filamentous influenza virus

Tatsuya Sakai, Mineki Saito (*Department of Microbiology, Kawasaki Medical School*)

Influenza virus motility is based on cooperation between viral hemagglutinin (HA) and neuraminidase, and is a major determinant of virus infectivity. The virus motility was recently found in influenza A virus (IAV) that was spherical in shape. Influenza virus is pleiomorphic, observed as both spherical and filamentous virion. Here, we report filamentous IAV motility. Using surface reflection interference contrast microscopy, we examined IAV behavior on glass surfaces with immobilized receptors. On the surface, filamentous virus moved in a random fashion. While moving, several domains of a filamentous virion attached to the surface and the attaching domains were changed temporally, demonstrating directly IAV motility employing exchange of HA-receptor cross-bridges.

2Pos137 外腕ダイニン中間鎖の点突然変異によるクラミドモナス鞭毛運動性の低下

A novel *Chlamydomonas* mutant harboring a point mutation in an intermediate chain gene of outer-arm dynein displays lowered motility

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Cilia and flagella beat through microtubule sliding powered by axonemal dyneins. Outer-arm dynein (OAD) is a large complex composed of 2-3 heavy chains (HCs), two intermediate chains (ICs), and ~10 light chains (LCs). Various OAD-deficient mutants (*oda*s) lacking the entire arms have been isolated in *Chlamydomonas*, and demonstrated the importance of OAD for flagellar beating at high beat frequency. Here we isolated a novel type of OAD mutant that displays moderately lowered beat frequency but no signs of reduction of HCs. Genetic analysis showed that it has a point mutation in the gene of IC2, a protein that anchors OAD to the outer-doublet microtubule. These results suggest an interesting possibility that IC2 regulates the entire motor activity of OAD.

2Pos138 システイン変異導入によるべん毛モーター固定子タンパク質 PomA のペリプラズムループ領域の解析

Characterization of periplasmic loop regions of PomA, a stator protein of flagellar motor, using cysteine mutagenesis

Hiroto Iwatsuki, Hiroyuki Terashima, Seiji Kojima, Michio Homma (*Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

In V. alginolyticus, the stator of the flagellar motor is composed of PomA and PomB, and is driven by sodium ion flow through the stator. The two loops located in the periplasmic region of PomA are involved in the ion flux in the stator channel. To gain structural insights into the PomA loops, cysteine mutants were generated in the loops and the accessibility of the substituted cysteine, in the purified PomA/PomB complex, was examined by the specific labeling by biotin maleimide. We found that only cysteines in loop 2 were labeled, consistent with the previous in vivo observation. Our results suggest that loop 1 is buried but loop 2 is exposed in the PomA/PomB complex. We are going to characterize more the loop regions by labeling under various conditions.

2Pos139 分散培養心筋細胞と心臓組織片の拍動同期
Synchronization of beating between dispersed culture of cardiomyocytes and cardiac tissue slice

Chiho Nihei, Tomoyuki Kaneko (*LaRC, Grad. Sch. Sci. & Eng., Hosei Univ.*)

Heart has systematic structures such as sinoatrial nod working as pacemaker. To validate the robustness of cardiac network for beating, we analyzed beating synchronization between dispersed culture of cardiomyocytes derived from chick embryos (E7) and cardiac tissue slice of chick embryos (E8-10) by multi electrode array system. We measured the extracellular potential of cardiomyocytes, and calculated the inter spike interval as beating intervals. Consequently, the beating of dispersed cardiomyocytes was influenced by the beating of cardiac tissue slice. In some cases, the dispersed cardiomyocytes beat in own rhythm irrespective of the beating of cardiac tissue slice. Therefore, cardiac tissue slice might be dominant, and might have robustness for the rhythm of beating.

2Pos140 シュードモナス属細菌の運動性およびべん毛回転測定
Measurements of motility and flagellar rotation in Pseudomonas species

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Members of the genus Pseudomonas swim by using a single polar flagellum or multiple polar flagella. Although the bacteria possess two sets of stator units, MotA/B and MotC/D, in common, both are believed to be proton-conducting stators. However, swimming speeds of Pseudomonas spp. are more than double of those of other proton-type bacteria such as Escherichia coli and Salmonella, and therefore the Pseudomonas stator units may have unprecedented output characteristics. In this study, we analyzed motilities and flagellar rotations of P. syringae and P. aeruginosa. Measurements of swimming speeds in various viscosities predicted that the maximum motor speed of Pseudomonas spp. reaches 500 Hz. We also show preliminary data of tethered-cell and bead assays.

2Pos141 Guanylate Cyclase mediates chemotaxis by transducing high-frequency signals for pseudopod formation

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Chemotaxis of eukaryotic cells is mediated by parallel signaling pathways including PIP3 and soluble guanylate cyclase (sGC), which transduce chemotactic signals by unidirectional localizations at a front pseudopod. Here, we report that sGC shows the localization to the pseudopod more frequently than PIP3 when cells moved up the chemical gradient. To characterize the dynamics of these pathways, we applied repetitive chemical stimuli with various intervals. sGC, not PIP3, was able to respond to the short interval stimuli, indicating that sGC localization has the short refractory period. Additionally, mutant cell with high cGMP level showed long refractoriness for sGC localization, suggesting that cGMP has an important role in high-frequency signaling for chemotaxis.

2Pos142 受容体の細胞膜上空間分布解析
Spatial distribution analysis of membrane receptors

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Cell can sense external signals through membrane receptors and respond properly. Then, how do receptors distributed on the cell surface? And what is the functional significance of such distributions? To answer these questions concerning with oligomerization, membrane lipid heterogeneity, and cell polarity, almost all cAR1 molecules (a GPCR that is essential for chemotactic signaling) in a Dictyostelium cell were spatially detected by super-resolution imaging PALM. Spatial statistical analysis showed that its distribution is significantly different from being random, more receptors clustered in the front side of the cell, and its frequency distribution is almost power-law. Possible mechanisms and functional significance of these findings will be discussed.

2Pos143 大腸菌温度感覚レセプター Tar-Tap キメラ体の温度受容能
Thermosensing abilities of Tar-Tap chimeric receptors of *Escherichia coli*

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Escherichia coli can sense temperature gradients and migrate toward warmer environments, a property called thermotaxis. Thermal stimuli are sensed by four chemoreceptors: Tsr, Tar and Trg function as warm sensors, which produce attractant and repellent signals upon increases and decreases in temperature, whereas Tap serves as a cold sensor, which elicits opposite signals. Here we constructed a series of Tar-Tap chimeric receptors to identify the region responsible for thermosensing. All the chimeras carrying the second transmembrane segment (TM2) of Tap functioned as cold receptors. Together with our previous finding that the periplasmic domain is dispensable for thermosensing, these results suggest that TM2 is the primary determinant for thermosensing.

2Pos144 脊椎動物の光受容タンパク質 Opn5 の分子特性の多様化とその変換
Comparison and conversion of diversified molecular properties in vertebrates Opn5 group

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Opn5s form one of independent groups in animal opsins and are responsible for non-visual photoreceptions. Vertebrate Opn5s are classified into four subgroups that are diversified based on the spectral sensitivity, preference for retinal isomers and photoreaction process. Opn5m and Opn5L2 subgroups contain UV light-sensitive bistable opsins, Opn5n contains visible light-sensitive opsins, and Opn5L1 contains photocyclic opsins to regulate their activities. Additionally, opsins within some of the subgroups have been further diversified from each other. In this study, we tried to convert the molecular properties among and within Opn5 subgroups by mutational analyses. From the results, we discuss amino acid residues responsible for the diversification of Opn5 subgroups.

2Pos145 Rc-PYP の光依存的複合体種の形成機構
Light dependent multiple complex formation of Rc-PYP

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Rhodobacter capsulatus PYP (Rc-PYP) is a light receptor protein which binds with PYP binding protein (PBP) in a light-dependent manner. Titration small angle X-ray scattering (tiSAXS) experiments have suggested that Rc-PYP and PBP can form several complexes depending to PYP/PBP molar ratio. Complexes mass identified by native MS measurement in several molar ratio conditions of PYP/PBP are stepwisely increased with 60KDa corresponding to two PYP molecules and one PBP dimer. Complex formation model was constructed from above results and applied to analysis of the result of tiSAXS. Two different Kd value were identified for these complexes formation, this is an essential factor to form different complexes in different molar ratio of PYP/PBP.

2Pos146 Light-Driven Cl^- Transport Mechanism of *Nonlabens marinus* Rhodopsin-3 Studied by Static and Time-Resolved Spectroscopy

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Nonlabens marinus rhodopsin-3, NM-R3, is a member of bacterial NTQ-type rhodopsins with light-driven inward Cl^- transport activity <Yoshizawa et al., *Proc. Natl. Acad. Sci. USA* 111, 6732-37, 2014>. In this study, to investigate the photoreaction dynamics directly connected to the Cl^- transport function of NM-R3, we performed static and time-resolved spectroscopic measurements. As a result, we found that NM-R3 passed through 5 or 6 photochemically distinct intermediates during the cyclic reaction called photocycle and the Cl^- was released and then taken up in the L or N – O_1 and O_2 – NM-R3' transitions in the photocycle. We propose the Cl^- transport mechanism of NM-R3 based on our results with other findings <Tsukamoto et al., *J. Phys. Chem. B* 121, 2027-38, 2017>.

2Pos147 The photochemical properties of archaerhodopsin and its mutants found in *Halorubrum* sp. ejinoor

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Haloarchaea *Halorubrumc* sp. ejinoor (*He*) was isolated from Ejinoor salt lake in Inner Mongolia of China. Three ORFs of retinal proteins (AR-like, HR-like and SRII-like) were identified in *He* genome DNA. Measurements of light-induced ion transport by *He*-membrane vesicles indicate the existence of proton pumping and chloride pumping activities.The AR-like retinal protein of *He* (*He*AR) was expressed in *E. coli* and it was confirmed that *He*AR is a light-driven outward proton pump. We made several amino acid displaced mutants of *He*AR and performed flash photolysis and ion pump activity measurements. The flash photolysis measurements show that the photocycle time constant of *He*AR-S164A is obviously different from that of the wild type.

2Pos148 桿体・錐体外節膜における脂質組成の解析
Analysis on lipid compositions in outer segment membranes of rod and cone photoreceptor cells

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Vertebrates have two types of visual photoreceptor cells, rods and cones. It is well known that the characteristics of the photoresponses are different between rods and cones. For example, rods show higher light sensitivity than cones. Due to this difference, rods mediate night vision and cones mediate daylight vision.
Both rods and cones have a cellular site, called outer segment (OS), responsible for generation of photoresponses. We succeeded to purify rod- and cone-OS from purified carp rods and cones, respectively. This enabled us to study the molecular bases of rod- and cone-specific responses. In this study, we analyzed the lipid compositions in rod- and cone-OS, and found some differences between them. The effect of the differences on responses will be discussed.

2Pos149 脊椎動物の視物質とピノプシンの熱活性化効率の比較解析
Comparison of thermal activation rates between vertebrate visual pigments and pinopsin

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Most vertebrate retinas have two types of photoreceptor cells, rods and cones. Rods are responsible for scotopic vision and cones are for photopic vision. Scotopic vision requires high sensitivity and low threshold to be able to detect a few photons. This can be achieved by the fact that rhodopsins in rod cells exhibit much lower thermal activation rates than cone pigments. In this study, to explore the molecular origin of vertebrate visual pigments, we compared the thermal activation rates between pinopsin and visual pigments. Pinopsin was originally identified from chicken pineal gland and is most closely related with visual pigments in the phylogenetic tree. We would like to discuss the diversification model of visual pigments and pinopsin.

2Pos150 光駆動ナトリウムポンプ KR2 の多量体形成に重要なアミノ酸残基
Aromatic amino acids of a light-driven sodium pump KR2 are important to form an oligomer

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Microbial rhodopsins form various oligomeric structures. A light-driven proton pump bacteriorhodopsin (BR) and chloride pump halorhodopsin (HR) form a trimer, which is important for thermal stability and function. On the other hand, a light-driven sodium pump KR2 forms a pentamer in 3-D crystal, whose role has been unclear. In this study, we found that F27A, Y154A and F158A mutants of KR2 showed different elution profiles from KR2-WT by size-exclusion chromatography in DDM solution. It suggested that these aromatic amino acids are important to form an oligomeric structure. The role of oligomerization for the function of KR2 will be discussed based on various methods including flash photolysis and high-speed atomic force microscopy.

2Pos151 紫外共鳴ラマン分光法によるオレンジカロテノイドタンパク質の光活性化機構

Evidence for close-to-open photoactivation of orange carotenoid protein from ultraviolet resonance Raman spectroscopy

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Orange carotenoid protein (OCP) is a soluble carotenoid-binding protein which plays an important role in photoprotection of cyanobacteria. Under strong blue-green light, OCP undergoes photoconversion from the orange dark state (OCPO) to the red active state (OCPR), by which OCP can absorb and release the excess excitation energy from the light-harvesting antenna for photoprotection. In this photoactivation process, the protein structural change from close to open form has been proposed in biochemical and spectroscopic studies. In this study, we use ultraviolet resonance Raman spectroscopy to directly observe the protein structure and examine the photoactivation mechanism. The Raman spectroscopic evidence for the close-to-open photoactivation of OCP will be presented.

2Pos152 霊長類青感受性視物質の極大吸収波長における内部結合水の役割

The role of internal water molecules in λ_{max} of primate blue-sensitive visual pigment

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Protein-bound waters are essential for the structure and function of many membrane proteins, including GPCRs. Here we report FTIR spectra of primate blue-sensitive visual pigment (MB), revealing the presence of internal waters possessing unique water vibrational signals which are reminiscent of the water cluster (Katayama et al. Sci. Rep. 2017). These vibrational signals of the waters are influenced by mutations at position Glu113 and Trp265 in Rh, suggesting that these waters are situated in between these two residues. Tyr265 being the key residue for achieving the spectral blue shift in λ_{max} of MB, we propose that these waters are responsible for increasing polarity toward the retinal Schiff base, leading to the blue shift of λ_{max}.

2Pos153 Na^+ポンプ型ロドプシンのNa^+輸送過程の解析

Analysis of Na^+ transfer reactions of Na^+-pumping rhodopsin

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The Na^+ transfer reactions were examined by a Na^+ selective membrane. The lipid-reconstituted *Gillisia limnaea* rhodopsin (GLR) was dried on the surface of Na^+ selective membrane, which was prepared with an ionophore Bis(12-crown-4) and PVC. After immersion in the buffer solution, the membrane potential was measured. Under continuous illumination, we observed the potential upshift, indicating the decrease of Na^+ concentration. When employing proteorhodopsin and a disabled GLR mutant, no potential shift was observed. We also attempted the time-resolved detection by using a laser pulse. The detected potential change almost matched the concentration change of O intermediate, suggesting that Na^+ is captured and released during the formation and decay of O intermediate.

2Pos154 *Gloeobacter* rhodopsin の多量体構造における機能的役割の解明

Functional importance of trimer formation of light-driven H^+pump*Gloeobacter* rhodopsin

Azusa Iizuka[1], Takashi Kikukawa[1,2], Kousuke Kajimoto[3], Tomoki Fujisawa[3], Takashi Tsukamoto[1,2], Tmoyasu Aizawa[1,2], Naoki Kamo[1], Masashi Unno[3], Makoto Demura[1,2] ([1]*Glad. Sch. Life Sci., Hokkaido Univ*, [2]*GSS, GI-CoRE, Hokkaido Univ.*, [3]*Grad. Sch. Sci. Eng., Saga Univ.*)

Many microbial rhodopsins are known to self-oligomerize, whereas the roles of oligomeric structures have not been well clarified. Here, we examined the role for a H^+ pump *Gloeobacter* rhodopsin (GR) by using the nanodiscs containing the GR trimer and the monomer. The monomerization appeared not to affect the dark state, but largely distorted the photocycle. The transient absorption and resonance Raman spectroscopies showed no M intermediate formation, and the pH indicator dye detected only negligible H^+ transfer reaction. Thus, monomeric GR probably loses the H^+ pumping activity. The trimeric assembly might enable the primal H^+ transfer reaction through adjusting the protein conformation around the Schiff base region.

2Pos155 Challenge for direct observation of bacterial growth and death in long-term starvation

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In most organisms, depletion of resources causes death of a majority of population, but in some bacteria, a minority of population can survive in starvation for years. Previous studies suggested that the surviving population is not static, and balancing of death and growth using nutrients from dead cells is essential for long-term survival in starvation. However, no study has yet directly observed death and recovery of viability that would occur in small fraction of cells upon prolonged starvation.
Here, we combined microscopy and fluidic chamber, and aimed to estimate death and growth rate of starved bacterial population quantitatively in single-cell level. This experimental system would enable us to understand more clearly resilience of starved microbial population.

2Pos156 運動性シアノバクテリアのコロニー形成による増殖活性の解析

Analysis of proliferation rate depending on colonial morphologies in motile cyanobacteria, Pseudanabaena sp

Keita Mizoe, Atsuko Takamatsu, Taku Kimura (*Waseda University*)

Motile cyanobacteria, Psedanabaena sp., are considered to adapt to environmental by forming various types of colonial morphologies. By measuring cell size distribution in each colony, the relation between cell proliferation rate and colony morphology was investigated. The distributions for colonies consisting of dense population included smaller cells than those for single bodies or aggregations of several bodies. The result suggests that proliferation rate become higher by forming dense population. It is known that bacteria secretes slime material, which would promote cell proliferation. Another possible candidate for promoter of cell division is direct interaction of bodies through pilli. To examine those more detailed analysis of small size aggregations is ongoing.

2Pos157 微生物生態系における種の共存と代謝ネットワーク
Metabolic network enables to live together in microbial ecosystems

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What is the mechanism of coexistence in microbial ecosystems? Theoretically, a microbial strain overcomes the other strain but not live together under competitive conditions. However, phenol-degrading bacteria strains P-10 and R2 had lived together under chemostat conditions supplied with phenol as sole carbon and energy source. The gene encoding phenol hydrogenase was expressed in only strain P-10 under a condition, whereas a dominant strain and expression of genes related to phenol-metabolism changed corresponding to changes of phenol-loading rates. These results suggested that the change of metabolic network reflected the process of adaptation to environmental changes, resulting in coexistence of microbial strains in competitive relationships.

2Pos158 フグ種別鑑別システムのためのフグ模様再現モデルの構築
Skin patterns replicate model of puffer fish for the crossbreed puffer fish identification system

Takeshi Ishida, Daiki Tadokoro (*National Fisheries University*)

Identification of puffer fish for edible use is conducted by expert who holds the cooking license of puffer fish. On the other hand, it is difficult to identify the poisoned part in case of crossbreed puffer. Therefore the entire doubtful crossbreed puffer is discarded at fishery harbor. If it could be established the crossbreed puffer fish identification system, it will be decreased the disposal puffer fish. In this study, replicate model of puffer fish skin patterns was constructed with cellular automata (CA) model. Here, our CA model can emerge Turing patterns through via the exchange of binary values between neighboring cells. In spite of a simple model, this model can produce characteristic skin pattern of all puffer fishes of Takifugu.

2Pos159 NMDA 受容体を介した Ca2+上昇による情報伝達の小体積効果
Small-Volume Effect of Information Transmission by NMDA receptor-mediated Ca2+ increase

Takehiro Tottori[1], Masashi Fujii[2], Shinya Kuroda[2] ([1]*Fac. Sci., Univ. Tokyo*, [2]*Grad. Sch. Sci., Univ. Tokyo*)

The spine is a small compartment of a neuron, which can contain only small numbers of molecules. Reactions inevitably become stochastic in the spines, and it is intuitively disadvantageous for information transfer. We previously found the small-volume effect, which the smallness of the spine of the cerebellar Purkinje cell realizes robust, sensitive, and efficient information transfer by mGluR-mediated Ca2+ increase. However, it is unknown whether this small-volume effect is observed for NMDA receptor-mediated Ca2+ increase in other spines such as cerebrum pyramidal cells. Here, we analyze small-volume effect of information transfer by NMDA receptor-mediated Ca2+ increase and examined the generality of the small-volume effect in the spines.

2Pos160 A Modified Sequence-Dependent Coarse-Grained Elastic-Network Model for DNA

Yan Zhao, Akinori Awazu, Hiraku Nishimori (*Grad. Sch. Sci., Univ. Hiroshima*)

Human nucleosome forming sequence and excluding sequence have significant impact on nucleosome positioning, observing the dynamical differences of these sequences can help with the identification of them. We used an accurate enough 3SPN.2C model to simulate and found their principle moving directions by using PCA. Considering the simulation is time consuming, we modified the simpler ENM to fit the sequence dependent property of DNA. In our modified ENM, we took base pairing and base stacking energies into account by giving different base pairs different spring constants, making simulation of sequence dependent dynamics of DNA possible. We also compared the anisotropic fluctuations of our model with 3SPN.2C model to verify the reasonability and efficiency of our model.

2Pos161 A stochastic simulation study on the mechanism of correlation between circadian oscillation and ATPase activity of KaiC hexamer

Sumita Das[1], Shota Hashimoto[1], Tomoki P. Terada[1,2], Masaki Sasai[1,2] ([1]*Department of Computational Science and Engineering, Nagoya University*, [2]*Department of Applied Physics, Nagoya University*)

KaiC is a hexameric protein, and each of its six subunits shows the slow ATPase activity. We developed a model of single KaiC hexamer and simulated the coupled oscillation of ATP hydrolysis and phosphorylation/dephosphorylation to explain the experimentally observed correlation between the ATPase activity and oscillation frequency. Because a single molecular simulation shows the large stochastic fluctuation, we examined the statistical distribution of the simulated frequency by running several thousand trajectories. Through such statistical analysis, we showed that the above correlation can be found in a single-molecular level when both the negative-feedback and positive-feedback mechanisms coexist within a single KaiC hexamer.

2Pos162 Extraction of statistical dynamics of a stochastic neuronal model

Takanobu Yamanobe (*Sch. Med., Hokkaido Univ.*)

In this study, we tried to extract the mathematical structure in a stochastic neuronal model. We used non-negative matrix factorization with sparseness constraints to reduce the linear operator that describes the statistical dynamics of a stochastic neuronal model. By using the given kernel function of the linear operator, this method allows us to construct a set of basis functions and the coefficients that describe the contribution of each basis function. We evaluated whether the kernel of the linear operator can be approximated by non-negative matrix factorization and showed that the kernel of the linear operator can be reproduced by using the set of basis functions and the corresponding coefficients.

2Pos163 DNA 損傷認識タンパク質による核内哨戒効率の理論的考察
Theoretical study of nuclear patrol efficiency by DNA damage recognition protein

Takamasa Yamamoto, Hiraku Nishimori, Akinori Awazu (*Dept. Math and Life Sci. Hiroshima Univ.*)

In nucleotide removal repair, which is one of key mechanisms for repairing DNA damage, XPC plays a role of damage recognition. XPC can find and bind to various DNA damages induced by ultraviolet rays or various chemical substances. A recent study reported that XPC and DNA damage sites are accumulated in deacetylated sites when DNA damage due to ultraviolet rays occurs. However, the mechanism and physiological roles of such processes were still unclear. In this study, we constructed a mathematical model of patrol behaviors of XPC in chromosomes using spring-beads model. We focused on the relationship between chromosome density and nuclear patrol efficiency to unveil functional meanings of such damage induced XPC-chromosome accumulations.

2Pos164 核膜変形と核内流体を考慮した分裂酵母減数分裂期染色体のモデル
Model of fission yeast meiotic chromosome considering nuclear envelope deformation and intranuclear hydrodynamics

Kazutaka Takao, Hiraku Nishimori, Akinori Awazu (*Dept. Math and Life Sci., Hiroshima Univ.*)

Homologous recombination (HR) in meiosis contributes to the genetic diversity within the same species. For the correct HR, the homologous chromosomes(HC) pairing must be formed correctly. However, the mechanism how chromosome search and recognize HC is not clear. In S.pombe, nuclear reciprocation with its deformation in cell is observed in meiosis prophase. Here, nuclear deformation induces intranuclear fluid flows and influences on the chromosome motions through the hydrodynamic effects. So in this study, we constructed a mathematical model considering nuclear deformation and hydrodynamic effects among chromosomes and nuclear envelope. As a result, we obtain pairing is formed from the part near SPB and HC takes a layered structure during nuclear reciprocations.

2Pos165 Understanding the Selection Effect through Lineage-Removal Operations

Shunpei Yamauchi, Yuichi Wakamoto (*Graduate School of Arts and Sciences, The University of Tokyo*)

Statistics of cellular phenotypes and dynamics obtained by single-cell measurement methods are generally different from those of large cellular populations in batch cultures because of the bias from the manual or automatic cell removal operations that are unavoidable in those methods. In this study, we have developed a theoretical framework that explicitly takes the effects of cell removal into account and quantifies fitness landscapes for phenotypic traits on lineages and selection strength in heterogeneous population. We whereby show that the increase of the selection strength caused by a certain type of cell removal operation is proportional to the fitness variance of the phenotype, a relation analogous to Fisher's Fundamental Theorem.

2Pos166 ヌクレオソーム排他的 DNA 配列のインスレーター機能の解析
Analysis of insulator function of nucleosome exclusive DNA sequence

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Insulator sequence is known to plays a role of genome domain boundary. CTCF binding site is one of the typical insulators that forms chromatin individual loop domain by binding CTCF and cohesion. Recently, nucleosome exclusive sequences like Poly-A or CCGNN repeat sequences and Ars-insulator identified in Sea Urchin also show insulator activity.
Then, in this study, we consider the mechanism of the insulator activity of such nucleosome exclusive sequences. We constructed a model that assumes nucleosome-containing regions can deform more flexibly on average than nucleosome exclusive region because of the influences of chromatin remodeling factors. Simulation result suggested the nucleosome exclusive sequence exhibits insulator activity due to its rigidness.

2Pos167 Theoretical study of YAP-dependent actomyosin network contribution to morphogenesis under gravity

Kazunori Takamiya, Seirin Ri, Hiraku Nishimori, Akinori Awazu (*Hiroshima University Graduate Graduate School of Science Department of Mathematical and Life Sciences*)

Multicellular organisms form their specific body shapes against the gravity. Recently, YAP protein was reported as a key transcriptional regulator to keep their body shape under gravity, where the YAP knockout mutant of medaka exhibits flattened body shape and misalignment of the organ. Furthermore, YAP knockout spheroid formed group of retinal cell cultured in human also showed the flattened body shape. Then, we construct a model of spheroid considering the dynamics of YAP-dependent actomyosin network and interactions among cells to unveil the mechanism of the abovementioned phenomena. We particularly focus on the roles of the interplays among intra-molecular dynamics and the translation and deformation of cells for their body shape regulations.

2Pos168 緑色光が及ぼす水素化アモルファスシリコン薄膜上のアミノ酸含有ゲルの電圧電流特性への効果
Green light effect on voltage current property of amino acid containing hydrogel on hydrogenated amorphous silicon film

Makoto Horigane[1], **Kouki Kagawa**[1], Mahoko Sano[1], Honoka Endo[1], Hiroshi Masumoto[2], Takashi Goto[3], Yutaka Tsujiuchi[1] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary*, [3]*Institute for Materials Research, Tohoku University*)

On an attempt for fabrication of biosensor using photo-controlled film system, we have been researching, by using ionic conduction in laminated gels on hydrogenated amorphous silicon film. In this study, voltage current analysis of amino acid containing hydrogel photo-controlled on hydrogenated amorphous silicon film (a-Si:H), are done using cottrell equation system, using several amino acids that are the elementally elements of bio molecule and has potential of diversity to electro chemical device. Recently we achieved an effective light controlling of gel on a-Si:H.

2Pos169 オンチップ 1 細胞計測系によるマクロファージの貪食試料の最適化

Optimization of antigen of macrophage phagocytosis using on-chip single cell measurement assay

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For understanding regulation of phagocytosis on a surface of single macrophage, optimization of antigen is important for reliable interpretation of multiple stimulation experiments. We examined and compared phagocytosis of three kinds of antigens as standard model candidates; 2-μm polystyrene (PS) beads, BSA coated PS beads (BSA-PS), and IgG coated PS beads (IgG-PS). Antigens were captured and attached on the surface of a macrophage by using of optical tweezers. IgG-PS showed the highest phagocytic efficiency, ca. 90% within 5 min after contact, whereas PS 30%, and BSA-PS 50%. The results indicate that IgG-PS is recognized by macrophages with almost 100% and is suitable for the studies on multi-stimulation phagocytosis mechanism of macrophages.

2Pos170 強制拍動刺激周期の変化に応答した心筋細胞集団の細胞外電位変化

Adaptation of field potential duration in cardiomyocyte clusters under forced electrical stimulation intervals

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External field potential is one of the powerful measurement technologies for analyzing the long-term change of their properties like adaptation. The QT interval on electrocardiogram is a key factor for the prediction of arrhythmogenicity, and is thought to equivalent to the field potential duration (FPD). To evaluate the FPD flexibility and hysteresis in cardiomyocytes, the change of FPD caused by the forced beating intervals was investigated using cardiomyocyte clusters in on-chip electrophysiological screening assay. When the faster electrical interval stimulation than spontaneous beating rate was applied, the FPD was exponentially shortened depending on the rate of stimulation intervals similar to the Bazett's manner.

2Pos171 オンチップ 1 細胞計測系によるマクロファージの同一点連続貪食の応答解析

Analysis of sequential single point phagocytosises in macrophages using on-chip single cell measurement assay

Yoshiki Nakata[1], Yuya Furumoto[2], Masao Odaka[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Hideyuki Terazono[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*Waseda Biosci. Res. Ins. in Singapore (WABIOS)*)

For understanding the recognition and response mechanism of phagocytosis for antigens in macrophage, we observed phagocytic response to sequential stimulations of antigens on single identical position of isolated single cells. We contacted an IgG coated 2-μm microbead as antigen on the surface of J774.2 cells by using optical tweezers. Once the microbead activated the cell for phagocytosis and was engulfed, the next microbead was attached at the identical point immediately. Then a series of phagocytosises occurred sequentially on identical position of isolated cells. However, the maximum engulfed number of microbeads for phagocytosis existed, and seems to be caused by the limit of acceptable engulf volume, i.e., the existence of volume-sensing phagocytosis mechanism.

2Pos172 心筋細胞クラスターの拍動周期の起源：心筋細胞ネットワークの拍動周期の選択ルールの解明

Origin of cardiomyocyte cluster beating intervals: Elucidation of selection rule of interbeat intervals of cardiomyocyte network

Naoki Takahashi[1], Natuki Seki[2], Masao Odaka[3,4], Hideyuki Terazono[3,4], Kenji Matsuura[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*, [4]*Waseda Biosci. Res. Ins. in Singapore (WABIOS)*)

We examined the hidden mechanism of interbeat interval (IBI) selection of the cell cluster from variety of different IBI of component cells during their clustering. We compared the IBIs and its stabilities of cardiomyocyte clusters and those of isolated single cells. Some isolated cardiomyocytes showed faster IBI than the clusters. In addition, the IBI of the clusters has stability equivalent to the most stable isolated cells. These results showed experimentally that only the concept of conduction in cardiomyocyte network is not enough to explain IBI selection rule in a spontaneous beating cell networks. Furthermore, we suggest that the IBI of cardiomyocyte network is determined depending on the stability of the IBI of the component cells before synchronization.

2Pos173 Study of the Structure change in protein using Polarization-dependent Fluorescence Correlation Spectroscopy (Pol-FCS)

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Polarization-dependent Fluorescent Correlation Spectroscopy (Pol-FCS) detects molecular rotational and translational diffusion dynamics of fluorophore, simultaneously. The purpose of this study is to confirm the fraction of rotational diffusion in Pol-FCS measurement relates orientation of fluorophores and shape of molecules. The relationship has been suggested by previous report and simulation (Oura *et al*. Sci Rep 2016). For this purpose, a new Ca^{2+} censor YY3.60 was constructed and measured by home-build Pol-FCS system. The relationship was confirmed in the different concentration of Ca^{2+}. Moreover, these results suggested that the Pol-FCS will be a convenient and powerful tool to analyze structure change of molecules such as protein and nucleic acids oligomer.

2Pos174 角度ダイナミックレンジ広範化に向けたサンプル傾斜角度走査型 X 線 1 分子追跡法の開発

Development of Sample Angular Scanning Diffracted X-ray Tracking for Enhancing Angular Dynamic Range

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Diffracted X-ray tracking is one of single molecule techniques for detecting atomic motion of the protein with microseconds level. A protein is labeled with a nanocrystal and the motion of the crystal coupled with the protein's motion is recorded as the trajectory of diffraction spot from the crystal. The narrow dynamic angular range is one of big problem for this method. The wider energy width of incident X-ray enhances the dynamic angular range; however, such incident X-ray has serious radiation damage for samples. We addressed these issues by recording diffraction images with fast sample scanning in tilting direction. The motion of the sample is elucidated by considering the sample angular position, and the apparent dynamic range is enhanced as sample scanning range.

2Pos175 SQUID とネオジウム磁石片を用いて，繊毛運動を測定する
Measurement of ciliary movement using SQUID gradiometer and a small neodymium magnet piece

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Ciliary movement in the choroid plexus in the mammalian ventricle causes cerebrospinal fluid circulation. In many studies on ciliary movement in the choroid plexus ciliated cells are taken out from the ventricle and studied in vitro; i.e., the ciliary movement in the choroid plexus has not been studied non-invasively in the animal. Superconducting quantum interference device (SQUID) is an ultra-sensitive magnetic sensor. We detected a signal (ca. 12 Hz and ca. 10 pT amplitude) from a small neodymium magnet piece attached on the cilia in the mantle of clams with a SQUID gradiometer placed ca. 30 mm above the specimen. This successful detection will lead to a new sensing platform that enables non-invasively measurement of ciliary movement from an intact animal.

2Pos176 冷却 HPD による広視野 1 分子蛍光寿命測定
Wide-field single-molecule fluorescence lifetime measurement by a cooled hybrid photo-detector (HPD)

Atsuhito Fukasawa[1], Gaku Nakano[1], Takayasu Nagasawa[1], Shigeru Ichikawa[1], Minako Hirano[2], Toru Ide[3], Yasuharu Negi[1], Tomohiro Ishizu[1], Hiroaki Yokota[2] ([1]*Hamamatsu Photonics K. K.*, [2]*Grad. Sch. Creation Photon. Indust.*, [3]*Grad. Sch. Nat. Sci. Tecnol., Okayama Univ.*)

We presented in the 2014 annual meeting that a cooled Hybrid photo-detector (HPD) (Hamamatsu Photonics) consisting of a photocathode and an avalanche photodiode enables low-background wide-field sub-millisecond single-molecule fluorescence detection. Here, we demonstrate that the HPD enables wide-field single-molecule fluorescence lifetime measurement with nanosecond temporal resolution. We will present time courses of single-molecule fluorescence lifetime of a fluorophore such as a Qdot whose fluorescence images were simultaneously monitored by an EM-CCD. The HPD based time-resolved single-molecule fluorescence detection, which is unlike fluorescence intensity based single-molecule detection, provides us with a new approach to dynamics of mobile single biomolecules.

