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生物物理

SEIBUTSU BUTSURI

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第58回年会予稿集

2020.9.16（水）～ 18（金）

オンライン開催

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　https://www.biophys.jp

第58回日本生物物理学会年会

The 58th Annual Meeting of the Biophysical Society of Japan

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開催概要／General Information

The 58h Annual Meeting of the Biophysical Society of Japan (BSJ2020)
第58日本生物物理学会年会（2020年度）

会期／Period
2020年9月16日（水）－18 日（金）
16 (Wed) – 18 (Fri), September, 2020

会場／Venue
オンライン開催
Online Conference

年会長・実行委員長／Chair of the Organizing Committee
大澤 研二（群馬大学大学院理工学府）
Kenji Oosawa, Ph.D.（Gunma University）

Website https://www2.aeplan.co.jp/bsj2020
※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）
※下記サイトからダウンロードいただけます。
http://www.biophys.jp/dl/pro/58th_proceedings.pdf
ID: ambsj58 Password: webgunma2020

年会長挨拶

第58回年会　年会長・実行委員長
大澤 研二
(群馬大学大学院理工学府)

第 58 回日本生物物理学会年会を、2020 年 9 月 16 日（水）から 18 日（金）までの 3 日間、群馬県高崎市の G メッセ群馬を会場として開催しようと、関東支部の委員により準備を進めてまいりました。しかし、新型コロナウイルス感染症の発生により、世界各地が甚大な被害を受け、日本国内でも人の往来が制限されたり、大規模な催しの開催が中止に追い込まれたりする事態となりました。

開催予定施設の G メッセ群馬は 2 ヶ月延期の後 6 月 1 日に開業されましたが、3 つの密が発生するイベントの開催は厳しく制限されることになりました。年会を主催する立場として、当然ながら、参加者の安全と健康を第一とする必要がありますので、今回は現地での開催ではなく、オンライン開催とすることを決定しました。

オンライン方式での開催となれば、参加者の皆さんにも多大な影響を及ぼすものと考えます。特に、発表にあたっては、情報伝達における障害の発生はもとより、発表内容の情報漏洩に関しても、多くの懸念があるものと思います。従来の方式でも、年会の発表においては撮影や録音は固く禁じられておりました。参加者の皆さんには研究に携わる者の倫理として、そのようなことは一切起きていないと信じておりますが、ネット上に情報が流れるとなれば、懸念が生じるのも致し方ないものと思います。そのため、第 58 回年会では、発表者の判断で発表内容を制限することに対しては、そのお考えを尊重します。

本年会のオンライン方式ではシンポジウムは一部を除き Zoom ミーティングでの開催とします。Zoom ミーティングでは通常の学会の講演と同じように、スライド上映などを行うことができますが、質疑応答に関してはチャット形式に限定することとします。一方、ポスター発表においては、アトラス社の Confit というシステムを使うことを決めました。このシステムではポスターを PDF 形式で掲示し、希望者は説明動画をつけることができます。こちらも質疑応答についてはチャット形式に限りますが、ポスター閲覧は各参加者が自由な時間に行えます。これらの方式で、日本生物物理学会独特の活発な議論の雰囲気ができることを期待しています。

今回は多くの高校生が参加しポスター発表いたします。高校生の発表者も、学会員の皆さんに混じって自由に議論ができるように配慮したいと考えています。

オンライン形式となりますが、会場でお会いするのを楽しみにしています。

第58回日本生物物理学会年会実行委員会
Organizing Committee

年会長・実行委員長	**Chair**
大澤 研二　（群馬大学）	Kenji Oosawa (Gunma University)
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会場（主担当）	**Venue**
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懇親会（主担当）	**Banquet**
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石川 良樹　（群馬県立県民健康科学大学）	Ryoki Ishikawa (Gunma Prefectural College of Health Sciences)
太田 善浩　（東京農工大学）	Yoshihiro Ohta (Tokyo University of Agriculture and Technology)
大沼 清　（長岡技術科学大学）	Kiyoshi Onuma (Nagaoka University of Technology)
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優 乙石　（前橋工科大学）	Isseki Yu (Maebashi Institute of Technology)

1日目 9月16日（水）				2日目 9月17日（木）	
9:00~11:30	12:00~13:00	13:30~16:00	16:30~18:30	9:00~11:30	12:00~13:00
<特別シンポジウム> 1SP コロイドから生体分子まで： 生物物理学の誕生と発展 （岡本 祐幸、 郷 通子）	キャリア支援説明会	<市民公開シンポジウム> 待ったなしの高大接続教育、いま学会は何をなすべきか？ （大澤 研二、 安藤 晃）		2S-1 生命現象の情報物理学 （石島 秋彦、 岡田 康志）	会員総会 （オンデマンド） 総会シンポジウム （オンライン）
	BPPB Editors' Choice Awardの発表 第9回BPPB 論文賞受賞講演	1S-1 生体機能の分子動画を撮像する革新的アプローチ （庄司 光男、 久保 稔）		2S-2 光操作による生命機能研究の新展開 （片岡 幹雄、 永田 崇）	
	バイオフィジックスセミナー クロマテクノロジジャパン合同会社	1S-2 最先端計測技術で拓く「生命金属科学」の新たなフロンティア研究」 （石森 浩一郎、 澤井 仁美）		2S-3 細胞の力学受容による多細胞システム恒常性の発現 （平田 宏聡、 野々村 恵子）	
		1YA 若手招待講演	ポスタービューイング & チャットタイム	2S-4 中国ー日本交流シンポジウム：膜分子ダイナミクスの最前線 （Junjie Hu、 Rikiya Watanabe、 Hiroko Bannai）	
				2S-5 光受容体の構造と機能を分光学で解き明かす （海野 雅司、 田母神 淳）	
				2S-6 タンパク質のフォールディング・ミスフォールディング・凝集の物理科学研究とその生命科学的背景 （黒田 裕、 新井 宗仁）	
				2S-7 免疫とがんにおけるシンギュラリティの検出と新たなイメージング技術 （花岡 健二郎、 竹馬 俊介）	

2日目 9月17日（木）		3日目 9月18日（金）		
13:30~16:00	16:30~19:00	9:00~11:30	12:00～13:00	13:30~16:00
2S-8 Happyな細胞に聞いた生命のしくみー井上信也博士に捧げる （谷 知己、 前島 一博）	2S-15 膜のリモデリングと組織化の分子基盤 （竹田 哲也、 末次 志郎）	3S-1 膜の海を旅するペプチド～ 脂質膜とペプチドの相互作用研究の新展開 （川村 出、 相沢 智康）	男女共同・若手支援シンポジウム	ポスタービューイング & チャットタイム
2S-9 膜タンパク質を「生きた」状態で再構成・解析・利用するための新しい脂質膜テクノロジー （安原 主馬、 森垣 憲一）	2S-16 新時代に突入したDNA-タンパク質研究 （Vaclav Brazda、 鎌形 清人）	3S-2 リニアモーターと細胞骨格が生む秩序と制御 （古田 健也、 矢島 潤一郎）	科研費説明会	
2S-10 Biomolecular Design to Control their Functions (門之園 哲哉、 DuyPhuoc Tran)	2S-17 もっと面白くなる細菌べん毛研究 ～残された宿題への挑戦～ （中村 修一、 加藤 貴之）	3S-3 磁覚と磁気応答生体物質の生物物理学 （新井 栄揮、 安達 基泰）	バイオフィジックスセミナー 株式会社 ニコン 株式会社 ニコンインステック	
2S-11 光生物学研究の多様性～分子から生物個体まで～ （小島 慧一、 山田 大智）		3S-4 タンパク質の多様な存在形態 ー その機能状態、動態から病態まで ー （谷中 冴子、 小川 覚之）		
2S-12 生体分子と薬剤の構造ゆらぎの生命機能科学 （米澤 康滋、 宮下 尚之）		3S-5 クロマチンの物理生物学 （木村 暁、 坂上 貴洋）		
2S-13 核酸が拓く新・生物物理研究 （片岡 幹雄、 永田 崇）		3S-6 光圧操作の新展開：生物物理学のための新しいアプローチ （細川 千絵、 西山 雅洋）		
2S-14 多様な細胞外微粒子の生体機能を探る （白崎 善隆、 田代 陽介）				