2Pos177 PC12 細胞の神経分化における細胞内温度イメージング
Imaging of intracellular temperature in PC12 cell nerve differentiation

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Neurite outgrowth is a key process in the development of the nerve differentiation. It has been reported that nerve differentiation is influenced by extracellular factors (e.g. cytokine) or intracellular factors (e.g. DNA methylation or histone modification). Recent studies showed that physical factors such as temperature (e.g. extracellular heat shock) also affects the neurite outgrowth ability. However, the detail mechanism remain elusive. Here, we characterize the intracellular temperature in relation to nerve differentiation by using a fluorescent polymeric thermometer and fluorescence-lifetime imaging microscopy (FLIM). We found the difference of the local temperature exists in the PC12 cells after NGF stimulation, and we would present our recent trial.

2Pos178 蛍光イメージング定量解析で明らかになった ATP に依存した INO80 クロマチン再構成複合体の核内動態
ATP dependent dynamics of INO80 chromatin remodeling complex revealed by quantitative fluorescence imaging

Yuma Ito[1], Masahiko Harata[2], Kumiko Sakata-Sogawa[2], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

ATP-dependent chromatin remodeling complex INO80 plays an important role in the structural changes of chromatin by sliding on DNA and evicting nucleosomes. Although INO80 complex contains several ATP binding subunits, including scafford Ino80 protein and actin related proteins (Arps), the role of ATP on the dynamics of the INO80 complex remains pooly understood. Here, we investigated the dynamics of Ino80, Arp4, Arp5 and Arp8 subunits in living cells using single-molecule tracking and FRAP. Quantitative image analysis of living cells with ATP depletion and ATP-binding mutants revealed distinct effects of ATP on the dynamics of these subunits. We will dissuss a quantitative model for the contribution of ATP on the dynamics of INO80 complex.

2Pos179 Screening of chemical compounds to find new inhibitors against ATP synthesis in mitochondria by MASC assay

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Several lines of evidence have suggested the relationship between ATP level change and extension of lifespan of nematode. For instance, the addition of metabolite alpha-ketoglutatate extends lifespan of worm with decrease of ATP level due to inhibition of ATP synthesis by oxidative phosphorylation.
In this study, we carry out the screening of chemical library to find inhibitor against ATP synthesis by MASC (Mitochondrial Activity of SLO-permeabilized Cells) assay. Up to date, we found 14 kinds of compounds by screening of ~200 chemical compounds. We will plan to investigate whether these inhibitors change the ATP level of cultured cells or nematode using ATP sensor protein ATeam.

2Pos180 線形ゼロモード導波路を用いたアクチン重合の 1 分子観察
Single-molecule analysis of actin polymerization mechanism using linear zero-mode waveguides

Soichiro Fujii[1], Ryo Iizuka[1], Masamichi Yamamoto[1], Makoto Tsunoda[1], Takashi Tanii[2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [2]*Fac. Sci. Eng., Waseda Univ.*)

Actin polymerization occurs through nucleation, elongation, and the steady-state phase. A previous study showed that ends of actin filaments grow and shorten faster than expected from the measured rate constants of monomer association and dissociation. However, the reason of the discrepancy has not been clarified. Actin polymerization using single-molecule fluorescence imaging with linear zero-mode waveguides was observed to investigate the oligomeric state of actin incorporated into the filament ends. We found that the monomers were associated with the filament ends in elongation phase, but small oligomers (dimer to trimer) were also associated with filaments in the steady-state phase. Furthermore, cooperative binding of actin at the filament ends was not observed.

2Pos181 ストレス顆粒内内在性 mRNA のナノスケール構成
Nanoscale Organization of Endogenous mRNAs in Stress Granules

Ko Sugawara[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., Univ. Tokyo*, [2]*JST, PRESTO*)

Stress granules (SGs) are RNA granules found in the eukaryotic cytoplasm under stress. Although it is indicated that the formation of SGs is related to translation regulation, the mechanism on how mRNAs are organized inside SGs remains unclear. Here, we visualized nanoscale localization and dynamics of endogenous mRNAs in stressed mammalian cells. Fluorescence super-resolution localization microscopy revealed that mRNAs inside SGs are distributed heterogeneously and form small clusters with a diameter of ~70 nm. Single mRNA tracking showed that mRNAs inside SGs are dominantly immobile. These results suggest that SGs are highly organized structure built up with small clusters composed of tethered mRNAs, which might contribute to translation regulation under stress.

2Pos182 酸化ストレス応答における Nrf2 動態の生細胞 1 分子イメージング
Dynamics changes of transcriptional factor Nrf2 in living cells upon exposure to oxidative stress using single-molecule imaging

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NE-E2-related factor 2(Nrf2) is a transcription factor that regulates oxidative stress genes. When cells are exposed to oxidative stress, Nrf2 accumulates in the nucleus and activates transcription of target genes as a heterodimer with MafG. However, the dynamic mechanism remains unclear. Here, we employed single-molecule tracking of SNAP-tagged Nrf2 and MafG in living cells. MafG molecules were found mainly to be immobile or following a slow diffusion, while Nrf2 diffused rapidly in the nucleus. Our results suggest that Nrf2 and MafG are governed by distinct molecular mechanisms. We will discuss the relationship between dynamics and function of heterodimerization based on simultaneous multi-color single-molecule imaging.

2Pos183 金，銀ナノ粒子を用いたマルチカラー 1 分子イメージング法の開発
Development of multi-color single-molecule imaging method using gold and silver nanoparticles

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Gold nanoparticles (AuNPs) have been used as optical contrast agents for single-molecule imaging of various biomolecular machines. Here we used silver nanoparticles (AgNPs) with AuNPs to develop multi-color single-molecule imaging method. Peak wavelength of AgNPs in the scattering spectra locates at ~400 nm, which is more than 100 nm shorter than that of AuNPs. With two lasers at 404 nm for AgNPs and 520 nm for AuNPs, we constructed total-internal reflection dark-field (DF) microscope. Through dual-view optics with a dichroic filter, DF images of AuNPs and AgNPs were projected on the different portion of same EMCCD camera. Frame rate and localization precision of the system, and application toward multi-color single-molecule imaging of protein motors will be discussed.

2Pos184 RNA 顆粒形成過程の細胞内温度測定
Intracellular temperature measurement during RNA granule formation

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RNA granules are non-membranous ribonucleoprotein aggregates that regulate translation to control the timing of protein synthesis. However, it is unknown how translating mRNAs initiate forming RNA granules. Previously, we showed that temperature variation inside cells is essential for this phenomenon. In this study, we performed temperature imaging during formation process of various physiological RNA granules by introducing fluorescent polymeric thermometer and antisense RNA probe into both cells and tissues. As well as stress granule in mammalian cells, we succeeded in observing P granule while visualizing temperature distribution in germ line cells of C. elegans. These imaging techniques will help to clarify the mechanism of RNA granule formation.

2Pos185 金ナノ粒子を利用した単一細胞内局所加熱法の開発
Development of a method of local heating a single cell using gold nanoparticles

Takaaki Honda[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharma. Sci., Univ. Tokyo*, [2]*JST, PRESTO*)

Although recent studies have shown that the intracellular temperature is heterogeneous, the mechanism and significance of intracellular heat generation are still unknown. Therefore, we aimed to develop a method to control intracellular local temperature for investigation of heat-related cell functions. In this study, we used gold nanoparticles (GNPs) for heating the cells. We investigated the incorporation of GNPs into cells and irradiated them with a laser. We succeeded in manipulating intracellular temperature increase in a quantitative manner and inducing local heat-mediated stress granules. These results show that this method is useful for comprehension of cell responses to the local intracellular temperature change.

2Pos186 相平衡状態にある核小体内領域における核小体構成タンパク質の 1 分子動態解析
Single-molecule dynamics of nucleolar proteins in different compartments of nucleolus

Daiki Matsumoto[1], Yuma Ito[1], Noriko Saitoh[2], Kumiko Sakata-Sogawa[3], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Dept. of Cancer Biol., The Cancer Inst. JFCR.*, [3]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

Nucleolus maintains its structure without being surrounded by biological membranes, and is divided into different compartments, including FC, DFC and GC. Although its importance in ribosome synthesis, the mechanism of its structural phase separation is still unclear. To investigate the physical properties of these compartments, we analyzed the single-molecule dynamics of constituent proteins in these compartments. In contrast to the simple diffusion behavior of NPM1 protein in GC region, FBL protein in DFC region slowly diffused with staying in one place frequently. Mean-square displacement analysis of single-molecule trajectories demonstrated the confined movement of FBL. We will discuss the effects of ribosomal proteins on the dynamics of these nucleolar proteins.

2Pos187 蛍光イメージングによる転写伸長メディエーター MED26 のダイナミクス解析

Molecular dynamics analysis of Mediator subunit MED26 controlling transcription elongation by fluorescence imaging in the nucleus

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Promoter-proximal pausing of Pol II is an rate-limiting step in transcription. Mediator subunit MED26 plays an important role in releasing from pausing. To elucidate the relationship between intracellular dynamics and its function, we performed FRAP analysis using domain deletion mutants of MED26. Fluorescence recovery of the N-terminal domain (NTD) deleted mutant was faster than that of the wild type, but slower than the C-terminal region (CTR) deleted mutant. Furthermore, wild-type was localized only in the nucleus, whereas a mutant lacking the intermediate region localized in the cytoplasm. Our results indicate that the interaction of CTR with the nuclear structure is stronger than that of NTD, and that the intermediate region is required for nuclear localization.

2Pos188 X 線自由電子レーザーを用いたコヒーレント X 線回折イメージングによる異なる細胞周期にある酵母細胞核の三次元構造解析

3D structural analyses of yeast nuclei in different cell phases by coherent X-ray diffraction imaging using X-ray free electron laser

Takahiro Yamamoto[1,2], Yuki Sekiguchi[1,2], Amane Kobayashi[1,2], Mao Oide[1,2], Asahi Fukuda[1,2], Koji Okajima[1,2], Tomotaka Oroguchi[1,2], Masaki Yamamoto[2], Masayoshi Nakasako[1,2] ([1]*Grad. Sci. Tech., Keio Univ.*, [2]*RSC, RIKEN*)

Coherent X-ray diffraction imaging (CXDI) is a technique for visualizing internal structures of sub-micrometer-sized biological particles without sectioning and chemical labeling. A 2D electron density map of a particle projected along the direction of the incident X-ray is obtained by phase-retrieval methods. By collecting a number of diffraction patterns from particles with similar structures in different orientations, an averaged 3D map of the particles can be reconstructed by applying the single particle analysis to the retrieved density maps. In this study, we reconstructed the 3D maps of yeast nuclei in the G2/M and G1 phases from a large number of diffraction patterns collected by CXDI experiments using X-ray free electron laser pulses at SACLA.

2Pos189 Photoregulation of Calmodulin using bifunctional Photochromic compound

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Calcium binding protein Calmodulin (CaM) has an important role in intra-cellular signal transduction. In this study, photochromic compounds as an artificial regulatory device were incorporated into the functional site of CaM to control CaM function photoreversibly. We employed the thiol group reactive photochromic compounds, PAM (N-(4-phenylazophenyl)maleimide), ABDM (Azobenzene-di-maleimide) as switching devices in CaM functional area. The CaM mutants, D24C-N60C and T28C-D64C were modified with the photochromic compounds. The modified CaM showed absorption spectral changes accompanied by photoisomerization of photochromic molecule upon UV and visible light irradiations. The photoreversible interaction of the photochromic CaM with M13-YFP was examined.

2Pos190 Introducing mitochondria to heterologous cells by electrofusion of giant unilamellar vesicles into cells

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Mitochondria are a cellular powerhouse in a live body. Defects in this energy generator results in metabolic disorders. Mitochondrial diseases are caused by maternally inherited mutations in mitochondrial DNA. Although an experimental animal is long-awaited, its reproduction has never been successful. To overcome this, we have invented a novel organelle transfer method. Fresh mitochondria were enclosed in giant unilamellar vesicles (GUVs) and these were subsequently fused with living cells transiently. Therefore, we successfully introduced human mitochondria into living rodent cells. Our results would be a potential milestone for developing a model mouse of human mitochondrial diseases and even for direct organelle transfer into heterologous species.

2Pos191 Photocontrol of interaction between small G protein Ras and its regulatory factor SOS using water soluble azobenezene

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Previously we have shown that guanine nucleotide exchange activity of SOS for Ras is photoreversibly regulated by the peptide mimicking SOSαH helix region, which is modified with hydrophobic azobenzene-di-maleimide (ABDM). However, the efficiency of photoregulation was not sufficient to utilize as a photo-switching. In this study, we employed water soluble azobenzene 2,2'-bis(sulfonate)-4,4'-bis(chloroacetamide)azobenzene (BSBCA22) to introduce photo-switching into SOSαH peptide. The SOSαH peptide modified with BSBCA22 showed absorption spectral change accompanied by UV and visible light irradiation. Photoreversible control of GDP-GTP exchange of Ras using SOSαH peptide modified with BSBCA22 was studied using fluorescent GDP analog.

2Pos192 Development of an automated microarray system for rapid microRNA profiling

Ryo Iizuka[1,2], Shoichi Tsuchiya[2], Taro Ueno[3], Takanori Ichiki[2,4], Takashi Funatsu[1] ([1]*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*, [2]*iCONM*, [3]*Nikon Corp.*, [4]*Grad. Sch. of Eng., The Univ. of Tokyo*)

Extracellular microRNAs (miRNAs) in body fluids such as serum, plasma, saliva, and urine have been identified as promising biomarkers for various human diseases. High-throughput profiling of these miRNAs is highly beneficial for the rapid and accurate diagnosis of diseases. To this end, we are developing an automated microarray system for rapid miRNA profiling. This system is based on ligase-assisted sandwich hybridization on a microfluidic mixing device, which allows the rapid and label-free detection of miRNAs. We demonstrated that 30 fmol of hsa-miR-143 was quantitatively detected in just 10 min after sample introduction. Our system enables to drastically reduce the time required to complete the assay compared with conventional microarray assays.

2Pos193 **Function control of vitamin D_3 hydroxilase toward efficient bio-sensing and bio-production**

Hikari Sasaki, **Yasuhiro Mie**, Yoshiaki Yasutake, Tomohiro Tamura (*Bioproduction Res. Inst., AIST*)

Vitamin D_3 hydroxylase (Vdh) is a cytochrome P450 monooxygenase that catalyzes the two-step hydroxylation of vitamin D_3 (VD_3) and produces 25-hydroxyvitamin D_3 ($25(OH)VD_3$) and 1α,25-dihydroxyvitamin D_3 ($1\alpha,25(OH)_2VD_3$). These hydroxylated derivatives are useful and currently used as pharmaceuticals for the treatment of symptoms associated with VD_3 deficiency and metabolic disorder. As the chemical synthesis of the hydroxylated VD_3 is inefficient, use of Vdh is promising for the efficient production. The electron supply step to the enzyme is a key process to utilize it effectively. In the present study, we developed the electrochemical system to drive the Vdh reaction with the electron transfer mediator and observed the catalytic signals.

2Pos194 **一分子検出のための生体ナノポアと固体ナノポアの特性比較**
CHARACTERISTICS COMPARISON OF BIOLOGICAL AND SOLID-STATE NANOPORES FOR A SINGLE MOLECULE DETECTION

Natsumi Takai[1], Masaki Matsushita[1], Kan Shoji[1], Tei Maki[2,3], Ryuji Kawano[1] ([1]*Dept. Biotech. Life Sci., TUAT*, [2]*Res. Ctr. for Sci. Tech., TUAT*, [3]*EM Biz. Unit, JEOL. Ltd*)

Nanopore sensing has attracted attention as a powerful tool for identifying unknown molecules. Types of nanopores are divided into biological and solid-state nanopores. It is important to select an appropriate nanopore for a single molecule detection with high sensitivity. However, the differences between these nanopores have not been discussed enough. Therefore, in this study, we compared streptolysin O and carbon-based nanopores as biological and solid-state nanopores which have same pore size. As a result, we evaluated the pore diameter and I-V characteristics and found that ion selectivity and shape of pores are different between these nanopores. We believe these findings contribute to select the optimal nanopore that depends on target molecules.

2Pos195 **人体システムにおける線形性と非線形性**
Linearity and Non-linearity in Human Body System

Susumu Ito[1], Izumi Kuboyama[2], Katsuhiko Hata[2] ([1]*High-Tech Res. Cent., Kokushikan Univ.*, [2]*Sch. Emerg. Med. Sys. Kokushikan Univ.*)

Linear system is relatively easy to analyse or simulate since it can be determined by the outputs to inputs which contain all frequency components. Biological systems such as human being, however, inevitably show non-linear behaviour since they cannot respond linearly to the unlimitedly large inputs.
Assumption of linearity, therefore, only can be applied to relatively small range of the inputs for a biological system, and even if the input range is sufficiently small, it sometimes shows quite evident non-linearity to input polarity. We discuss behaviour of biological system from the viewpoint of linearity and non-linearity, using respiratory and cardiovascular responses to load inputs of healthy adults in cycling exercise as a typical example.

2Pos196 **Automated cell manipulation system by using high-speed two fingered micro-hand**

Masaru Kojima[1], Eunhye Kim[1], Yasushi Mae[1], Tatsuo Arai[2,3] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Glob. Alliance Lab., The Univ. of Electro-Communications*, [3]*Beijing Inst. of Tech.*)

Recently, researches on manipulation method for biological cells are actively examined. For cell manipulation, probe type manipulator was used from a long time ago. However, manual operation with such device is difficult for beginner, and in order to improve the experimental efficiency, manipulation technic has to be improved for high speed and stabilize manipulation. From such viewpoint, cell manipulation support systems using micro robotics have been actively researched. We also developed two-fingered micro-hand systems, which realize high efficiency operation of micro objects. In here we demonstrate our developed system and show automated high-speed manipulation.

2Pos197 **ヘリックス相互作用認識を利用したエクソソームの細胞受容体標的**
Receptor clustering and activation using artificial coiled-coil peptide-modified exosomes

Natsumi Ueno[1,2], Miku Katayama[1,2], Kosuke Noguchi[1,2], Tomoka Takatani-Nakase[3], Nahoko Bailey Kobayashi[4,5], Tetsuhiko Yoshida[4,5], Ikuo Fujii[2], Shiroh Futaki[6], Ikuhiko Nakase[1] ([1]*N2RI, Osaka Prefecture Univ.*, [2]*Grad. Sch. Sci., Osaka Prefecture Univ.*, [3]*Sch. of Pham. Pham. Sci., Mukogawa Women's Univ.*, [4]*KARC, Keio Univ.*, [5]*Toagosei Co., Ltd.*, [6]*ICR, Kyoto Univ.*)

In this presentation, we demonstrate a novel system for inducing clustering of cell surface receptors using artificial leucine zipper peptides (E3/K4) [1], which form heterodimeric coiled-coils, and exosomes. Modification of the exosomal membrane with K4 peptide allowed for the recognition of E3-fused epidermal growth factor receptor (EGFR) on the cell membrane. With this system, targeting of receptor-expressing cells and facilitating the endocytic uptake of exosomes, which contained the anti-cancer protein saporin, were successfully achieved, leading to cell death [2].
[1] Litowski, R. J., *et al., J. Biol. Chem*., **277**, 37272-37279 (2002), [2] Nakase, I., Ueno, N., *et al., Chem. Commun*., **53**, 317-320 (2017).

2Pos198 **希釈がもたらす生命システムの非線形濃度応答とその人工細胞技術への応用**
Nonlinear concentration dependence of biosystems on dilution and its application on artificial cell technology

Kei Fujiwara (*Department of Biosciences and Informatics, Keio University*)

Because of nonlinear behavior of biosystems, the rate of the output from the initial substrate is not necessarily proportional to the concentration of the components in the system. By utilizing this fact, we developed a switch to regulate gene circuits by the shift of the system concentration, and realized an efficient bio-conversion system using a small amount of enzymes inside artificial cells. In this presentation, we show the results of numerical simulation and wet experiments targeting cell-free protein expression system and an artificial ethanol synthesis pathway. The results indicate the existence of threshold of the system concentration at the origin of life, and raise the possibility of fermentation using artificial cells.

2Pos199 **Interaction of HVR domain of small GTPase Ras with catalytic domain**

Takashi Hashimoto[1], Nobuhisa Umeki[2], Yasunobu Sugimoto[3], Shinsaku Maruta[1] ([1]*Grad. Sci. Bioinfo., Univ. Soka*, [2]*Wako Inst., RIKEN*, [3]*NUSR*)

The lipid-anchored small G protein Ras has hypervariable region (HVR) at the C-terminal, which is believed as a physiologically important region. We have previously shown that chemical modification of the cysteine residues in the HVR with hydrophobic SH group reactive reagents induced multimerization of Ras. The multimerization phenomenon may reflect the physiological function of Ras. In this study, we analyzed the interaction between HVR and catalytic domain by chemical cross-linking, small angle X ray scattering and FRET. Small angle X-ray scattering data suggested that Ras modified with fluorescent probe DACM forms multimer. Furthermore, we analyzed the FRET efficiency from the tryptophan residue in HVR domain to the fluorophore in the GTP binding site.

2Pos200 **撹拌操作が引き起こすゲノム DNA の二本鎖切断：新規実験手法の提案**

How to keep genome-sized DNA safe against stirring stress: Quantitative analysis through single DNA observation

Hayato Kikuchi, Yuko Yoshikawa, Rinko Kubota, Kenichi Yoshikawa (*Lab. Biol. Phys., Facul. Life Med. Sci., Doshisha Univ.*)

Currently, it has been difficult to eliminate and analyze giant DNA molecules above the size of hundreds kilo base pairs (kbp). Establishment of experimental methodology to treat giant DNA molecules without any damage during experimental analysis in a laboratory is essentially important. Here, by use of fluorescence microscopy we report our results on the quantitative evaluation of double-strand breaks, DSB, on giant DNA molecules under mechanical agitation, such a mixing procedure in a sample tube. And more, we will propose a novel method of mixing of DNA solution to decrease the DSB probability in a significant manner.

2Pos201 **Protocol to optically measure pH in nanopores of protein crystals**

Kazuo Mori, Bernd Kuhn (*OIST*)

Fluorescence probes and imaging techniques can help to study key characteristics of water/salt/buffer filled nanopores in protein crystals. Here, we use the crystals of lysozyme and thaumatin to develop a protocol for measuring pH accurately in the crystal nanopores. In our perfusion protocol we measure at first the crystal autofluorescence, then wash in the dye. The fluorescent dye diffuses into the nanopores and allows local measurement. To avoid the melting of the perfused crystal we also add dissolved protein to the perfusion solution. pH is measured simultaneously in the crystal and, for reference, in the bath solution with confocal or two-photon microscopy. Our perfusion system allows us to change pH smoothly and to record for many hours.

2Pos202 **高周波磁場によるナノ粒子の加熱効果の検証**

Heat production of bio-synthesized nano-particles in altering magnetic field

Daisuke Katayama[1], Naoki Takashima[1], Hideyuki Yoshimura[2] ([1]*Biophysics Third Lab., Physics Major, Grad. Sch. Science and Technology, Univ. Grad. Sch. Meiji*, [2]*Univ. Meiji*)

Hyperthermia therapy has attracted attention in recent years as minimally invasive treatment for cancer. Magnetic particles are known to generate heat in a high-frequency magnetic field, and sometimes utilized as a heat source for hyperthermia. Ferritin is known to produce magnetite nano-particles in the cavity in anaerobic condition and is called magneto-ferritin. We succeeded to synthesize single crystal magnetite nanoparticles with homogenous diameter of 8nm. To utilize magneto-ferritin for hyperthermia, we have tested heat production of different sizes of synthesized magnetite particles in altering magnetic field. The heat production efficiency was investigated against particle size, frequency of magnetic field, applied voltage and design of the solenoids.

2Pos203 **生命構造の維持・形成に関わる力場についての一考察**

A concept for understanding biological dynamics, which would maintain and reproduce biological structure

Ryutaro Izumi (*Nihon University*)

In biological creature on Earth, organized and integrated structure would be maintained and reproduced from cellular to whole body level, against randomization, as long as they are in living status. This phenomenon exists under the flow of energy and materials, and never violate the second law of thermodynamics. However, neither physical nor biochemical law is clarified to explain this biological pattern formation universally. In this presentation, molecular-molecular interaction (MMI) is proposed as minimum unit for consisting the dynamics of this biological pattern formation.

2Pos204 **ゼロモード導波路(ZMW)の量産化と生体分子観察への応用**

High-throughput fabrication of Zero-Mode Waveguide (ZMW) and its application to observation of bio-molecules

Kimiko Nakao[1], Hisashi Tadakuma[1], Yong-Woon Han[2], Kodai Fukumoto[1], Yoshie Harada[1] ([1]*Inst. for Protein Res. Osaka Univ.*, [2]*School of Life Science and Technology, Tokyo Tech.*)

Zero-mode waveguides (ZMWs) are powerful tool for single-molecule imaging at physiological concentrations. However, fabrication process of ZMWs using single beam electron lithography is time consuming and thus hinders wide application of ZMWs. In this study, we used character projection (CP) masks for drawing electron lithographic patterns and succeeded in high-throughput fabrication of ZMWs. Using these CP-ZMWs, we observed fluorescently labeled bio-molecules at single molecule level.

2Pos205 **Combining a docking software with a ligand-based virtual screening method, VS-APPLE**

Daisuke Kobayashi, George Chikenji (*Nagoya University*)

With the rapid development of computer, Virtual screening (VS) is becoming a more and more powerful tool in drug discovery. We have been developing a ligand-based VS method, VS-APPLE (Virtual Screening Algorithm using Promiscuous Protein-Ligand complExes), which yields great performance. A disadvantage of VS-APPLE is that it demands at least one resolved target protein structure bound to a ligand for VS calculation, which means when there are no structurally resolved protein-ligand complexes, VS-APPLE can not be employed. In dealing with this issue, we have been developing a hybrid VS method which combines a protein-ligand docking software with VS-APPLE so that the virtual screening can be performed even when there is no protein-ligand complex structure information.

3Pos001 L グルタミン酸酸化酵素の基質特異性変換の構造基盤
Structural basis of the conversion of substrate specificity of L-glutamate oxidase

Nanako Ito[1], **Masaki Kitagawa**[1], Shinnsaku Matsuo[2], Michiko Nemoto[2], Takashi Tamura[2], Hitoshi Kusakabe[3], Kennji Inagaki[2], Katsumi Imada[1] ([1]*Dept. MacroMol., Grad. Sch. Sci., Osaka Univ*, [2]*Grad. Sch. Env. & Life Sci., Okayama Univ*, [3]*Enzyme Sensor Co. Ltd*)

L-glutamate oxidase (LGAO) is a flavoenzyme that catalyzes oxidative deamination of L-glutamate to produce 2-oxoglutaric acid with ammonia and hydrogen peroxide. LGOX shows strict substrate specificity for L-glutamate, whereas most of known LAO show broad specificity for various amino acids. Recently, single mutation at Arg-305 to Glu has been found to convert the substrate specificity of LGOX to L-arginin. To elucidate the molecular mechanism of the substrate specificity conversion, we determined the crystal structures of LGOX (R305E) and its substrate complex at 2.65 Å and 2.7 Å, respectively. The structures indicate that the R305E mutation induces a large change in the side chain recognition pocket but does not affect the catalytic site structure.

3Pos002 Development of the software with an intelligent strategy for serial data analysis measured by SEC-SAXS/UV-Vis. Spectroscopy

Kento Yonezawa, Masatsuyo Takahashi, Keiko Yatabe, Shinya Saijo, Nobutaka Shimizu (*Photon Factory, IMSS, KEK*)

SEC-SAXS is the latest world standard method in BioSAXS. The target molecule in the polydisperse solution can be measured while isolating it by gel filtration. The SEC-SAXS system at the Photon Factory is designed to measure SAXS and UV-Vis. spectroscopy simultaneously in order to evaluate the sample concentration. Since hundreds of data are acquired during the serial measurement, we developed the software to analyze such a lot of data automatically. This algorithm can perform the data process in consideration of the interparticle interference by combining the scattering intensities with the UV-Vis. absorbances, and it finally outputs an appropriate profile extrapolated to zero concentration. We will present details and examples in this poster.

3Pos003 二重スピンラベルたんぱくの cwEPR 距離測定に対するウエーブレット変換の応用
An application of wavelet transform to distance measurement by continuous wave EPR of doubly spin labeled protein

Yasunori Ohba[1], Shoji Ueki[2], Toshiaki Arata[3] ([1]*IMRAM, Tohoku Univ.*, [2]*Fac. Pharm. Sci., Tokushima Bunri Univ.*, [3]*Grad. School of Sci., Osaka City Univ.*)

The EPR distance measurement method measures the distance between the two aminoacid residues that labeled by spin labels by analyzing spectral broadening caused by the dipolar interaction between the two labels. In the case of continuous wave EPR, the analysis consists of extraction of dipolar line shape form the doubly labeled spectrum by deconvoution with singly labeled spectrum. This is a typical ill-posed problem that needed some stabilization of the calculation. At present, three methods are used in EPR: regularization based on Fourier transform (FT) or singular value decomposition (SVD) and nonlinear spectrum fitting. In this paper, we examined an application of wavelet decomposition that has advantages over FT and SVD in some specific cases.

3Pos004 *Porphyromonas gingivitis* の線毛蛋白質 FimA の構造
Structure of FimA, a major component protein of fimbriae of *Porphyromonas gingivitis*

Kodai Okada[1], Koji Nakayama[2], Mikio Shoji[2], Katsumi Imada[1] ([1]*Grad. Sch. Sci. Osaka Univ.*, [2]*Grad. Sch. Biomedical Sci. Nagasaki Univ.*)

Porphyromonas gingivitis, a gram-negative anaerobic bacterium, is a major periodontal pathogen. *P. gingivitis* fimbriae interact with host cells, function as a major virulence factor and are involved in biofilm formation. FimA is a major component of the fimbriae of *P. gingivitis* and are classified into at least five different subtypes (FimA1-FimA5) based on sequence and immunogenic properties. The virulence highly depends on the type of fimbriae expressed on bacteria. To elucidate the molecular basis of fimbriae virulence, we determined the crystal structure of FimA2 at 1.6 Å resolution. We will discuss the structural difference between FimA2 and other types of FimA whose structures have previously determined.

3Pos005 タンパク質の構造コンプライアンス適合運動の解析
Analysis of SC (Structural Compliance) Consistent Motion in Proteins

Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)

Linear interpolation between two different conformations of a protein often generates unrealistic motion (e.g., a part goes through other parts). Based on the structural compliance (SC) properties of proteins, we propose a method for generating a more realistic motion, termed as SC consistent motion. In this method, an elastic network model that focuses on the main chain structure is employed. SC consistent motion is generated via a type of feedback in which the motion directed toward the other conformation is the reference and the intensities of softer-mode motions are inputs. Moreover, by constraining the parts in the protein model and by evaluating changes in SC consistent motion, we can identify the parts that significantly affect the SC consistent motion.

3Pos006 GPI アンカー型タンパク質におけるシグナル配列の二次構造解析
Secondary structural analysis of signal sequence in GPI-anchored protein

Keiya Inoue, Tomonao Iibuchi, Daiki Takahashi, Tatsuki Kikegawa, Kenji Etchuya, Yuri Mukai (*Dept. Electronics, Grad. Sch. Sci. & Tech., Meiji Univ.*)

GPI transamidase is considered to recognize the specific tertiary structures around GPI attachment signals (GPI-ASs) in the premature GPI-anchored proteins (GPI-APs). However, even though the tertiary structural data of mature GPI-APs have been reported in the PDB, the structures of GPI-ASs are not included in the data, because the GPI-ASs are separated from the mature proteins.

The purpose of this study is to uncover the recognition and digestion mechanisms of GPI transamidase based on analyzing the secondary structures. The secondary structures of GPI-ASs which were fused GFP proteins and were expressed in E.coli, were analyzed by circular dichroism (CD). The function of GPI-AS in the GFP fusion protein expressed in HeLa cells was confirmed by PI-PLC treatment.

3Pos007 蛍光異方性解消法を用いたタンパク質の構造変性時における回転拡散係数および局所構造動きに関する研究

Rotational diffusion coefficients and the fluctuation of local structure of proteins along denaturation curve

Tomoyuki Yoshitake, Masahide Terazima (*Kyoto University*)

Protein structure and its dynamics are certainly important information for understanding protein reactions and functions. To probe protein conformation changes and movements, we are trying to develop a new method based on the depolarization rate of fluorescence. Here, we investigated relationship between rotational diffusion coefficients, which were measured by the fluorescence polarization decay, and the secondary structures of proteins along the denaturation curves measured by the CD method. For this purpose, we prepared lysozyme mutants with a fluorescent molecule at various positions. The probe position dependence of the depolarization rate should provide information on a local movement (fluctuation) during denaturation.

3Pos008 レプリカ交換分子動力学シミュレーションによる酸性条件下でのポリグルタミン酸の最安定構造

The dominant structure of polyglutamic acids under an acidic conditions analyzed by replica-exchange molecular dynamics simulations

Ryosuke Iwai[1], Tetsuro Nagai[2], Kota Kasahara[3], Takuya Takahashi[3] ([1]*Grad. Sci. Life Sci., Ritsumeikan Univ*, [2]*Dept. Of Phys., Nagoya Univ*, [3]*Coll. Life. Sci., Ritsumeikan Univ*)

Polyglutamic acids (PGA) have been studied for a long time in order to comprehend the protein structure changes depending on solvent pH. However, the dominant structure of PGA under acidic condition is unclear at the atomic level. To evaluate the dominant structures of PGA, we performed replica exchange molecular dynamics (REMD) simulations with a 20-residue PGA model, by using various combinations of force field and GB/SA models. The best combinations were determined in terms of reproducibility of circular dichroism values and we analyzed the dominant structure of PGA under an acidic condition. As a result, we revealed that the single helix structure is dominant and the C-terminal side of the helix is less stable than the other region.

3Pos009 Nontargeted parallel cascade selection molecular dynamics using convex hull for structure selection

Kenichiro Takaba[1,2] ([1]*Asahi Kasei Pharma Co., Ltd.*, [2]*Grad. Sch. Sci., Univ. Tokyo*)

Nontargeted parallel cascade selection molecular dynamics (nt-PaCS-MD) is a method to enhance the conformational sampling of proteins. Nt-PaCS-MD comprises multiple cycles each of which consists of two major steps: (i) selection of initial structures significantly deviated from the average structure for multiple independent MD simulations and (ii) conformational sampling by the independent MD simulations. Here, we propose a new selection method based on the principal component analysis and convex hull calculation. The new selection method was successful in observing the open-closed transitions of glutamine binding protein within a nanosecond time scale and is expected to be more efficient than the original nt-PaCS-MD.

3Pos010 位相板を用いたクライオ電子顕微鏡法での腸内連鎖球菌 V-ATPase 単粒子構造解析

Single Particle Analysis of *Eh*V-ATPase by Phase-Plate electron cryo-microscopy

Jun Tsunoda[1,2], Chihong Song[2], Takeshi Murata[3], Hiroshi Ueno[4], Naoyuki Miyazaki[5], Kenji Iwasaki[5], Ryota Iino[6], Kazuyoshi Murata[1,2] ([1]*SOKENDAI*, [2]*NIPS*, [3]*Dept. Chem., Chiba Univ.*, [4]*Dept. Appl. Chem., Sch. Eng., Univ. Tokyo*, [5]*IPR*, [6]*OIIB/IMS*)

V-ATPases are large membrane protein complexes to transport ions through cell membranes. *Eh*V-ATPase isolated from Enterococcus hirae consists of 24 subunits from 9 different proteins, and uniquely shows an ATP-driven Na^+-pump. The architecture is similar to other V-ATPases (which show a H^+-pumping). So far, the structures of *Eh*V-ATPase's individual subunits have been revealed by X-ray crystallography, however the whole structure of the complex is still unclear. In this study, we applied phase-plate cryo-erectron microscopy equipped with a direct electron detector to visualize the detergent (0.05% DDM)-solubilized *Eh*V-ATPase and analyze the data by RELION. We successfully reconstruct the whole 3D structure of *Eh*V-ATPase.