参加者へのご案内

１．参加方法

◇概要

本年会ホームページ（https://www2.aeplan.co.jp/bsj2020/index.html）のリンクからConfitにログインします。ログインには、IDとパスワードが必要になります。Confit内にもプログラムや抄録があり、それらを検索できます。Confit内で、参加するシンポジウムや、閲覧したいポスターを選択して先に進んでください。シンポジウムへの参加は、Zoomを使います。特別シンポジウム等の一部では、Zoomのwebinar機能を使いますが、通常のシンポジウムはZoomのmeeting機能を使います。**Zoomに参加する際には、参加登録番号＋氏名を参加者の名前として下さい。オーガナイザーから特別な許可がない限り、ご自身のマイクおよびカメラはオフにして下さい。**講演者への質問・コメントは、原則Zoomのチャット機能を使って伝える様にして下さい。

一般演題発表はポスターのみで、ポスターの画像ファイル（上限10MB）とともに希望者は動画ファイル（上限100MB、時間10分以内）を使って発表を行います。Confitにポスターが掲載されます。閲覧者は、その画像ファイルを自由に拡大縮小できます。質疑応答は、チャット形式で行います。時間に縛られることなく24時間好きな時間に、質問や、質問に対する回答を随時書き込んで下さい。ポスター発表者による説明義務時間帯は設定しませんが、代わりにチャットによる意見交換に集中する時間帯（初日9月16日（水）16:30~18:30および3日目9月18日（金）13:30~16:00）を設定します。活発な意見交換がなされることを期待しています。また、ポスター掲示・閲覧は、9月30日まで可能です。その間、チャット形式での質疑応答も可能です。

◇言語

特別シンポジウム、市民公開シンポジウムを除き、使用言語は原則英語です。

◆事前配布物

参加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、オンライン参加用ID、パスワードが事前にメールで送られます。また、プログラム集冊子も事前に送付されます。

注意1）参加登録は年会参加登録費（参加費）の振込後に完了します。振込がない場合登録は無効となります。

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、オンライン参加用ID、パスワードが送付されません。年度会費をお支払いください。

注意3）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、参加登録費は免除されます。

◇参加証

本年会は、オンライン開催のため参加証は送付いたしません。代わりに、オンライン参加用ID、パスワードをご登録いただきましたメールアドレスにお送りいたします。

◇領収書の発行

参加費の領収書が必要な場合は、年会事務局までご連絡下さい。

◇プログラム集冊子/オンライン予稿集【8月末　公開予定】

プログラム集冊子（前付・シンポジウムプログラム）は日本生物物理学会会員および事前登録が完了された非会員に事前に送付いたします。なお予稿本文はプログラム集冊子には掲載されません。ポスタープログラムと予稿本文は、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/58th_proceedings.pdf ダウンロードID：ambsj58 パスワード：webgunma2020

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（https://www.jstage.jst.go.jp/browse/biophys/-char/ja）

◇プログラム検索（ウェブ版）【8月24日(月) 公開予定】

年会ホームページで「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、発表日等を表示します。

◇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、会員としての参加をみとめません。また、日本生物物理学会への新規入会も受け付けます。

2．禁止事項

◇撮影・録音・スクリーンショット保存

PC画面のカメラ、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。またPCのスクリーンショット保存も厳禁とします。実行委員会は、理事会・組織委員会等の承認を得て、記録用として録画を行う場合があります。

3．年会についての問い合わせ

◇問い合わせ先

◆年会事務局

〒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 内
Tel: 06-6350-7163 FAX: 06-6350-7164
E-mail: jbp2020@aeplan.co.jp（年会全般）
E-mail: e_jbp58@aeplan.co.jp（広告・展示関連）

◆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: bsj2020sys-sprt@e-naf.jp

◆会期中の問い合わせ先 Tel: 080-4137-9158

謝 辞

本年会の開催・運営にあたり，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を申し上げます。

共催／協賛（敬称略）
JSTさきがけ「生命機能メカニズム解明のための光操作技術」
JSTさきがけ「生体における微粒子の機能と制御」
新学術領域研究「高速分子動画」
新学術領域研究「「生命金属科学」分野の創成による生体内金属動態の統合的研究」
新学術領域研究「発動分子科学：エネルギー変換が拓く自律的機能の設計」
新学術領域研究「情報物理学でひもとく生命の秩序と設計原理」
新学術領域研究「遺伝子制御の基盤となるクロマチンポテンシャル」
新学術領域研究「光圧によるナノ物質操作と秩序の創生」
新学術領域研究「シンギュラリティ生物学」

第５８回日本生物物理学会年会
年会長 大澤 研二

Greeting

The 58th Annual Meeting of the Biophysics Society of Japan
Chair of the Organizing Committee

Kenji Oosawa, Ph.D.

(Gunma University)

The conference committee had been preparing the 58th Annual Meeting of the Biophysical Society of Japan, to be held at G Messe Gunma in Takasaki, Gunma, from 16th to 18th of September, 2020. The current situation of a novel coronavirus disease (COVID-19) in and out of Japan, however, does not allow having social activities like the ones we used to have. Many restrictions have been imposed on everyday life and on big events to minimize impact of disease all over the world.

G Messe Gunma was opened at the beginning of June, but there are many types of restrictions imposed on a meeting held in the place for a certain time period. Under this condition, we have decided that the meeting should be held as the format of online conference, instead of physical conference at the G Messe Gunma prioritizing the safety and health of participants.

A lot of concerns may arise on an online style conference, especially on the data disclosure level of the presentation. Many concerns such as troubles on information transmission and information leakages have been already suggested. The past annual meetings have prohibited photography and recording of any formats during presentation, and hence this rule is applied to the online conference letting all the participants stay away from such conducts. However, we also understand that the concern remains and the decision on the presentation style and contents by the participants is highly esteemed.

We will use Zoom meeting style for symposia in the conference. We can use slide show for presentation, but we have to use chat system for comments and discussion. For poster presentation, we will use Confit developed by Atlas Co., Ltd. In this system, presenters can hang out their poster PDF with voice explanation. The posters can be visited any time. For comments and discussion for posters, chat system will be introduced. We are looking forward to having exciting meeting as usual in the Biophysics Society of Japan.

We invite high school students for poster presentations in this conference as well. And those high school students will participate in the poster session without any difference from the standard participants.

We look forward to seeing all of you at the 58th Annual Meeting of the Biophysics Society of Japan online in September.

16 (Wed.) September Day 1				September 17 (Thu.) Day 2	
9:00~11:30	12:00~13:00	13:30~16:00	16:30~18:30	9:00~11:30	12:00~13:00
<Special Symposium> 1SP From Colloids to Biomolecules: the Birth of Biophysics and its Development (Mitsuo Shoji, Minoru Kubo)	Career Support Events	<Public Symposium> Relationship of Scientific Societies to Partnerships between High Schools and Universities (Kenji Oosawa, Akira Ando)	Poster Viewing & Chat Discussion Time	2S-1 Information Physics of Living Matters (Akihiko Ishijima, Yasushi Okada)	General Meeting (On-demand) General Meeting Symposium (Online)
	The 9th Award Seminar of Outstanding Biophysics and Physicobiology Paper	1S-1 New Approaches Towards Molecular Movies of Biological Functions (Mitsuo Shoji, Minoru Kubo)		2S-2 New Horizon of Bio-function Studies by Light Control (Mikio Kataoka, Takashi Nagata)	
	<Biophysics Srminar> Chroma Technology Corporation	1S-2 New Frontiers of "Bio-metal Science" Opened with Cutting-Edge Techniques (Koichiro Ishimori, Hitomi Sawai)		2S-3 Cell Mechanosensing Underlies Homeostasis of Multicellular Systems (Hiroaki Hirata, Keiko Nonomura)	
		1YA Early Career Award in Biophysics Candidate Presentations		2S-4 China-Japan Joint Symposium (Junjie Hu, Rikiya Watanabe, Hiroko Bannai)	
				2S-5 Spectroscopic Approach for Exploring Structure andFunction of Photoreceptor Proteins (Masashi Unno, Jun Tamogami)	
				2S-6 Biophysical Studies on Protein Folding / Misfolding and Aggregation with Regard to Life Sciences (Yutaka Kuroda, Munehito Arai)	
				2S-7 Detection of Singularity in Immunity and Cancer by Novel Imaging Techniques (Kenjiro Hanaoka, Shunsuke Chikuma)	

September 17 (Thu.) Day 2		September 18 (Fri.) Day 3		
13:30~16:00	16:30~19:00	9:00~11:30	12:00~13:00	13:30~16:00
2S-8 Listening to Happy Cells Through the Microscope -A Tribute to Shinya Inoué (Tomomi Tani, Kazuhiro Maeshima)	2S-15 Molecular Basis for Membrane Remodeling and Organization (Tetsuya Takeda, Shiro Suetsugu)	3S-1 New Developments in Studies on Interactions between Membranes and Peptides (Izuru Kawamura, Tomoyasu Aizawa)	Gender Equality and Young Researchers Support Symposium	Poster Viewing & Chat Discussion Time
2S-9 New Lipid Membrane Technologies for Reconstitution, Analysis, and Utilization of 'Living' Membrane Proteins (Kazuma Yasuhara, Kenichi Morigaki)	2S-16 Beginning of a New Era for Investigation of DNA-Protein Systems (Vaclav Brazda, Kiyoto Kamagata)	3S-2 Order and Control: Linear Motors and Cytoskeleton 2020 (Ken'ya Furuta, Junichiro Yajima)	KAKENHI Guide Meeting	
2S-10 Biomolecular Design to Control their Functions (Tetsuya Kadonosono, DuyPhuoc Tran)	2S-17 Past, Present, and Future of the Bacterial Flagella~ Towards the Remaining Challenges~ (Shuichi Nakamura, Takayuki kato)	3S-3 Biophysics of Magnetoreception and Magnetic Responsive Biomaterials (Shigeki Arai, Motoyasu Adachi)	<Biophysics Srminar> NIKON CORPORATION / NIKON INSTECH CO.,LTD	
2S-11 Diversity of Photobiology ; From Molecules to Organisms (Keiichi Kojima, Daichi Yamada)		3S-4 The Multiple Modes of Proteins – From Molecular Dynamics to Pathogenesis (Yanaka Saeko, Tadayuki Ogawa)		
2S-12 Biofunctional Science of the Structural Fluctuations of Biomolecules and Drugs (Yasushige Yonezawa, Naoyuki Miyashita)		3S-5 Physical Biology of Chromatin (Akatsuki Kimura, Sakaue Takahiro)		
2S-13 Frontier of Nucleic Acid Biophysics (Kohki Okabe, Masahiro Takinoue)		3S-6 Frontiers in Optical Manipulation: New Approach for Biophysics (Chie Hosokawa, Masayoshi Nishiyama)		
2S-14 Open Up Extracellular Nanoparticles! -Their Diversity and Biodynamics (Yoshitaka Shirasaki, Yosuke Tashiro)				

Information for Participants

1. How to participate

◇Overview

Log in to Confit from the link on the Annual Meeting website (https://www2.aeplan.co.jp/bsj2020/index.html). ID and password are required an delivered to the participants beforehand via Email. The program and the abstracts are available on Confit.

For the symposium, select the symposium you want to attend on Confit. The symposium is held on Zoom, a web conferencing system. Some special symposia will use the webinar function of Zoom, and general symposium will use the meeting function of Zoom. **When joining the symposium through Zoom, please set your registration number + your name as the name of the participant. Please turn off your own microphone and camera** unless the organizer gives you specific permission. Questions and comments to the speakers should be communicated using the chat function of Zoom in principle.

The poster session is carried out on confit, too. The presenter can also use an additional movie file (no more than 100MB, 10 min) together with a poster image file (no more than 10MB) that must be prepared as a PDF format. Viewers can freely scale the image file using Confit's viewer system. Questions and answers are performed by the chat system of Confit. This is an online chat-type Q&A session, and the questions and answer can be written anytime. There is no compulsory presentation hour this year, but there is an intensive Q&A hour (the first day, September 16 (Wednesday) 16:30-18:30 and the third day (Friday, September 18 13:30~16:00)). We look forward to an active exchange of opinions. Also, posters can be displayed and viewed until the end of September. During that time, you can also ask and answer questions by chat function of Confit.

◇Language

The language used will be in English in principle, except for special and public symposia.

◇Receipt

If you need a receipt for your participation fee, please contact the Annual Meeting Secretariat.

◇Program booklet / Abstract online system【Release date: Aug. 31 (Mon.)】

A program booklet (general information of the annual meeting, and symposium program) will be sent in advance to BSJ members and non-members with advance registration. The abstracts and poster program will be released only on the online system. No printed abstract booklet will be issued. On the online system, the participants can browse, search and download abstracts.

Abstract online system :
http://www.biophys.jp/dl/pro/58th_proceedings.pdf
Download ID : ambsj58
PW : webgunma2020

The program(presentation title, presenter's name and affiliation) and the online abstracts will be released on the BSJ2020 web site. Half a 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. 24 (Mon.)】

Program search system will be released on the BSJ2020 web site.

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

If the annual membership fee of the Biophysical Society of Japan has not been paid, one cannot participate as a member. For non-members, we welcome you 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. Prohibited Items

◇ Photography & recording including screenshot saving

Photography and recording with camera, video, mobile phone and any device including screenshot saving is NOT allowed at the online meeting and poster sessions. The organization committee will record symposia as implementation evidence with the approval of the society board.

第 7 回会員総会シンポジウム：学会員のメリットとは？―賞推薦と受賞報告

オーガナイザー：日本生物物理学会　理事会
日　時：9 月 17 日（木）12:00 〜 13:00

概　要：本学会の法人化（2014 年）以降，それまで年会中に開催されていた会員総会の役割は，代議員による社員総会に移った。以後，会員総会では会長発案によるシンポジウムを開催することで，通常のシンポジウムとは異なる話題や課題を会員とともに考える場とすることとしている。学会の大きな役割と学会員のメリットの一つに，学会員の賞への推薦がある。受賞につながることは受賞者本人だけでなく，学会のプレゼンスを高める意味でもとても喜ばしいことである。普段あまり身近に感じることもないかも知れないが，今年度の年会では，2019 年度に内藤記念科学振興賞を受賞された神取秀樹氏（名古屋工業大学）と，中谷賞大賞を受賞された野地博行氏（東京大学）に受賞記念講演をお願いした。両氏のお祝いの場となるとともに，後に続く学会員がでることを強く願っている【会長・原田慶恵，副会長（賞・助成金担当）・須藤雄気】。

講演者・プログラム：
1. 神取秀樹氏（名古屋工業大学）「光遺伝学ツールとしての新規ロドプシンの開発」
2. 野地博行氏（東京大学）「デジタルバイオ分析法」

一般社団法人日本生物物理学会　第 9 回 Biophysics and Physicobiology 論文賞受賞講演会

The 9th 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 16 日（水）12:20 ～ 13:00 ／ Sep.16 Wed.
会　場：オンライン開催／ Online
形　式：講演会／ Lecture

第 9 回 Biophysics and Physicobiology 論文賞受賞者

坂野貴子，Md. Iqbal Mahmood，山下雄史，藤谷秀章
Takako Sakano, Md. Iqbal Mahmood, Takefumi Yamashita, Hideaki Fujitani
東京大学先端科学技術研究センター
Research Center for Advanced Science and Technology, The University of Tokyo

MD シミュレーションによるタンパク質－リガンド相互作用の研究
Molecular dynamics study on protein-ligand interaction

Understanding of the protein-ligand interaction is a key issue for the drug development [1]. Thus, many drug design software suites have been developed to predict the binding affinity based on the docking method. In the standard docking method, the binding affinity is predicted as an empirical binding score, following the protein-ligand complex structure prediction. Accordingly, the accurate prediction of the protein-ligand complex structure is quite important. Here, we utilized the molecular dynamics (MD) simulation to check the stability of the predicted complex structure. Although in the docking we used protein structures obtained by the high-resolution X-ray crystallography experiments, we often observed the complex structures were largely changed in the MD simulations, which indicated that the predicted complex structures were not the most stable. When the complex structure was unstable, we further observed that the ligand was dissociated from the protein. In this sense, we consider that the MD simulation can provide the information about the protein-ligand complex structure and modify the complex structure predicted by the docking [2]. Today, due to the advancement of computer power, as symbolized by the supercomputers, K and Fugaku, the MD simulation becomes a popular method and is applied to more challenging problems. This seminar will review and discuss the recent MD studies on the ligand-protein simulation.