3Pos011 HIV-1 プロテアーゼにおける触媒的加水分解反応に関する理論化学的研究

Theoretical study on catalysis of HIV-1 protease

Masahiro Kaneso, Masahiko Taguchi, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

HIV-1 protease is necessary for virus growth and thus is one of the important targets for treatment of AIDS. The protease is a homodimer and the catalytic site with two aspartic acids exists at the interface of the dimer. Protein flexibility and proton translocation of the catalytic aspartic acids therefore play a crucial role in the catalytic activity.
In this study, we first performed molecular dynamics (MD) simulations to examine the protonation states of the aspartic acids. Based on the structures obtained by the MD simulations, we then carried out QM/MM calculations to investigate catalytic reaction profile. Using the calculated reactant and product structures, we performed QM/MM free energy optimizations to examine effect of protein flexibility in the reaction.

3Pos012 Improved method for soluble expression and rapid purification of yeast TFIIA

Naruhiko Adachi[1,2,3], Kyohei Aizawa[2], Shinya Saijo[1], Nobutaka Shimizu[1,2], Toshiya Senda[1,2] ([1]*SBRC, IMSS, KEK*, [2]*Soken Univ.*, [3]*PRESTO, JST*)

Purified RNA polymerase II (pol II) and general transcription factors (GTFs) are required for the in vitro reconstitution of eukaryotic transcription systems. Among GTFs, TFIID and TFIIA play critical roles in the early stage of transcription initiation; TFIID first binds to the DNA in transcription initiation and TFIIA regulates TFIID's DNA binding activity. Despite the important roles of TFIIA, the time-consuming steps required to purify it have hampered the preparation of in vitro transcription systems. Here, we report an improved method for soluble expression and rapid purification of yeast TFIIA. Our improved method provides highly purified TFIIA of sufficient quality for biochemical, biophysical, and structural analyses of eukaryotic transcription systems.

3Pos013 クライオ電顕を用いた好熱菌プロトン回転型 ATPase の単粒子解析

Cryo EM structure of intact rotary H+-ATPase/synthase from Thermus thermophilus

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([1]*Department of Molecular Biosciences, Kyoto Sangyo University*, [2]*Research Center for Ultra-High Voltage Electron Microscopy*)

H+- translocating rotary ATPases couple ATP hydrolysis/synthesis, taking place in the soluble domain, with proton flow through the membrane domain via a rotation of the common central rotor complex against the surrounding peripheral stator apparatus. Here we present the cryo-EM single particle structures of three rotational states of the V/A type H+-rotary ATPase from Thermus thermophilus. These three states differ in the orientation of the rotor subunit and provide important insights into how the surrounding stator subunits dynamically deform and reposition during rotation. These new maps are higher resolution than any obtained previously, and provide the detailed molecular basis for how the rotary ATPase allows turning of the stator relative to the rotating rotor.

3Pos014 分子動力学法による緑色蛍光タンパク質のフォールディングとアグリゲーション

Folding and Aggregation of Green Fluorescent Protein Studied by Molecular Dynamics Simulation

Mashiho Ito[1], Shoji Takada[2] ([1]*Nagoya Univ.*, [2]*Kyoto Univ.*)

Green Fluorescent Protein (GFP) is a widely used bioimaging tool. GFP forms its chromophore in cells by autocatalytic cyclization without cofactor. To reduce the aggregation propensity of wild-type GFP, various mutants have been developed by random mutation methods. Here we investigated the mechanism that these mutants work by coarse-grained molecular dynamics simulation. Firstly, we used the multicanonical ensemble method and determined the folding energy surface of GFP. Secondly, we performed the constant-temperature simulation and clustered folding pathways. Finally, we introduced fragments that interfere with folding and studied misfolding and aggregation. This study can contribute to the development of stable functional proteins.

3Pos015 Flexible docking and affinity calculation between CDK2 and its inhibitor CS3 using multicanonical MD and thermodynamic integration

Gert-Jan Bekker[1], Narutoshi Kamiya[2], Mitsugu Araki[3], Ikuo Fukuda[1], Yasushi Okuno[3], Haruki Nakamura[1] ([1]*IPR, Osaka Univ.*, [2]*Grd. Sch., Univ. Hyogo*, [3]*Grd. Sch. Med., Kyoto Univ.*)

Enhanced sampling using McMD simulation and TI were combined as a general drug docking method in order to predict the accurate binding configuration as well as the binding affinity for a flexible protein receptor and its inhibitor drug. CDK2 is involved in the cell cycle regulation. Malfunctions in CDK2 are thought to cause tumorigenesis, and is thus considered a potential drug target. Here, we performed a long McMD simulation for docking of one CDK2's inhibitors, CS3, starting from the unbound state. Next, a potential binding/unbinding pathway was obtained from the ensemble, and the binding free energy was computed by TI along this pathway. Using this combination, the correct binding pose was obtained, and the affinity coincided well with the experimental value.

3Pos016 A structural study of the novel chemokine receptor-binding protein, R1-15

Hiroko Takasaki[1], Sosuke Yoshinaga[1], Soichiro Ezaki[1], Mitsuhiro Takeda[1], Yuya Terashima[2], Etsuko Toda[2], Kouji Matsushima[2], Hiroaki Terasawa[1]
([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*Grad. Sch. Med., Univ. Tokyo*)

The chemokine receptor CCR1 is an anti-inflammatory therapeutic target for rheumatoid arthritis and lung diseases. We newly identified R1-15 as a cytoplasmic binding protein of CCR1. Since R1-15 regulates signal transduction from CCR1, chronic inflammatory diseases may be cured by controlling R1-15. The aim of this study is to develop inhibitory compounds of the CCR1—R1-15 interaction, based on the protein structures. A R1-15 expression and purification procedure was established. NMR and CD analyses revealed that R1-15 has an α-helical structure. A protease-resistant fragment of R1-15 also retains the α-helical structure. The identification of the chemokine receptor-binding domain and the structural analysis will be reported.

3Pos017 ユニークな Coiled-coil 構造を有する VSOP の電気生理学的および構造学的研究

Electrophysiological and structural studies of a unique coiled-coil region of VSOP

Akima Yamamoto[1], Takashi Tanibayashi[1], Satomi Shibumura[1], Yuichirou Fujiwara[4], Yasushi Okamura[4,5], Atsushi Nakagawa[1,5], Kohei Takeshita[1,2,3]
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VSOP is a proton channel depending on membrane potential changes. It consists of a voltage sensor and a cytoplasmic coiled-coil (CC) regions. The CC is not only responsible for dimerization of VSOP but also essential for cooperative gating in a plasma membrane. Moreover, gating kinetics of a dimeric VSOP is slower than that of a monomeric VSOP deleted CC. This suggested the importance of dimerization of VSOP for reduction of rapid changes of pH in vivo. Most of know CC show the I/L hydrophobic packing pattern in the interface of the dimer. On the other hand, unique interactions between dimer in CC were found in several species of VSOP. In this presentation, we will discuss the electrophysiological property and the approach for the structural studies of a gorilla VSOP.

3Pos018 小角散乱によるヒト α-シヌクレインのアミロイド線維の構造解析

Structural characterization of amyloid fibrils of human α-synuclein by small-angle scattering

Fumiaki Kono[1], Tatsuhito Matsuo[1], Shin-ichi Takata[2], Yasunobu Sugimoto[3], Satoru Fujiwara[1] ([1]*QuBS, QST*, [2]*J-PARC Center*, [3]*SR Center, Nagoya Univ.*)

Amyloid fibrils of α-synuclein (α-Syn) (and/or its intermediate structures toward the mature fibrils) is involved with pathogenesis of Parkinson's disease. Structural characterization of amyloid fibrils is important for elucidation of the mechanism of the fibril formation of α-Syn and thereby elucidation of the mechanism of the pathogenesis. Here we characterize the structure of amyloid fibrils of α-Syn by small-angle X-ray and neutron scattering (SAXS and SANS). Combined analysis of the SAXS and SANS curves shows that the diameter of the fibrils is about 15 nm, and the density of the fibril increases towards its outer region. It is also suggested that significant hydration occurs in the α-Syn molecules within the fibrils.

3Pos019 A SAXS study of thermal denaturation and coagulation of a major soybean storage protein β-conglycinin

Nobuhiro Sato[1], Yuki Higashino[2], Rintaro Inoue[1], Masaaki Sugiyama[1], Reiko Urade[2] ([1]*Res. React. Inst., Kyoto Univ.*, [2]*Grad. Sch. Agric., Kyoto Univ.*)

β-conglycinin (7S) is a major soy protein responsible for the physical properties of soy foods. The denaturation and coagulation of 7S that occurred along with the heat treatment and the addition of a coagulant were investigated by small-angle X-ray scattering (SAXS). Little structural change was observed below 50 °C, but partial denaturation occurred above 60 °C and finally reached random structures above 70 °C. By adding a coagulant glucono-δ-lactone after the preheat treatment at 50 °C, a large structural change over a 30 nm scale was observed but there was no change in a 5-10 nm scale, indicating that coagulation occurs via small structural changes on the surface of 7S molecules while keeping its original subunit structure.

3Pos020 ガウス関数入力型混合正規分布モデルによる３次元密度マップの近似表現
Gaussian-input Gaussian mixture model for approximate representation of 3D density map

Takeshi Kawabata, Haruki Nakamura (*Inst. Prot. Res., Osaka U.*)

A Gaussian mixture model (GMM) is one of shape approximation methods for fitting and comparing density maps and atomic models. The standard GMM algorithm (EM algorithm) used an input set of 3D points with weights, corresponding to voxel or atomic centers, ignoring their grid width or atomic radius. It also had a singularity and slow-computation problems. To solve these problems, we introduced a Gaussian-input GMM algorithm, considering the input atoms or voxels as a set of Gaussian functions. For a fast computation, we introduced a down-sampled Gaussian-input GMM where neighboring voxels are merged into an input anisotropic Gaussian function. The new algorithm can be also applied to generate an initial model for the 3D-reconstruction from 2D projection images.

3Pos021 バックグラウンドイメージより抽出した CTF を使ったネガティブ染色電子顕微鏡像の CTF 補正
The CTF correction of negative-staining electron micrographs by using the CTF extracted from the background image

Hitoshi Sakakibara (*Nat. Inst. Inf. Com. Tech. Bio-Function Sec.*)

In order to improve the image quality of electron micrographs, CTF correction is generally performed. We propose here a new method for accurate and easy CTF correction of negative staining electron microscope images. In negative staining electron microscopy, we observe the same heavy metal particles when observing the observation object and the background image. These particles are convoluted with the same CTF. We thought that we could produce a good filter for CTF correction when the CTF component was extracted from the background image. The CTF component was extracted by obtaining the autocorrelation of the background image. The square root of the autocorrelation FFT was used as a filter for CTF correction. The correction seemed well done judging from the FFT image.

3Pos022 細胞内のアクチン構造は細胞への機械刺激により変化する。
Atomic structure of actin within cells is changed by external mechanical stimulus

Urara Tokuishi[1], Q.P. Taro Uyeda[2], Q.P. Taro Noguchi[1] ([1]*National Institute of Technology, Miyakonojo College*, [2]*Waseda University*)

Changes of the atomic structure of actin are speculated to play important roles in mechanical response of cells. In the 2014 meeting, we reported that FRET actin, of which the two domains were attached with acceptor and donor dyes and introduced into PtK2 cells, showed that the atomic structure of actin changed in the region pushed by another cell. This result suggested that actin structure is affected in response either to external mechanical force or to chemical signaling from the cell in contact.
To distinguish between the two possibilities, PtK2 cells containing FRET actin were pushed by a glass needle. FRET index at the pushed site significantly increased, indicating clearly that the atomic structure of actin in cells changes in response to mechanical force.

3Pos023 Shootin1 の複数のリン酸化体とその構造
Multiple phosphorylated species of shootin1 and their solution structure

Shoki Nakata[1], Kentarou Baba[2], Yugo Hayashi[1], Yoichi Yamazaki[1], Naoyuki Inagaki[2], Hironari Kamikubo[1] ([1]*Grad. Sch. of Mater. Sci., NAIST.*, [2]*Grad. Sch. of Biol. Sci., NAIST.*)

Shootin1 can bind to both of an F-actin binding protein and a cell adhesion molecule to promote nerve axon-elongation. The binding affinities of shootin1 with the two proteins are controlled by phosphorylation of S101 and S249 in shootin1. Here, we focused on the reactivity of the two serines and its effect on the structure of shootin1. Monitoring the phosphorylation reaction induced by PAK1, the two serines showed different reaction rates, resulting in accumulation of two major spices of S101*/S249 and S101*/S249* during the reaction. CD and SAXS measurements revealed that the two phosphorylated species take distinct structures. From these results, we postulate that shootin1 realizes selective binding depending on its phosphorylation level.

3Pos024 アシル CoA の分子力学力場パラメータの改良
Refinement of molecular mechanics force field of acyl-CoA

Kyosuke Sato (*Dept. Mol. Physiol., Fac. Life Sci., Kumamoto Univ.*)

A preliminary MD simulation of substrate-bound acyl-CoA dehydrogenase, where the general amber force field 2 was used for the acyl-CoA topology, showed a problem that the adenosine moiety of acyl-CoA deviates from the correct position and finally is detached from the protein. To refine the force field of acyl-CoA, all the dihedral parameters were redetermined by comparing the energies calculated by quantum chemical and molecular mechanical methods. The MD simulation using the new force field was successful: fluctuations of CoA atom positions were suppressed and the correct binding was quickly restored even after the adenosine moiety was occasionally detached from the enzyme.

3Pos025 ラン藻でのアルカン合成に必要な 2 つの酵素間の相互作用
Interaction between two enzymes essential for cyanobacterial alkane biosynthesis

Mari Chang[1], Keigo Shimba[2], Hisashi Kudo[2], Hidenobu Kawai[2], Yoshiki Oka[2], Manami Wada[2], Yuuki Hayashi[2], Munehito Arai[1,2] ([1]*Dept. Phys., Univ. Tokyo*, [2]*Dept. Life Sci., Univ. Tokyo*)

Cyanobacterial biosynthesis of alkanes is catalyzed by a two-step reaction involving acyl-(acyl carrier protein) reductase (AAR) and aldehyde deformylating oxygenase (ADO). Recently, both enzymes are reported to interact with each other, but their interactions are poorly understood. Here, by mutational studies we identified two amino acid residues of ADO essential for the AAR binding. We will report the forces involved in the AAR-ADO binding by measuring the salt concentration dependence of isothermal titration calorimetry and gel filtration experiments. Second, to elucidate the overall structure of the AAR-ADO complex, we measured small angle X-ray scattering of the complex. The analysis is under way.

3Pos026 クライオ EM マップ及び多階層構造を対象とした状類構造検索サービス「Omokage 検索」の改良
Improvement in Omokage search, shape similarity search for cryo-EM maps and multi-scale structure data

Hirofumi Suzuki[1,2], Takeshi Kawabata[1], Genji Kurisu[1,2], Haruki Nakamura[1,2] ([1]*IPR, Osaka-Univ*, [2]*PDBJ*)

Recent innovation in structure analysis methods, especially in cryo-EM, increase many values of structure data. Increasing data in different data types (atomic model, density map, or dummy-atom model) are stored in various structure databanks, such as EMDB, PDB and SASBDB. Their scales are widening from molecules to cells. We have been developed Omokage search, a Web-based service to search structures data based on the shape similarity through the three databanks, EMDB PDB and SASBDB. Recently, we have made some improvement in it. One of them is keyword and component similarity filters to narrow the search result. In the poster session, we will discuss about the improvement and some case studies using the new functionalities.

3Pos027 単分子動態計測によって明らかになる KcsA チャネル開閉構造変化の遷移過程における立体構造安定性
Structural Stabilities during Gating Transitions in the KcsA Potassium Channel Revealed by Single-Molecule Dynamics Recordings

Hirofumi Shimizu, Masayuki Iwamoto (*Univ. Fukui. Fac. Med. Sci.*)

We have refined the diffracted X-ray tracking method to measure conformational changes in the KcsA potassium channel at a single-molecule level. In this method, the conformational changes are recorded as a movie by tracking the motions of diffraction spots from a gold nanocrystal attached to the channel as a probe. Here, we report the stepwise twisting motions of the channel during gating with newly developed probes. The dwell time for each twisting angle differed significantly, which reflected the structural stability of the angle. This dwell time map, recorded at submillisecond timescale, provided a landscape for structural stabilities of transition states between open and closed conformations.

3Pos028 NMR と MRS による α-シヌクレインの生体内オリゴマー化の解析
NMR and MRS analyses of α-Synuclein oligomerization *in vivo*

Keika Saito, Mitsuhiro Takeda, Sosuke Yoshinaga, Hiroaki Terasawa (*Fac. Life Sci., Kumamoto Univ.*)

α-Synuclein (α-Syn) is the major component of Lewy bodies, found in the brains of dementia patients, and forms a neurotoxic oligomer. While an oligomer of α-Syn can be formed *in vitro* [1], the oligomers present *in vivo* may be affected by molecular crowding effects, as suggested by a recent in-cell NMR study of α-Syn [2]. We examined the oligomerization of α-Syn in an agarose gel, to explore the reconstitution of the *in vivo* oligomer. α-Syn embedded in the agar was incubated at 4°C, resulting in its accelerated oligomerization, as monitored by NMR. The α-Syn in the agar was also detected by ^{13}C MRS using a ^{13}C cryogenic probe, for comparisons with the α-Syn present *in vivo*.

[1] Dhiman G, *et al. Sci.Rep.* **5**, 9228 (2015)
[2] Theillet FX, *et al. Nature* **530**, 45-50 (2016)

3Pos029 リン酸化タンパク質におけるリン酸基周辺の水和水動態解析
Analysis of water dynamics around phosphorylated protein

Hiroya Yamazaki, Shige H. Yoshimura (*Grad. Sch. Biostudies., Univ. Kyoto*)

Hydration plays critical roles in protein structure and function. In this study, we analyzed the effect of phosphorylation, which is one of the most important post-translational modifications in the functional regulation of protein, on the dynamics of water molecules in hydration layer. We performed molecular dynamics simulation on phosphorylated and non-phosphorylated ubiquitin. The analysis of water molecules around the phosphoserine showed that both translational and rotational motions of water were restricted by phosphate. Dissecting molecular interaction in the first hydration layer revealed that the loss of entropy is compensated by a large gain of enthalpy from phosphate-water interaction.

3Pos030 アデニル酸キナーゼの反応機構に関する計算化学的研究
Computational Study on the Reaction Mechanism of Adenylate Kinase

Kenshu Kamiya (*Dept. Phys., Sch. Sci., Kitasato Univ.*)

We have been studying the theoretical model of the reaction of adenylate kinase:ATP+AMP->2ADP. The truncted model of the catalysis were use for the calculation with ONIOM method using AMBER99 force field and DFT, and the reactant, product, transition structures were optimized. Although some of the calculated results shows reasonable values, more accurate calculations tend to the product state unstable. With analysis using experimental data of the product, the global structural deformation of the molecule associated with the reaction process is found to be important. The details about the effect of the model including the global deformation, as well as that of rearrangement of water molecules of the reaction center, will be discussed.

3Pos031 T 細胞受容体による特異的および交差反応的な抗原認識機構の解明

Analyses of the structural mechanisms of specific and crossreactive recognitions of antigen peptide-MHC by TCRs

Yuko Tsuchiya[1], Yoshiki Namiuchi[2], Hiroshi Wako[3], Hiromichi Tsurui[4] ([1]*IPR, Osaka Univ.*, [2]*QBiC, RIKEN*, [3]*Sch. of Social Sci., Waseda Univ.*, [4]*Sch. of Med., Juntendo Univ.*)

T cell receptor (TCR) recognizes an antigen-peptide in complex with MHC, which lead to T cell activation. The complex structures between TCR and peptide-MHC (pMHC) show completely different interacting areas and binding affinities between TCR and pMHC. In addition, these interacting areas and binding affinities do not correlate to each other. To elucidate the reason of the non-correlation, we analyzed the recognition mechanisms of a pMHC by the different five TCRs, based on the MD simulations and the FMO quantitative energy calculations. Our analyses showed that the five TCRs recognize the pMHC by the mechanisms with different "specificity" levels, from peptide-specificity to cross-reactivity, which explained the reason of the non-correlation.

3Pos032 Virtual system coupled canonical molecular dynamics simulation to enhance sampling along a reaction coordinate

Bhaskar Dasgupta[1,2], Kota Kasahara[3], Haruki Nakamura[1], Junichi Higo[1] ([1]*IPR, Osaka University*, [2]*Technology Research Association for Next Generation Natural Products Chemistry*, [3]*College of Life Sciences, Ritsumeikan University*)

It is well-known that canonical sampling for large systems often fails when multiple conformational states exist in the conformational space. Here we introduce a simple method to enhance sampling along a reaction coordinate (RC), which improves sampling by modulating discrete transition probabilities defined along the RC. To define the transition probabilities we have used a virtual system including multiple virtual states (an arbitrary system with arbitrary states). We also devised a method to reconstruct canonical probability distribution along RC from the obtained data. We named our method "virtual system coupled canonical molecular dynamics" (Vc-MD) simulation. We applied Vc-MD to an antigen-antibody system for flexible binding of the ligand to the receptor.

3Pos033 シトクロム P450 還元酵素における荷電状態変化に応じた物理状態変化

Physical state change in NADPH-cytochrome P450 oxidoreductase in response to the charged state change

Mikuru Iijima, Takato Sato, Ryota Moritake, Tohru Sasaki, Mitsunori Takano (*Dept. of Pure. & Appl. Phys., Waseda Univ.*)

NADPH-cytochrome P450 oxidoreductase (CPR) is an enzyme that supplies electrons to heme proteins (redox partners). For the electron transfer from NADPH to redox partners via CPR, drastic conformational change of CPR depending on redox states of its cofactors (FAD and FMN) is required. Although previous studies suggested electrostatic interactions are important for the redox-dependent conformational change, the response mechanism is not clear. Thus we examined the structural and electrostatic response of CPR to redox state change by conducting molecular dynamics simulation. Then we discuss the observed responses from the viewpoint of the dielectric allostery (Sato et al., 2016, JPCB) induced by the electronic input.

3Pos034 タンパク質の協同的な折れたたみとループのつながり方の関係: 4α-2β タンパク質トポロジーに関する網羅的解析

Relation between cooperative protein folding and loop connections: comprehensive analysis over 2α-4β protein topologies

Nobu C. Shirai[1], Shintaro Minami[2] ([1]*Center for Information Technologies and Networks, Mie University*, [2]*Graduate School of Information Science, Nagoya University*)

In our previous study, we reported that there is a correlation between the number of families defined in ECOD database and cooperativity of protein folding calculated by coarse-grained simulations for small number of topologies with two α helices and four β strands. In order to extend the analysis into larger scale, we calculated all possible 2α-4β topologies except unpreferable topologies that violate known rules about loop connection. We still observed a correlation between the number of families and cooperativity.

3Pos035 MD シミュレーションを用いた ATP 作動性イオンチャネル P2X における競合的阻害剤 TNP-ATP の作用機序の解明

MD simulation of ATP-gated P2X receptors reveals the inhibitory mechanism of a competitive antagonist TNP-ATP

Ryoki Nakamura[1], Go Kasuya[1], Mizuki Takemoto[1], Motoyuki Hattori[2], Ryuichiro Ishitani[1], Osamu Nureki[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Sci., Fudan Univ.*)

P2X receptors are ATP-gated cation channels. The previous P2X structures in the apo, closed and in the ATP-bound open states revealed the activation mechanism. Recently, our group determined the crystal structure of P2X in complex with a competitive antagonist TNP-ATP. In this structure, TNP-ATP bound at the ATP binding site while the ion channel pore was closed. To investigate the inhibitory mechanism of TNP-ATP, we created the apo and ATP-bound structure models and performed the MD simulation. We observed the specific movement of the extracellular domain toward the pore opening in the ATP-bound model. In contrast, we did not observe any specific movement in the apo model. This result indicates that the TNP moiety of TNP-ATP blocks the movement toward the pore opening.

3Pos036 Real-time imaging of Na^+-induced structural transitions of MotPS stator complex of flagellar motor by HS-AFM

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The flagellar stator acts as a transmembrane ion channel to couple the ion flow through the channel with torque generation. Here, we report real-time imaging of structural dynamics of the Na^+-type stator complex MotPS by high-speed atomic force microscopy. The purified MotPS in a buffer containing 150 mM NaCl had two distinct ellipsoids linked by a flexible string. We succeeded in real-time imaging of a disorder-to-order transition of the PGB domain by exchanging the salt in a buffer. The center-to-center distance between these two ellipsoids were increased up to 5 nm, allowing the PGB domain to bind to the peptidoglycan layer. Based on the available information, we propose a model for the assembly-disassembly cycle of MotPS stator.

3Pos037 Comparison of amyloid fibrillation between wild type and I2E mutant of VL domains of antibody light chain

Takafumi Naito[1], Masahiro Noji[1], Masatomo So[1], Kenji Sasahara[1], Johannes Buchner[2], Goto Yuji[1] ([1]*IPR*, [2]*Technical University Munich*)

Amyloid fibrils are associated with numerous diseases such as Alzheimer's disease and form in a concentration-dependent manner. Antibody light chain also forms amyloid fibrils and causes AL amyloidosis. It is known that mutations of light chain variable domain (VL) promote AL amyloidosis. We studied the mechanism of fibril formation with wild WT and I2E mutant of MAK33 VL by performing fibrillation experiments under various conditions. In contrast to previous studies that WT did not form amyloids, both WT and I2E formed fibrils although their kinetics were quite different. The experiments at various NaCl concentrations suggested the underlying mechanism responsible for the differences between WT and I2E.

3Pos038 味覚受容体細胞外領域ヘテロ二量体の発現・精製および性状解析
Expression, purification, and characterization of the entire heterodimeric extracellular regions of fish taste receptor

Hiroki Maruhashi[1], Daisuke Noshiro[2], Norihisa Yasui[1], Toshio Ando[2], Atsuko Yamashita[1] ([1]*Grad. Sch. Med. Dent. Pharm. Sci., Okayama Univ.*, [2]*Bio-AFM FRC, Inst. of Sci. & Eng., Kanazawa Univ.*)

Taste receptor type 1 (T1R) family proteins are responsible for recognition of sweet and umami taste substances. The family functions as a heterodimer of T1R1/T1R3 or T1R2/T1R3. T1R consists of the extracellular domain (ECD), formed by the ligand binding domain (LBD) and the cysteine-rich domain (CRD), and the seven transmembrane domain. To elucidate the signal transduction mechanism after the tastant-binding at LBD, we addressed recombinant protein preparation of T1RECD. We succeeded the expression and purification of T1R2a/T1R3ECD from medaka fish, and found that the purified sample forms a dimer. Interestingly, T1R3ECD was turned out to form a homodimer at a higher rate than T1R3LBD did, suggesting the existence of interaction sites for dimerization in the T1R3CRD.

3Pos039 ポリリン酸による α-synuclein のアミロイド線維形成誘導のメカニズム
The mechanisms of polyphosphate-induced amyloid fibrillation of α-synuclein

Tatsuya Fujikawa, Masatomo Sou, Yuji Goto (*Osaka Univ. IPR*)

Amyloid fibrils are associated with serious diseases including Alzheimer's and Parkinson's diseases. Although it has been reported that various additives have effects on amyloid fibrillation: acceleration or inhibition, the mechanism of amyloid fibrillation is still unclear. We found that polyphosphates, which exists in our body as a phosphate-reserving substance, accelerated or inhibited fibrillation of various proteins including α-synuclein depending on the concentration of polyphosphates. Here, we investigated the molecular mechanisms of acceleration of polyphosphate-dependent α-synuclein fibrillation using NMR, revealing intermediates of fibrillation. We discuss the structure and dynamics of α-synuclein in the pre-amyloid states.

3Pos040 Structure elements are closely related to intramolecular residue-residue contacts

Yasumichi Takase, Yugo Hayashi, Yoichi Yamazaki, Hironari Kamikubo (*NAIST MS*)

We had previously found some segments in an amino acid sequence responsible for structure formation by using comprehensive Ala-insertion mutation analysis, termed structure elements. However, physicochemical determinants for the elements remain unclear. In this study, we investigated the relationship between the elements and intramolecular residue-residue contacts. For this purpose, we firstly developed software to calculate overlapped contact volume (CV) in every possible residue-residue contact. Comparing the structure elements and the CV profile of DHFR, it was found that they agree well with each other, suggesting that the structure element is a region densely packed with residues in proteins.

3Pos041 弱酸性条件における $A\beta_{1\text{-}40}$ のアミロイド線維化
Amyloid fibrillation of $A\beta_{1\text{-}40}$ under weak acidic conditions

Kaori Mageshi, Naoki Yamamoto, Takato Hiramatsu, Eri Chatani (*Grad. Sch. of Sci., Kobe Univ.*)

Amyloid β protein (Aβ) aggregates into amyloid fibrils and that is thought to cause Alzheimer's disease (AD). Many studies related to the formation of Aβ amyloid fibrils have been performed under physiological pH. However, it is suggested that diabetes, which has been found to be linked with AD, lowers the pH of interstitial fluid. To understand effects of weak acidic conditions on Aβ fibrillation, we incubated $A\beta_{1\text{-}40}$ at several pHs ranging from 7.4 to 6.0. The result showed that $A\beta_{1\text{-}40}$ aggregation proceeded under the acidic conditions, and all products showed fibrillar morphology with similar heights. However, CD spectra showed difference of secondary structure, suggesting that the structures of $A\beta_{1\text{-}40}$ amyloid fibrils vary depending on small differences in pH.

3Pos042 示差走査熱量測定によるマルチドメイン蛋白質の不可逆熱転移の速度論的解析
Kinetic analysis of the irreversible thermal transition of multi-domain proteins by Differential Scanning Calorimetry

Shigeyoshi Nakamura[1,2], Hiroka Suzuki[3], Pitchanan Nimpiboon[4], Priya Kaewpathomsri[4], Piamsook Pngsawasdi[4], Wataru Nunomura[4], Shun-ichi Kidokoro[4] ([1]*NIT, Ube College*, [2]*Nagaoka Univ. of Tech.*, [3]*Akita Univ.*, [4]*Chulalongkorn Univ.*)

The stability of protein is very important for the industrial application of proteins. DSC is a strong tool to evaluate the stability in the thermal transition of proteins. While DSC studies have performed frequently for the equilibrium thermal transition of proteins, many proteins show irreversible thermal transitions. In this study, we introduce the kinetic analysis for the complex irreversible thermal transition. We analyzed the thermal transition of calmodulin from human and amylomaltase from Thermus filiformis as examples of multi-domain proteins. Their thermal transitions are found to be explained by a multi-unit kinetic model. Their kinetic parameters, such as the denaturation constant and the standard activation enthalpy, were evaluated for each unit.

3Pos043 Conformational fluctuation of phosphorylated-ubiquitin studied by high-pressure NMR spectroscopy

Soichiro Kitazawa, Yu Aoshima, Junki Iga, Takuro Wakamoto, Ryo Kitahara (*Ritsumeikan Univ.*)

Ubiquitin (Ub) phosphorylated at Ser65(pUB) exists in conformational equilibrium between major and minor conformations. The major species have closely similar conformations with wild-type Ub. Surprisingly, the minor species were expected to have entirely different hydrogen bonding patterns at the b-sheet region, in which b5-strand has retracted into the core region by two amino acids [Wauer et al. EMBO J. 2015]. Here, we report analysis of conformational fluctuation of pUb using high-pressure NMR spectroscopy. Pressure-induced chemical shifts of amide protons and nitrogens were markedly different at the b-sheet region between the major and minor ones, indicating that pressure-induced changes in hydrogen bond length and torsion angles are different at the b-sheet region.

3Pos044 Solubilization and structural analysis of heat-aggregated keratin protein

Atsushi Baba[1], Momoko Furuta[1], Kentaro Shiraki[2], Len Ito[1] ([1]*MILBON Co., Ltd.*, [2]*Fac. Pure and App. Sci., Univ. Tsukuba*)

Proteins are generally sensitive to heat, and application of heat to proteins is known to induce aggregation through denaturation. We have found that hair cosmetic procedures in which the temperature exceeds 100°C, such as thermal ironing, cause aggregation of proteins in the hair and induce undesirable changes in the condition of hair, such as hardening. Here we explored various dispersing solvents that efficiently solubilize heat-aggregated keratin protein. We found that a kind of osmolytes could lead positive effect. We will discuss the molecular mechanism of additives on keratin protein.

3Pos045 マイクロ波照射環境での酵素反応のエントロピー低下
Entropy reduction of enzymatic reaction in microwave irradiated environment

Fujiko Aoki, Takeo Yoshimura, **Shokichi Ohuchi** (*Dept Biosci Bioinform, Kyushu Inst Tech*)

In the microwave assisted enzymatic reaction, it can be assumed that there is a microwave output range where the reaction rate increases. In this study, we attempted to calculate the thermodynamic quantity of the enzyme reaction system under microwave irradiation. A cavity resonant microwave irradiation device was used for the experiments. This device can be experimented under adiabatic conditions. The amount of microwave energy absorbed by the reaction system and the temperature rise of the reaction system can be precisely calculated. As a result, the entropy corresponding to the microwave output was estimated and the correlation with the frequency factor was compared.

3Pos046 統計力学モデルによるマルチドメインタンパク質のフォールディング経路の解析
Folding pathways of multi-domain proteins predicted by a statistical mechanical model

Koji Ooka[1], Munehito Arai[1,2] ([1]*Dept. Phys., Univ. Tokyo*, [2]*Dept. Life Sci., Univ. Tokyo*)

A coarse-grained statistical mechanical model called the Wako-Saito-Muñoz-Eaton (WSME) model has succeeded in theoretically explaining experimentally observed folding mechanisms of small globular proteins by predicting free energy landscapes. The model is suitable for small proteins, because it assumes that a native pair of residues is stabilized only when all intervening residues cooperatively form native-like configuration. However, this assumption may not be applicable to multi-domain proteins. To clarify the limitations of this model, here we calculated folding pathways of many multi-domain proteins using the WSME model and compared the results with experimental observations. We then attempt to modify the model to account for the topology of multi-domain proteins.

3Pos047 張力によって誘起されたアクチンの静電的変化：アクチンフィラメントの圧電性
Tension-induced electrostatic change in actin: piezoelectricity of an actin filament

Jun Ohnuki, Hideyo Okamura, Akira Yodogawa, Takato Sato, Taro Q.P. Uyeda, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

Mechanical stimuli applied to actin filaments alter the affinity with actin-binding proteins (ABPs). By conducting molecular dynamics (MD) simulation of a tension-applied actin filament, we discovered piezoelectricity by which the tension changes the electrostatic potential on the actin surface, suggesting that the affinity with ABPs is regulated electrostatically (Annu. meeting, 2016). We here reinforced the conformational sampling of the actin filament by using the accelerated MD method and confirmed the piezoelectricity. Moreover, we found that the tension suppresses the filament twisting fluctuation that should play a key role in the binding of the ABP cofilin. We discuss how these responses arise by focusing on the electrostatic (ionic and hydrogen) bond network.

3Pos048 トリガーファクターが補助するタンパク質フォールディングの 高速原子間力顕微鏡を用いたリアルタイム観測
Real time observation of Trigger Factor assisted protein folding using high-speed atomic force microscope

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Newly synthesized proteins are folded to their native structures, which is mainly driven by hydrophobic packing. The hydrophobic packing is supposed to be promoted by molecular chaperones such as Trigger Factor (TF), but the mechanism is poorly understood. Here, we exploited high-speed atomic force microscope (HS-AFM) to examine the interactions of TF with the substrate for the folding. Our HS-AFM experiments showed that TF interacts with the substrate only at the initial stage of the folding to form partially folded ‘substructures’, and these substructures are found to correspond to the hydrophobic core of the native structure. TF, therefore, promotes hydrophobic packing by forming substructures at the initial stage, resulting in acceleration of the protein folding.

3Pos049 対イオンで誘起されるアクチンの静電的変化：リエントラント重合における大域斥力と局所引力のバランス

Counter-ion-induced electrostatic change in actin: the balance between global repulsion and local attraction in reentrant polymerization

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Actin polymerization exhibits a reentrant(non-monotonic) dependence on the salt concentration. To clarify the reentrant mechanism, we calculated the polymerization energy, ΔE, using a continuum dielectric model with the counterion considered in a mean-field manner. The reentrant behavior was observed in ΔE, which was caused by the change in the electrostatic balance between the global repulsion (due to the net charges of the subunits) and the local attraction (due to ionic bonds at the subunit-subunit interface). Furthermore, by conducting molecular dynamics simulation including explicit counterions, we address the role of the specific binding of counterions, the salt-concentration dependence of the actin structure, and the temperature dependence of polymerization.

3Pos050 単一アクチンフィラメントの両末端におけるモノマー間の変動の差異

Differences of inter-monomer fluctuations of single actin filament at either ends

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Mutual configuration of monomers within a single filament of actin should be closely related with the flexibility of the filament. A uniform copolymer of either donor or acceptor labeled G-actin presents FRET fluorescence. FRET efficiencies and the fluctuation of them were calculated along the filament and demonstrated as false colors. This technique allows us to visualize local flexibility of the filaments superimposing their fluorescent images. Surprisingly, the local fluctuation of each filament edges differed. This difference might be originated by polymerization of F-actin or nucleotide exchange of monomers within the filament.

3Pos051 セルロース合成の時分割 X 線小角散乱による計測

Time-resolved SAXS measurement of cellulose synthesized in vitro

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Small angle X-ray scattering (SAXS) is a technique to analyze the structure within 1 - 100 nm. In this report, we observed cellulose synthesis by solubilized membrane preparation of a Gram-negative bacterium *Komagataeibacter xylinus* by time-resolved SAXS. Because cellulose is insoluble in water, time-resolved SAXS is suitable to observe cellulose formation. A temporal change of SAXS profile $I(q)$ was observed specifically in the presence of cellulose synthase activator c-di-GMP. This result indicates that SAXS can visualize the process of the synthesis of cellulose fiber.

3Pos052 タンパク質レベルでの発現が確認されていないスプライシングアイソフォームの機能性推定

Estimating functionality of expression-unconfirmed splicing isoforms at the protein level

Teerasetmanakul Pramote, **Masafumi Shionyu** (*Grad. Sch. of Bio-Sci., Nagahama Inst. Bio-Sci. Tech.*)

Papers reporting the functional significance of splicing isoforms increase every year, and many alternatively spliced isoforms are detected by high-throughput sequencing. On the other hand, it is argued that alternative splicing may not contribute the complexity of proteome because only a small number of splicing isoforms are confirmed to be expressed at the protein level by proteomics analyses. We have developed a method that estimates functionality of splicing isoforms based on the features of function-known splicing isoforms. To clarify whether expression-unconfirmed splicing isoforms are functional or not, the modified method is applied to them. We will discuss the contribution of alternative splicing to the diversity of protein function.

3Pos053 グラム陽性菌 *Bacillus subtilis* 由来 ferredoxin-NADP$^+$酸化還元酵素パラログ YcgT の酵素学的解析

Enzymatic characterization of ferredoxin-NADP$^+$ oxidoreductase paralogue YcgT from gram-positive bacterium *Bacillus subtilis*

Daisuke Seo[1], Masaharu Kitashima[2], Kazuhito Inoue[2], Hirofumi Komori[3] ([1]*Div. Mat. Sci., Grad. Sch. Nat. Sci. Tec., Kanazawa Univ*, [2]*Dep. Biol. Sci., Kanagawa Univ*, [3]*Fac. Educ., Kagawa Univ*)

In *Bacillus subtilis* cells, YumC catalyzes Fd reduction using NADPH as reductant. Interestingly, this bacterium contains *yumC* paralogue *ycgT* (50% amino acid identity) and its gene transcription increases under certain growth conditions. Here we report enzymatic characterizations of YcgT. The diaphorase assay demonstrated that catalytic efficiency toward NADPH was 1,000-fold less than that of YumC. Pre-steady studies suggested that the affinity of YcgT toward NADPH was lower. Fd reduction rate in the cytochrome *c* reduction assay was at least 10-fold less than that of YumC. Obtained results suggested that YcgT seems scarcely participate in Fd reduction under physiological conditions.

3Pos054 タウタンパク質に対する Pin1 由来のプロテアーゼの活性の定量的評価

Quantitative evaluation of activity of a protease derived from Pin1 for tau protein

Teikichi Ikura, Nobutoshi Ito (*Med. Res. Inst., Tokyo Med. Dent. Univ.*)

The Alzheimer's disease-related protein, tau, aggregates into neurofibrillary tangles when it is hyperphosphorylated. A peptidyl-prolyl isomerase, Pin1, targets a motif pS/T-P of the hyperphosphorylated tau and restores the function of tau. The function of Pin1 for tau, however, is not effective enough to prevent progress of dementia. Recently we succeeded in converting the PPIase activity of Pin1 into the proteolytic activity by a single mutation, and reported that this proteolytic activity of the mutant Pin1 worked on tau protein and its aggregate effectively. In the present study, we developed a novel method to kinetically evaluate this proteolytic activity by modifying the ELISA method. The activity of the mutant Pin1 will be discussed on the basis of this method.

3Pos055 拡張アンサンブル分子動力学シミュレーションを用いたヒストン脱メチル化酵素阻害剤のアイソザイム選択制に関する研究

Study for Isozyme Selectivity of Lysine Demethylase Inhibitor by Using Generalized Ensemble Molecular Dynamics Simulations

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Histone demethylases play key role in epigenetic regulation by controlling gene transcription and also have correlation with some diseases such as cancer. JARID1 family ,that is a member of histone demethylases, is one of potential targets for cancer therapy. But it is difficult to distinguish a member from JARID1 family because the strucutres and the amino-acid sequences of these enzymes are very similar.
In this study, we performed generalized ensemble molecular dynamics simulations to analyze the selectivity of JARID1 inhibitor. Some results obtained from our simulations agree and be able to explain the isozyme selectivity.

3Pos056 プラストシアニンとシトクロム *f* との反応過程に対する分子間静電相互作用の寄与に関する理論的研究

Theoretical study on contribution of electrostatic intermolecular interaction to reaction process of Plastocyanin with Cytochrome *f*

Satoshi Nakagawa, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Sch. Nat. Sci. Tech., Kanazawa Univ.*)

Plastocyanin (Pc) is a copper protein and has the function of the electron transfer from cytochrome f (Cyt*f*) in cytochrome b_6f to P700 in photosystem I. Pc diffuses in thylakoid lumen and associates with Cyt*f* by hydrophobic and electrostatic interactions. In this study, our purpose is to investigate the contribution of electrostatic interaction to reaction process of Pc with Cyt*f*. Therefore we solve the Langevin equation for Pc-Cyt*f* complex represented by Go-like model with effective intermolecular interactions. The electrostatic interaction is expressed as screened coulombic interaction. We discuss the reaction process of Pc with Cyt*f* in relation to the contribution from electrostatic intermolecular interaction to the process.

3Pos057 ADP/ATP 交換輸送体のミトコンドリアにおける活性調節の計測

Measurements of activity regulation of adenine nucleotide translocator in mitochondria

Mayu Yoneda, Saki Yamashita, Yoshihiro Ohta (*Ohta. Lab., Univ. Noko*)

Adenine nucleotide translocator (ANT) is a protein that functions as an antiporter of ATP and ADP in mitochondria. Since ATP synthesized in mitochondria is translocated from the matrix to the cytosol by ANT, the activity of ANT is important for supply of ATP to the cytosol. However, the mechanism of the regulation of ANT has not been clarified. In the present study, we measured ANT activity in mitochondria by expressing FRET-based ATP sensor, GO-ATeam in the mitochondrial matrix. Addition of ATP or ADP changed the intramitochondrial ATP concentration, and the several inhibitors of mitochondrial proteins affected the observed changes upon addition of ADP. The detailed conditions and results of the measurements will be discussed.

3Pos058 Single α-helix alone in a shaft of F_1-ATPase cannot fully transmit the torque but closely cooperate with the stator

Shou Furuike, Yasushi Maki, Hideji Yoshida (*Phys., Osaka Med. Col.*)

F_1-ATPase is an ATP-driven rotary molecular motor. The shaft of rotor, an antiparallel α-helical coiled coil of the N-ter and C-ter of the γ subunit, is set in the central cavity of the cylinder-like stator ($\alpha_3\beta_3$-ring).
We constructed F_1 mutants in which the shafts would retain nearly genuine shape and have less than half of torsional/bending rigidity. For example, the C-ter α-helix of a mutant is cut at the middle (the portion would not interact with the $\alpha_3\beta_3$-ring), and jointed together by three helix-breaker amino-acids. The rotation rates with and without drag became down ~1/4 and ~3/4 of wild type, respectively. The mutant would reserve the cooperativity between subunits, but lost ability of fully generating/transmitting the torque.

3Pos059 OPA1 プロテオリポソームによるミトコンドリア内膜形態制御機構の解明

Elucidating the regulation of mitochondrial inner membrane morphology using OPA1 proteoliposome

Tadato Ban, Naotada Ishihara (*Dept. of Protein Biochem., Inst. of Life Science, Kurume Univ.*)

OPA1 is an essential GTPase protein for both mitochondrial inner membrane fusion and cristae structure. However, little is understood about how OPA1 regulate the membrane morphology. We have developed methods to express and purify human OPA1 using the BmNPV bacmid-silkworm expression system, and found that OPA1 on one side of membrane, and CL on the other side are sufficient for the fusion. GTP-independent heterotypic membrane tethering through OPA1 and CL primes the subsequent GTP-hydrolysis-dependent fusion. In contrast, CL independent membrane tethering through a homotypic trans-OPA1 interaction might mediate the cristae structure. Thus, multiple OPA1 functions for regulation of mitochondrial morphology are modulated by the local CL conditions.

3Pos060 抗菌性ペプチドも進化するのか？：チャネル電流計測を用いたヒトとサルにおける抗菌ペプチドの膜障害活性評価からの推察

Do pore-forming activities of antimicrobial peptides change with evolution between Human and Gibbon?

Naoki Saigo, Yusuke Sekiya, Ryuji Kawano (*Dept. Biotech and Biosci*)

Antimicrobial peptides (AMPs) have a role of biological defense mechanisms in broad spectrum species. One of the antimicrobial function is pore-formation in cell membranes that induces the cell lysis. Previously, we observed AMPs channel currents of Ascidiacea, Frog and Human. From these results, we found hydrophilic region relate to pore diameter. In this study, we chose the two different AMPs of Human and Gibbon produced from same gene. As the results of AMPs properties, we found the AMPs pores are different with following the evolution of the species even if produced from same gene. About pore diameter, we found same tendency of hydrophilic region is similar to other AMPs. We believe this result is promising to reveal the molecular mechanism of AMPs.

3Pos061 結晶性多糖を分解する双方向性リニア分子モーターの計算機合理設計と構造解析

Computational design and structural analysis of bi-directional linear molecular motor hydrolyzing crystalline polysaccharide

Fumihiro Kawai[1], Akihiko Nakamura[1,2], Mayuko Yamamoto[1], Yasuko Okuni[1], Ryota Iino[1,2,3] ([1]*Okazaki Institute for Integrative Bioscience*, [2]*The Graduate University for Advanced Studies (SOKENDAI)*, [3]*Institute for Molecular Science*)

Serratia marcescens chitinase A (*Sm*ChiA) and B (*Sm*ChiB) are linear molecular motors moving to opposite directions, and hydrolyze crystalline chitin from reducing and non-reducing ends, respectively. *Sm*ChiA and *Sm*ChiB have a catalytic domain (CD) and a carbohydrate binding domain (CBM), and these domains are connected by a short linker. The CDs show almost identical fold (TIM barrel), while positions of the CBM relative to CD are different. In this study, we are trying to engineer bi-directional motor *Sm*ChiAB, a fusion protein carrying one CD and two CBMs from of *Sm*ChiA and *Sm*ChiB. Unfortunately, so far, crystal structures of eight *Sm*ChiABs showed significant differences from the designs by ROSETTA. We will discuss detail of the structural differences and future strategy

3Pos062 モモ由来システインリッチアレルゲン peamaclein の大量発現

Over expression of recombinant peamaclein, a cysteine-rich plant allergenic peptide derived from peach pulp

Hiromu Suzuki[1], Takasumi Kato[1], Mihoko Yasumoto[1], Kento Iwama[1], Akiho Okamura[1], Tomoya Kato[1], Naoya Kitada[1], Md. Ruhul Kuddus[1], Farhana Rumi[1], Takashi Tsukamoto[1,2], Takashi Kikukawa[1,2], Makoto Demura[1,2], Tomoyasu Aizawa[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*GI-CoRE, Hokkaido Univ.*)

Peamaclein is a cysteine-rich peptide (63 a.a, 12 cysteines) which was originally found as one of the allergenic peptides from peach pulp. In this study, we expressed recombinant peamaclein in the methylotrophic yeast *Pichia pastoris*, and then purified and characterized. Secretion vector was prepared and *P. pastoris* was transformed. After purification, we obtained a large amount of peamaclein from fermentation culture. Characterization of recombinant peamaclein was carried out by MALDI-TOF MS and ^{1}H NMR, and these results suggested that peamaclein was folded correctly. This peptide is highly homologous to snakin-1 which is an antimicrobial peptide from potato. Now we are trying to investigate whether peamaclein has antimicrobial activity.

3Pos063 V_1-ATPase 非活性界面を再設計することで分子モーターを理解する試み

An Attempt to Understand Molecular Motor by Redesigning Non-Catalytic Interface of V_1-ATPase

Takahiro Kosugi[1,2], Tatsuya Iida[2,3], Fumihiro Kawai[3], Minako Kondo[1], Mikio Tanabe[5], Ryota Iino[1,2,3], Nobuyasu Koga[1,2,5] ([1]*CIMoS, IMS*, [2]*SOKENDAI*, [3]*Okazaki. Inst. Integ. Biosci.*, [4]*KEK*, [5]*JST, PRESTO*)

Many of molecular motors work in complex state and regulate function through the complex interfaces. Redesigning the interfaces can be one of the approaches to understand mechanisms of the molecular motors. V_1-ATPase consisting of the asymmetrical ring-shaped A_3B_3 complex changes the conformational states of the interfaces upon ATP hydrolysis, resulting in the rotation of the central axis DF subunits. In this work, non-catalytic interface, which does not bind ATP, was redesigned to ATP bindable site with the P-loop, which was experimentally evaluated. We found that the non-catalytic interface is natively "designed" not to bind ATP for optimizing the ATP binding affinity at the catalytic site and the reconstitution rate of A_3B_3DF complex.

3Pos064 Generation of a ruthenium-binding peptide motif containing genetically encoded bipyridylalanine as ligand

Marziyeh Karimiavargani[1], Noriko Minagawa[2], Seiichi Tada[2], Takuji Hirose[1], Yoshihiro Ito[2], Takanori Uzawa[2] ([1]*Graduate School of Science and Engineering, Saitama University*, [2]*Nano Medical Engineering Laboratory, RIKEN*)

Unique phosphorescence property of tris(bipyridine) ruthenium, Ru(bpy)3, have attracted much attention. We aim to generate a derivative of this metal complex in a peptide motif containing genetically encoded bipyridylalanine (Bpy-Ala) as the ligand. Liposome-based in vitro compartmentalization was applied to express a Ru-binding motif containing 3 Bpy-Alas in a liposome. Because phosphorescence would be emitted from a liposome in which three Bpy-Alas coordinate to Ru-ion, we isolated fluorescence positive liposome by FACS. Following 3 rounds of selection, we synthesized 6 enriched peptides. All peptides with Ru ion exhibited similar phosphorescence spectra to Ru(bpy)3 and elongated lifetime from Ru(bpy)3, implying that we successfully generated Ru-binding motif.

3Pos065 人工設計タンパク質間結合面の移植による新規タンパク質間相互作用の創出

Development of a novel protein complex by grafting an artificial protein-protein binding interface

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Previously, we have constructed a de novo protein-protein interaction between two helical bundle proteins, sulerythrin and LARFH, through designing an inter-molecular helix-helix interaction. For design of the interface, leucine residues and charged residues were introduced onto the a-helix of these proteins. In this study, we created some 3-isopropylmarate dehydrogenase (IPMDH) mutants, which have LARFH-type binding interface onto its exposed a-helix. Pull-down assay was performed to analyze the interactions between the IPMDH mutants and the sulerythrin mutant. Some IPMDH mutants interacted to sulerythrin mutant. Thus, this protein-protein binding interface may be implantable to other proteins in order to generate novel protein materials.

3Pos066 リポソームディスプレイ法を用いた多剤排出トランスポーター EmrE の in vitro 機能進化

In vitro evolution of E. coli multidrug efflux transporter EmrE by using liposome display

Sae Uchida, Atsuko Uyeda, Hajime Watanabe, Tomoaki Matsuura (*Dep. Biotechnol, Grad. Sch. Eng., Osaka Univ*)

Liposome display is a method that enables the directed evolution of membrane proteins entirely in vitro. The method is based on syntheses of membrane proteins from a single copy of template DNA using an in vitro transcription-translation system inside a cell-sized liposome. We applied liposome display to an E. coli multidrug transporter EmrE. More than 10 rounds of screening were performed based on substrate (EtBr) transport activity of EmrE, starting from a random mutagenized gene library of wild-type EmrE. As a result, EmrE mutant gene pools that showed transport activation higher than that of the wild-type was obtained. Sequence changes during the screening rounds obtained from the next generation sequencing will also be presented.

3Pos067 アルカリフォスファターゼの変異導入率と酵素活性分布の関係

The relationship between mutation rate and enzymatic activity distribution of alkaline phosphatase

Makoto Kato[1], Yi Zhang[1,2], Hiroshi Ueno[1], Kazuhito Tabata[1], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*JAMSTEC*)

Fitness landscapes depict how genotypes manifest at the phenotypic level and important for understanding of natural evolution and library construction for directed evolution. It is expected that, in case of random mutagenesis, the higher the mutation rate is, the lower and broader the distribution of enzymatic activity becomes. It is in general difficult to analyze a large number of libraries in high throughput manner. In this study, we investigate fitness landscape of an enzyme by using femtoliter chamber array, which enables both quantitative and high-throughput assay. We constructed two mutant libraries of alkaline phosphatase with different mutation rate by error-prone PCR. In this meeting, we will report the results of assays of these libraries.

3Pos068 細胞内における脂肪酸アルデヒド生成量のリアルタイム検出とその応用

***In vivo* real-time measurement of fatty aldehyde and its application**

Yuuki Hayashi, Munehito Arai (*Dept. Life Sci., Univ. Tokyo*)

Alkanes produced by cyanobacteria are attractive candidates for alternative biofuels. Acyl-ACP reductase (AAR) catalyzes reduction of acyl-ACP into fatty aldehydes, which is an initial step in alkane biosynthesis. However, an enzymatic activity of AAR is very low and needs to be improved for practical use. Directed evolution of AAR requires high-throughput measurements of the AAR activity in cells. Nonetheless, current protocols to measure the AAR activity take time and labor for various steps. Here, we developed a non-invasive method to measure the AAR activity *in vivo*. This method can measure an amount of fatty aldehyde produced by AAR in an E. coli colony or cell culture as bioluminescence in real-time. Directed evolution of AAR using this method is ongoing.

3Pos069 ATP 結合型外向きヘム輸送体の計算的モデリング

Computational Modeling of the ATP-Bound Outward-Facing Form of a Heme Importer

Koichi Tamura[1], Hiroshi Sugimoto[2,3], Yoshitsugu Shiro[2], Yuji Sugita[1,4,5,6] ([1]*RIKEN AICS*, [2]*Grad. Sch. Life Sci., Univ. Hyogo*, [3]*RIKEN SPring-8*, [4]*RIKEN TMS*, [5]*RIKEN iTHES*, [6]*RIKEN QBiC*)

Heme importer belongs to the large family of type-II ATP-binding cassette (ABC) transporter. Transport of heme across the cell membrane involves large and global structural changes of the protein during which two ATPs are consumed. Recently, crystal structures of bacterial heme importer in the ATP-free inward-facing form have been solved. Based on the structures and biochemical experiments, a molecular mechanism for heme transport cycle was proposed. In this study, computational modeling approach was adopted to model the ATP-bound outward-facing (OF) form of the heme importer and thereby complement the molecular model of the transport cycle. An iterative remodeling approach yielded a structurally stable atomistic model and revealed a gating mechanism for the OF form.

3Pos070 呼吸鎖ヘム・銅酸素還元酵素 A タイプのプロトン移動経路の pKa 解析

pKa analysis of the proton transfer pathway in respiratory A-type heme-copper oxygen reductase

Kazumasa Muramoto (*Dept. Life Sci., Univ. of Hyogo*)

Respiratory chain generates proton motive force coupled to electron transfer at high energy efficiency. Respiratory O_2 reductases and NO reductases belong to evolutionally related heme-copper O_2 reductase superfamily. O_2 reductases are broadly classified into A, B and C-types based on their molecular structures.

A-type O_2 reductases contain one magnesium ion and one sodium or calcium ion. It has been suggested that these cation-binding sites contribute the proton translocation coupled to the oxygen reduction. In this study, to understand protonation state of the ligands of these cations, I performed pKa analysis. Preliminary results suggest that two carboxyl groups of the magnesium ligands and one carboxyl group of the sodium ligand are deprotonated.

3Pos071 ヘムタンパク質中のヘムの歪みの統計および量子化学計算による解析

Statistical and quantum-chemical analysis of heme distortion in hemoprotein

Yasuhiro Imada[1], Yusuke Kanematsu[2], Hiroko Kondo[2], **Yu Takano**[1,2] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sci. Info. Sci., Hiroshima City Univ.*)

Heme proteins have wide variety of functions that can be attributed to the modulability of the molecular and electronic structures of hemes. In order to clarify the relation between structural variety of hemes and their activities in protein, we first compared the structural distributions of oxidoreductases and oxygen transporter/storage proteins. We obtained the feature vector to distinguish the distributions of two groups obtained by the Fisher's linear discriminant analysis (LDA), and the oxidation potential and the oxygen adsorption energy computed by the quantum chemical calculation were linearly correlated with the displacement along the feature vector, implying the availability of LDA to approach the structural bias on heme for the functional differentiation.

3Pos072 金属還元酵素ヒト Steap3 の分子機能解明

Analyses on the molecular function of metalloreductase human Steap3

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Steap3 is known as a major ferric reductase in developing erythrocytes participating an important role in cellular iron uptake. Steap3 is comprised of an N-terminal cytosolic NADPH/flavin binding domain and a C-terminal heme-containing 6-transmembrane helices domain. Steap3 is predicted to receive electrons from cytosolic NADPH via flavin and to transfer them to heme. On the extracellular surface of Steap3, they are used to reduce Fe^{3+} to Fe^{2+}. However, little work has been done to describe its detailed functions. To clarify the details of the ferric reductase activity, we attempted to express and purify Steap3 by using *Picia pastoris* system. Analysis of the purified protein showed Soret, α and β peaks in UV-visible spectra, indicative of the binding of a b-type heme.

3Pos073 Computational design of heme-binding protein by remodeling NTF2-like structure

Minako Kondo[1], Yoshitaka Moriwaki[2], Takahiro Kosugi[1], Norifumi Muraki[1,3], Shigetoshi Aono[1,3], Rie Koga[1], Nobuyasu Koga[1,4] ([1]*CIMoS, IMS*, [2]*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [3]*Okazaki. Inst. Integ. Biosci.*, [4]*JST, PRESTO*)

NTF2-like proteins bind to various small molecules based on the shape and size of internal pocket of the structures. Computational design of steroid-digoxigenin-binding proteins based on a NTF2-like structure were previously reported. Here, we demonstrate that the NTF2-like structures can be widely applied as scaffolds to design of the small-molecule binding pocket. In the present study, we computationally designed a heme-binding protein using one of the NTF2-like structures by remodeling the main chain to enlarge the pocket and building a heme-binding interaction site. The design was found to show typical CD spectra of alpha-beta proteins and bind to heme in the 5 coordination with the designed histidine.

3Pos074 コスモトロープ溶質による多量体アロステリック蛋白質の解体とその機能への影響

Disassembly and Impact on Function of a Multimeric Allosteric Protein by Kosmotropes

Antonio Tsuneshige, Satoru Unzai (*Frontier Bioscience, Hosei University*)

We attempted to disassemble under non denaturing solution conditions a multimeric allosteric protein, namely, tetrameric α2β2 human hemoglobin A (Hb), by using amphipathic zwitterionic kosmotropic solutes, and tried to correlate changes in its quaternary structure with changes in its allosteric function. Allosteric theory dictates that when the tetramer splits into two αβ dimers, the allosteric function will be obliterated.
We used three kosmotropic solutes, trimethylglycine, 3-(1-pyiridino)-1-propane sulfonate, and dimethylbenzylammonium propane sulfonate, and correlated the concentration of each solute with quaternary structure and oxygenation properties.
Our results suggest that kosmotropes induce dimerization of Hb, but surprisingly, cooperativity was not abolished.

3Pos075 膜内在性一酸化窒素還元酵素 cNOR の保存されたバリン残基の役割

Functional roles of a conserved valine residue in membrane-integrated nitric oxide reductase, cNOR

Raika Yamagiwa[1,2], Hitomi Sawai[1], Takehiko Tosha[2], Hiro Nakamura[3], Hiroyuki Arai[4], Yoshitsugu Shiro[1] ([1]*Grad. Sch. of Life Sci., Univ. of Hyogo*, [2]*RIKEN, SPring-8*, [3]*RIKEN, Yokohama*, [4]*GSALS, Univ. of Tokyo*)

In denitrification, cytochrome c-dependent nitric oxide reductase (cNOR) catalyzes the reduction of nitric oxide to generate the major ozone-depleting gas, nitrous oxide. The cNOR is a membrane-integrated protein, and contains four redox active metal centers, hemes *b*, b_3 and *c* and a non-heme iron. Although the crystal structure of cNOR was determined, the molecular mechanism of nitric oxide transfer to the active center for the enzymatic reaction is not fully understood, because the recombinant cNOR expression system for site-directed mutagenesis was not established. Recently, we could overcome this point and investigated the functional roles of a conserved valine residue on the edge of the hydrophobic channel using newly established technique.

3Pos076 時間分解可視・赤外吸収分光法を用いた一酸化窒素還元酵素の NO 還元反応機構の解明

Elucidation of the NO Reduction Mechanism of Nitric Oxide Reductase Using Time-resolved Vis / IR Spectroscopy

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Nitric oxide reductase is a membrane protein that reduces NO to N_2O using two electrons and two protons. This reaction is catalyzed in the active center constituted by heme and non-heme irons, but the reaction mechanism is yet to be defined. Using time-resolved visible absorption spectroscopy with caged-NO as a reaction trigger, we have revealed that the NO reduction reaction proceeds with three kinetic phases (~μs, 100 μs, ~ms). Recently, to elucidate the reaction step involving proton transfer, we prepared the variant of proton pathway and compared its reaction kinetics to that of WT. The result suggests that the proton transfer contributes to the 3rd phase. Currently, we try to characterize each kinetic phase in more details using TR-IR spectroscopy.

3Pos077 ミオシンによるポリ三リン酸の加水分解とアクトミオシン運動への影響

Tripolyphosphate hydrolysis by myosin and its effect on the motility of actomyosin

Kuniyuki Hatori, Mitsuru Seino, Koji Ito (*Dept. Bio-Systems Eng., Yamagata Univ.*)

Skeletal muscular myosin is not only an ATPase but also a tripolyhosphatase. We examined the properties of myosin for hydrolysis of tripolyphosphate (TPP) either in Mg- or EDTA-conditions. TPPase activity was 3-fold lower than ATPase activity in the presence of Mg^{2+} (V_{max} = 0.02 /s, K_m = 0.1 mM), and EDTA condition increased the TPPase activity. This result indicates that TPP hydrolysis is the same fashion of ATP hydrolysis. The TPPase activity was competitively inhibited by adenosine. Interestingly, TPPase activity was activated by actin filaments in low concentrations (< 0.05 mg/ml actin), however high concentrations could not induce the actin-activation. The motility of actin filaments by HMM was not found in the presence of TPP without ATP.

3Pos078 溶液中のアクチンフィラメントは平面で運動するアクトミオシンに引き付けられる

A motility induced concentration effects detected by QCM-microscopy

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Filamentous protein such as microtubule or F-actin is known to move collectively at relatively high concentration in the presence of motor proteins on glass surfaces. We have found that those filaments in solution were induced onto the glass surface. The amount of filaments allocating on the glass surface were estimated both fluorescent microscope and direct measuring with QCM (Quartz Crystal Microbalance) simultaneously, which we have named as QCM-Microscopy. We have already reported the unexpected apparent mass change of actin filaments using this microscope. The rate of filament concentration on the glass was found to be faster than that expected from simple diffusion. The possible mechanism of induced concentration will be discussed.

3Pos079 Effects of E244D mutation of cardiac troponin T on the structure of thin filaments by small-angle x-ray scattering

Tatsuhito Matsuo, Fumiaki Kono, Satoru Fujiwara (*QuBS, QST*)

In order to investigate the effects of a cardiomyopathy-causing mutation E244D of troponin (Tn) T on the structure of thin filaments, small-angle x-ray scattering measurements were carried out on bovine cardiac thin filaments, in which the endogenous Tn was exchanged with human cardiac Tn containing the wild-type (WT) or E244D mutant (MT) of TnT, in the $-Ca^{2+}$ and $+Ca^{2+}$ states. Analysis by model calculation shows that while there are no structural differences between the WT and MT in the $-Ca^{2+}$ state, tropomyosin (Tm) of the MT moves closer to the fiber axis than that of the WT in the $+Ca^{2+}$ state. Since Tm directly controls myosin binding, this change would modulate the force production process, leading to functional aberration reported for the E244D mutation.

3Pos080 ヒトβ-アクチン発現系の構築と変異体の解析
System for Expressing and Purification of Human β-Actin and Analysis of Mutants

Mizuki Matsuzaki[1], Sae Kashima[1], Kayo Maeda[1], Tomoharu Matsumoto[1], Mahito Kikumoto[1], Motonori Ota[2], Akihiro Narita[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Grad. Sch. Info. Sci., Nagoya Univ.*)

We constructed the expression system for recombinant human β-actin by using a baculovirus-based system in insect cells. The construct of the human β-actin included a Strep-Tag II affinity tag at N-terminus, the tag was removed in purification. The recombinant WT β-actin had polymerization and depolymerization activities. On the observation of the WT β-actin filament by EM, its diffraction pattern showed that the actin had native fold.
In this poster we will report the result of mutant β-actin which is prepared by this expression system.

3Pos081 Structural analysis of human cardiac muscle thin filament by electron cryomicroscopy

Yurika Yamada[1], Keiichi Namba[1,2], Takashi Fujii[2] ([1]*Grad. Sch. of Frontier Biosci., Osaka Univ.*, [2]*RIKEN QBiC*)

Muscle contraction is driven by cyclic interactions of myosin in the thick filament with the thin filament composed of actin, tropomyosin (Tm) and troponin (TnC, TnI, TnT). It is thought that the binding of Ca2+ released from sarcoplasmic reticulum to TnC causes a conformational change of Tm on the actin filament to allow actin-myosin interaction. To understand this regulatory mechanism, the structure of the thin filament at high resolution is necessary. We made an E. coli expression system of the human cardiac troponin complex and slightly modified tropomyosin, purified them, and reconstituted the thin filament. We were able to obtain the structure of reconstituted thin filament by CryoEM.

3Pos082 心筋リン酸化調節に関与するトロポニン I と T の動的構造：双極子 ESR を用いた距離測定法による研究
Structural dynamics of cardiac troponin I and T regulated by phosphorylation, as studied by distance measurement using dipolar ESR

Toshiaki Arata[1,2,5], Kouichi Sakai[1], Chenchao Zhao[1], Hiroaki Yamashita[1], Takayasu Somiya[1], Shinji Takai[1], Masao Miki[3], Shoji Ueki[4] ([1]*Dept. Biol. Sci., Grad. Sch. Sci., Osaka Univ.*, [2]*Ctr. Adv. High Mag. Field Sci.*, [3]*Univ. Fukui*, [4]*Tokushima Bunri Univ.*, [5]*Dept. Biol., Grad. Sch. Sci., Osaka City Univ. (Present Address)*)

Heart muscle beating is fine-tuned by phosphorylation. ESR spectra from two spin labels attached on i and i+4 residues of the N-extension (NxTnI) of full-length TnI were well fitted by narrow 8-10 and broad 10-20Å distributions. Upon binding with TnC causing higher Ca affinity, PKC region of NxTnI exhibited only former distribution, α-helix, and PKA region showed the latter distribution made narrower, stabilizing an extended conformation. Upon PKC phosphorylation of C-domain TnT in the thin filament, the mobility of spin label bound to N-domain TnT (NTnT) was markedly enhanced and the interspin distance between NTnT and tropomyosin (Tm) was markedly increased from < 8Å to 15-20Å. The loosening of NTnT-Tm upon phosphorylation may reduce tension and ATPase in the heart.

3Pos083 Rotation of the engineered F_1-ATPase with α-type P-loop on catalytic β subunit

Hiroshi Ueno[1], Rie Koga[2], Tomoko Masaike[3], Nobuyasu Koga[2], Hiroyuki Noji[1,4] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*CIMoS, IMS*, [3]*Dept. Appl. Biol. Sci., Tokyo Univ. of Sci.*, [4]*ImPACT, JST*)

Rotation of F_1-ATPase (F_1) has been studied extensively, but its design principle remains elusive. To investigate it, we focused on the P-loops located at the nucleotide binding sites of α and β subunits. ATP is bound to α without catalysis for a regulatory role whereas β hydrolyzes ATP for torque generation. Interestingly, the P-loop sequences of α and β are distinctly different, but completely conserved among species respectively. Crystal structures of F_1 suggest large conformational changes of P-loop in β during catalysis in contrast to the counterpart in α. Therefore, we substituted the P-loop sequence of β with that of α and analyzed the rotation of these engineered F_1s. We report the impact of such radical mutations on the chemomechanical coupling of F_1.