[1] Yamashita, T. et al. (2015). *Chem. Pharm. Bull.,* 63: 147-155.
[2] Sakano, T., Mahmood, M. I., Yamashita, T., & Fujitani, H. (2016). *Biophys. Physicobiol.*, 13: 181-194.

男女共同参画・若手支援委員会企画シンポジウム
今だから，今こそ，今なら言いたい，「博士を取ろう！」

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：2020 年 9 月 18 日（金）12:00 〜 13:30
会　場：オンライン開催
言　語：日本語
形　式：講演会
司　会：大上雅史（東工大）
シンポジスト：池田宗太郎（文部科学省 研究振興局 基礎研究振興課），上村みどり（帝人ファーマ 生物医学総合研究所），落合陽一（筑波大学／ピクシーダストテクノロジーズ）

概　要：「博士課程に進んでも取ってくれる企業が減って就活に不利になるから〜」，「最近は任期付きのアカデミックポジションしかなくて不安定だから〜」，「27 歳にもなって学生でいるのもなあ〜」。博士課程・博士の学位を取ることへのネガティブな話題は事欠きません。周りの先生は博士取得を勧めてくるのだけど，いまいちメリットがピンと来ないという方も多いでしょう。でもそれは仕方がないことかもしれません。周りの先生はアカデミアに就職した人というサンプルに過ぎなく，企業や官公庁で働く博士の人たちにはなかなか出会う機会がないのですから。

私たち日本生物物理学会 男女共同参画・若手支援委員会でも，多様なキャリアパスを目指せるよう，企画シンポジウムを年会で開催して話題提供を続けています。直近では，『キャリアデザインの第一歩―大学院生・研究者のための自己分析ワーク―』（2016 年つくば年会），『20 代 , 30 代を駆け抜けて：伝えたいこと，聞きたいこと』（2019 年宮崎年会）など，講演会やワークショップを通じて参加者と一緒にキャリアパスを考える機会を作ってきました。しかしながら，それでも実際に博士を取ってアカデミア以外で活躍される方の話は，依然として聞けるチャンスは少なかったと思います。

そこで今年は，（せっかくのオンライン開催なのですから！）アカデミア以外の場にも焦点を当て，実際に企業や官公庁で活躍されている方々に，博士を取ること・取ったことのメリット・デメリットを含めた率直な話を聞いてみたいと思います。「産官学」，産＝産業界から帝人ファーマで創薬研究開発を進められている上村みどりさん，官＝官公庁から文部科学省で科学技術政策や研究人材育成に関わる池田宗太郎さん，産学＝大学・アカデミアと産業界を跨いで活躍されている筑波大／ピクシーダストテクノロジーズの落合陽一さんより，良かったことを（もしかしたら悪かったことも）存分に語って頂きましょう。本シンポジウムが若手研究者の皆さんのキャリアを考える一助になれば幸いです。

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 16 日（水）12:00 ～ 13:00
形　式：オンライン開催（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，今年度も「キャリア支援説明会」を開催します。昨年の反響を受けて本年会は，（株）アカリクから講師を迎えて大学院生やポストドクター向けの就職支援活動セミナーを実施します。また，昨年度と同様に今年度も個別キャリア相談会を実施いたしますので，是非ご活用ください。博士課程出身のアカリク社員が何でも質問に答えます！

プログラム：理系大学院生や研究者の就活・転職について，「専門外就職」や「博士人材向け」の情報も交えてお話しいたします。

【Part 1】12:00 ～ 12:20　博士・PD の方の為の就活ガイダンス
徐々に企業の採用対象として存在感を増してきている博士人材ですが，研究実績があっても状況の把握や伝え方を誤れば機会を逃してしまいます。そこで，①企業の採用活動の現在，②博士や PD の就職活動の実態，③博士人材が活躍できる企業の探し方を中心に紹介します。

【Part 2】12:20 ～ 12:40　理系大学院生の就活ケーススタディ
周りを見れば大枠としてどのように就職活動しているか見えてくるかと思いますが，自身に最適な方法や目標を見つけるのは至難の業です。ここでは実際にアカリクで支援した方の情報をもとにして，状況に応じてどのような戦略や戦術が有効なのかを解説します。

【Part 3】12:40 ～ 13:00　専門外就職へ向けて何をすべきか
専門性が高いほど技術や知識がそのまま活用できる仕事は少なくなりますが，その専門性を構成する要素を紐解くことで「専門外」の領域で幅広く活躍することが視野に入ってきます。専門外就職を目指す上で特に注意すべき「一貫性」を中心に書類の書き方や面接対策などのノウハウを解説します。

個別キャリア相談会：就職活動・キャリアに関する悩みや不安を気軽にご相談ください。また就活ノウハウや企業での待遇面など分からないことがあれば遠慮なくお尋ねください。お申込方法は年会ウェブサイトをご確認ください。

科学研究費助成事業について
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主任研究員）

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

日　時：9 月 18 日（金）12:00 〜 13:00

会　場：オンライン開催

言　語：日本語

形　式：プレゼンテーション

概　要：今，日本が将来にわたって卓越した研究成果を持続的に生み出し続け，世界の中で存在感を保持できるかが問われています。こうした中，科学技術･学術審議会において，学術研究への現代的要請として，「挑戦性・総合性・融合性・国際性」の四つを挙げ，科研費制度の抜本的改革が提言されました。これを踏まえ，文部科学省では「科研費改革の実施方針」を策定し，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（「審査システム改革 2018」）が行われ，平成 30 年度科研費（平成 29 年 9 月公募）において，新たな審査システムによる審査を実施しました。今回は，このシステム改革の内容のほか，その他の改善や充実を図った点等について，日本学術振興会から講演者をお招きしてご説明をいただきます。

第 1 日目（9 月 16 日（水））／Day 1（Sep. 16 Wed.）

13:30〜16:00
1YA　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

Biophysical Society of Japan (BSJ) grants “Early Career Award in Biophysics” and “Early Career Presentation Award” to young BSJ members for their excellent presentations that show great potential to contribute to the progress of biophysics. In this 16th year, we received 25 highly qualified applications. After the first round of competitive screening based on submitted documents, the 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 awardees of the Early Career Award in Biophysics will be selected. The Early Career Presentation Award will be given to the rest of the excellent invited speakers.

13:30　Jakia Jannat Keya　20227G
1YA1330　Autonomous molecular swarm robots realized by sequential transfer of DNA signal
Jakia Jannat Keya[1], Yuta Yamasaki[2], Kazuki Sada[1], Akinori Kuzuya[2], Akira Kakugo[1] ([1]*Hokkaido University*, [2]*Kansai University*)

13:45　村上　光　20250H
1YA1345　1 細胞自律的な細胞内温度制御の分子機構
A cell-autonomous control of intracellular temperature by mitochondrial thermogenesis
○村上 光 [1,2], 長尾 耕治郎 [1], 坂口 怜子 [1], 岡部 弘基 [2], 原田 慶恵 [3], 梅田 眞郷 [1]（[1]京大・院工・合成・生物化学, [2]東大・院薬, [3]阪大・蛋白研）
Akira Murakami[1,2], Kohjiro Nagao[1], Reiko Sakaguchi[1], Kohki Okabe[2], Harada Yoshie[3], Masato Umeda[1] ([1]*Dept. of Synth. Chem. And. Biol. Chem., Grad. Sch. of. Eng., Kyoto Univ.*, [2]*Grad. Sch. of Pharm. Sci., Univ. of Tokyo*, [3]*Inst. for Protein Res., Osaka Univ.*)

14:00　大貫　隼　20121A
1YA1400　非リボソーム分子機械によるペプチド合成の静電的ラチェット機構
Electrostatic ratcheting mechanism of peptide synthesis by non-ribosomal molecular machine
○大貫 隼, 高野 光則（早大・物理応物）
Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

14:15　岡畑　美咲　20343K
1YA1415　線虫 *C. elegans* を用いた異なる感覚情報の統合に関わる神経回路モデル
The model of neural circuit integrating different sensory information in *C. elegans*
○岡畑 美咲 [1], Wei Aguan D.[2], 太田 茜 [1], 久原 篤 [1,3] ([1]甲南大統合ニューロバイオロジー研究所, [2]SEA Children’s Research Inst., [3]日本医療研究開発機構）
Misaki Okahata[1], Aguan D. Wei[2], Akane Ohta[1], Atsushi Kuhata[1,3] ([1]*Inst. for Integrative Neurobio., Konan Univ.*, [2]*SEA Children’s Research Inst.*, [3]*AMED-PRIME*)

14:30　佐藤　航　20086A

1YA1430　シトクロム *c* が仲介する多段階電子伝達反応における呼吸鎖超複合体形成の機能的意義

Functional significance of formation of respiratory supercomplex for multiple electron transfer reaction mediated by cytochrome *c*

○佐藤 航, Brzezinski Peter（ストックホルム大 院理）

Wataru Sato, Peter Brzezinski (*Stockholm Univ. Fac. of Nat. Sci.*)

14:45　志甫谷　渉　20042A

1YA1445　ヘリオロドプシンおよびシゾロドプシンの構造から明らかになった微生物型ロドプシンの多様性

Structures of heliorhodopsin and schizorhodopsin elucidate the structural diversity of microbial rhodopsins

○志甫谷 渉[1], 井上 圭一[2], マニッシュ シン[3], 樋口 昌光[1], 今野 雅恵[2], 吉住 玲[3], 内橋 貴之[4], 神取 秀樹[3], 濡木 理[1]（[1]東大院理生物, [2]東大物性研, [3]名工大院工生命, [4]名大院理物理）

Wataru Shihoya[1], Keiichi Inoue[2], Singh Manish[3], Akimitsu Higuchi[1], Masae Konno[2], Rei Yoshizumi[3], Takayuki Uchihashi[4], Hideki Kandori[3], Osamu Nureki[1] ([1]*Dept. of Biol., Grad. Sch. Sci, Univ. of Tokyo*, [2]*ISSP, Univ. of Tokyo*, [3]*Life Sci. Appl. Chem., Grad. Sch. Eng., NIT*, [4]*Dept. of Phys., Grad. Sch. Sci, Nagoya Univ.*)

15:00　下林　俊典　20248H

1YA1500　細胞内脂肪滴の普遍的相挙動

Liquid-liquid crystal phase transitions in intracellular lipid droplets

○下林 俊典[1], 大崎 雄樹[2]（[1]プリンストン大・化学生物工学, [2]名大・院医学）

Shunsuke F. Shimobayashi[1], Yuki Ohsaki[2] ([1]*Chemical Biological Engineering, Princeton Univ.*, [2]*Grad. Sch. Med., Nagoya Univ.*)

15:15　田村　康一　20025A

1YA1515　Theoretical Study on the Transport Cycle of the Heme ABC Transporter BhuUV-T

Koichi Tamura[1], Yuji Sugita[1,2,3] ([1]*RIKEN R-CCS*, [2]*RIKEN BDR*, [3]*RIKEN CPR*)

15:30　植木　紘史　20530S

1YA1530　2 光子生体イメージングでみるインフルエンザウイルス感染肺

In vivo imaging of the cellular pathophysiology in influenza virus-infected mouse lung

○植木 紘史[1], 河岡 義裕[1,2,3]（[1]東大医科研 ウイルス感染分野, [2]東大医科研 感染症国際研究センター 高病原性感染症系, [3]Department of Pathobiological Sciences, School of Veterinary Medicine, University of Wisconsin-Madison.）

Hiroshi Ueki[1], Yoshihiro Kawaoka[1,2,3] ([1]*Division of Virology, Department of Microbiology and Immunology, Institute of Medical Science, University of Tokyo*, [2]*Department of Special Pathogens, International Research Center for Infectious Diseases, Institute of Medical Science, University of Tokyo*, [3]*Department of Pathobiological Sciences, School of Veterinary Medicine, University of Wisconsin-Madison*)

15:45　山本　詠士　20326I

1YA1545　Effect of lipid quality on the association of membrane bound proteins with phosphoinositide-containing membranes

Eiji Yamamoto[1], Junko Sasaki[2], Takehiko Sasaki[2], Mark S. P. Sansom[3] ([1]*Department of System Design Engineering, Keio University*, [2]*Medical Research Institute and Graduate School of Medical and Dental Sciences, Tokyo Medical and Dental University*, [3]*Department of Biochemistry, University of Oxford*)

9:00〜11:30
1SP　**コロイドから生体分子まで：生物物理学の誕生と発展**
From Colloids to Biomolecules: the Birth of Biophysics and its Development

オーガナイザー：岡本 祐幸（名古屋大学），郷 通子（長浜バイオ大学/中部大学）
Organizers: Yuko Okamoto (Nagoya University), Mitiko Go (Nagahama Institute of Bio-Science and Technology/ Chubu University)

One of big flow of biophysics research in Japan was started by Professor Fumio Oosawa. His first research field was colloids, which led to the depletion force of Asakura-Oosawa Theory. He then moved to study the transitions between the G-actin and F-actin, which gave one of the earliest results of biophysics research in Japan. In this Symposium, leaders of colloid and biophysics research will look back the paths that Professor Oosawa took and present their latest results that came out from Oosawa's works.

はじめに
Opening Remarks
岡本 祐幸（名古屋大学大学院理学研究科物質理学専攻(物理系)）
Yuko Okamoto (*Department of Physics, Nagoya University*)

1S-P-1　**ソフトマター物理と大沢**
Contribution of Fumio Oosawa to Soft Matter Physics
○栗原 和枝（東北大, 未来科学技術共同研究センター）
Kazue Kurihara (*NICHe, Tohoku Univ.*)

1S-P-2　Asakura-Oosawa **理論とその広がり**
Variations on a Theory by Asakura and Oosawa
○秋山 良（九州大学大学院理学研究院化学部門）
Ryo Akiyama (*Department of Chemistry, Kyushu University*)

1S-P-3　**生物運動の仕組みを解く：大沢さんから学んだもの**
Unraveling the Mechanism of Biological Movement: What I Learned from Oosawa-san
○石渡 信一（早稲田大学理工学術院物理学科）
Shin'ichi Ishiwata (*Waseda University, Faculty of Science and Engineering, Department of Physics*)

1S-P-4　**アクチン ATP 加水分解反応のメカニズム：ATPase 蛋白質の共通性と独自性**
Reaction mechanism of actin ATP hydrolysis: as compared with other ATP hydrolysis proteins
○前田 雄一郎（名古屋大学大学院情報学研究科）
Yuichiro Maeda (*Nagoya University, Graduate School of Informatics*)

1S-P-5　**筋収縮とイオン能動輸送**
Muscle contraction and ion active transport
○神山 勉（名古屋大学大学院理学研究科物理学専攻）
Tsutomu Kouyama (*Nagoya Univ. Graduate School of Science*)

1S-P-6 揺らぎと生命機能
Fluctuation and the function of life
○柳田 敏雄 [1,2]（[1]大阪大学大学院生命機能研究科, [2]情報通信研究機構 脳情報通信融合研究センター）
Toshio Yanagida[1,2] ([1]*Osaka University Graduate school of Frontier Biosciences*, [2]*NICT CiNet*)

1S-P-7 アクチン重合の熱力学測定～ギブスの平行論に沿って～
Thermodynamic quantities of actin polymerization ~along Gibbs' equilibrium theory~
○菊本 真人 [1], 大澤 文夫 [2,3]（[1]名大理生命分 3 成田 G, [2]名大／阪大名誉教授, [3]故人）
Mahito Kikumoto[1], Fumio Oosawa[2,3] ([1]*NaritaG, Bio., Sci., Nagoya-u.*, [2]*Prof.Emertis,Nagoya/Osaka-u.*, [3]*Deceised*)

1S-P-8 筋収縮とその制御におけるアクチン繊維の構造と役割
Actin filament in muscle contraction and regulation
○難波 啓一 [1,2,3]（[1]大阪大学大学院生命機能研究科, [2]理研生命機能科学研究センター・放射光科学研究センター, [3]大阪大学 日本電子 YOKOGUSHI 協働研究所）
Keiichi Namba[1,2,3] ([1]*Graduate School of Frontier Biosciences, Osaka University*, [2]*RIKEN Center for Biosystems Dynamics Research and Spring-8 Center*, [3]*JEOL YOKOGUSHI Research Alliance Laboratories, Osaka University*)

おわりに
Closing Remarks
郷 通子（長浜バイオ大学、中部大学）
Mitiko Go (*Nagahama Institute of Bio-Science and Technology/Chubu University*)

13:30～16:00
1S-1 共催：新学術領域研究「高速分子動画」
生体機能の分子動画を撮像する革新的アプローチ
New Approaches towards molecular movies of biological functions

オーガナイザー：庄司 光男（筑波大学），久保 稔（兵庫県立大学）
Organizers: Mitsuo Shoji (University of Tsukuba), Minoru Kubo (University of Hyogo)

Time-resolved (TR) crystallography using X-ray free electron lasers (XFEL) is being established as a technique for making “molecular movies” of biological molecules over the past few years. As a next step, to deepen our understanding of how dynamically proteins work, the collaborative analyses of “molecular movies” with various kinds of biophysical methods, including the latest theoretical approaches, are required. In this session, we will share recent challenges and achievements of TR-crystallography and other state of the art experimental and theoretical techniques, to build up the dynamic pictures of proteins from the microscopic to macroscopic points of view.