3Pos084 光ピンセットで停止させたバクテリアべん毛モーターのトルク
Stall torque of the bacterial flagellar motor measured by optical tweezers

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The bacterial flagellar motor couples ion flux to mechanical work. It consists of a rotor surrounded by multiple stator units. The stator units dynamically exchange between the motor and a pool in the cell membrane, and their number incorporated in the motor depends on the external mechanical load to it. In this study, we measured the motor torque in the stalled condition by optical tweezers, i.e. under the maximum load condition. The stall torque was estimated to be about 1,800 pN nm, 40% greater than the torque generated by a motor rotating at 70 Hz. This increase of the generated torque might reflect the increase of the incorporated efficiency of stator units in the motor.

3Pos085 人工筋肉の創成に向けたサルコメアユニットの設計
Designing of sarcomere unit from microtubules and kinesins for construction of artificial muscles

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Biomolecular motor protein kinesin transforms chemical energy of ATP into kinetic energy in the presence of microtubules. They are nanosized motors that can perform mechanical work with a high efficiency. Therefore, considerable efforts have been devoted to develop artificial devices through self-assembly of microtubules/kinesin. Here we aim at developing artificial muscle using microtubule/kinesin and photo responsive DNA. In this system, microtubule-kinesin-DNA conjugate will contract upon visible right irradiation, but the conjugate will relax upon UV right irradiation through DNA duplex formation and dissociation. This artificial muscle is expected to widen the range of potential applications of biomolecular motor in nanotechnology.

3Pos086 Na^+と K^+で駆動するバクテリアべん毛モーターの発生トルク
Torque-IMF relationship of Na^+- and K^+-driven bacterial flagellar motor

Kenta Arai[1], Taishi Kasai[2], Yuka Takahashi[3], Masahiro Ito[3], **Yoshiyuki Sowa**[1,2] ([1]*Dept. Frontier Biosci, Hosei Univ.*, [2]*Reserch Center for Micro-Nano Tech., Hosei Univ.*, [3]*Fac. Life Sci., Toyo Univ.*)

The bacterial flagellar rotary motor consists of a rotor surrounded by multiple ion-conducting stator units. The motor of *Escherichia coli* cells expressing MotPMotS of *Bacillus alcalophilus* (BA-MotPS) as stator components is known to be driven by both Na^+ and K^+, although natural *E. coli* motor runs by H^+ flux.
In this study, we measured the motor speed of BA-MotPS motor in *E. coli* under various ion-motive force conditions. The torque generated by single stator units increased linearly with increasing ion-motive force. We found that the slope estimated by linear fit to the data for K^+ driving states is identical to that for Na^+ driving states. These results suggest that the motor running on any type of ion-motive force generates torque at the constant efficiency.

3Pos087 ハイブリッド F_1-ATPase の１分子回転観察
Rotation of hybrid F_1-ATPase from bacterial rotor and mammalian stator ring

Ryo Watanabe, Hiroshi Ueno, Toshiharu Suzuki, Ryohei Kobayashi, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

F_1-ATPase is a rotary molecular motor which has the rotor γ subunit and the stator $\alpha_3\beta_3$-ring. Previous studies revealed that F_1 from Bacillus PS3 (TF_1) and bovine mitochondorial F_1 (bMF_1) rotate at different speed with different substep size. Which subunit causes this difference of rotation schemes? In this study, we investigate the rotation substeps of the hybrid F_1s composed of the subunits of TF_1 and bMF_1. We constructed the hybrid F_1-ATPase, rotor γ subunit of TF_1 inserted into stator $\alpha_3\beta_3$-ring of bMF_1, and succeeded in observing the rotation of this hybrid F_1-ATPase. The rotation speed of the hybrid F_1-ATPase was about 573±45 rps at 1 mM ATP, closed to the rotation speed of bMF_1 than that of TF_1.

3Pos088 駆動力と集積力に依存するアクチン線維流の配向
Alignment of actin-streams driven by myosin motors: Dependence on driving force and packing force

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We have reported to change the alignment patterns of streams of actin filaments by changing KCl concentration in the presence of 1% methylcellulose (Iwase et al., BSJ 2016). Increase in both KCl and actin concentrations decreased the space intervals between aligned streams. Here, we attempted an agent-based simulation, which individual filaments can change their moving direction when some filaments are encountered. Fluctuations of movement were imitated on the basis of actual movement of single filaments. Magnitude of changing direction (constraint), density of filaments, and velocity were variable. At high constraint, filaments tended to align with bi-directional streams. The decrease in velocity could lead to the convergence of streams and narrow space intervals.

3Pos089 Novel photochromic inhibitor of mitotic kinesin Eg5 composed of spiropyran and azobenzene

Md Alrazi Islam[1], Ryouta Shimoyama[2], Shinsaku Maruta[1] ([1]*Soka University, Department of Bioinformatics, Graduate School of Engineering*, [2]*Dept. of Sci. and Eng. Faculty of Bioinfo.*)

The mitotic kinesin Eg5 is essential for the formation of bipolar spindles during eukaryotic cell division and has been considered as a potential target for cancer treatment. In this study, to control Eg5, we have synthesized a novel photochromic compound composed of photo-responsive azobenzene and Spiropyran derivatives. The photochromic compound SP-AB showed three different isomerization states Mero-Cis, SP-Trans and Mero-Trans upon ultraviolet (UV) irradiation, visible (Vis) light irradiation and in the dark respectively. We introduced thiol reactive Iodoacetyl group into SP-AB. Subsequently, the Iodoacethyl-SP-AB was reacted with N-acetyl-cystein to synthesize photochromic inhibitor. Eg5 ATPase activity was significantly decreased in the presence of the inhibitor.

3Pos090 Structural basis of the mechanical properties of the flagellar distal rod and the hook

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The bacterial flagellar distal rod and hook are directly connected to each other, but show distinct mechanical properties. The distal rod is a helical assembly of FlgG and rigid as a drive shaft. The hook is a helical assembly of FlgE and flexible in bending as a universal joint. We determined a crystal structure of a 20kDa fragment of FlgG from Salmonella. The structure is greatly similar to the structure of FlgE from Campylobacter. The structural similarity allowed us to construct a novel atomic model of the distal rod using the crystal structure and the EM map of the distal rod that had been previously reported. The model suggests that the subunit interaction mediated by the L-stretch is one of the keys that generate distinct mechanical properties.

3Pos091 Structural analysis of the NATIVE state flagella hook by electron cryomicroscopy

Takayuki Kato[1], Tomoko Miyata[1], Peter Horvath[1], Keiich Namba[1,2] ([1]*Grad. Front. Biosci, Osaka Univ*, [2]*QBiC, RIKEN*)

The bacterial flagellum is a motile protein complex composed with a rotary motor, hook and flagella. The hook is flexible in bending as universal joint to smoothly transmit torque produced by the motor to the filament. So far, the hook structure was solved by cryoEM after its straighten. Since bending structure are not known from the result, then conformational change during rotation in bending was analyzed by molecular dynamics simulation. We solved the bending structure of the hook by cryoEM at 6A resolution. The resolutional map was sufficient to reveal the conformational difference between hook proteins in tight and loose subunit packing in bending. I want to discuss about interactions and conformational changes when hook transmits the torque.

3Pos092 細菌べん毛モーターの回転方向変換制御機構の解明
Elucidation of the directional switching mechanism of the bacterial flagellar motor by electron cryomicroscopy

Tomoko Miyata[1], Takayuki Kato[1], Akihiro Kawamoto[1], Keiichi Namba[1,2] ([1]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [2]*QBiC, RIKEN*)

Many bacteria swim by reversibly rotating flagella. The three switch proteins, FliG, FliM and FliN, form the C-ring on the cytoplasmic face of the MS ring and control counterclockwise-clockwise (CCW/CW) switching of the motor rotation. To understand the switching mechanisms in detail, we analyzed the C ring structures of wild type (CCW form) and CW-locked mutants by electron cryomicroscopy. We suceeded to analyze the C-ring structure at 9 Å resolution. The crystal structures of the switch proteins were well fitted into the 3D map. We will report the structural change and interaction of the each proteins between the CCW and CW forms and discuss about the switching mechanism of flagellar motor rotation.

3Pos093 High resolution structural analysis of the flagellar hook of Salmonella Typhimurium

Peter Horvath[1], Takayuki Kato[1], Tomoko Miyata[1,2], Keiichi Namba[1] ([1]*FBS Osaka Uni.*, [2]*QBiC, RIKEN*)

Equipments and techniques for CryoEM methods for structural studies of macromolecules have rapidly advanced in recent years. These developments allow near-atomic resolution structure determination, which is inevitable for understanding underlying biological mechanisms. The bacterial flagellar hook functions as a universal joint. The highest resolution structure available so far is 7.1 Å, and this was achieved with a CCD camera. To gain more detailed information about the flexible mechanism of the hook, we tried to analyse the hook structure by electron cryo microscope with direct electron detector camera. Finally, we succeeded to solve the structure at 4A resolution and constructed the whole atomic model of hook. We will discuss the flexible mechanism.

3Pos094 pH-indicator を用いた好熱菌 *Bacillus* PS3 由来 F_oF_1-ATP 合成酵素の ATP 加水分解と H^+輸送の共役機構
Analyses of coupling mechanism between ATP-hydrolysis and H^+-translocation of *Bacillus* PS3 F_oF_1-ATP synthase using pH-indicator

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F_oF_1-ATP synthase (F_oF_1) synthesizes ATP by the energy of H^+-flow across membranes. The energy conversion is achieved with a dual-rotary motor architecture of F_oF_1 composed of F_1, which converts chemical potential of ATP to rotation, and F_o, which is rotated by H^+-flow. We have established an analytical system for F_o to investigate the coupling mechanism between F_o and F_1, using pH-sensitive fluorescence dye. Proteoliposomes were prepared by reconstituting *Bacillus* PS3 F_oF_1 into the liposomes including the pH-indicator. ATPase activity and inside pH of the proteoliposomes were analyzed in real time under several conditions. The coupling mechanism will be discussed from time-dependent changes in activities of ATPase and H^+-translocation, and also in H^+/ATP-ratio.

3Pos095 Regulation of dynein motility by NDEL1

Toshiaki Saito[1], Takuya Kobayashi[1], Takayuki Torisawa[2], Takashi Murayama[3], Yoko Y Toyoshima[1] ([1]*Grad. Sch. of Arts & Sci., Univ. Tokyo*, [2]*Bio ICT Lab, NICT*, [3]*Dept. Pharmacol., Juntendo Univ. Sch. of Med.*)

Cytoplasmic dynein is a molecular motor that moves along microtubules. It is composed of multiple subunits, and involved in intracellular transport. NDEL1 is known to control dynein function in the cell, and previous in vitro studies revealed that dynein was dissociated from microtubules by NDEL1. Although NDEL1 is suggested to have two dynein binding sites one of which is involved in the regulation of dynein motility, the mechanism by which NDEL1 dissociates dynein from microtubules is unclear. To elucidate the mechanism, we made the truncated mutants of NDEL1 and investigated the subunits of dynein complex as the binding partner of those mutants. Including the results of in vitro motility assay, we will discuss the binding property of NDEL1 to dynein.

3Pos096 F_O モーターの回転ブラウン運動の数値解析
Computational Analysis of the Brownian rotation of F_O motor

Daiki Yamakoshi, Dan Parkin, Kota Tezuka, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

F_O motor, which is the membrane-embedded portion of ATP synthase, is composed of the stator subunits *a* and *b* and the rotor *c*-ring. The unidirectional rotation of *c*-ring coupled to proton motive force (PMF) is explained by the half-channel model, in which protonation states (PS) of the conserved acidic residues in the *c*-ring is changed according to PMF, which biases the direction of Brownian rotation. However, the atomistic mechanism by which the *c*-ring unidirectionally rotates is still unclear. In this study, to observe the rotation of a c_8-ring over a rotational period (45°), we conducted molecular dynamics simulations starting from several angles and PSs. We found that change in PS affects the rotational behavior. Based on this, we discuss how PMF drives the rotation.

3Pos097 微小管のグライディング運動における蛍光 ATP の Linear zero-mode waveguides を利用した 1 分子観察
Single molecule observation of fluorescent ATP in microtubule gliding motility enabled by linear zero-mode waveguides

Kazuya Fujmoto[1], Ryota Iino[2], Michio Tomishige[3], Hirofumi Shintaku[1], Hidetoshi Kotera[1], Ryuji Yokokawa[1] ([1]*Kyoto Univ.*, [2]*Institute for Molecular Science*, [3]*Aoyama Gakuin Univ.*)

Recently, zero-mode waveguides (ZMWs) have been used for single molecule observation with μM order of fluorescently labelled molecules by confining excitation light in cylindrical apertures with 100 nm of diameter. However, ZMWs was not compatible with motor proteins that interact with filamentous biomolecules such as microtubules or actin filaments, despite those proteins are the major targets of single molecule fluorescent experiments.
Here, we propose a linear-shaped zero-mode waveguides (LZMWs) that enables use of linear motor proteins and single molecule observation with 100 nM order of labelled molecules. Using 150 nm width of LZMWs track, single molecule observation of labelled ATP in microtubule motility with 500 nM of concentration was realized.

3Pos098 Probing cell-wall synthetic dynamic using bacterial membrane protein-complex

Yi-Ren Sun, Chien-Jung Lo (*Department of Physics and Graduate Institute of Biophysics, National Central University*)

Bacteria have to elongate their cell body as the preparation for division. As cell elongate, elongasome, a group of enzymes, carry out the PG insertion on the cell-wall which is guided by the cytoskeletal protein MreB filament. We aim to understand the cell-wall synthetic dynamic as cells reproduce by observing the interaction among the PG insertion, elongasome/divisome and MreB/Ftsz filaments.
We observe the dynamics of fluorophore labeled hook of flagella during the duplication process. That is, when the new PG strand been inserted, the original cell-wall with the motors embedded in it will be pushed away from its original location. Therefore, by observe the movement of the motors as cells reproduce, we can observe the spatiotemporal coordination of the PG insertion.

3Pos099 足場の形状によるアクチン波と細胞極性の制御
Actin waves and cell polarity regulated by substrate geometry

Gen Honda[1], Akihiko Nakajima[2], Satoshi Sawai[1,2] ([1]*Department of Basic Science, Graduate School of Arts and Sciences, University of Tokyo*, [2]*Research Center for Complex Systems Biology, Graduate School of Arts and Sciences, University of Tokyo*)

Formation of dendritic F-actin that spreads along the cortical layer of the plasma membrane, the so-called “actin wave”, is known in diverse cell types from neurons, fibroblasts to amoebae. Here we show that micrometer-scale curvature of the cell-substrate dictates propagation of actin waves in Dictyostelium. Characteristic cell movements observed that correlated with actin waves were: 1) persistent wave propagation and directional cell migration along a straight or winding ridge, 2) wave termination and reflection and concomitant migration reversal at T-junctions, and 3) wave splitting at Y-junctions that induced bifurcating leading edges. These observations suggest how regulation of actin waves can transform the topography of the substrate into migratory modes.

3Pos100 Manipulation and Detection of Ca^{2+} Concentration Change of Single Immotile Cilium in Mammalian Node

Takanobu A Katoh[1], Katsutoshi Mizuno[2], Hiroshi Hamada[2], Takayuki Nishizaka[1] ([1]*Dept. Phys., Gakushuin Univ.*, [2]*CDB, RIKEN*)

Immotile cilia are solitary hair-like protrusions that extend from the surface of cells. It is now established that the nodal immotile cilia sense a flow-dependent signal to determine the L-R patterning of the embryo. To quantify the relationship between the deformation of the cilia and intraciliary [Ca^{2+}], we constructed the optical system to manipulate a single cilium by optical tweezers. The system is applied to nodal immotile cilia of a Tg mouse that expresses Ca^{2+} indicator GCaMP6. The rise of the GCaMP6 intensity was often detected after multiple bending (40% in n = 14) with the delay of ～10 s, while the single bends did not induce intensity change. Our observations support the idea that the nodal cilium increases intraciliary [Ca^{2+}] via mechanical stimulation.

3Pos101 リニアモータータンパク質によるミトコンドリアの形態変化
Mitochondrial Shape Changing by Linear Motor Proteins

Keitaro Shibata[1,2], Luca Scorrano[1,2] ([1]*Dept. of Biol., Univ. of Padua*, [2]*VIMM*)

Mitochondria are essential organelles that provide ATP and regulate housekeeping processes. They undergo dynamic morphological changing and make a complex network in eukaryotic cells. The dynamics is linked to their functional versatility so deeply that it is important to elucidate the mechanisms by which they change their shape. Some motor proteins moving along cytoskeletons are linked to mitochondria. Mitochondria use force from the motors for movement and transformation. However, it is not known how motor proteins regulate the complex morphology of mitochondria. Here, we try to show positional relationship between the motor proteins and mitochondria by morphometric analysis in living cells, and demonstrate how motor proteins control mitochondrial morphology.

3Pos102 生体ゲル内ナノ粒子の移動量に基づく細胞浸潤時の力場計測
Force map of collective cells invading into biological matrix gels

Yuto Sano, Seohyun Lee, Hideo Higuchi (*University of Tokyo, School of Science, Department Physics*)

Epithelial cancer cells metastasize and form secondary tumors. To analyze force acted on matrix around the cells during invasion, cells are incubated on matrix gel in which fluorescence beads were embedded and force was calculated from displacement of the beads. As it is known that multiple cells invade collectively in vivo, we calculated force map at collective invasion by measuring two-dimensional displacement of beads. To reduce error of displacement by microscope stage drift, we developed the system measuring three-dimensional stage drift. As a result, we found that force generated by collective invasion is much higher than single cells.

3Pos103 Universal glass-forming behavior of living cytoplasm

Masahiro Ikenaga, Kenji Nishizawa, Daisuke Mizuno (*Dept. of Phys., Univ. Kyushu*)

It was found in our prior study that in vitro cytoplasm that lacks metabolism shows a mechanical property typical for “fragile” glass formers that is universally conserved in different species and developmental stages. In this study, the mechanics of the living cell interiors were investigated. We measured probe fluctuations suspended in eukaryote cells taken from different tissues by laser interferometry. The intracellular viscosity was obtained from the fluctuation at high frequencies (~ 4kHz). Controlling the biomacromolecules concentrations in cells by adjusting the osmotic pressure of the culture medium, we found that metabolic activity fluidized the living cytoplasm and turned their universal glass-forming behavior from that of fragile to strong glass formers.

3Pos104 超解像顕微鏡で観察された、ラメリポーディア領域のファシンとアクチンメッシュ ワークの相互作用

Interaction between fascin and actin meshwork in lamellipodial region revealed with superresolution microscopy

Minami Tanaka[1,2], Ryoki Ishikawa[3], Kaoru Katoh[2] ([1]*Grad. Sch. Life & Env. Sci., Univ. Tsukuba*, [2]*Bio Mes Res. Inst., AIST*, [3]*Gunma Pref. Coll. Health Sci*)

Growth cones, at the tip of growing neurites, play important roles in neuronal path finding and target recognition. Their movement is controlled by actin dynamics. Their actin cytoskeleton is made up of actin bundles in filopodia and actin meshwork in lamellipodia. Fascin is well known to bind actin filaments in the filopodia but was not well studied in the lamellipodia, because it was difficult to observe lamellipodial actin meshwork with conventional optical microscopes. Here, we visualized lamellipodial actin meshwork and fascin simultaneously with 2 color SIM. We clearly showed co-localization of fascin with actin filaments in the lamellipodia. Moreover, we visualized effect of unbinding of fascin from actin meshwork on the movement and shape of the lamellipodia.

3Pos105 Live-cell analysis of actin network by high-speed atomic force microscopy

Yoshitsuna Itagaki, Yanshu Zhang, Aiko Yoshida, Masahiro Kumeta, Shige H. Yoshimura (*Grad. Sch. Biostudies, Kyoto Univ.*)

Actin plays critical roles in various cellular functions such as cell cycle, cell migration and mechano-sensing and responses. Here, we visualized and analyzed dynamics of actin filaments in lamellipodium of living COS-7 cells by high-speed atomic force microscope. Dynamic rearrangement of actin filament network and its retrograde flow was observed at the edge of the cell. The rate of the flow is constant (~10 nm/sec) and is driven mainly by actin polymerization at the barbed end, but not by acto-myosin system. Inhibition of Arp2/3 complex and formin affected the dynamics of actin and morphology of the cell edge, suggesting that the numbers of branching and active barbed ends are critical determinants of the force balance at the cell edge.

3Pos106 原子間力顕微鏡による正常および肺高血圧症の肺動脈平滑筋細胞の弾性率測定

Elastic modulus of pulmonary arterial smooth muscle cells in normal and pulmonary arterial hypertension patient by atomic force microscopy

Nao Tatsumi[1], Shinichi Katsuragi[2], Ryosuke Tanaka[1], Hidekazu Ishida[2], Shigetoyo Kogaki[2], Takaharu Okajima[1] ([1]*Grad. Schl. Inform. Sci. and Technol., Hokkaido Univ.*, [2]*Dept. Ped., Grad. Schl. Med., Osaka Univ.*)

Pulmonary arterial hypertension (PAH) is a life-threatening disease causing right ventricular dysfunction. Recently, the stiffening of pulmonary artery in PAH is noted as a new predictor of mortality due to right ventricular overload [1], but the detailed mechanism of the tissue stiffening at the single cell level is unclear. Here we investigated the Young’s modulus, E, of pulmonary artery smooth muscle cells from PAH patients (P-PASMC) and non-patients (N-PASMC) by atomic force microscopy (AFM). We observed that E of P-PASMC cells exhibited a large variation compared with N-PASMC. We also succeeded to measure with a customized AFM the mechanical property of ex vivo pulmonary arteries of rat, the results of which will be presented. [1] Wang, et al. PLoS ONE (2013).

3Pos107 細胞競合現象における細胞内部環境のダイナミクス

The dynamics of intracellular environments under cell competition

Katsuhiro Umeda[1], Wataru Nagao[1], Kenji Nishizawa[1], Shunsuke Kon[2], Yasuyuki Fujita[2], Daisuke Mizuno[1] ([1]*Grad. Sch. Sci., Univ. Kyushu*, [2]*Grad. Sch. Sci., Univ. Hokkaido*)

Most of newly-emerging transformed cells in our body are eliminated from tissues via competition against surrounding normal cells. Such “cell competition” can be artificially prepared in an in vitro model by culturing normal MDCK epithelial cells with those mutated to express constitutively-active oncogenic Ras (RasV12) after induction with tetracycline. In this study, we investigate the mechanical aspect of cell competition. The mutated cells were tracked in the model system and their mechanical properties and activities were measured by using the dual-feedback microrheology technique. By comparing the changes made after inducing transformation, we found that mutated cells surrounded by normal cells became more active and that their cytoplasm were fluidized.

3Pos108 光ゆらぎ法による酸化ストレスを受けた動物細胞の損傷度の計測

Evaluation of oxidative stress in mammalian cell by intensity fluctuation method

Morito Sakuma, Yuichi Kondo, Hideo Higuchi (*Department of Physics, Graduate School of Science, The University of Tokyo*)

Removal of cancer cell or undifferentiated iPS cell is necessarily for therapy. Reactive oxygen species (ROS) induced by photoactivating fluorescent dyes has been applied, but surviving cancer cells from the damage can obtain resistant to ROS. Here to understand the effects of ROS, we developed an intensity fluctuation method to measure cell damages from intracellular organelles movement. The motility of cell organelles gradually decreased with a progression of cell damage. ROS also damaged kinesin and dynein activity in vitro motility assay, therefore, ROS may be a primary factor for causing decrease of organelles motility. These results suggested that the cell organelles motility change is a primary indicator of cell damage.

3Pos109 On bending rigidity of microtubules measured from in vitro motility assay with external force

Takahiro Nitta (*Applied Physics Course, Gifu Univ.*)

Microtubules (MTs) serve as mechanical basis of cells. While their mechanical properties have been intensively investigated, values of bending rigidities reported so far vary over orders of magnitude. In measuring the bending rigidities, in vitro motility assays with external force were used, as well as observing thermal fluctuation of free standing MTs and bending MTs with optical tweezers. One of advantages of the use of the methodology is that owing to microfabrication technology, well-controlled force can be simultaneously applied to MTs. Here, by using our own developed computer simulation, we investigated the validity of the methodology, providing insights on interpretations of bending rigidity of MTs measured from in vitro motility assay with external force.

3Pos110 GPI アンカー型受容体プリオンタンパク質と Thy1 の動的メゾスケール拡散停止：1 分子追跡による検出
Dynamic mesoscale anchorage of GPI-anchored receptors prion protein and Thy1 in the cell membrane as revealed by single molecule tracking

Yuri L. Nemoto[1,2,4], Roger J. Morris[3], Hiroko Hijikata[1], Taka A. Tsunoyama[4], Akihiro C. E. Shibata[1,2], Rinshi S. Kasai[2], Akihiro Kusumi[1,2,4], Takahiro K. Fujiwara[1] ([1]*Center for Meso-Bio Single-Molecule Imaging (CeMI), Institute for Integrated Cell-Material Sciences (WPI-iCeMS), Kyoto Univ.*, [2]*Institute for Frontier Life and Medical Sciences, Kyoto Univ.*, [3]*Department of Chemistry, King's College London*, [4]*OIST*)

The transmission of the prion protein (PrP) misfolding from one to another occurs by the structural conversion of the normal cellular PrP to the pathogenic one, by its interaction with the misfolded PrP. Here, using single-molecule imaging and tracking, we found that PrP exhibited intermittent immobilizations lasting for a few seconds within an area of 3.5 nm in diameter in cultured hippocampal neurons, which are likely induced by temporary association with PrP clusters. Thy1 exhibited less immobilization. PrP molecules might be newly recruited to PrP clusters all the time, and simultaneously, PrP molecules in the cluster might be departing continuously. Such dynamic interactions of normal PrP molecules would strongly enhance the spreading of misfolded PrP.

3Pos111 Stiffness measurement of bacterial cell using high-resolution imaging tracking

Chih-Chao Liao, Chien-Jung Lo (*National Central University*)

Bacterial cell stiffness is mainly maintained by cell wall. During the cell growth and division process, cell wall is remodeled. However, there is no reliable experimental method to probe the dynamics of cell wall. Here, we present a method to investigate the bending dynamic of bacterial cell with shape fluctuation in time evolution. The position localization of bacterial cell in this method can be occurred with subpixel accuracy. For bacterial cell in swarming colony, the persistence length can be reduced to micrometers by the interaction between swarming cell.

3Pos112 べん毛 III 型分泌装置のある構成因子は膜内部で Rhomboid プロテアーゼ GlpG による切断を受ける
A component of the flagellar type III secretion system receives proteolytic cleavage by rhomboid protease GlpG inside the membrane

Yohei Hizukuri, Kosuke Terushima, Yoshinori Akiyama (*Inst. Front. Life Med. Sci., Kyoto Univ.*)

Rhomboid family intramembrane proteases are ubiquitously found in all kingdoms of life. They are known to be involved in various important cellular events in eukaryotes, such as the proteolytic activation of EGF signaling or the development of Parkinson's disease. In contrast, their physiological roles and substrates in prokaryotes remain largely unknown. In the last meeting, we have presented the result of a screening to explore a proteolytic substrate of an *Escherichia coli* rhomboid homologue, GlpG, and identified a component of the flagellar type III secretion apparatus as a possible candidate. We are now trying to investigate the physiological significance and the molecular mechanism of this cleavage.

3Pos113 単一細胞におけるミトコンドリアのダメージと活性酸素発生の同時観察
Simultaneous measurements of mitochondrial damages and ROS generation in single cells

Emika Shida, Yoshihiro Ohta (*Ohta. Lab., Univ. Noko*)

Oxidative stress are frequently observed in damaged cells. Mitochondria are considered to have a significant contribution to oxidative stress, because mitochondria get easily damaged by reactive oxygen species (ROS) and damaged mitochondria have an tendency to produce more ROS. The aim of this study is to know the correlation between mitochondrial damages and ROS generation. To observe mitochondrial damage and ROS generation, C6 cells were simultaneously stained with mitochondria selective dye and ROS indicator. Mitochondrial damages were induced by adding the inhibitors of respiratory chain to cells and were evaluated in terms of mitochondrial membrane potential and shape. The detailed conditions and results will be discussed.

3Pos114 Molecular mechanism of T cell signaling termination

Hiroaki Machiyama, Tadashi Yokosuka (*Dept. Immunol, Tokyo Med. Univ.*)

T cell activation triggers adaptive immune system. Since aberrant immune response involves autoimmune diseases, the termination signaling for T cell activation is required. However, its molecular mechanism is unclear. Using TIRF microscopy and planar lipid bilayer that is embedded essential molecules in T cell activation pMHC, CD80 and ICAM-1, we identified the recruited molecules at TCR microclusters that serve as a signalsome in T cell activation. Upon T cell activation, TCR microclusters are ubiquitinated by E3-ubiquitin ligase Cbl-b and endocytosis-related molecules EPS15, clathrin and dynamin are recruited at TCR microcluster. These findings suggest that ubiquitination of TCR microclusters lead to clathrin-dependent endocytosis to terminate T cell activation.

3Pos115 Small GTPase, F-actin and cell morphology dynamics in migrating cells under well-defined noisy chemoattractant gradients

Yoichi Irie[1], Taihei Fujimori[1], Akihiko Nakajima[2], Satoshi Sawai[1,2] ([1]*Grad. Sch. Arts Sci., Univ. Tokyo*, [2]*Res. Ctr. Complex Sys. Biol., Univ. Tokyo*)

The occurrence of pseudopods in chemotactic cells is thought to be stochastically biased in a shallow chemoattractant gradient. However, its exact nature and the relation to the input signals are unclear. Here, by employing live-cell imaging and microfluidics in migrating Dictyostelium cells, we show that biasing of Ras activity towards the gradient direction is strengthened by F-actin as evidenced by the weakening of such features in latruculin A treated cells. In a reorienting gradient, cells whose Rac activity was temporary reset showed denovo formation of leading edge, while those with persistent Rac activity underwent a U-turn motion. We will also discuss how the 3-D morphology affects the readout of the noisy input based on the light-sheet 3D imaging data.

3Pos116 Investigating contribution of transcription to temperature in nucleus

Shunsuke Takeda[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., The Univ. of Tokyo*, [2]*PRESTO, JST*)

According to recent intracellular temperature distribution measurement, the temperature in the nucleus was higher than that in the cytoplasm. However, its mechanism and its significance are unknown. Here, we focused on transcription because it is one of the highest activities in the nucleus. Furthermore, RNA is highly susceptible to temperature-dependent structure change. In this study, we measured the temperature in the nucleus using a fluorescent polymeric thermometer and fluorescence lifetime imaging. Temperature imaging in cells in which transcription was inhibited showed that the temperature in the nucleus was lower than that in normal cells, suggesting that transcription is involved in the heat production in the nucleus of cells.

3Pos117 細胞性粘菌のアメーバ運動のブレブモードへの移行は、細胞外からの Ca^{2+}流入に依存しない
Motility of *Dictyostelium* amoebae switches to the bleb mode without Ca^{2+} influx

Naoto Yoshinaga, Taro Uyeda (*Dept. Phys., Waseda Univ.*)

Amoeboid cells are known to migrate in two distinct modes, depending on either pseudopods or blebbing. Starved *Dictyostelium* amoebae switch to the bleb mode when flattened by an agarose block, but the mechanosensor for this mode switching has not been identified. Here, we examined the possibility that the mode switching depends on Ca^{2+} influx through stretch-activated Ca^{2+} channels (SACs) in the cell membrane, since intracellular Ca^{2+} is known to affect cell motility. However, cells switched to the bleb mode normally when flattened by an agarose block, even in the presence of 100 μM Gd^{3+} or 100 μM EGTA, demonstrating that SACs are not the mechanosensor for the mode switching. We are carrying out experiments to identify the responsible mechanosensor in this mechanism.

3Pos118 前後運動する神経幹細胞における力測定
Traction Force working on Reversive Motion of Neural Stem Cells

Masahito Uwamichi, Masaki Sano (*Dept. of Phys, Univ. of Tokyo*)

Neural stem cells stochastically changes the direction of its motion.

3Pos119 微速度撮影によるユーカリ苗の根生長速度における電界応答測定
Electric response measurement of E. camaldulensis in seedling root growth by time lapse photography

Kazuki Sugawara[1], Yutaro Mukai[1], Hideki Suganuma[2], Shigeru Kato[1], Takuya Ito[1], Toshinori Kojima[1], **Seiichi Suzuki**[1] ([1]*Faculty of Science and Technology, Seikei University*, [2]*Kawasaki Environment Research Center*)

Root growth rate of Eucalyptus camaldulensis seedling was measured by time lapse photography with/without application of AC electric field in aqueous culture vessel. Stimulation of 50 Hz AC electric field is known to enhance growth rate of R. sativus root in a moderate range of field intensity. However, electric response of E. camaldulensis was difficult to measure for it's small size. In this study, mutual correlation analysis with modulated electric field stimulation revealed the response of the plant to electric stimulation. Response time of the root growth is within the range of some minutes, which seems very quick compared with plant growth. This result suggests the existence of some high speed information processing system in plant body.

3Pos120 繊毛虫テトラヒメナの空間の広がりに対する適応能
Adaptive capacity in response to spatial expansion in the ciliate protozoan Tetrahymena

Itsuki Kunita[1], Tatsuya Yamaguchi[2], Atsushi Tero[2], Masakazu Akiyama[3], Shigeru Kuroda[3], Toshiyuki Nakagaki[3] ([1]*University of The Ryukyus*, [2]*Kyushu University*, [3]*Hokkaido University*)

Bramstedt reported in 1935 that the ciliate Paramecium could memorize spatial configurations, such as a triangle or rectangle. Concerning the spatial memory capacity in ciliates, there have been both supporting and opposing opinions. We here examined experimentally whether the ciliate Tetrahymena could memorize a spherical shape and its size. Half of the specimen showed circular movement in an open space after the motion experienced in a tiny spherical droplet. The remaining half behaved similar to control. We accepted the hypothesis of spatial memory capacity and explain the mechanism of spatial memory in ciliates on the basis of membrane potential dynamics, which controls the ciliary movement.

3Pos121 モジホコリ変形体における行動決定の揺らぎ
Fluctuation in decision-making of Physarum plasmodium

Yuya Mitsutake, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

To know how Physarum plasmodium, primitive giant unicellular organism, makes a decision under complicated environment, the behavior during selecting from two alternatives was investigated. A plasmodium was placed at the boundary between two different conditions of culture media, then its development process and movement were observed. To quantify the behavior, centroid, growth rate (GR) and maximum reachable distance (RD) were analyzed. The movement of the organism first fluctuated around the boundary, finally moved toward one of the media. The fluctuating period increased as the difference of the two conditions were closer. Contrarily, GR and RD seemed to depend only on the condition of the selected media.

3Pos122 モジホコリ変形体における周期刺激に対する輸送管ネットワークの適応
Adaptation of transportation network against periodic stimuli in Physarum plasmodium

Akira Ishizaki, Satoshi Toyoda, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

An adaptation process to environmental change by transportation network morphology of Physarum plasmodium was investigated. Periodically switching lights were given as repulsive stimuli, then the network formation process was analyzed. No remarkable response was observed under short period of stimuli. When the period exceeded a certain length, the number of the transportation tubes decreased during the stimulation, then the extension direction of the progressing ends was reversed. Under intermediate period of stimuli, dense meshed network was formed. This network formation could be the most robust against the inbetween and complex environment.