1S-1-1 Protein dynamics structures revealed by time-resolved serial femtosecond crystallography
Eriko Nango[1,2] ([1]*IMRAM, Tohoku Univ.*, [2]*RIKEN RSC*)

1S-1-2 分子動画に基づく量子分子動力学シミュレーションによるバクテリオロドプシンにおけるプロトン移動の微視的機構の解明
Microscopic mechanisms of proton transfers in bacteriorhodopsin revealed by quantum molecular dynamics method based on molecular movies
○小野 純一 [1,2]（[1]京大学際融合センター, [2]早大理工総研）
Junichi Ono[1,2] ([1]*C-PIER, Kyoto Univ.*, [2]*WISE, Waseda Univ.*)

1S-1-3 分子シミュレーションによるタンパク質の機能活性化過程の原子論的解明
Atomistically Deciphering Functional Activation Processes of Proteins with Molecular Simulations
○林 重彦（京大院理）
Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

1S-1-4 Observation of protein dynamics with solution scattering
Masaaki Sugiyama, Rintaro Inoue (*Kyoto University*)

1S-1-5 SPring-8 におけるシリアル放射光結晶解析法の開発
Develpment of serial synchrotron crystallography at SPring-8
○熊坂 崇（（公財）高輝度光科学研究センター タンパク質結晶解析推進室）
Takashi Kumasaka (*Prot. Cryst. Anal. Div., Jpn. Sync. Rad. Res. Inst.*)

1S-1-6 SACLA を用いたチャネルロドプシンの時分割構造解析によって明らかになったイオン透過経路形成の初期構造変化
Time-resolved serial femtosecond crystallography reveals early structural changes in channelrhodopsin
○西澤 知宏（東京大学）
Tomohiro Nishizawa (*The Univ. of Tokyo*)

13:30〜16:00
1S-2 共催：新学術領域研究「「生命金属科学」分野の創成による生体内金属動態の統合的研究」最先端計測技術で拓く「生命金属科学」の新たなフロンティア
New Frontiers of “Bio-metal Science” Opened with Cutting-Edge Techniques

オーガナイザー：石森 浩一郎（北海道大学），澤井 仁美（兵庫県立大学）
Organizers: Koichiro Ishimori (Hokkaido University), Hitomi Sawai (University of Hyogo)

Trace amounts of “bio-metals” are essential for maintaining our life, but we have not yet fully understood molecular mechanisms of how they function in proteins, cells, organs, and bodies. Extensive researches of “bio-metals” have been explored by the development of precise biophysical measurements and visualization of trace metals in biological materials. Cuttingedge developments of NMR, EPR, mass spectrometry, chemical imaging, and nuclear resonance vibrational spectroscopy (NRVS) are now opening the door for new strategies to understand “bio-metals” and establish “bio-metal science”. In this symposium, pioneers of the measurements and exploitation of “bio-metals” are invited to introduce their marvelous techniques and discuss recent achievements toward medical and environmental applications.

1S-2-1 Native mass spectrometry for Bio-Metal Science
Satoko Akashi (*Grad. Sch. Med. Life Science, Yokohama City Univ.*)

1S-2-2 X-ray Crystallography and EPR Spectroscopy Reveal Active Site Rearrangement of Cold-Adapted Inorganic Pyrophosphatase
Masaki Horitani[1], Hiroshi Sugimoto[2], Keiichi Watanabe[1] ([1]*Saga Univ., Dept of Appl Biochem & Food Sci*, [2]*RIKEN, SPring-8 Center*)

1S-2-3 Exploiting paramagnetic metal ions for protein structural study in solution
Tomohide Saio, Koichiro Ishimori (*Faculty of Science, Hokkaido University*)

1S-2-4 **複数の異なる NMR データの統合解析によるタンパク質 multi-state 立体構造解析**
Multi-state protein structure determination by integrated analysis of several NMR data sets
○池谷 鉄兵, 伊藤 隆（東京都立大学理学研究科）
Teppei Ikeya, Yutaka Ito (*Graduate School of Science, Tokyo Metropolitan University*)

1S-2-5 **核共鳴振動分光法による鉄含有酵素の元素選択的測定 -世界最強強度の放射光源を利用した最近の進展-**
Atom-selective measurement of iron enzymes by nuclear resonance vibrational spectroscopy
○依田 芳卓（（公財）高輝度光科学研究センター 精密分光推進室）
Yoshitaka Yoda (*Japan Synchrotron Radiation Research Institute*)

1S-2-6 **量子ビームによる細胞内生命金属動態**
Application of quantum beam elemental analyses for dynamics of cellular distribution of bio-metals
○武田 志乃（量子科学技術研究開発機構放射線医学総合研究所）
Shino Homma-Takeda (*National Institutes for Quantum and Radiological Sciences*)

2 日目（9 月 17 日（木））／Day 2（Sep. 17 Thu.）

9:00〜11:30
2S-1 **共催：新学術領域研究「情報物理学でひもとく生命の秩序と設計原理」**
生命現象の情報物理学
Information physics of living matters

オーガナイザー：石島 秋彦（大阪大学），岡田 康志（東京大学）
Organizers: Akihiko Ishijima (Osaka University), Yasushi Okada (The University of Tokyo)

Information or signaling has been one of the core concepts to understand the biological systems. Recent progress in technologies has enabled quantitative measurements of biological phenomena even at a single molecule level. However, theoretical framework(s) are still missing that can handle information in biological systems in a quantitative and unified manner. Meanwhile, a new physics theory is emerging at the interface of the thermodynamics and the information theory. Now, information can be treated as a physical quantity just like heat or mechanical works. In this symposium, we aim to establish a new interdisciplinary research field by applying this new information physics to biological systems.

はじめに
Opening Remarks
岡田 康志（東京大学）
Yasushi Okada (*The University of Tokyo*)

2S-1-1 Thermodynamic inequalities and applications to biological systems
Andreas Dechant, Shin-ichi Sasa (*Grad. Sch. Sci., Kyoto U.*)

2S-1-2 **ERK MAPK 活性化の熱力学コストを定量化する情報幾何学的手法**
Information-geometric method to quantify the thermodynamic cost of ERK MAPK activation
芦田 慶太 [1], 青木 一洋 [2], ○伊藤 創祐 [1,3]（[1]東京大学 理学系研究科 生物普遍性研究機構, [2]自然科学研究機構 生命創成探究センター, [3]JST 戦略的創造研究推進事業, さきがけ）
Keita Ashida[1], Kazuhiro Aoki[2], **Sosuke Ito**[1,3] ([1]*Universal Biology Institute, the University of Tokyo*, [2]*Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences*, [3]*JST PRESTO*)

2S-1-3 高密度バクテリア集団研究のための広域マイクロ灌流系と、それによる細胞集団の統計物理学・情報物理学実験の試み
Extensive microperfusion system for dense bacterial populations and its applications for statistical physics of cells with information
○竹内 一将（東大・理 物理）
Kazumasa A. Takeuchi (*Dept. Physics, Univ. Tokyo*)

2S-1-4 バクテリア走化性の情報物理学
Information Physics of Bacterial Chemotaxis
○小林 徹也 [1,2], 中村 絢斗 [2]（[1]東京大学 生産技術研究所 小林(徹)研究室, [2]東京大学 情報理工学系研究科 数理情報学専攻）
Tetsuya Kobayashi[1,2], Kento Nakamura[2] ([1]*Institute of Industrial Science, the University of Tokyo*, [2]*Department of Mathematical Informatics, Graduate School of Information Science and Technology, the University of Tokyo*)

2S-1-5 アクティブマター系でのレヴィ・フライトのミクロ導出
Microscopic theory for Levy flights in active suspension
○金澤 輝代士（筑波大学システム情報系）
Kiyoshi Kanazawa (*Faculty of Engineering, Information and Systems, University of Tsukuba*)

2S-1-6 Condensed matter concepts in collective cell dynamics
Kyogo Kawaguchi[1,2,3] ([1]*RIKEN CPR*, [2]*RIKEN BDR*, [3]*UBI, Univ. Tokyo*)

9:00〜11:30
2S-2 共催：JST さきがけ「生命機能メカニズム解明のための光操作技術」光操作による生命機能研究の新展開
New horizon of bio-function studies by light control

オーガナイザー：片岡 幹雄（奈良先端科学技術大学院大学），永田 崇（東京大学）
Organizers: Mikio Kataoka (NAIST), Takashi Nagata (The University of Tokyo)

The recent remarkable advances in optogenetics, which are not limited to brain research, made it possible to further advance our understanding of many biological systems and functions. In addition to optogenetics utilizing light-sensitive proteins, various other techniques to observe, measure, analyze and control biological processes by light have also been developed one after another. In this symposium, researchers who are making remarkable contributions to life sciences by developing or applying light control techniques will discuss the present and future of the light control techniques to shed new light on their possibilities and expandability from basic biology to medical application.