3Pos123 Cloning of cryptochrome 2 gene from honey bee

Yuhei Hosokawa, Shigenori Iwai, Junpei Yamamoto (*Grad. Sch. Eng. Sci., Univ. Osaka*)

Cryptochromes (CRYs) are blue-light receptors involved in regulation of the circadian clock, and also considered to function as magnetoreceptors. CRYs share high homology with DNA repairing enzyme photolyases, but CRYs have lost DNA repair activity during evolutional process. Two isoforms of CRYs are found, namely CRY1 and CRY2, and the both are normally required to maintain the biological clock. Interestingly, only a CRY2 gene was found in honey bee and reportedly homologous to mouse CRY. Therefore, their functional roles remain unclear and are of interest.
In this study, we cloned the CRY2 gene from total RNA extracted from honey bee. The predicted amino acid sequence of honey bee CRY2 (HbCRY2) shared high similarity with mouse CRY and animal (6-4) photolyase.

3Pos124 ナトリウムイオンポンプ型ロドプシンの細胞外側表面に位置する酸性残基の機能解析
Functional analyses of Na^+-pumping rhodopsin focusing on acidic residues on the extracellular surface

Akiko Okamura[1], Takashi Kikukawa[1,2], Takashi Tsukamoto[1,2], Tomoyasu Aizawa[1,2], Naoki Kamo[1], Makoto Demura[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*GSS, GI-CoRE, Hokkaido Univ.*)

Na^+-pumping rhodopsin from *Indibacter alkaliphilus* was functionally analyzed through the mutations of acidic residues. Here we present the topics relating to D101 and E10. Previous reports suggest that D101 residue binds Na^+, and E10 residue connects the N-terminal helix to the protein core by forming a hydrogen-bonding complex with E160 and R242 residues. The obtained results are summarized as follows: 1) Not only Na^+ but also K^+ binds near the D101 residue. These bindings weaken the Na^+-pumping activity but enhance the structural stability. 2) E10Q lost the Na^+-pumping activity. But, it was restored in E10Q/R242Q. Thus, E10 residue is probably essential to neutralize the charge of R242 residue. Without this interaction, R242 residue might inhibit the Na^+ transport.

3Pos125 *Natronomonas pharaonis* halorhodopsin T126E 変異体の機能解析
Functional analysis of T126E mutant of *Natronomonas pharaonis* halorhodopsin

Shuhei Abe[1], Takashi Kikukawa[1,2], Takashi Tsukamoto[1,2], Tomoyasu Aizawa[1,2], Naoki Kamo[1], Makoto Demura[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*GSS, GI-CoRE, Hokkaido Univ.*)

We attempted to convert a Cl^- pump *Natronomonas pharaonis* halorhodopsin (NpHR) into a H^+ pump like bcteriorhodopsin (BR). Two key residues D85 and D96 in BR correspond to T126 and A137 in NpHR, respectively. We observed the M intermediate in the mutant T126E but not in T126D. However, the prolonged M decay could not be accelerated by the mutations of A137 and other several residues. Next, we examined the "azide effect" to probe a difference between NpHR and BR. For D96N-BR, azide accelerated the M decay up to 1900-fold. For T126E-NpHR, however, only 9-fold acceleration was observed. The smaller conformational change in NpHR might disable the embedded H^+ donor residue.

3Pos126 NTQ 型アニオンポンプの輸送機能と構造解析
Functional and Structural Analysis of NTQ type Anion Pump Rhodopsins

Miwako Teranishi[1], Shota Ito[1], Manish Singn[1], Keiichi Inoue[1,2], Hideki Kamitori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*,, [2]*PRESTO, JST*)

Bacteriorhodopsin (BR) and Halorhodopsin (HR) are well known ion pumping microbial rhodopsins which transport H^+ and Cl^- actively by using light energy, respectively. In addition to them, novel ion pumping rhodopsins have been found in eubacteria by genomic analysis. These rhodopsins possess the conserved amino acid motif in the helix C: DTE in H^+pump, NDQ in Na^+pump, NTQ in Cl^-pump.
Here we analyzed the NTQ anion pumps to reveal the anion-dependent structural changes, which must be correlated to the anion pump function. To this aim, we measured pumping activity, anion binding selectivity, photocycle and structural changes with various anion conditions. The obtained results will be useful for understanding biological energy production system.

3Pos127 二量体化がロドプシンの光構造変化に与える影響
Effect of dimerization on the light-induced helical rearrangement of visual rhodopsin

Yasushi Imamoto[1], Keiichi Kojima[2], Toshihiko Oka[3], Ryo Maeda[4], Yoshinori Shichida[5] ([1]*Kyoto Univ.*, [2]*Okayama Univ.*, [3]*Shizuoka Univ.*, [4]*RIKEN*, [5]*Ritsumeikan Univ.*)

The physiologic relevance of dimerization of G-protein-coupled receptors is long-standing issue. In rhodopsin, it is reported that dimerization is not essential for its function, but the difference in photoresponse between monomeric and dimeric rhodopsin has not been investigated in detail. Here we prepared nanodiscs containing one or two rhodopsin molecule(s), and light-induced helical rearrangement of rhodopsin was monitored by high-angle X-ray scattering. The intensity difference curve obtained by monomeric rhodopsin agreed with that calculated from the crystal structures of dark state rhodopsin and metarhodopsin II. However, that of dimeric rhodopsin was significantly reduced, suggesting that the interaction between rhodopsin molecules modulates structural changes.

3Pos128 ^{13}C NMR 化学シフト値計算によるセンサリーロドプシンの光中間体におけるレチナール構造の解析
Quantum chemical calculation of ^{13}C NMR chemical shifts for retinal at photo-intermediates in the photocycle of sensory rhodopsin

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Sensory rhodopsin I (SRI) and II (ppR) are a photoreceptor with a retinal chromophore and function as positive/negative and negative photo-taxis. When the chromophore absorbs light, the retinal isomerizes from all-trans to 13-cis configurations. We have obtained ^{13}C NMR chemical shift values of retinal at several functional photo-intermediates during photocycle by in-situ photo-irradiation solid-state NMR. In particular, there are unusual NMR signals of C20-methyl carbon in retinal at N'-intermediate of ppR and P-intermediate with of SrSRI. Here, we calculated the chemical shift values of retinal configurations at dark state, M and N'-intermediate of ppR to investigate detailed conformation of twisted retinal state by means of quantum chemical calculation.

3Pos129 ショウジョウバエ Rh7 の特徴的な幅広い吸収スペクトルの解析
Drosophila melanogaster Rh7 is a UV-to-visible light sensor having extraordinarily broad absorption spectrum

Kazumi Sakai[1], Kei Tsutsui[1], Takahiro Yamashita[1], Naoyuki Iwabe[1], Keisuke Takahashi[1], Akimori Wada[2], Yoshinori Shichida[1] ([1]*Grad. Sch. Sci., Kyoto Univ.*, [2]*Organic Chemistry for Life Science, Kobe Pharm. Univ.*)

Fruit fly, Drosophila melanogaster, has seven rhodopsins. Six of them are known to function as visual pigments in the eyes. Recently, the last one, Rh7, has been found to function in circadian photoentrainment in the brain. However, its detailed molecular properties have not been characterized yet. Here we successfully prepared a recombinant protein of fly Rh7. It could bind both 11-cis-retinal and 11-cis-3-hydroxyretinal and absorb UV light. UV light irradiation caused the formation of the G protein activating state. Interestingly, Rh7 exhibited an unusual broad spectrum with a longer wavelength tail reaching 500 nm. We would like to discuss the putative molecular mechanism and the physiological relevance of the unique spectral property of fly Rh7.

3Pos130 青色光センサー PixD の光反応とその多様性
Study on diversity of photoreactions among various homologous PixD proteins

Shunrou Tokonami, Yusuke Nakasone, Masahide Terazima (*Grad. Sch. Sci., Univ. Kyoto*)

PixD is one of cyanobacterial BLUF (sensor of Blue Light Using FAD) proteins regulating a positive phototaxis. So far, structures and photochemical reactions of PixD proteins from two different species (SyPixD and TePixD) have been studied. Interestingly, although SyPixD and TePixD have high similarity in crystal structure, they show quite different photoreaction especially in the dependence on excitation light intensity. In this study, we newly purified two other PixDs to investigate the origin of the difference in photoreaction among different organisms. At the symposium, we would like to discuss what makes the diversity of photoreactions of PixD proteins.

3Pos131 緑藻の光駆動プロトンポンプであるアセタブラリアロドプシン II のフォトサイクルにおける２つの O 中間体の存在
Existence of two O intermediates in the photocycle of *Acetabularia* rhodopsin II, a light-driven algal proton pump

Jun Tamogami[1], Takashi Kikukawa[2,3], Toshifumi Nara[1], Makoto Demura[2,3], Tomomi Kimura-Someya[4,5], Mikako Shirouzu[4,5], Shigeyuki Yokoyama[4,6], Seiji Miyauchi[7], Kazumi Shimono[7,8], Naoki Kamo[2] ([1]*College Pharm. Sci., Matsuyama Univ.*, [2]*Fac. Adv. Life Sci., Hokkaido Univ.*, [3]*Glob. Sta. for Soft Mat., Glob. Ins. for Col. Res., Edu., Hokkaido Univ.*, [4]*RIKEN SSBC*, [5]*RIKEN CLST*, [6]*RIKEN Structural Biology Laboratory*, [7]*Grad. Sch. Pharm. Sci., Toho Univ.*, [8]*Fac. Pharm. Sci., Sojo Univ.*)

In the photocycle of microbial rhodopsins, the sequence of two molecular events during the transition from N to O: thermal reisomerization of retinal and accessibility switch of the protonated Schiff base (PSB) has not been clarified even in well-characterized bacteriorhodopsin. In this study, we investigated the photocycle of *Acetabularia* rhodopsin II (ARII), a light-driven proton pump from *Acetabularia acetabulum*, under acidic conditions (pH < 5.5). Kinetic analysis of the flash photolysis data revealed the formation of two sequential O-states (termed O1 and O2) with different molar extinction coefficients during the photocycle, implying the possibility of the following isomerization of retinal upon the O1-O2 transition after switching of PSB.

3Pos132 Quantitative evaluation of UV-induced cell death and its resistance by drug in human epidermal keratinocytes

Noritaka Masaki, Shigetoshi Okazaki (*Dept. Med. Spec., Hamamatsu Univ. Sch. Med.*)

UV is necessary for living organisms such as for synthesis of vitamin D. On the other hand, its high energy is useful for sterilization and eliminating contamination of DNA. However, UV also threatens our healthy life such as by causing skin cancer. None the less, there is no medical treatment for UV damage otherwise than prevention. It is because UV damage is still largely unknown.

In the present study, we aimed to establish quantitative evaluation of cell viability against UV irradiation vs drug treatment using normal human epidermal keratinocytes-adult. Effect of UV and drug in cell viability was evaluated by varying delay of drug treatment and its duration to understand underlying mechanism.

3Pos133 Comparison of chromophore environments between rhodopsin and cone visual pigment using Fourier transform infrared spectroscopy

Naoto Noguchi[1], Takahiro Yamashita[1], Yoshinori Shichida[2], Yasushi Imamoto[1] ([1]*Kyoto University*, [2]*Ritsumeikan University*)

Rod cells and cone cells work in dim light and daylight conditions, respectively. In accordance, the nature of rod pigment rhodopsin is significantly different from that of cone pigments. E122Q/I189P mutant of bovine rhodopsin shows cone-like characteristics such as high thermal activation rate, suggesting that the alternation of chromophore environment induced by these mutations makes visual pigment rhodopsin. To probe the chromophore environment, we introduced a cysteine residues, whose SH vibrational band is sensitive to the local environment, in vicinity of chromophore, and measured the SH stretching mode using Fourier transform infrared (FTIR) spectroscopy. The difference in the chromophore binding pocket between rhodopsin and cone pigment will be discussed.

3Pos134 FTIR 分光電気化学法による光化学系 II 第一キノン Q_A の酸化還元電位計測：Mn 除去の影響

Influence of Mn depletion on the redox potential of the primary quinone Q_A in photosystem II as revealed by FTIR spectroelectrochemistry

Ayaka Ohira, Ryo Nagao, Takumi Noguchi, Yuki Kato (*Grad. Sch. Sci., Nagoya Univ.*)

The redox potential of the primary quinone Q_A, $E_m(Q_A)$, in PSII has been estimated to be -100 mV in intact samples and shown to be shifted by ca. +150 mV upon Mn depletion. These values have been obtained by a fluorescence method, which indirectly monitors the redox state of Q_A. In this work, we measured the $E_m(Q_A)$ in intact and Mn-depleted PSII preparations using FTIR spectroelectrochemistry, which can directly detect the redox reaction of Q_A. The $E_m(Q_A)$ in intact PSII was determined to be -100 mV in agreement with that by the fluorescence method. However, the $E_m(Q_A)$ value was little affected by Mn depletion. It is thus suggested that the large $E_m(Q_A)$ upshift by Mn depletion found in previous works can be an artifact due to the fluorescence method.

3Pos135 ATR-FTIR 解析による光化学系 II における非ヘム鉄のヒスチジン配位子のプロトン化状態

ATR-FTIR study on the protonation state of a histidine ligand to the non-heme iron in photosystem II

Masakazu Kimura, Shin Nakamura, Yuki Kato, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Univ.*)

It is known that the redox potential (E_m) of the non-heme iron, which is located between Q_A and Q_B in PSII, is pH dependent. However, the cause of this pH dependence remains unresolved. In this study, to clarify the mechanism of the pH dependence of $E_m(Fe^{2+}/Fe^{3+})$, we investigated the protonation structure around the non-heme in PSII using light-induced ATR-FTIR spectroscopy. Fe^{2+}/Fe^{3+} FTIR difference spectra at pH 5.0-7.5 showed that bands of His around 1100 cm^{-1} changed depending on pH. SVD analysis revealed a band shift from 1101 to 1094 cm^{-1} with pK_a of about 6, indicative of the formation of a deprotonated His anion. It was concluded that deprotonation of D1-His215, a ligand to Fe interacting with Q_B, is responsible for the pH dependence of $E_m(Fe^{2+}/Fe^{3+})$.

3Pos136 光化学系 II 結晶における水分解 S 状態遷移の ATR-FTIR 解析

ATR-FTIR analysis of the S-state transitions during water oxidation in photosystem II crystals

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Clarification of the high-resolution crystal structures of the S-state intermediates in the water oxidation center in PSII is crucial in full understanding of the water oxidation mechanism. Whether the intermediate structures in crystal retain the native ones in solution is another important question. In this study, we analyzed the reactions in the S-state transitions in PSII crystals using ATR-FTIR spectroscopy. FTIR difference spectra of the PSII crystals upon 2 flashes showed very similar features to those of PSII in solution. This observation indicates that the S_1->S_2 and S_2->S_3 transitions proceeded with relatively high efficiencies even in crystals, and the structures of the S_1, S_2, and S_3 states were virtually unchanged between those in crystals and in solution.

3Pos137 ヘリオバクテリア光合成反応中心のドナー側とアクセプター側における電子伝達反応の解析

Analyses of electron transfer reactions on donor and acceptor sides in heliobacterial photosynthetic reaction center

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The reaction center of heliobacteria (hRC) is the homodimeric type 1 RC, and its electron transfer scheme is analogous to that in photosystem I. The PetJ protein, a membrane-anchored cytochrome *c*-553, is supposed to function as the electron donor to the P800, and the PshB, an iron-sulfur protein holding centers A and B (F_A/F_B), as the electron acceptor from the F_X. In the present study, PetJ and two dicluster ferredoxins (Fd1 and Fd2), the latter two of which were candidates for PshB, were obtained by overexpressing them in *E. coli*. We measured Xe-flash-induced absorption changes of the P800 after reconstitution with each of them. While both Fd1 and Fd2 functioned as the acceptor, PetJ, even if it added in excess molar ratios, could not donate electrons to P800.

3Pos138 光化学系 II における Mn クラスターの光活性化過程の FTIR および量子化学計算による解析

FTIR and quantum chemical calculation study of the photoactivation process of the Mn cluster in photosystem II

Shin Nakamura, Akihiko Sato, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Univ.*)

The initial step of construction of the water-oxidizing Mn_4CaO_5 cluster (photoactivation) in PSII is binding of one Mn^{2+} ion to a high-affinity site in the protein. Identification of this high-affinity Mn^{2+} site has been under debate. In this study, to clarify the photoactivation mechanism, we investigated the initial process of the Mn^{2+} binding using quantum chemical calculation and FTIR spectroscopy. Quantum chemical calculation showed that binding of Mn^{2+} to the Mn2 site with two carboxylate ligands is the most stable out of the four Mn sites (Mn1-Mn4). This model of Mn^{2+} binding was supported by the presence of two symmetric COO^- bands in a Mn^{3+}/Mn^{2+} FTIR difference spectrum upon single-flash illumination on Mn-depleted PSII in the presence of Mn^{2+}.

3Pos139 北海道の河川から採取した紅色非硫黄細菌による水素生成に対する pH と基質濃度の影響

Effect of pH and substrate concentration on hydrogen production by purple non-sulfur bacteria from rivers in Hokkaido

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Hydrogen has been extensively considered to replace fossil fuels as the energy source of the next generation. Biological hydrogen production processes are renewable and alternative energy sources, and less energy-intensive and more environmentally-friendly as compared to thermochemical and electrochemical processes. Purple non-sulfur photosynthetic bacteria (PNS) is a major field of research for biological hydrogen production. Herein, we investigated the effects of initial medium pH and organic acid concentration on H_2 production in batch-type photobioreactor experiments using the PNS bacteria collected from rivers in Hokkaido. High-yield H_2 production was obtained around neutral pH (15-60 mM acetate or succinate).

3Pos140 構造解明されている 2 種類の紅色光合成細菌の LH2 タンパク質からの B800 バクテリオクロロフィル a の脱離挙動解析

Analysis of removal of B800 bacteriochlorophyll a from structure-determined LH2 proteins derived from two purple photosynthetic bacteria

Yoshitaka Saga[1,2], Keiya Hirota[1], Kokomi Doi[1] ([1]*Kindai Univ.*, [2]*PRESTO, JST*)

Light-harvesting complex 2 (LH2) in purple photosynthetic bacteria has two types of bacteriochlorophyll (BChl) a called B800 and B850. These BChl a pigments play crucial roles not only in the photosynthetic functions but also in folding and maintaining the LH2 protein structure. We report large differences in the removal behaviors of B800 BChl a from two structure-determined LH2 proteins derived from Rhodoblastus (Rbl.) acidophilus and Phaeospirillum (Phs.) molischianum. The LH2 protein from Rbl. acidophilus smoothly released B800 BChl a, whereas B800 BChl a was hardly removed from LH2 of Phs. molischianum under the same conditions as in the case of LH2 from Rbl. acidophilus. In addition, we report physicochemical properties of LH2 proteins without B800 BChl a.

3Pos141 新奇クロロフィルを持つシアノバクテリアにおけるクロロフィル *f* 蓄積過程のエネルギー移動の解析

Spectral characterization of new chlorophyll containing cyanobacterium in the accumulation process of chlorophyll *f*

Toshiyuki Shinoda[1], Keishi Arai[2], Hiroki Tabushi[2], Seiji Akimoto[3], Tatsuya Tomo[1,2] ([1]*Grad. Sch. Sci., Tokyo Univ. Sci.*, [2]*Fac. Sci., Tokyo Univ. Sci.*, [3]*Fac. Sci., Kobe Univ.*)

Recently, red-shifted Chlorophyll (Chl) *f* was found in a novel cyanobacterium. The Chl content of this cyanobacterium depends on the cultivation light. Chl *f* is synthesized only in cells grown under far-red (FR) light (>700 nm). The photochemical and photophysical functions of Chl *f* are not known in photosystems in accumulation process. Therefore, this cyanobacterium was cultured under white to FR light transition. We analyzed steady and time-resolved fluorescence spectroscopies for investigations of cells in the accumulation process of Chl *f*. We will discuss characteristics of energy transfer within Chl *f* containing cyanobacterium.

3Pos142 Spectral characterization of Photosystem II reaction center in a chlorophyll d-dominated cyanobacterium

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Chlorophylls (Chls) play essential roles in energy transfer, charge separation and electron transfer in bPhotosystem (PS) I and II. Acaryochloris marina is a unique cyanobacterium that differs from the majority of photosynthetic organisms by having Chl d as the major pigment (>95%). In our previous analyses, a small number of Chl a were bound in PS II complex. If the Chl a is involved in the charge separation process, our current understanding of the overall energetic of the PS II would need to be modified. In this study, we isolated the PS II RC, which is the minimum complex capable of charge separation., from A. marina. We characterized the spectral properties of PS II RC. We will discuss the site energies of Chls in isolated PS II RC.

3Pos143 ヘリオバクテリア反応中心の初期電荷分離スピン相関解析ラジカル対の捕捉

Initial charge separated spin-polarized radical pair in reaction center of *Heliobacterium modesticaldum*

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Heliobacterial RCs constitute the ancestral form of photosystem I (type I RC). The heliobacterial RCs' structure and function is still unclear. In this work, we measured *Heliobacterium modesticaldum* RC core was measured by time resolved electron spin resonance (ESR). The signal centered at g = 2 with the A/E (A: absorption, E: emission) polarized pattern was observed in the presence of A_1^- radical, which was assigned to the radial pair $P800^+A_0^-$. The simulated result showed that the exchange interaction J and dipole interaction D between electron spins in the radical pair were -0.2 and -0.6 mT, respectively. The small J-coupling would explain the slow electron transfer in the RC.

3Pos144 光合成における電子伝達体のダイナミックスに関する理論的研究

Theoretical studies on dynamics of electron carriers in photosynthesis

Hidemi Nagao, Satoshi Nakagawa, Isman Kurniawan, Koichi Kodama, Muhammad Arwansyah, Kazutomo Kawaguchi (*Kanazawa University*)

Plastocyanin(PC) is one of type I copper proteins which have one copper ion in their active site. In photosynthesis, PC transfers one electron from cytochrome f in cytochrome b6f complex to P700 in Photosystem I by diffusing in the lumen side of the thylakoid membrane. We discuss the association and diffusion processes of PC with cytochrome f by using all-atom molecular dynamics simulation and a simple coarse-grained model for describing intermolecular interaction between proteins in solvent to investigate the association, self-assembly behavior, and binding modes with complex configurations in relation to the free energy profile for the association, the reaction constant of the electron transfer, and so on.

3Pos145 光化学系複合体と炭素ナノ材料間の電子移動反応
Linear electron transfer between photosystems and carbon nanomaterials

Shota Tanaka[1], Mariko Miyachi[2], Yoshinori Yamanoi[2], Akihide Iwase[1], Akihiko Kudo[1], Hiroshi Nishihara[2], Tatsuya Tomo[1] ([1]*Grad. Sch. Sci., Tokyo Univ. of Sci.*, [2]*Grad. Sch. Sci., Tokyo Univ.*)

Novel carbon materials, such as graphene, carbon nanotubes, and fullerene, often lead to the development of new materials in the area of bioscience. Graphene exhibits excellent electrical conductivities, strength, and stiffness. The quantum yield of photosynthetic energy and electron transfer is nearly 100%. Therefore, the conjugates between graphene and photosystem complexes can expect the useful electronic device. In this study, we isolated photosystem complexes from thermophilic cyanobacterium and applied the graphene oxide as conjugates. Linear electron transfer between photosystems and graphene oxides was successfully obtained by visible light irradiation. We attempt to evolve hydrogen molecules by using the conjugates.

3Pos146 高等植物の光化学系 II における効率的な電荷分離反応のメカニズム
The mechanism of efficient charge separation reaction in photosystem II of higher plants

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In the primary event of the photosynthesis, the light energy is transferred to the reaction center (RC) of the photosystem II. The charge separation state is formed between Chl a pair and Pheo. Many studies have been performed to understand mechanisms of the charge separation process, however, roles of cofactor geometries on the electronic interaction of the charge-separated state is still unknown. In this study, we measured time-resolved EPR and analyzed geometry of charge separation state using a novel method, "3D spin polarization imaging". The results also showed that the electronic coupling between the charges (Pheo- and P+) is significantly weak although the tunneling route is geometrically active after the charge separation.

3Pos147 The dynamics of photosystem 2 and light-harvesting complex 2 in spinach grana membrane revealed by high-speed AFM

Risa Mutoh, Takahiro Iida, **Daisuke Yamamoto** (*Faculty of Science, Fukuoka Univ.*)

In chloroplast, photosynthesis initiates with absorption of light by pigments bound to photosynthetic proteins, such as photosystem 2 (PS2) and light-harvesting complex 2 (LHC2). The configuration and their interaction of PS2, LHC2, and other photosynthetic protein complexes in grana membrane still remain unclear. In this study, we isolated grana thylakoid membrane derived from spinach, and performed high-speed atomic force microscopy analysis. We observed dimer particles in grana membrane, of which the height was approximately 15 nm from the mica surface. This was consistent with the height of PS2. We also detected LHC2 trimer in vicinity to PS2. We will discuss the structural dynamics by environmental changes such as non-photochemical quenching.

3Pos148 ステート遷移における光捕集系の膜内移動の検証
Verification of Shuttling of Light-Harvesting Complexes upon State Transition

Yuki Fujita, Yutaka Shibata (*Tohoku University*)

Photosystem I (PSI) and PSII play central roles in the photochemical reactions in photosynthesis. A mechanism called state transition (ST) is known as a function to control the excitation ballance between PSs in vivo, which assures an efficient photosynthesis. Although it is believed that ST is caused by shuttles of light harvesting complex of PSII (LHCII) between the PSs, there has been no direct observation of its movement within a cell. Here, we examined the movement of LHCII by using a newly developed cryogenic microscope. By the measurement, we could obtain the intracellular distributions of PSI, PSII, and LHCII components. From the obtained result, We propose a revised model that ST is induced by reversible isolation of LHCII from PSs.

3Pos149 水晶振動子微量天秤による光制御型 bZip モジュール photozipper 及び N131 変異体の DNA 結合の解析
DNA-binding of a light-regulated bZIP module, photozipper and Asn131 mutants analyzed by quartz crystal microbalanc

Samu Tateyama, Osamu Hisatomi (*Grad. Sch. Sci., Univ. Osaka*)

Photozipper (PZ) is a light-regulated basic leucine zipper (bZIP) module composed of a bZIP domain and a light-oxygen-voltage-sensing domain of aureochrome-1. Blue light induces the dimerization and the subsequent binding of PZ for the target DNA sequence. In this study, we attempted to quantify the DNA binding of PZ and its site-directed mutants by quartz crystal microbalance. Dissociation constant of PZ for the target DNA sequence was estimated to be ~ 50 nM in the presence of 140 mM KCl, which was consistent with the data obtained from electrophoretic mobility shift assay. Moreover, PZ mutants in which Asn131 in the basic region were substituted to Ala, Ser and Gln, showed higher K_d values, suggesting that Asn131 plays a crucial role on DNA binding of PZ.

3Pos150 フォトジッパーにおける Q317 の機能解明
Function of Q317 in Photozipper

Itsuki Kobayashi, Yuki Yabe, Yoichi Nakatani, Osamu Hisatomi (*Grad. Sci., Univ. Osaka*)

Photozipper (PZ) is an engineered protein containing a basic region/leucine zipper (bZIP) domain and a light-oxygen-voltage-sensing (LOV) domain of Aureochrome-1. We have reported that blue light induces dimerization of PZ and increases its affinity for the target DNA. To elucidate the role of a highly conserved Gln residue (corresponding to Q317 of PZ) closely located at C(4a) of FMN, we prepared recombinant proteins in which Q317 was replaced to Val, Leu, Ser, Asn and Glu. These substitutions greatly affected the time course of dark regeneration and the monomer-dimer equilibrium in the dark state. Our data suggested the Q317 plays a crucial role on the PZ function.

3Pos151 アニオンチャネルロドプシン 2(ACR2)の線虫における超高感度光神経抑制活性

Ultrasensitive neural silencing activity of Anion channelrhodopsin-2 (ACR2) in *Caenorhabditis elegans*

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Anion channelrhodopsin-2 (ACR2) has been recently discovered from the cryptophyte algae *Guillardia theta* as a light-gated anion channel. A truncated variant of ACR2 can be heterologously expressed both in mammalian and *E. coli* cells with the anion channel function and strong hyperpolarization activity. Here we expressed ACR2 in *C. elegans* cells and examined its neural silencing activity as a model for an in vivo system. Transgenic *C. elegans* expressing ACR2 in neurons stopped the locomotion at much lower light intensity (several tens of $\mu W/cm^2$) than those expressing Archaerhodopsin-3 (several mW/cm^2), one of the most efficient neural silencers reported so far. Our results indicate that ACR2 works as an ultrasensitive neural silencer even in a living animal.

3Pos152 光駆動ナトリウムポンプロドプシンの活性中心の水素結合構造

Hydrogen-bonding network in the active site of light-driven sodium pumping rhodopsins

Shota Ito, Sahoko Tomida, Hideki Kandori (*Nagoya Inst. Tech.*)

Water molecules inside protein play important roles, not only to occupy the empty space of protein interior, but also to construct the specific hydrogen-bonding network for function. To investigate such water-containing hydrogen-bonding network of the active site, Fourier-transform infrared (FTIR) spectroscopy is a powerful method. In this study, we analyzed hydrogen-bonding interaction between Schiff base and the counterion in light-driven sodium pumping rhodopsin (KR2), by use of active site mutants (D116E, N112A, S70A) and Schiff base ^{15}N-labeled protein. Based on our FTIR results and X-ray structure, we will propose detailed hydrogen bonding network around the retinal Schiff base region in dark state and changes during its photocycle.

3Pos153 光捕集カロテノイドアンテナと相互作用する光駆動プロトンポンプ TR の創出

Production of a light-driven proton pump TR interacted with light-harvesting carotenoid antennae

Keigo Nishikawa[1], Keiichi Kojima[1], Shigeko Kawai-Noma[2], Sayaka Nemoto[3], Takeshi Murata[3], Daisuke Umeno[1,2], Yuki Sudo[1] ([1]*Grad. Med. Den. Pha., Univ. Okayama*, [2]*Dep. Applied Chemistry and Biotechnology., Univ. Chiba*, [3]*Grad. Sci., Univ. Chiba*)

Recently, we identified Thermophilic rhodopsin (TR) as a light-driven proton pump with high thermal stability [1] and estimated to have a putative carotenoid-binding cavity by its crystal structure (5AZD) [2]. It is expected that, in the TR-carotenoid complex, functional and photochemical properties of TR are modulated by interaction with carotenoids. Here we constructed coexpresseion system of TR and carotenoids (astaxanthin and canthaxanthin) in Escherichia coli and analyzed the stoichiometry, efficiency of energy transfer, functional and photochemical characteristics of the TR-carotenoid complex. Based on the results, we will discuss the significance and mechanism of the binding of the carotenoid with TR.
[1] (2013) JBC, 288, 21581. [2] (2016) JBC, 291, 12223.

3Pos154 光誘起チャネルロドプシンに関する理論研究

Theoretical study on molecular mechanism of photo-induced gate opening of channelrhodopsin

Cheng Cheng[1], Motoshi Kamiya[1], Norio Yoshida[2], Shigehiko Hayashi[1] ([1]*Grad. of Science, Kyoto Univ.*, [2]*Grad. of Science, Kyushu Univ.*)

Channelrhodopsins (ChR) are light-sensitive cation channels formed by seven-transmembrane helices, which have shown experimental utilities in optogenetics. However, although the crystal structure of the closed-state of ChR was determined in 2012, the ion conducting open-state structure and the molecular mechanism of the ion conduction remain unknown. In this study, the gate-opening conformational changes of ChR induced by photo-isomerization of the retinal chromophore were studied in atomic detail with molecular dynamics (MD) simulations and QM/MM RWFE-SCF free energy geometry optimization. Water/ion distributions of the channel in the photo-activation process are then examined by 3D-RISM theory with conformational samples obtained by MD simulations.

3Pos155 光制御型 bHLH-ZIP 転写因子の開発

Development of a light-regulated bHLH-ZIP transcription factor

Yoichi Nakatani, Osamu Hisatomi (*Grad. Sch. of Sci., Osaka Univ.*)

To understand the functions of endogenous transcription factors, light-controlling their activities could be powerful methods. Max is a member of the basic helix-loop-helix leucine zipper (bHLH-ZIP) transcription factors. Max forms homo- or heterodimer and binds to the target sequence (E-box), and regulates the gene expression related to cell proliferation, differentiation and apoptosis. Here, to tune DNA-binding of Max by using light, we fused its bHLH domain to Photozipper which is a blue light-regulated dimerizing module based on Aureochrome-1. The engineered chimeric proteins reversibly bound to DNA in a sequence-specific and a light-dependent manner. This work can provide a novel design to optically control the activities of transcription factors.

3Pos156 光駆動イオントランスポーターハロロドプシンの理論的研究

Theoretical study on molecular mechanism of a light-driven ion transport of Halorhodopsin

Ryo Oyama, Taisuke Hasegawa, Shigehiko Hayashi (*Grad. Sch. Sci., Univ. Kyoto*)

Halorhodopsin from Natronomas pharaonis functions as an inward light-driven chloride pump and is utilized to silence neurons in optogenetics technique in neuroscience. The chromophore retinal isomerizes from all-tran conformation to 13-cis one upon photoabsorption, and triggers a photocycle during which one chloride ion is transported across the membrane. In this study, we performed QM/MM RWFE-SCF calculations to examine the functional coupling of the structural change of the chromophore isomerizing from all-trans conformation to 13-cis one described at the quantum chemistry level of theory with protein large conformational changes of alternating access for the active transport of the ion described with MD simulations with a MM force field.

3Pos157 Effect of interaction between IP6 and NOX2 on monocytic differentiation

Asuka Kato[1], Yuki Hirakawa[2], Wakako Hiraoka[2] ([1]*Department of Obstetrics and Gynecology, Fujita Health University School of Medicine*, [2]*Department of Physics, Graduate School of Science and Technology, Meiji University*)

Inositol hexaphosphate (IP6) is a potent metal chelator, and is known as an anti-cancer reagent. We have studied the role of reactive oxygen species (ROS) from NADPH oxidase (NOX2) in monocytic differentiation of IP6-treated human leukemia PLB-985 and gp91phox knockout X-CGD. Cell growth was assayed with cell counter. Anti-microtubule-associated-protein-light-chain-3 (LC3) antibody-FITC was used as a marker of autophagy. Exposure to IP6 for 24h led PLB-985 cells to induce LC3, and the cells acquired monocytic properties such as adhesion activity after 72h. The results by comparing with X-CGD experiments shows that there is some cross talk between IP6 and NOX2 through ROS reaction on monocytic differentiation.

3Pos158 放射線照射がミトコンドリア電子伝達系酸化還元関連分子に与える影響の電子スピン共鳴法を用いた評価。
Estimating physiological transition of electron transport chain with ESR in whole cell culture

Yukihaya Watanabe, Naoya Matsunaga, Wakako Hiraoka (*Dept. Phys., Grad. Sch. of Sci. & Tech., Meiji Univ.*)

A mitochondrial electron transport chain (mETC) is a series of complexes that transfer electrons from electron donors to electron acceptors via redox reactions. To estimate physiological transition of mETC in whole cell culture, hydrogen peroxide treated PLB-985 cells and HeLa cells were analyzed with electron spin resonance (ESR). Cells incubated with hydrogen peroxide for 1-24 hours were analyzed with flow cytometer to measure cell damage such as apoptosis and necrosis. Harvested cells (-10^8) were resuspended into 200 µl PBS(-) containing 30% glycerol. Cell suspension was transferred to 5 mm Φ cylindrical quartz cell. ESR spectra (20K - 300K) containing signals from Fe-S, complex I, and semi quinone radical was altered by oxidative stress.

3Pos159 Cross talk between mitochondria and NOX2 in vitamin D_3-induced monocytic differentiation

Naoya Matsunaga, Yukihaya Watanabe, Wakako Hiraoka (*Dept. Phys., Grad. Sch. Sci. & Tech., Meiji Univ.*)

To elucidate the mechanism of reactive oxygen species (ROS) in immune enhancement, we focused on the signal transduction in vitamin D_3-induced monocytic differentiation. In the 54th meeting, we reported that hydroxyl radical and hydrogen peroxide had a significant role in vitamin D_3-induced differentiation. Human myeloid PLB-985 was incubated with 200 nM vitamin D_3 and/or 100 nM phorbol 12-myristate 13-acetate. After 3 days, induction of CD11b was assayed with flow cytometer. Vitamin D-stimulated cells with diphenyleneiodidonium (NOX2 inhibitor) and actinomycin D (mitochondrial inhibitor) were analyzed with ESR spin trapping. Our results showed the cross talk between mitochondria and NOX2 in monocytic differentiation.

3Pos160 Phenotypic Constraints Shaped by Evolution: Numerical and Experimental Approaches

Chikara Furusawa[1,2], Kunihiko Kaneko[2,3] ([1]*QBiC, RIKEN*, [2]*UBI, Univ. Tokyo*, [3]*Grad. Sch. Art Sci., Univ. Tokyo*)

Constraints on phenotypic changes in adaptation and evolution have recently been discussed both experimentally and theoretically. Here, by using a cell model which reproduce itself via a catalytic reaction network, we analyzed how the degree of constraint changes through evolution. As a result, we found that after evolution the concentration changes across all components in response to environmental and evolutionary changes are constrained along a one-dimensional major axis within a huge-dimensional state space. Based on the observations, we proposed a theory of phenotypic constraint shaped by evolutionary dynamics. The related experimental results of bacterial laboratory evolution will be discussed.

3Pos161 Polymerization and information selection in template-directed ligation of information polymers

Yasuhiro Magi, Shoichi Toyabe (*Appl. Phys., Tohoku Univ.*)

We have previously demonstrated that template-directed ligations of DNA implement a hyperbolic frequency-dependent selection of information under appropriate nonequilibrium setting. The nonlinear selection provides a mechanism to stably keep complex sequence like the hypercycle proposed by Eigen and possibly leads to the emergence of molecular species in the prebiotic environment. Here, we report our experiments and simulations about the dynamics of the polymerization and the information selection in the template-directed ligations. We used the ligations of short DNA strands by DNA ligase as the model system. We discuss how the system can suppress the error catastrophe and preserves information.

3Pos162 鋳型ライゲーションにおける拡散混合に対する情報保持の実験的証明
Experimental demonstration of information retention against diffusional mixing in templated ligation

Kazuki Hata, Yasuhiro Magi, Syoichi Toyabe (*Tohoku University, Applied Physics*)

In the previous study, we experimentally demonstrated that (i) the templated ligation of information polymers such as DNA and RNA copies information not exponentially but hyper-exponentially like the hyper cycle, (ii) this growth selects information in the frequency-dependent way. The results imply that the information can be sustained at different locations against diffusional mixing and shows a possibility of the emergence of "individuality" without compartments in the prebiotic environment. In this presentation, we report our experiments to demonstrate this information retention against diffusional mixing. We used a model experimental system based on the templated ligations of DNA strands by DNA ligase in microfluidic device.

3Pos163 アルカリ性熱水噴出孔における硫化鉄を触媒にした還元的炭素化合物生成過程の第一原理分子動力学シミュレーション
***Ab initio* molecular dynamics study of reducible carbon compounds production catalyzed by iron sulfides at an alkaline hydrothermal vent**

Kohei Shimamura[1], Fuyuki Shimojo[2], Aiichiro Nakano[3], Shigenori Tanaka[1] ([1]*Kobe Univ.*, [2]*Kumamoto Univ.*, [3]*Univ. of Southern California*)

Alkaline hydrothermal vents have attracted attention as a possible place of birth of life. It is experimentally considered that the potential difference caused by a pH gradient between the hot water side and primordial ocean and a catalysis of iron sulfide membranes formed by the pH gradient supported to dissociate hydrogens (emitting from the vents) and to release electrons, which reduced oxidative carbon compounds such as carbon dioxides present in the ocean. To investigate the microscopic mechanisms related to the hypothesis, we perform *ab initio* molecular dynamics simulations. In the presentation, we will report in detail the dissociation process of hydrogens on the iron sulfide surfaces and the accompanied reduction process of carbon dioxides.

3Pos164 凍結融解によるリポソーム融合を介した人工細胞への栄養供給法の確立
Sustainable biochemical reactions in liposoems by liposome fusion via the freeze-thaw

Gakushi Tsuji[1,2], Takeshi Sunami[1,2], Satoshi Fujii[1], Norikazu Ichihashi[1,3] ([1]*Grad. Sch. of IST, Osaka University*, [2]*IAI, Osaka University*, [3]*Grad. Sch. of FBS, Osaka University*)

Reconstitution of life-like structure is one of the most challengeable themes for society to elucidate the border between life and non-life. Recently, many scientists have reported reconstruction of biochemical reactions in lipid bilayer compartment called liposomes. However, liposomes couldn't take in substrates for reactions because of robust membrane. In this study, we reported the freeze-thaw method which can induce liposome fusion and supply substrates via inner solution mix. Using this method, we established the sustainable biochemical reaction such as RNA replication in liposome with proliferation of compartment. Also we achieved supplying in vitro translation system by liposome fusion to realize protein synthesis in liposomes.

3Pos165 出芽酵母の tRNA 遺伝子の転写量と核内における空間配置との相関解析
Analysis of Correlation Between tRNA Levels and Spatial Arrangement of tRNA Genes in the Budding Yeast Nucleus

Naoko Tokuda, Masaki Sasai (*Grad. Sch. Eng., Nagoya Univ.*)

Budding yeast tRNA genes have long been considered to be localized near the nucleolus. However, recent Hi-C data and confocal microscopic data (Belagal et al., 2016) have shown that tRNA genes near the tethering elements are away from the nucleolus and localized at around centromeres or the nuclear periphery. Relationship between this spatial arrangement and functions of tRNA genes is not known, and the biological meaning of this variety of spatial distribution of tRNA genes remains unclear. By comparing the observed expression levels and the results simulated by a computational model of 3D genome conformation, we will analyze the correlation between the tRNA levels and the spatial distribution of tRNA genes.

3Pos166 A quasi-harmonic approach to investigating chromatin domains

S.S Ashwin[1], Tadasu Nozaki[2], Kazuhiro Maeshima[2], Masaki Sasai[1] ([1]*Department of Applied Physics, Nagoya University*, [2]*Structural Biology Center, National Institute of Genetics*)

Mammalian genomic DNA is conjectured to be organized into domains such as topologically associating domains (TADs) based on Hi-C data. Direct detection of such domains is an area of intense activity, and it is important to examine their cell to cell heterogeneity. Based on the experimentally observed trajectories of nucleosomes in single cells, we empirically calculate dynamical matrix and cage size distribution to calculate frequencies and effective temperature of the nucleosomes. We then model quasi-harmonic trajectories for the nucleosomes participating in positive frequency modes, which should distinguish the distribution of chromatin domains in the nucleus. Visualization of these trajectories is used to understand domains and other packing features of the genome.

3Pos167 The phase-separation principle of human genome architecture

Shin Fujishiro, Masaki Sasai (*Dept. Comp. Sci. & Eng., Nagoya Univ.*)

Mammalian genomic DNA folds non-randomly in nucleus by forming chromosome territories, A and B compartments, and various types of chromatin domains; such spatial organization has been suggested as bases of gene regulation. To clarify the principle of genomic organization, we modeled human chromosomes as chains of heterogeneous chromatin beads; active and silenced chromatins were assumed to be softer and harder beads, respectively. Simulated chromosomes showed phase separation of active and silenced chromatins in nucleus, which well reproduced the experimentally observed contact maps and nuclear lamina interactions. We discuss the minimum amount of ChIP-seq or Hi-C data to suitably identify active and silenced chromatin regions for the proper modeling of genome folding.

3Pos168 Transient local contacts and meta-stable global organization of human interphase chromosomes

Lei Liu, Changbong Hyeon (*Sch. Comp. Sci., KIAS*)

By using a coarse-grained polymer model that incorporates Hi-C contact frequency information, we constructed a conformational ensemble of human interphase chromatin, and studied the dynamics of loci by molecular simulations. The mean squared displacement of DNA loci reveals a loci property dependent sub-diffusion with a diffusion exponent about 0.4, which is determined by local chain organization. Movement of loci are correlated with each other across a large length scale. While local chromosome structures such as chromatin loops (< 1Mb) are highly dynamic, the structure of a larger length scale (> 5Mb) are characterized with a much slower (> 10^3) relaxation dynamics, leading to the cell-to-cell variability and meta-stability of human chromosome in interphase.

3Pos169 遺伝子発現におけるポリアミンの促進と阻害の二面性
Dual effect of polyamines on gene expression: Acceleration and inhibition

Ai Kanemura[1], Yuko Yoshikawa[1], Takahiro Kenmotsu[1], Wakao Fukuda[2], Kenichi Yoshikawa[1] ([1]*Doshisha University*, [2]*Ritsumeikan University*)

Polyamines are known to play important roles on various biological functions. We have studied the effect of polyamines on gene expression in relation to their effect on DNA conformation. Gene activity was evaluated by in vitro luciferase assay. It was found that polyamines accelerate the gene expression at low concentrations, whereas, at high concentrations, a significant inhibition is marked. We also examined DNA higher order structure at different concentration of polyamines by use of AFM. It becomes clear that DNA takes compact conformation at the polyamine concentrations to cause the inhibition. At lower concentrations, loosely condensed state of DNA is observed. Possible interpretation underlying the structure-activity relationship will be discussed.

3Pos170 Microdroplet-based screening method for microbes producing polymer-degrading enzymes

Kai Saito[1], Ryo Iizuka[1], Eiji Shigihara[1], Wataru Kawakubo[2], Dong Hyun Yoon[2], Tetsuji Sekiguchi[3], Shuichi Shoji[2], Yuji Hatada[4], Takashi Funatsu[1] ([1]*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*, [2]*Dept. of Nanosci. and Nanoeng., Waseda Univ.*, [3]*Res. Org. for Nano & Life Innov., Waseda Univ.*, [4]*Dept. of Life Sci. and Green Chem., Saitama Inst. of Technol.*)

Today, various enzymes that degrade natural and synthetic polymers are needed to protect the global environment. We envisioned a method for screening microbes that produce polymer-degrading enzymes using water-in-oil (W/O) microdroplets. W/O microdroplets in which macromolecules gradually degrade into smaller molecular units increase deformability. Screening is therefore accomplished by using a microfluidic device that allows passive sorting of deformable W/O microdroplets. We have demonstrated the identification of agarose microdroplets with or without enzymatic degradation on the device. By adopting this method, we are trying to screen agarose-degradable microbes obtain novel agarases.

3Pos171 機械学習を用いたタンパク質と薬のドッキング予測
A new prediction method for complex structures of protein and small molecule with machine learning

Fumiaki Sato, Kota Kasahara, Takuya Takahashi (*Col. Life Sci., Ritsumeikan Univ*)

It takes enormous time and cost to develop new medicine. To enhance the drug development, machine learning (ML) is a promising technique. A major problem to apply ML is how to find the optimal definition of the feature vector.
Here, we developed a novel definition of the feature vector for predicting complex structures of proteins and small molecules. We extracted knowledge about the known structures of protein-ligand complexes from the PDB by using our original feature vector. In the prediction pipeline, first, candidate structures of complex are predicted by using "Auto-dock" program. Second, our ML technique evaluated the predicted structures. This works as a post-docking filter.

3Pos172 拡張アンサンブル分子動力学法のサンプリング効率向上のための最適条件の探索
Investigation of appropriate conditions for enhancing sampling efficiency of multi-canonical molecular dynamics

Takuya Shimato[1], Kota Kasahara[1], Junichi Higo[2], Takuya Takahashi[1] ([1]*Col. Life Sci., Ritsumeikan Univ.*, [2]*IPR, Osaka Univ.*)

The multicanonical molecular dynamics (McMD) is a promising method to calculate ensemble of protein conformations in an equilibrated state. However, this requires appropriate settings of adjustable parameters and there is no standard way to determine them. Here, we investigate relationships between these parameters and simulation results of the McMD. We aim to clarify settings which obtain highly accurate result with fewer amount of computation resources. We applied the McMD method to the 20-residue protein, Trp-cage, under various conditions: the number of independent runs of simulation and the simulation time for each run. As a result, we confirmed that relationships between the parameters and convergence of free energy landscape.

3Pos173 Statistical analysis of correlation between amino acid sequence and protein function based on using Protein Data Bank

Ryohei Kondo, Kota Kasahara, Takuya Takahashi (*Col. Life Sci., Ritsumeikan Univ.*)

Recently, it is increasing in protein structure data due to innovation in structural biology. However, the relationship between sequences of amino acid and protein structure has not been fully clarified. The purpose of this study is to elucidate this relationship by analyzing the large-scale data and utilizing the machine learning. Specifically, we first decomposed sequences of many proteins in Protein Data Bank into short sequences consisting of several residues. Then, we statistically analyzed the characteristics in short sequence responsible for the structure and interactions with other peptides. In addition, it is predicted that structure and interactions of the short sequence by the machine learning based on deep neural network.

3Pos174 MEGADOCK-WEB: タンパク質間相互作用予測の統合データベース
MEGADOCK-WEB: an integrated database of structure-based protein-protein interaction predictions

Masahito Ohue[1,2], Takanori Hayashi[1,3], Yuri Matsuzaki[3], Keisuke Yanagisawa[1,3], Yutaka Akiyama[1,2,3] ([1]*Dept CS, Sch Comput, Tokyo Tech*, [2]*ACDD, IIR, Tokyo Tech*, [3]*ACLS, Tokyo Tech*)

We constructed an integrated database of protein-protein interaction (PPI) predictions by our MEGADOCK tool, named MEGADOCK-WEB. The 7,564 proteins and predicted PPIs are registered. Each protein is annotated with PDB ID, chain, UniProt AC, KEGG Pathway and known PPI pairs. MEGADOCK-WEB provides the four functions, 1) Searching PPI predictions, 2) displaying known PPI, 3) visualizing candidate of interaction with query protein on biochemical pathway, and 4) visualizing predicted complex structure by 3D molecular viewer. Since MEGADOCK-WEB integrates comprehensive PPI predictions, the number of registered PPI predictions is more than 10 times more than other databases. MEGADOCK-WEB is freely available for use at http://bi.cs.titech.ac.jp/megadock-web.

3Pos175 生体膜系におけるヘリックス間の相互作用パターン解析
Analysis of helix interaction pattern in each biological membrane environment

Masato Sakai[1], Masami Ikeda[2], Makiko Suwa[1,2] ([1]*Biol. Sci., Grad. Sci. Eng., Aoyama Gakuin Univ.*, [2]*Chem. Biol. Sci., Sci. Eng., Aoyama Gakuin Univ.*)

For structure prediction of membrane protein (MP), it's necessary to decide mutual arrangement of transmembrane helices (TMHs) based on their amino acid (a.a) interactions. Since kind of the interactions should be affected from chemical properties of the surrounding environment, we aimed to pick out the a.a interaction pattern of 726 MP structures in different subcellular localization. The TMH regions were shred with 3 areas (core membrane, extracellular, and cytoplasmic) and we counted the interacting a.a pairs in each area. Many hydrophobic a.a pairs were observed at the core area while in each organelle, the a.a pairs were different in the extracellular/cytoplasmic areas. These results suggest that constitution of fatty acid may influence on the a.a pair patterns.

3Pos176 ポリグルタミン酸のヘリックスコイル転移における末端の安定性に関する分子動力学法による検討
Study on helix-coil transition stability of the termini of poly-glutamic acid using molecular dynamics method

Naoki Ogasawara[1], Ryosuke Iwai[1], Kota Kasahara[2], Takuya Takahashi[2] ([1]*Grad. Life. Sci., Ritsumeikan Univ.*, [2]*Col. Life. Sci., Ritsumeikan Univ.*)

Helix-coil equilibrium of poly-glutamic acid (PGA) has been studied from both experiments and theoretical approaches. Although differences in the helix stability between the center and the termini of PGA have been shown, the differences between the N- and C-terminus are still unclear. To elucidate this point, we performed all-atom molecular dynamics (MD) simulations with 20-residue PGA. As a result, we found that helical structure at the C-terminus was easily broken than that at the N-terminus. In order to elucidate the mechanisms of this stability difference between the termini, we analyzed the time course of MD simulations by using a Markov model of helix-coil transitions in each residue.

3Pos177 What are the structural features of superfolds? a case study of beta-sheet proteins

George Chikenji[1], Hayao Imakawa[1], Shintaro Minami[2] ([1]*Dep. App. Phys., Nagoya Univ.*, [2]*CIMoS, IMS*)

The number of families that encode a protein fold is termed the “designability” of the fold. It has been shown that designability differs drastically from fold to fold: only a small fraction of protein folds have high designability while majority of folds have low designability. Although a great deal of effort has been devoted in the past two decades, the question of what makes particular protein folds more designable is still unsolved. Here, we propose a simple theoretical framework that can predict the designability of beta-sheet proteins. The framework is based on the empirical rules of protein structures which we have recently discovered. We show that the framework is useful to understand the origin of designability of beta-sheet proteins.

3Pos178 Annotation of missense genomic variations based on various protein 3D structures

Matsuyuki Shirota[1,2,3] ([1]*Grad. Sch. Med., Tohoku Univ.*, [2]*ToMMo, Tohoku Univ.*, [3]*Grad. Sch. Inform. Sci. Tohoku Univ.*)

Recent population genomics projects have discovered millions of missense single nucleotide variations (SNVs) in human genome. To estimate the biological significance of a missense SNV, 3D structures of the protein that is affected by the SNV play a crucial role. Here I developed an annotation pipeline of SNVs based on protein 3D structures in PDB by considering all the available structures for the given protein in various conditions, e.g. in combination with other proteins and ligands. The effect of an SNV was evaluated using the structure in which the mutation is assumed to be most deleterious by affecting interaction sites with other molecules. This pipeline was effective to evaluate the SNVs of Exome Aggregation Consortium for selecting damaging SNVs.

3Pos179 機能に関する選択圧による P-loop 蛋白質のフォールド多様性についてのシミュレーション
Simulated diversification of the P-loop protein fold through functional selection

Kohei Inukai, Masaki Sasai, George Chikenji (*Department of Applied Physics, Nagoya University*)

In general, the protein fold, which is defined by the spatial arrangement and connectivity of secondary structure elements, is highly conserved during the course of evolution. However, contrary to the general rule, great variety of protein folds are observed in the phosphate binding loop (P-loop) protein family, which binds to nucleotide. An interesting question here is how the P-loop family has diversified protein folds while conserving the function in its evolution. To understand the evolutionary events of the P-loop family, using a course grained protein model, we computationally carried out evolutionary simulations imposing the functional selection pressure. In the presentation, we will report the detailed description of the method and the results.

3Pos180 Neo-logistic model precisely predicting a bacteria growth curve

Tohru Tashiro[1], Fujiko Yoshimura[2] ([1]*Dept. Sci., Ochanomizu Univ.*, [2]*Sch. Comput., Tokyo Tech.*)

In this lecture we propose a mathematical model precisely describing a growth curve of bacteria in a batch culture. The traditional approach for the system has utilized the logistic or the Gompertz model. However, it is not clear what kind of behavior of bacteria they are based on. Moreover, these models cannot be used as they are and need a modification. In this lecture, therefore, firstly we unveil the behaviors of bacteria which yield the logistic model and then point out the unnatural. Next, we construct a new model from more natural behavior. Finally, we predict both the saturation number of bacteria and the start time of stationary phase from the data during the logarithmic phase and show that the accuracy of predictions are considerably better than others.

3Pos181 細胞間および基質との接着を考慮した細胞集団の粒子モデル
Individual cell-based model for cell population considering cell-cell and cell-matrix adhesion

Seiya Nishikawa, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

Biological function of tissues would emerge through cell clustering. Existence of extracellular matrixes (ECM) plays an important role for cell to clustering. To elucidate the effect of ECM, an individual cell-based model was constructed, where cell-cell and cell-matrix adhesion were considered with the following assumption; cells adhere stochastically to the adjacent cells and the matrix; cytoskeletons expressed by springs are coupled to adhesion molecules; a growth factor is produced intracellularly depending on the sum of the tensions generated by the springs. The results suggested that higher cell-matrix affinity promotes cell proliferation. This model would be applicable to more complex behavior of cell population.

3Pos182 ストレスを受けた概日時計における位相変動の数理モデル
A mathematical model for stress induced phase shift in mammalian circadian systems

Yosuke Someya, Atsuko Takamatsu (*Dept. of Elec., Eng. & Biosci., Waseda University*)

Stress is known to initiate secretion of glucocorticoid (GC) in humans and rodents, then to induce phase shift in their circadian clocks. To clarify the effect of GC on the clocks, a mathematical model, consisting of coupled two-oscillators, was proposed. A brain oscillator couples to a peripheral (adrenal gland; AG) oscillator via nerves and hormones. AG oscillator couples to the brain oscillator via GC secretion, which is assumed to be received through a phase response function. Stress is expressed as an increase of GC secretion, additional to basal oscillation of GC. The simulation results suggested the phase response function for GC input is a key factor for reproducing the experiment result.

3Pos183 Mathematical model for motor-filament aster locomotion on motor-coated substrate

Masahiro Sawada[1,2], Takayuki Torisawa[2,3], Kazuhiro Oiwa[2,3], Shuji Ishihara[1,2] ([1]*Grad. Sch. Arts and Sciences, Univ. Tokyo*, [2]*CREST, JST*, [3]*Advanced ICT Inst., NICT*)

The self-organization in motor-filament system plays critical role in various cellular processes. We recently observed novel dynamics of the radial microtubule array (aster) in vitro experiment; The asters formed in the mixture of kinesin and microtubule displayed a cell-like crawling when they interacted with motor-coated surface. To research how such behavior arises, we construct the theoretical model in 2D space, considering the balance of contractile force exerted motor in an aster and traction force by motor on the surface. Our model displays asymmetric states arise from circularly symmetric states, which involves translational movement of the aster. The results show the simple feedback between the aster and the environment alone can cause a cell-like locomotion.

3Pos184 Probability eddy currents in a coupled genetic and epigenetic network

Bhaswati Bhattacharyya, Masaki Sasai (*Nagoya University*)

Gene expression in eukaryote is controlled by processes involving transcription factor (TF) binding/unbinding and epigenetic modification of histones. We present a model of the coupled stochastic dynamics of TF and histone states by using a self-activating gene network as an example. From a time-dependent master equation, we derive the dynamics of joint probability of the order parameters representing protein copy number, histone states, and TF states. We find two basins of attraction in the probability landscape for a range of parameters, and the probability current flows between them in the form of eddy currents. We analyze the currents in two and three dimensional order-parameter spaces to study the effects of timescale separation between TF and epigenetic dynamics.

3Pos185 ヒト血糖値調節におけるホルモン・代謝物の血中動態の数理モデルを用いた解析
Mathematical model analysis for blood glucose homeostasis regulated by blood hormones and metabolites in humans

Kaoru Ohashi[1], Masashi Fujii[1], Shinsuke Uda[2], Hiroyuki Kubota[2], Hisako Komada[3], Kazuhiko Sakaguchi[3], Wataru Ogawa[3], Shinya Kuroda[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Med. Ins. of Bioreg., Kyushu Univ.*, [3]*Grad. Sch. Med., Kobe Univ.*)

Homeostatic control of blood glucose is regulated by a complex feedback between glucose and hormones (e.g. insulin). Blood insulin also affects the concentration of blood metabolites (mainly amino acids / fats), and conversely, blood metabolites influence the sensitivity of insulin actions. This complex and dynamic interaction network between blood hormones and metabolites should be elucidated to understand the blood glucose homeostasis. We construct the mathematical model, based on our previous models for blood glucose and insulin, to reproduce the blood hormones and metabolites, and discuss the analysis of time changes and interaction between them.

3Pos186 ErbB シグナル転写ネットワークの新規統合数理モデルの構築と制御反応の同定
A new integrated mathematical model of the ErbB signaling and transcriptional network reveals key reactions determining the ErbB response

Hiroaki Imoto, Mariko Okada, Kazunari Iwamoto (*IPR, Osaka Univ.*)

The growth factor-triggered activation of ErbB signaling pathway mediates gene expression to regulate the cell proliferation and differentiation, and dysregulation of ErbB signaling drives malignant transformation. Hence, it is important to understand the quantitative relationship between the ErbB signaling activity and the downstream transcriptional activity.
In this study, we constructed a new mathematical model of ErbB signaling network integrating the process from the interaction between ligands and receptors to the activation of transcription factor c-Fos. The simulation result agreed with the experimental data, indicating that our model is biologically appropriate. Sensitivity analysis identified several key reactions that control the output of the ErbB network.

3Pos187 真性粘菌変形体の細胞運動が有する Lévy-walk 的性質
Levy-walk nature in the cell migration of Physarum plasmodium

Tomohiro Shirakawa[1], Takayuki Niiato[2], Hiroshi Sato[1], Ryota Ohno[1] ([1]*Department of Computer Science, School of Electrical and Computer Engineering, National Defense Academy of Japan*, [2]*Department of Intelligent Interaction Technologies, Graduate School of Systems and Information Engineering, University of Tsukuba*)

The plasmodium of Physarum polycephalum is a unicellular and multinuclear giant amoeba that has a kind of computational ability. Many studies have already been done on its optimization behavior in a closed space, however, there are not so many studies on the behavior of the plasmodium in an open space, though we believe that to study the adaptability of biological entity in such a condition is biologically more important. We thus established an experimental setup with very large and strictly homogeneous substrate, and observed the long term cell migration of the plasmodium. As a result, we found in the behavior of the plasmodium the pattern that is similar to Levy-walk but with anisotropic property.

3Pos188 細胞知覚の位相推定モデル
Phase Detection Model of Cellular Sensing

Ryo Yokota, Tetsuya, J. Kobayashi (*Institute of Industrial Science, The University of Tokyo*)

Oscillations are widely observed in various cellular signaling such as gene expressions for circadian rhythms, neural population coding, and chemical signals of microorganisms. Some of these systems utilize phases of oscillations as an information carrier to communicate temporal environmental changes. However, when the oscillations include stochastic noises, it is not so easy to decode the temporal changes from the phase signals, because the time differentiation of the signals is much more sensitive to noises than to signals. To address this problem, we formulated a cellular phase-detection mechanism by using a sequential bayesian inference algorithm. As a result, we analytically obtained the differential equation that is similar to the Kuramoto oscillator model.

3Pos189 ３次元フェイズフィールドモデルによるアメーバ細胞動態の解析
Cellar 3D phase-field model for amoeboid movement

Nen Saito[1], Satoshi Sawai[2] ([1]*Graduate School of Science, University of Tokyo*, [2]*Department of Basic Science, Graduate School of Arts and Sciences, University of Tokyo*)

Ameboid cell shows various dynamic behaviors such as formation of filopodia, lamellipodia and phagocytosis, which are inherently 3-dimensional. To capture and model these behaviors, model framework for 3D simulation are required.
In this talk, we introduce 3D phase-field model for amoeboid movement. This model with the help of GPU computation enables us to simulate dynamics of cell membrane and membrane localized proteins successfully.

3Pos190 Imaging of cysteic acid produced in ultraviolet-irradiated hair using synchrotron radiation

Kosuke Watanabe[1], Chinami Ariji[2], Daisuke Yoshida[2], Sho Kobayashi[1], Takaaki Maeda[1], Kazuyuki Suzuta[1], Len Ito[1] ([1]*MILBON CO., LTD.*, [2]*COSMOS TECHNICAL CENTER CO., LTD.*)

Ultraviolet rays are known to cause hair damage, and consumers are looking for products that can repair this damage. It has been reported that cysteic acid, an indicator of hair damage, is produced as an effect of ultraviolet irradiation on hair. Although it is important to understand the distribution of cysteic acid produced in ultraviolet-irradiated hair for developing treatments, there is little knowledge about how cysteic acid is produced in the hair. In the present study, we succeeded in capturing the distribution of cysteic acid produced in ultraviolet-irradiated hair using BL43IR of SPring-8. We will present these details on the day of presentation.

3Pos191 光第二高調波顕微鏡によるタンパク質構造解析
Optical second-harmonic generation microscope as a tool for protein structure analysis

Junichi Kaneshiro[1], Yasushi Okada[1,2], Tomohiro Shima[2], Mika Tsujii[3], Katsumi Imada[3], Taro Ichimura[1], Tomonobu M. Watanabe[1] ([1]*RIKEN QBiC*, [2]*Grad. Sch. Sci. Univ. Tokyo*, [3]*Grad. Sch. Sci. Osaka Univ.*)

Second-harmonic generation (SHG) is one of nonlinear optical scattering phenomenon occurs in materials with polar structures. Polarization-resolved SHG (PSHG) measurement enables us to detect SHG tensor components which characterize protein structures without any labeling. Here we demonstrate that structures of single microtubules (MT) in various nucleotides states are distinguished by PSHG technique. Precise analysis using MT bundles reveals that the angles of tubulin dimers depend on nucleotide state. We also show that PSHG exhibits dynamic change of structural state in a crystal of photo-switchable protein, Kohinoor. Temporal developments of SHG tensor components measured in both activation and deactivation processes indicate nonlinear processes occur in the crystal.

3Pos192 Continuous fluorescence observation without oxygen scavengers using a LED-based fluorescence microscope

Shin Yamaguchi[1], Kazuki Nakajima[1], Junichiro Yajima[2], Yuichi Inoue[1] ([1]*SIGMAKOKI Co., LTD*, [2]*Dept. of Life Sciences, Graduate School of Arts and Sciences, The Univ. of Tokyo*)

We have developed a LED-based fluorescence microscopy, called “Core Unit”, as a future foundation in the advanced research of biological sciences. The Core Unit can be used to observe single filamentous molecules as rhodamine-labeled microtubules with approximately half price of conventional microscope. Furthermore, fluorescence observation by Core Unit was continuous over several minutes (time constant > 300 s) even in the absence of oxygen scavengers, which are essential for conventional microscope to prevent phototoxic effects on biomolecules. The low phototoxicity of the Core Unit would be helpful to visualize the live activities of various biomolecules in vivo. Additional results about motor-related activities would be discussed at the meeting.

3Pos193 初期胚発生過程における細胞弾性率と細胞骨格構造の時空間変動
Spatiotemporal change in elastic modulus and cytoskeletal structure of cells in early embryonic development

Yuki Fujii[1], Taichi Imai[2], Wataru Koizumi[2], Kohji Hotta[2], Kotaro Oka[2], Takaharu Okajima[1] ([1]*Grad. Schl. Inform. Sci and Tech. Hokkaido Univ.*, [2]*Grad. Schl. Biosci. and Bioinfo. Keio Univ.*)

Cell division and morphogenesis of embryo are mechanically regulated in the developmental stage [1]. Using atomic force microscopy (AFM), we observed that the elastic modulus, E, of cells in ascidian embryo was significantly different between animal and vegetal poles, and the E increased at cell division [2]. Here, we investigated E and cytoskeletal structures of cells during embryogenesis by AFM and confocal microscopy to understand these mechanical behaviors. We found that actin filaments are localized close to cell membrane at the onset of cell division where E increases. This implies that the stiffness of embryonic dividing cells was increased by localization of cortical actin.

[1] C-P. Heisenberg, et al. Cell (2016)
[2] Y. Fujii, et al. 54th Annu. Meet. BSJ (2016)

3Pos194 Analysis of the number density distribution of colloidal particles on a substrate before solidification: A study of biomineralization

Amano Ken-ichi, Taira Ishihara, Nishi Naoya, Tetsuo Sakka (*Grad. Sch. Eng., Kyoto Univ.*)

Biomineralization is one of recent hot topics in biophysics. Shells, pearls, corals, and bones are fabricated by biomineralization, where colloidal particles, proteins, and organic-inorganic substances are systematically assembled. Chemical composition of the material and its microscopic structure have already been clarified, but the microscopic structure before solidification has not been elucidated. Hence, in this study, as a first step, we analyze the number density distribution of the colloidal particles on a substrate before solidification. Data from colloidal-probe atomic force microscopy and our analytical method are used to calculate it. In the poster, we discuss relationship between the obtained microscopic structure and mechanism of the biomineralization.

3Pos195 改良型蛍光 ATP センサーを用いた細胞内代謝変化の可視化
Visualization of intracellular metabolic changes using an improved fluorescent ATP indicator in mammalian cells

Hideyuki Yaginuma, Yasushi Okada (*QBiC, RIKEN*)

Adenosine triphosphate (ATP) provides energy to intracellular reactions. Demand for ATP and other metabolites changes depending on cell state, but how the different pathways for ATP synthesis is controlled inside cell during differentiation is not clear. We have developed an improved version of “QUEEN”, a fluorescent ATP indicator protein for quantification of ATP inside cells. The new QUEEN is suitable for visualization of ATP concentrations in mammalian cells at 37C. By timelapse QUEEN imaging combined with the use of several metabolic inhibitors, we succeeded to visualize metabolic changes during cell differentiation. Our results highlight the importance of monitoring metabolism in single cells even in an apparently uniform population.

3Pos196 蛍光相互相関分析に及ぼすヘモグロビン光吸収の影響
Effects of hemoglobin absorption on fluorescence cross correlation analysis

Atsushi Matsuo, Yasutomo Nomura (*Maebashi Institute of Technology*)

The feasibility of FCCS application to diagnosing with HbA1c was assessed. In the high throughput clinical examination, light absorption by Hb in the tested solution is inevitable. In this study, when Hb absobed fluorescence in the solution, we examined the effect on FCCS parameters. Prior to using the antibody, the test sample was formed by mixing 100 nM avidin Q-dot 655 conjugate as the red fluorescent dye and 100 nM biotinylated Alexa Flour 488 as the green one. Although count per particle was decreased by absorption due to Hb, number of molecule and diffusion coefficient were independent of the coexistence up to 50 μM Hb, which the hemolysate in clinical examination often contained. Using FCCS, we plan to evaluate the immunocomplex formation of HbA1c.

3Pos197 単一細胞中でのミトコンドリア電子伝達の計測
Measurements of mitochondrial electron transfer in a single cell

Hiroko Kashiwagi, Yoshihiro Ohta (*Ohta. Lab., Univ. Noko*)

Mitochondrial electron transfer is important for ATP synthesis. So far, to test the electron transfer, dissolved oxygen level in the cell suspension has been measured. However, since this measurement requires a lot of cells, it is difficult to measure electron transfer in minority cells included in cell population. The aim of this study is to develop the novel technique to measure the electron transfer in a single cell. For this purpose, we measured the generation of mitochondrial membrane potential instead of the decrease in the dissolved oxygen level with fluorescence microscopy. After permeabilizing the plasma membrane of the cell, we added substrates for electron transfer sequentially. The detailed conditions for the measurements are investigated.