2S-2-1 Optogenetic control of intracellulary expressed functional antibodies
Fuun Kawano[1,2] ([1]*The University of Tokyo*, [2]*JST PRESTO*)

2S-2-2 オプトメカニカル画像走査による高速ライトシート顕微鏡
High-speed light-sheet microscopy using optomechanical image scanning
○三上 秀治 [1,2,3]（[1]北大電子研, [2]東大理, [3]JST さきがけ）
Hideharu Mikami[1,2,3] ([1]*RIES, Hokkaido Univ.*, [2]*Sc. Sci., UTokyo*, [3]*PRESTO, JST*)

2S-2-3　フェムト秒レーザー誘起衝撃力による細胞操作とその物理
Single cell manipulations utilizing femtosecond laser impulse and the physics
○細川 陽一郎（奈良先端科学技術大学院大学物質創成科学領域）
Yoichiroh Hosokawa (*Divison of Materials Science, Nara Institute of Science and Technology*)

2S-2-4　Optogenetic control of phospholipids flipping and related biomembrane functions in budding yeast
Tomomi Suzuki[1,2], Tetsuo Mioka[3], Kazuma Tanaka[3], Akira Nagatani[1] ([1]*Grad. Sch. Sci, Kyoto Univ.*, [2]*JST, PRESTO*, [3]*Genetic Medicine Inst., Hokkaido Univ.*)

2S-2-5　植物の高速シグナル伝達を視る
Shining light on rapid signal transduction in plants
○豊田 正嗣（埼玉大・院理工）
Masatsugu Toyota (*Dept. Biochem. & Mol. Biol., Saitama Univ.*)

2S-2-6　光による不随意運動疾患根治法
Optogenetic neuromodulation for movement disorders
○吉田 史章（佐賀大・医）
Fumiaki Yoshida (*Saga Univ.Med.Sch.*)

おわりに
Closing Remarks

9:00〜11:30
2S-3　細胞の力学受容による多細胞システム恒常性の発現
Cell mechanosensing underlies homeostasis of multicellular systems

オーガナイザー：平田 宏聡（名古屋大学），野々村 恵子（基礎生物学研究所）
Organizers: Hiroaki Hirata (Nagoya University), Keiko Nonomura (NIBB)

Development and homeostasis of tissues depend on spatiotemporal control of constituent cell behaviors. Cells in tissues interact not only chemically but also mechanically with their surrounding environments including interstitial and vascular fluids, neighboring cells, and extracellular matrices. In this symposium, we discuss, from both experimental and theoretical viewpoints, how cells detect mechanical inputs from surroundings and integrate them with chemical information to achieve homeostatic regulation of multicellular systems.

2S-3-1　角化細胞の増殖の接触阻害には接着結合の引張力が必須である
Tensile force at adherens junctions is responsible for contact inhibition of keratinocyte proliferation
○平田 宏聡, Dobrokhotov Oleg, 曽我部 正博（名大・院医）
Hiroaki Hirata, Oleg Dobrokhotov, Masahiro Sokabe (*Grad. Sch. Med., Nagoya Univ.*)

2S-3-2　細胞間シグナル–上皮リモデリングのフィードバックループが制御する神経管閉鎖ジッパリング
Dynamic integration of signaling, force generation and tissue remodeling control zippering and neural tube closure
○橋本 秀彦[1], ロビン フランソワ[2], シェラード クリスティン[1], ムンロ エドウィン[1]（[1]シカゴ大学, [2]ソルボンヌ大学）
Hidehiko Hashimoto[1], Francois Robin[2], Kristin Sherrard[1], Edwin Munro[1] ([1]*University of Chicago*, [2]*Sorbonne University*)

2S-3-3 Strain-triggered mechanical feedback in self-organizing epithelial morphogenesis
Satoru Okuda (*Nano Life Science Institute, Kanazawa University*)

2S-3-4 Cell dynamics under high hydrostatic pressure conditions
Masatoshi Morimatsu[1], Masayoshi Nishiyama[2], Keiji Naruse[1] ([1]*Grad. Sch. of Med., Dent. and Pharma. Sci., Okayama Univ.*, [2]*Department of Physics, Kindai Univ.*)

2S-3-5 Mechanical stress by extracellular confinement trigger a mode transition of neuronal migration
Naotaka Nakazawa[1], Gianluca Grenci[2], Mineko Kengaku[1,3] ([1]*iCeMS, Kyoto University*, [2]*Mechanobiology Institute, National University of Singapore*, [3]*Graduate School of Biostudies, Kyoto University*)

2S-3-6 リンパ管の弁の形成における Piezo1 を介した空間的に規定されたメカノトランスダクション
Spatially defined mechanotransduction via Piezo1 involved in lymphatic valve formation
○野々村 恵子 [1], 勝田 紘基 [2], 蟹江 朱美 [1], Patapoutian Ardem[3], 藤森 俊彦 [1] ([1]基礎生物学研究所, [2]名古屋大学大学院医学系研究科, [3]スクリプス研究所)
Keiko Nonomura[1], Hiroki Katsuta[2], Akemi Kanie[1], Ardem Patapoutian[3], Toshihiko Fujimori[1] ([1]*National Institute for Basic Biology*, [2]*Nagoya Univ. Grad. Sch. Med.*, [3]*The Scripps Institute*)

9:00〜11:30
2S-4 中国-日本交流シンポジウム：膜分子ダイナミクスの最前線
China-Japan Joint Symposium: Frontline of membrane dynamics

Organizers: Junjie Hu (Institute of Biophysics, CAS), Rikiya Watanabe (RIKEN), Hiroko Bannai (Waseda University)

Basic principle underlying the membrane self-assembly, membrane fusion, and membrane transport between different organella, has been a long-time question in the field of biophysics. In this symposium, we aim to exchange knowledge and cutting-edge technologies on membrane dynamics between researchers from China and Japan, to opening up new horizons in membrane dynamics research. Four leading biophysicists from China will present their recent studies on intracellular membrane trafficking, organella shaping and remodeling, and membrane protein interactions. Researchers from Japan will introduce imaging and simulation studies at single-molecule resolution contributing to elucidate the molecular mechanism underlying membrane dynamics and membrane protein functions.