3Pos198 蛍光分子薄膜の紫外可視光変換システム解析
Ultra violet visible light conversion system analysis of fluorescent molecular thin film

Shotaro Minato[1], Taiyo Tsurugai[1], Miku Kaneta[1], Honoka Endo[1], Hiroshi Masumoto[2], Takashi Goto[3], **Yutaka Tsujiuchi**[1] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary*, [3]*Institute for Materials Research, Tohoku University*)

For the purpose of functional film fabrication for biosensor using photo-controlled film system, we have been researching, by using ionic conduction system in laminated gels on hydrogenated amorphous silicon film, and using ultra violet visible light conversion system. In this study, Langmuir Blodgett films of different fluorescent molecules were fabricated using wilhelmy equations onto customized original apparatus. And emission spectrum analysis and voltage current analysis of the films on hydrogenated amorphous silicon film, are conducted. These systems function as the new detection method of sample properties.

3Pos199 Quantitative imaging analysis of microtubule-organizing center repositioning mediated by CLIP-170 phosphorylation during T cell activation

Wei Ming Lim[1], Yuma Ito[1], Kumiko Sakata-Sogawa[2], Makio Tokunaga[1] ([1]*Sch. Lif. Sci. Tech., Tokyo Ins. Tech.*, [2]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

At the initial phase of T cell activation, microtubule-organizing center (MTOC) repositioned to the center of immunological synapse and drives T cell signaling. However, our understanding of the underlying molecular mechanism remains limited. We investigated how CLIP-170 mediates MTOC repositioning. Fluorescence imaging and quantitative analysis showed that microtubule dynamics and the T cell immune response were impaired when CLIP-170 phosphorylation was inhibited. Further investigation using dual-colour imaging revealed that CLIP-170 colocalizes with dynactin and moves toward the cell surface. These results indicate that MTOC repositioning depends on dynactin localization mediated by CLIP-170, and that CLIP-170 plays a crucial role in T cell activation.

3Pos200 Comparison of the analgesic effects of different types of therapeutic agents on allodynia-specific pain using fMRI

Yuri Kitamoto[1], Sosuke Yoshinaga[1], Naoya Yuzuriha[1], Hiroshi Sato[2], Mitsuhiro Takeda[1], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Univ. Kumamoto*, [2]*Bruker Biospin*)

Fibromyalgia and neuropathic disorders characterized by chronic pain induce the pathological condition “allodynia”, in which a stimulus that is normally not painful causes pain sensations. The aim of this study is to observe the allodynia-specific responses in an animal model of fibromyalgia, using functional Magnetic Resonance Imaging (fMRI), and to evaluate the effects of analgesic agents. We observed the brain responses of fibromyalgia model rats that were evoked by a green laser, using fMRI. Based on a group analysis (n=5), the primary somatosensory cortices, insura and thalamus regions contributed to the allodynia-specific pain responses. These brain responses were suppressed or decreased by the analgesics that are currently used for fibromyalgia.

3Pos201 １分子イメージングによる機能性 RNA TERRA の動態・局在解析
Dynamics and localization of a non-coding RNA TERRA in living cells revealed by single molecule imaging

Hideaki Yoshimura, Toshimichi Yamada, Rintaro Shimada, Takeaki Ozawa (*Sch. Sci., Univ. Tokyo*)

Telomere-repeat containing RNA (TERRA) is a ncRNA containing a telomeric repeat, and implicated in telomere maintenance. To reveal the true mechanism of TERRA function, we developed a fluorescent probe to visualize TERRA in living cells and performed single molecule fluorescence imaging of TERRA. From the results, there are two modes in TERRA diffusion motion: the diffusive mode and the stationary mode. In addition, the two modes frequently switch to each other around a telomere. The stationary TERRA were intensively localized on and around telomeres. The stationary TERRA around a telomere frequently colocalize with a protein hnRNPA1. This result implies that TERRA remove hnRNPA1 from a telomere to maintain the telomere.

3Pos202 生物発光イメージング法を用いたグルカゴン分泌の可視化解析系の構築
Video rate bioluminescence imaging of glucagon secretion from pancreatic alpha cells

Satoru Yokawa[1], Takahiro Suzuki[2], Satoshi Inouye[3], Yoshikazu Inoh[1], Ryo Suzuki[4], Naohide Hirashima[4], Tadahide Furuno[1] ([1]*Sch. Pharm., Aichi Gakuin Univ.*, [2]*Sch. Dent., Aichi Gakuin Univ.*, [3]*JNC Co., Yokohama*, [4]*Grad. Sch. Pharm. Sci., Nagoya City Univ.*)

We have firstly visualized glucagon secretion using a method of video-rate bioluminescence imaging. The fusion protein of proglucagon and Gaussia luciferase (PGCG-GLase) was used as a reporter to detect glucagon secretion from mouse pancreatic α cells. Luminescence signals of the secreted PGCG-GLase were detected by a microscope with EM-CCD camera. The images showed an increase in glucagon secretion from clustered cells in response to stimulation by KCl. The secretory events were observed at the intercellular contact regions. The localization and frequency of glucagon secretion might be regulated by cell-cell adhesion. Here, we demonstrated that the imaging method is a powerful tool for spatiotemporal analysis of glucagon secretion in pancreatic islet.

3Pos203 遊走細胞からの分泌を実時間で可視化する
Real-time secretion tracking system for migrating single cells

Yoshitaka Shirasaki[1], Yosuke Yasuzawa[1], Yumiko Tanaka[1], Nobutake Suzuki[1], Sotaro Uemura[1], Kazuyo Moro[2] ([1]*Dep. Biol. Sci., Grad. Sch. of Sci., The Univ. of Tokyo*, [2]*IMS, RIKEN*)

We observed secretion dynamics from single mouse type-2 innate lymphoid cells (ILC2s) arranged in nano-litter wells. Activated ILC2s secreted enormous amount of type 2 cytokines, often associated with active migration and high mitotic rate. To focus on the relationship between secretion activity and migration or mitotic activity, we developed the real-time single cell secretion tracking system without nanowell structures. We succeeded in monitoring the secretion dynamics and their movement of ILC2s every 4 seconds. We are trying to develop a long-term tracking system with a feedback of acquisition position to the center of the target cell. This system will uncover the details of relationships among cell migration, shape, mitotic activity, and secretion.

3Pos204 細胞・組織内生体分子の動態を可視化する逆ラマン顕微測定システムの開発
Development of inverse Raman micro spectroscopic system toward visualizing the dynamics of biomolecule *in vivo* and *in cellulo*

Yuka Kawahara-Nakagawa, Satoru Nakashima, Takashi Ogura (*Grad. Sch. Sci., Univ. Hyogo*)

Raman miscroscope has been acknowledged as a powerful tool to visualize dynamics of molecules in vivo and in cellulo based on vibrational finger print without any labeling or staining. However, it ordinarily takes longer than a minute to obtain 2D molecular image (i.e. 128×128 pixel) with a fine quality sufficient for identifying classifications of molecules. To drastically reduce the time required to scan the area and to realize a video-rate (30 frames/s) observation, we propose to adopt the “inverse Raman” instead of the “spontaneous Raman”. As a first step, we have developed a proto-type of an inverse Raman spectrophotometer and successfully applied it to water and some organic solvents.

3Pos205 細胞内温度変化による細胞機能制御の分子機構の解明
Investigating molecular mechanism of intracellular temperature dependent cell functions

Yu Bi[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pha. Sci., Univ. Tokyo*, [2]*JST-PRESTO*)

Intracellular temperature was found to distribute inhomogeneously inside a living cell. In this study, we investigate the molecular mechanism of cell function controlled by the change of intracellular temperature. We used a recently-developed cell-permeable fluorescence polymeric thermometer, which will allow the thermometry in a number of cells. Using our optimized protocol, we confirmed the application of this thermometer to various cell lines and revealed that fluorescence intensity and lifetime imaging can detect the intracellular change in numerous cells at a time. This technique will serve as a platform for investigating the contribution of molecule on the intracellular temperature, and aid the future discoveries of the molecular mechanism of thermal signaling.

3Pos206 振動和周波検出赤外超解像顕微鏡法による爪・毛髪中のケラチンタンパク質の分布・配向観察
Molecular distribution and orientation of keratins in human nails and human hairs observed by VSFG-detected IR super-resolution microscopy

Yuichiro Iwasaki, Maho Hata, Mitsuki Fujiwara, Ryo Morimoto, **Hirona Takahashi**, Makoto Sakai (*Okayama University of Science*)

Keratin is one of the most important structural proteins, and is often discussed in terms of α- and β-keratins. For example, wool and human hair are composed of α-keratins, but the main components of feather and human nail are β- keratins. Recently, we developed a vibrational sum-frequency generation (VSFG) detected IR microscope and applied it to observe the distribution and orientation of keratin proteins in various biological samples. And it is found that the intensity of VSFG signals depends on the angles between the polarization of IR light and the extending direction of α- and β-keratins. In the presentation, we will discuss the results of orientation-sensitive molecular imaging of human nail β-keratins and human hair α-keratins by IR super-resolution microscopy.

3Pos207 振動和周波検出赤外超解像顕微鏡法による羽毛 β-ケラチンの分子配向イメージング
Orientation-sensitive molecular imaging of feather β-keratins by a VSFG-detected IR super-resolution microscopy

Kota Yamamoto, Kosuke Tatekabe, Tomoya Miyake, Yuya Kimura, Hirona Takahashi, **Makoto Sakai** (*Okayama University of Science*)

Feather is generally known to consist of rachis, barb and barbule regions from the root to the tip, and it has been reported that main components of feather are β-keratins with β-sheet structures. On the other hand, the spatial inhomogeneity of β-keratins could not be disclosed because of a lack of the spatial resolution of previous analytical methods. In this study, we aim to elucidate the spatial distribution and orientation of β-keratins at each region of feather in the amide I band and verify those differences at each region by a vibrational sum-frequency generation (VSFG) detected IR super-resolution microscopy that has the ability to measure the orientation-sensitive molecular image with sub-micrometer scale spatial resolution.

3Pos208 Evaluation of anesthesia conditions for detecting odor responses in the mouse whole brain

Fuyu Hayashi, Hirotsugu Funatsu, Sosuke Yoshinaga, Naoya Yuzuriha, Shunsuke Kusanagi, Mitsuhiro Takeda, Hiroaki Terasawa (*Fac. Life Sci., Kumamoto Univ.*)

BOLD analysis is the main method to track real-time odor responses. BOLD responses are susceptible to the anesthesia conditions, thus preventing us from determining the odor discrimination system especially in the mouse whole brain, in which is difficult to obtain sufficient signals. This study compared the odor responses of mice under some anesthetizing procedures, using the t-test and independent component analysis (ICA). Under urethane, the t-test and ICA both detected the regions activated by isoamyl acetate. However, under medetomidine, ICA could not detect them. The respiratory depressant action of Med may have extended the delay between odor administration and inhalation, and thus it was harder for ICA to detect the activation based on the stimulated frequency.

3Pos209 １分子軌跡追跡により時空間動態と結合解離を定量する解析法
An analysis method for quantification of spatiotemporal dynamics and kinetics using single-molecule tracking

Yuma Ito[1], Kumiko Sakata-Sogawa[1,2], **Makio Tokunaga**[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Grad. Sch. Agr. Sci., Tohoku Univ.*)

We introduced a method to quantify dynamics and kinetics spatiotemporally in living cells using single-color single-molecule tracking. Combining with three-color simultaneous single-molecule imaging, we quantified the dynamics and kinetics of molecules in spatial relation to T cell receptor (TCR) microclusters that activate TCR signaling. CD3ε, a component of the TCR/CD3 complex, and CD45, a phosphatase regulating signaling, were each found in two mobility states. The TCR microclusters were loosely composed of heterogeneous nanoregions. Kinetic analysis quantified the association and dissociation rates of interactions with the microclusters. On the inside of the microclusters, the association was accelerated, and the stable association was increased.

3Pos210 マウスノロウイルス MNV-S7 のクライオ電顕単粒子構造解析
Capsid Structure of Murine Norovirus S7 revealed by cryo-electron microscopy

Chihong Song[1], Naoyuki Miyazaki[2], Kenji Iwasaki[2], Motohiro Miki[3], Reiko Todaka[4], Kei Haga[4], Akira Fujimoto[4], Kazuhiko Katayama[4], Kazuyoshi Murata[1] ([1]*NIPS*, [2]*IPR*, [3]*Denka Co., Ltd.*, [4]*Kitasato Univ.*)

Human norovirus (HuNoV) is the major cause of epidemic nonbacterial gastroenteritis worldwide, but the mechanism producing the antigenic diversity is almost unknown. We generated murine norovirus S7 strain (MNV-S7) VLPs using baculovirus expression system as a surrogate of HuNoV, and investigated the 3D structure of MNV-S7 by single-particle cryo-electron microscopy (CryoEM). The capsid structure of MNV-S7 was compared with that of Murine norovirus 1 strain (MNV-1) previously reported. Although the difference of the amino acids is only 6% in the two genotypes, the whole structure of the capsids was drastically changed. Especially, the residues forming the interaction in the neighboring protrusion (P)-domains were switched between these genotypes.

Name Index (索引)

名字（Family Name）のアルファベット順にソートしています。すべて、オンラインで入力されたデータのまま、表示しています。

㈱情報数理バイオ / ㈱アフィニティサイエンス / ㈱京都コンステラ・テクノロジーズ / ㈱バイオモデリングリサーチ

国産無償創薬ソフトを使った臨床からの新薬再開発の提案

Proposal for redevelopment of existing drugs in line with clinical needs using free drug development software suite of Japanese origin

日　時：2017年 9月19日（火）　11：50 ～ 12：40
会　場：A会場（熊本大学 黒髪北　全学教育棟 E107）

■　講演者：大池 正宏　先生　（九州大学大学院医学研究院　生体情報薬理学分野）

既存の疾患治療薬に新しい適応疾患を見出す既存薬再開発は、薬物開発の新しい可能性として注目されています。医師など臨床に携わる者は自らの臨床知見や入手可能な臨床データをもとに既存薬再開発に貢献できる可能性がありますが、手がかりとなる情報がなければ偶然の機会を待つしかありません。

九州大学医学部医学科では、希望する学生を対象に、国産の無償創薬ソフト群myPrestoを使用したインシリコ既存薬再開発の実習を行っています。学生は、主に製薬企業の創薬対象になりにくい希少疾患を対象に各自で標的蛋白を設定して13,000種の既存市販薬から候補化合物を検索し、その過程でプログラム操作法や背景理論を習得しています。確率上はそれらの候補化合物が実際に奏功する可能性は高いものではないと思われますが、多くの医学生が習得することで、将来、臨床の要請に沿った既存薬再開発が国産創薬ソフトによって臨床主導で行われることを期待しています。

本セミナーでは、myPrestoの応用例としてのインシリコ既存薬スクリーニングと今後の展望についてご紹介いたします。

■　スポンサー企業のサービス紹介1　（株式会社バイオモデリングリサーチ 代表取締役 中村 寛則）

myPrestoには、年々、新しい機能が追加されています。Amberで使われている新しい低分子用の分子力場GAFF2の導入やタンパク質周辺の水分子配置プログラムの改良等、最新のmyPrestoの状況について説明し、myPrestoの機能をマウス操作で簡単に利用することができ、分子の立体構造を詳細に観察できるグラフィック・ユーザー・インターフェース(GUI)ソフトウェアMolDeskの操作デモを行います。MolDeskは、(株)情報数理バイオが開発した有料のソフトウェアです。

■　スポンサー企業のサービス紹介2　（株式会社アフィニティサイエンス　営業部 沖 みゆき）

ACISS(Affinity-Constella In Silico Support)サービスは、創薬やその他関連分野における計算科学支援を目的として、アフィニティサイエンスと京都コンステラ・テクノロジーズが共同で提供する受託研究・解析サービスです。両社のコア技術・各種ソフトウェアを組み合わせることにより、優れた費用対効果でトータルに創薬研究をサポートいたします。本サービスの中では、myPrestoも利用させていただいております。

2015年春に開始したACISSサービスですが、既に数十のプロジェクトに携わらせて頂いており、繰り返しご利用いただいているお客さまも多くいらっしゃいます。これまでの実績を交えながら、本サービスの概要についてご紹介させて頂きます。

お問合せ先

株式会社情報数理バイオ IMSBIO Co., Ltd. TEL. 03-6907-0315, http://www.imsbio.co.jp
株式会社アフィニティサイエンス Affinity Science Corporation TEL. 03-6417-3695, http://www.affinity-science.com
株式会社京都コンステラ・テクノロジーズ Kyoto Constella Technologies Co., Ltd. TEL. 075-241-9672, http://www.k-ct.jp
株式会社バイオモデリングリサーチ Biomodeling Research Co., Ltd. TEL. 052-720-7704, http://www.biomodeling.co.jp

Malvern　第55回　日本生物物理学会年会ランチョンセミナー

蛋白質科学に向けた様々な溶液拡散解析手法の紹介

発表日：9月19日（火） 11:50～12:40　会場： D会場

スペクトリス株式会社　マルバーン事業部

志波　公平

蛋白質は構造を持ち、構造と機能の間には密接な関係性があることは周知の事実であり、現在数多くの蛋白質の構造をベースとした研究が盛んに行われています。とりわけ蛋白質の構造解析は、X線結晶構造解析技術の発展によって大きく進歩し、次の関心として溶液中における物性解析が取り上げられています。例えば蛋白質の代表的な機能の1つに特定分子との特異的結合がありますが、この活性を示すときに対象の蛋白質がどのような構造を示しているのかは大変大きな関心事です。溶液中における結合活性と分子サイズを合わせて議論することの重要性はこの点に存在します。また、高分子科学の観点から、蛋白質そのものの性質を知る上でも溶液物性は重要になってきます。

物性測定の中で、溶液中の拡散計測は様々な情報を与えます。その中で代表的なものが流体力学的径(Hydrodynamic Size)で、動的光散乱（Dynamic Light Scattering; DLS）法や分析超遠心(Analytical Ultracentrifuge; AUC)法などによって計測できます。この拡散係数を用いた計測法の場合、測定対象物への負荷をほとんど与えることなく計測できる一方、サンプル量や再現性、スループットが課題とされています。

一方、Taylor分散（Taylor Dispersion）法は1950年代にG. I. Taylorらによって提唱され、1980年代にH. Brennerらによって確立された手法で、キャピラリ内に生じる流体速度分布によって高分子の拡散係数を導く手法です。この手法の特徴はUVによる検出が可能であり、ごく微量で計測できる点にあります。再現性に優れており、1 nm以下のサイズ変化の議論も可能になります。
本発表では、Taylor分散法を用いたいくつかのアプリケーションを、他の物性測定と合わせながら紹介していきます。また、後半では当社が持つ物性解析装置の紹介も併せて行います。

粒子径・ゼータ電位・分子量測定装置
ゼータサイザーナノZSP

微量粘度・サイズ測定装置
ビスコサイザーTD

第 55 回日本生物物理学会年会

ニコンインステック ランチョンセミナー（1LSF）

多次元画像計測が可能とする先端バイオサイエンス
～1分子シークエンサー技術・1細胞分泌動態可視化技術への応用例

上村 想太郎 先生 （東京大学 大学院理学研究科）

白崎 善隆 先生 （東京大学 大学院理学研究科）

日時 2017年9月19日（火）11:50～12:40

会場 熊本大学黒髪北地区 F会場（全学教育棟E205）

多次元画像計測を可能とする安定した電動顕微鏡技術は、溶液制御や微細加工チップ、画像解析など様々な先端技術を組み込むことで新たな生物学的価値を生み出す測定プラットフォームとして機能する。今回のランチョンセミナーではニコン Ti-E 顕微鏡をベースに講演者が開発している１分子シークエンサーシステム、１細胞分泌リアルタイムイメージングシステムおよび１細胞リアルタイムピックアップシステムの技術紹介と共に、顕微鏡を高度にシステム化することによる今後の技術発展についても議論したい。

****

株式会社ニコン インステック

バイオサイエンス営業本部

電話 03−6433−3982 URL http://www.nikon-instruments.jp/jpn/

第55回日本生物物理学会年会

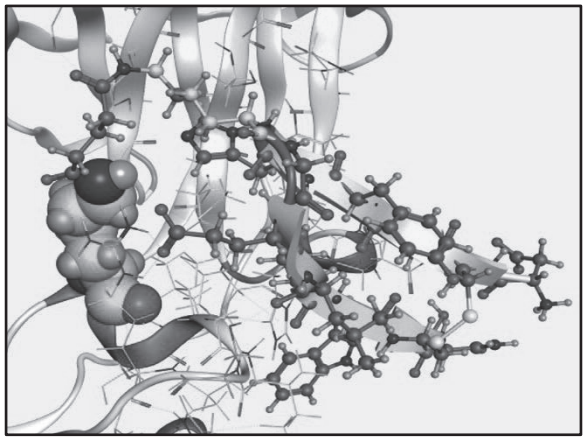
株式会社モルシス ランチョンセミナー
計算化学的手法によるペプチド創薬の効率化

日時： 9月19日（火）　11:50 ～ 12:40

場所： G 会場（全学教育棟 C301）

部位特異的修飾による抗体の高機能化に向けた親和性ペプチド試薬のデザイン

鹿児島大学　大学院理工学研究科　教授　**伊東 祐二**



抗体の高機能化、例えば、ビオチン化や蛍光標識、近年では、抗体医薬品の中の抗体薬物複合体の作製には、化学修飾の一つであるアミンカップリング法が汎用されている。しかし、この修飾は、通常、アミノ基にランダムに起こるため部位特異的な修飾は不可能である。演者は、最近、抗体に対する親和性ペプチド試薬を用いて、部位特異的に特定のアミノ酸残基を修飾する CCAP（Chemical Conjugation by Affinity Peptide）法を開発した。この方法では、抗原結合部位への修飾による抗体の抗原結合能の低下を避け、Fc 領域に種々のリガンドを容易にかつ定量的に導入することができる。本講演では、医薬品開発に向けた本手法による抗体の高機能化とともに、MOE の利用による CCAP 法のための親和性ペプチド試薬のデザインについて紹介する。

MOE によるペプチド創薬支援

株式会社モルシス　**木村 嘉朗**

統合計算化学システム MOE は、計算化学者から実験研究者まで幅広いユーザーの研究をサポートする創薬・生命科学研究のための分子シミュレーションソフトウェアです。MOE はペプチドデザインをはじめ、突然変異体モデリング、バーチャルファージディスプレイ、表面パッチ解析、ドッキングシミュレーションなどのペプチド創薬を支援するさまざまな機能を搭載しています。本セミナーでは、MOE のペプチド創薬を支援する機能の応用例を紹介します。

MOLSIS

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URL: https://www.molsis.co.jp/

第55回 日本生物物理学会年会

浜松ホトニクス株式会社
ランチョンセミナー

◇ **プログラムNo. 1LSI**

◇ **日時:2017年9月19日(火) 11:50 ～ 12:40**

◇ **会場:I会場(全学教育棟 E305)**

演題1

「sCMOSカメラとW-Viewによって明らかになった生細胞の核内環境」

"Nuclear environment in living cells revealed by sCMOS camera and W-View system"

前島 一博 先生

国立遺伝学研究所 構造遺伝学研究センター 生体高分子 前島研究室

演題2

「浜松ホトニクスの最新イメージング技術」

- 高速イメージング技術とその展望 -

"The latest imaging technology of Hamamatsu Photonics"
- High speed imaging technologies and perspectives -

伊東 克秀

浜松ホトニクス株式会社 システム事業部

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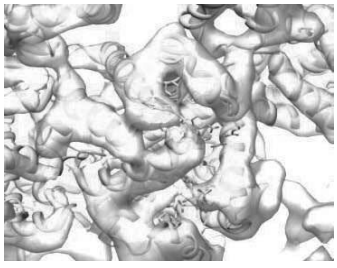
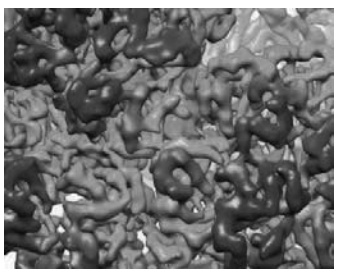
第55回日本生物物理学会年会ランチョンセミナー

The Revolution of Cryo-EM

日時: 9月20日（水）11:30 – 12:20
場所: D会場（全学教育棟 E201）
演者: 岩崎　憲治　先生 (Dr. Kenji Iwasaki)
（大阪大学蛋白質研究所, Institute for Protein Research）
演題: 自動クライオ電顕撮影による高速近原子分解能解析
~ ボルタ位相板の進展 ~
High-Throughput Near Atomic-resolution Cryo-EM
- Utilizing Volta Phase Plate -

本講演では、タンパク質複合体の立体構造解析手法として欠かせないツールとなったクライオ電子顕微鏡法、特に単粒子解析法をテーマに、FEIのユーザー様である大阪大学蛋白質研究所の岩崎先生をお招きし、技術的革新の詳細と実際の共用運営体制の現状について、所内で解析されたデータ例を踏まえご講演いただく。





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第55回 日本生物物理学会年会
オプトライン ランチョンセミナー

ライトシート・ライトフィールド顕微鏡が実現する細胞・組織レベルの超高速3Dイメージング

日　時　9月20日（水）　11:30 ～ 12:20

会　場　G会場（全学教育棟 C301）

演　者

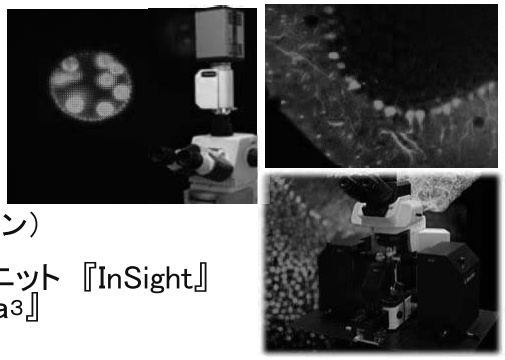
野中 茂紀　先生

自然科学研究機構　基礎生物学研究所
イメージングサイエンス研究領域 時空間制御研究室　准教授

細胞や組織といった数十～数百μmレベルの厚みを持った生物試料を観察する手法として、ライトシート顕微鏡は、低褪色・低光毒性とともに高速性が大きな特長である。 しかし現在、大手顕微鏡メーカーから市販されているライトシート顕微鏡はZスキャンのために試料自体を移動させるため、高速性を求める上では、このことがしばしば足かせとなる。試料の代わりにシート光と焦点面を動かせばより高速な画像取得が可能になる。さらに焦点面の移動に高速な液体レンズを用いることで最大限の高速化が達成される。

これに対してライトフィールド顕微鏡は、そもそもZスキャンを行わず、マイクロレンズアレイを通して撮影した1枚の像から立体情報を取り出す。カメラのフレーム取得速度そのものがボリューム取得速度になり、究極の高速化が可能である。

本セミナーではそれぞれの顕微鏡法で撮られた生物動画を紹介しつつ、その長所と限界について議論する。またこれらの顕微鏡観察を実現するPhaseView社のラインナップについて紹介する。



演　者

岩井　亮一　（株式会社オプトライン）

ライトフィールド 3Dイメージングユニット 『InSight』
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日本マイクロソフト株式会社　ランチョンセミナー　（プログラム No. 3LSA）

日時：9 月 21 日（木）11:45 ～ 12:35

会場：A 会場（全学教育棟 C206）

myPresto on Azure—クラウドコンピューティングを利用した分子設計統合システム

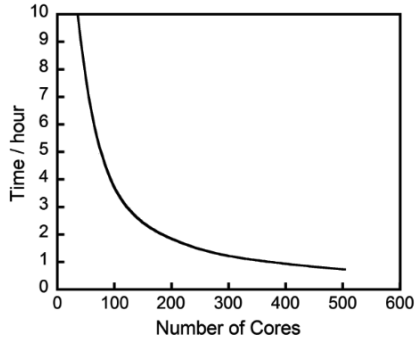
次世代天然物化学技術研究組合　和田 光人

日本マイクロソフト株式会社　林 勝典

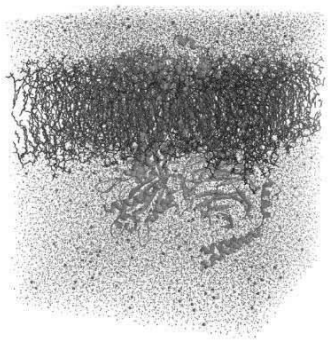
次世代天然物化学技術研究組合は、大阪大学中村春木教授の指揮のもと、分子設計システム *myPresto* を長年に渡って開発してきました。低分子化合物の三次元構造構築、力場パラメータ割当、溶解度/LogP などの物性予測から、タンパク質へのドッキング、分子動力学計算による分子の動的挙動の解析に至るまで分子設計に必要なツールは一通り *myPresto* に揃っています。また、800 万件の低分子化合物の 3 次元データベースも兼ね備えているので、ユーザが標的分子を設定すればスクリーニング計算の機能を使ってすぐにリード化合物の探索にとりかかることができます。

創薬探索を中心として、myPresto は世界中の数多くの研究者に利用されてきましたが、課題はその多彩な機能ゆえに生じるソフトウェア環境設定の複雑さでした。この問題を解決するために、マイクロソフトのクラウドである Azure 上に myPresto のすべての機能を搭載した仮想マシン環境を準備いたしました。ユーザは myPresto 環境が全て整った Azure 上の仮想マシンにアクセスすれことにより、薬物スクリーニングや分子動力学計算を即座に実行することができます。多数のコアを搭載した仮想マシンを使えば、200 化合物を対象としたスクリーニング計算を最短で 30 分、約 3,000 円のコストで実行することが可能です。また、Azure では絶えず最新の GPU が搭載されたマシンが準備されているので、Gタンパク質共役受容体(GPCR)などの複雑な膜タンパク質の分子動力学計算も高速に実行することが可能です。

本セミナーでは、myPresto on Azure の利用方法の説明と、Azure 上で計算を実行した GPCR に関する研究成果についてご紹介いたします。



200 万化合物のスクリーニングに要する計算時間



β2アドレナリン受容体/G タンパク質複合体の分子動力学計算におけるスナップショット

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Malvern　第55回　日本生物物理学会年会ランチョンセミナー

Thermodynamicsの生化学的応用（酵素反応など）および光散乱を用いた蛋白質の構造解析

発表日：9月21日（木） 11:45～12:35　会場： D会場

スペクトリス株式会社　マルバーン事業部

廣瀬　雅子、志波　公平

等温滴定型熱測定（Isothermal Titration Calorimetry、ITC）は、蛋白質-蛋白質間、および蛋白質-低分子リガンド間の相互作用といった、様々な生体分子の相互作用解析の基礎的な研究から創薬研究まで幅広く用いられています。ITC測定では、溶液中での相互作用をその反応熱の滴定トレンドから解析していくものであり、相互作用に限らず反応熱を観察することができます。

一方、酵素反応は、例えばMichaelis-Menten式を用いて議論が展開されますが、その触媒機能によってもたらされた熱量もまた検出することができることがわかりました。前半では、ITCの基本原理から酵素反応への応用に関して触れていきます。

蛋白質のサイズ解析に関しては、SEC (Size Exclusion Chromatography)が広く使用されています。SECは分子（粒子）体積の違いによって分画し解析するものですが、分子密度が不明である点、得られる分子量が相対的なものである点などが問題とされています。

一方、SECの検出部分に光散乱および粘度検出を導入すると、絶対分子量、固有粘度といった物性に関連が深いデータを取得することができます。後半では、SECに光散乱、粘度検出器をつけた際に得られるデータを通じてわかることを、事例を交えながらご紹介します。

分子間相互作用解析装置

MicroCal PEAQ-ITC

SEC/GPC用マルチ検出システム

OmniSEC

https://pdbj.org/

PDBj Protein Data Bank Japan

Luncheon Seminar at the 55th Annual Meeting of Biophysical Society of Japan

September 21(Thu), 11:45 ～ 12:35, Room I（Room E305, General Education Bldg. 3F）

1. Recent activities of PDBj and wwPDB

PDBj と wwPDB の最近の活動について

Genji Kurisu, Institute for Protein Research, Osaka University

The PDBj (PDB Japan, https://pdbj.org/) is the representative archive of macromolecular structural data by X-ray crystallography, NMR and cryo-EM, processing the deposited data from researchers in Asian and Middle-east regions, as one of the four members of the wwPDB (worldwide PDB, https://wwpdb.org/). In order to promote the recent “Data Science,” the wwPDB is introducing several new policies: (i) Collection of ORCID (Open Researcher and Contributor ID: http://orcid.org/) that is implemented in 2016 and will expand to all entry authors, (ii) Introduction of a versioning system that allows depositors of record to update their own previously released entries. Upon introduction of the file versioning system, the current 4-characters PDB ID will change. These issues will be introduced at the Seminar.

2. Querying the PDBj Mine2 relational database

PDBj Mine2 関係データベースを検索する

Akira R. Kinjo, Institute for Protein Research, Osaka University

PDBj Mine2 RDB is the relational database for PDBj. It can be directly accessed via the interactive web interface at https://pdbj.org/mine/sql or via the REST API at https://pdbj.org/rest/mine2_sql (see https://pdbj.org/help/rest-interface for the details of the REST API). Furthermore, a complete database dump is available at ftp://ftp.pdbj.org/mine2/ for local installation using PostgreSQL (https://www.postgresql.org/) version 9.3 or higher (see https://pdbj.org/help/mine2-rdb-local-install for the instruction). Most of the tables in PDBj Mine2 RDB correspond to the categories defined in the PDBx/mmCIF dictionary (http://mmcif.wwpdb.org/). For a complete description of the database schema, see https://pdbj.org/mine-rdb-docs. We have also integrated the SIFTS resource (https://www.ebi.ac.uk/pdbe/docs/sifts/). Currently, only the "quick access" files of SIFTS are incorporated in the PDBj Mine2 RDB, the table structures of which reflect the tab-separated format of the original SIFTS files (see https://pdbj.org/help/sifts for the detail). A comprehensive list of examples are available at https://pdbj.org/help/mine2-sql. In this seminar, I will explain the basic structure of the database as well as effective ways to query it.

3. Situation, utilization and visualization of cryo-EM structure data

クライオ電子顕微鏡データの現状、見方、使い方

Hirofumi Suzuki, Institute for Protein Research, Osaka University

Recent innovation in cryo-EM methodology gave significant impact to structural biology and databanks for its data, EMDB and PDB. To utilize such the multiscale hybrid structure data, PDBj provide Web-based services, EM Navigator, Yorodumi, and Omokage search. New version of PDBx/mmCIF format supports better-organized information especially about experimental information of EM. In the seminar, we will introduce news about the structure data, improvement of the tools, and our new collaborative effort with wwPDB members.

Protein Data Bank Japan
https://pdbj.org/

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6. 日本生物物理学会のホームページ
   http://www.biophys.jp

本誌記事の動物実験における実験動物の扱いは,
所属機関のルールに従っています.

生物物理 SEIBUTSU BUTSURI
日本生物物理学会 THE BIOPHYSICAL SOCIETY OF JAPAN

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