Opening Remarks
Rikiya Watanabe[1], Hiroko Bannai[2] ([1]*RIKEN*, [2]*Waseda University*)

2S-4-1 Molecular mechanisms that regulate secretion of sonic hedgehog
Yusong Guo (*Division of Life Science, Hong Kong University of Science and Technology*)

2S-4-2 自己組織化による細胞極性形成の 1 分子粒度シミュレーション
Self-organization in cellular polarity signaling reconstituted by single-molecule-imaging based single-particle simulation
○松岡 里実 [1,2,3], 上田 昌宏 [1,2] ([1]阪大・院生命機能, [2]理研・生命機能科学, [3]科学技術振興機構さきがけ)
Satomi Matsuoka[1,2,3], Masahiro Ueda[1,2] ([1]*Grad. Sch. Frontier Biosciences, Osaka Univ.*, [2]*BDR, RIKEN*, [3]*PRESTO, JST*)

2S-4-3 Towards the mechanism of mitochondrial outer membrane fusion
Song Gao (*Sun Yat-sen University Cancer Center*)

2S-4-4　1 分子イメージングによる生細胞膜中の GPCR シグナロソーム計測
Single-molecule imaging of GPCR signalosome in living cell membrane
○柳川 正隆（独立行政法人 理化学研究所 佐甲細胞情報研究室）
Masataka Yanagawa (*Cellular Informatics Lab., Riken*)

2S-4-5　A proximity labeling method to resolve membrane protein interaction networks
Min Zhuang (*School of Life Science and Technology, ShanghaiTech University*)

2S-4-6　1 分子イメージングで明らかになったラフト組織化と機能
Raft organization and function as revealed by single-molecule imaging
○鈴木 健一 [1,2]（[1]岐阜大・G-CHAIN, [2]東海国立大学機構糖鎖生命コア研究拠点）
Kenichi Suzuki[1,2] ([1]*G-CHAIN, Gifu Univ.*, [2]*Tokai National Higher Education System, iGCORE*)

2S-4-7　Fusion of the inner mitochondrial membrane
Junjie Hu (*Institute of Biophysics, CAS*)

Closing Remarks
Junjie Hu (*Institute of Biophysics, CAS*)

9:00〜11:30
2S-5　光受容体の構造と機能を分光学で解き明かす
Spectroscopic approach for exploring structure and function of photoreceptor proteins

オーガナイザー：海野 雅司（佐賀大学），田母神 淳（松山大学）
Organizers: Masashi Unno (Saga University), Jun Tamogami (Matsuyama University)

Understanding protein function at the atomic level is an important challenge for biophysics. Such an attempt requires the high-resolution structural information including protons as well as an electronic structure of a cofactor molecule embedded in protein environments to realize how proteins work. Spectroscopic and theoretical studies are crucial to gather these insights. In this symposium, recent state-of-the-art investigations of photoreceptor proteins such as cyanobacteriochromes, microbial rhodopsins, and flavin-containing BLUF proteins are presented, and we will discuss future perspectives of the related research fields.

はじめに
Opening Remarks
海野 雅司（佐賀大学）
Masashi Unno (*Saga University*)

2S-5-1　ビリン結合光受容体の多様な吸収波長の分子基盤
Molecular basis of spectral tuning of the bilin-based photosensors
○広瀬 侑（豊橋技術科学大学）
Yuu Hirose (*Toyohashi Univ. of Tech.*)

2S-5-2　GAF ドメインの結晶構造解析と NMR 解析
Crystallography and NMR Studies of GAF domain
○三島 正規（東京都立大学 理学研究科）
Masaki Mishima (*Grad. Sch. Sci., Tokyo Metro. Univ.*)

2S-5-3 フラッシュフォトリシス法を用いた微生物ロドプシンの光反応解析
Photoreaction analysis of microbial rhodopsin by flash photolysis techniques
○菊川 峰志 [1,2]（[1]北大・院先端生命, [2]北大・国際連携研究教育局）
Takashi Kikukawa[1,2] ([1]*Fac. Adv. Life Sci., Hokkaido Univ.*, [2]*GI-CoRE, Hokkaido Univ.*)

2S-5-4 ラマン光学活性を利用したプロトンポンプ型ロドプシンにおける発色団の立体構造解析
Three-dimensional chromophore structures in proton-pumping microbial rhodopsins from Raman optical activity
○藤澤 知績（佐大理工）
Tomotsumi Fujisawa (*Fac. Sci. Eng., Saga Univ.*)

2S-5-5 FTIR 分光法で示されたフラビン結合光受容体における特異的な水素結合の形成
Unique hydrogen-bonding formation in Flavin-binding photoreceptors revealed by FTIR spectroscopy
○岩田 達也（東邦大学薬学部）
Tatsuya Iwata (*Phar. Sci. Toho Univ.*)

2S-5-6 分光学による光受容体の構造・機能解析：将来展望
Future perspective of spectroscopic study on structure and function of photoreceptor proteins
○田母神 淳（松山大・薬）
Jun Tamogami (*College Pharm. Sci., Univ. Matsuyama*)

9:00〜11:30
2S-6 タンパク質のフォールディング・ミスフォールディング・凝集の物理科学研究とその生命科学的背景
Biophysical studies on protein folding / misfolding and aggregation with regard to life sciences

オーガナイザー：黒田 裕（東京農工大学），新井 宗仁（東京大学）
Organizers: Yutaka Kuroda (Tokyo University of Agriculture and Technology), Munehito Arai (The University of Tokyo)

Because most proteins can function only when they are natively folded, protein aggregation and folding/misfolding is indeed deeply associated to most aspects of life sciences and research in this field is attracting a renewed attention. In this symposium, we will discuss new concepts of protein aggregation, folding and misfolding from a biophysical, conformational and structural viewpoint, and discuss their possible consequences on the biological/physiological function of a protein.

2S-6-1 デング・エンベロープ蛋白質第 3 ドメインのミスフォールディングと凝集
Misfolding and aggregation of the dengue envelop protein domain 3
○黒田 裕, 早乙女 友則（東京農工大学工学研究院）
Yutaka Kuroda, Tomonori Saotome (*Tokyo Univ Agr and Tech*)

2S-6-2 再構築型無細胞タンパク質合成系を用いたタンパク質凝集の網羅解析
Comprehensive analysis of protein aggregation by using a reconstituted cell-free translation system
○丹羽 達也, 田口 英樹（東京工業大学 科学技術創成研究院）
Tatsuya Niwa, Hideki Taguchi (*Institute of Innovative Research, Tokyo Institute of Technology*)

2S-6-3 Molecular basis for diversification of amyloid conformation
Yumiko Ohhashi[1], Motomasa Tanaka[2] ([1]*Grad.Sch.Sci., Kobe Univ.*, [2]*CBS, RIKEN*)

2S-6-4　6 M 塩化グアニジニウム中で変性したユビキチンの DMSO-停止 2D NMR 法による H/D 交換反応解析
The H/D-Exchange Kinetics of Unfolded Ubiquitin in 6 M Guanidinium Chloride Studied by the DMSO-Quenched 2D NMR Techniques
○桑島 邦博 [1,2], 矢木-内海 真穂 [3,4], 谷中 冴子 [3,4], 加藤 晃一 [3,4]（[1]東大・理, [2]韓国高等科学院, [3]分子研, [4]生命創成探究セ）
Kunihiro Kuwajima[1,2], Maho Yagi-Utsumi[3,4], Saeko Yanaka[3,4], Koichi Kato[3,4] ([1]*Univ. Tokyo*, [2]*KIAS*, [3]*IMS*, [4]*ExCELLS*)

2S-6-5　タンパク質のフォールディングとデザインへの理論的アプローチ
Theoretical approaches to protein folding and design
○新井 宗仁 [1,2]（[1]東大・総合文化・生命環境, [2]東大・理・物理）
Munehito Arai[1,2] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Dept. Phys., Univ. Tokyo*)

9:00〜11:30
2S-7　共催：新学術領域研究「シンギュラリティ生物学」
免疫とがんにおけるシンギュラリティの検出と新たなイメージング技術
Detection of Singularity in Immunity and Cancer by Novel Imaging Techniques

オーガナイザー：花岡 健二郎（東京大学），竹馬 俊介（慶應義塾大学）
Organizers: Kenjiro Hanaoka (The University of Tokyo), Shunsuke Chikuma (Keio University)

It is known that a very small number of cells that can be counted in the fingers become singularities and dramatically change the biological system. In this symposium, we focused on the establishment of the immune response and the carcinogenic process, approached the essential understanding of the mechanism from the viewpoint of singularity. We also selected the topics of the latest imaging technologies that enable the detection of rare events in the body. Using these as inputs, we will comprehensively discuss the singularity in biology.

2S-7-1　Singularity in Immunity: Immune-aging associates with a defect in Chromatin Regulation on Immune Cells
Shunsuke Chikuma (*Microbiology and Immunology, Keio University School of Medicine*)

2S-7-2　Which cells initiate lymph node formation?
Shinichiro Sawa (*Medical Institute of Bioregulation, Kyushu University*)

2S-7-3　Live imaging of epidermal sensory nerves and keratinocyte tight junctions
Takaharu Okada[1,2] ([1]*RIKEN IMS*, [2]*Grad School of Med Life Sci, Yokohama City Univ*)

2S-7-4　がん細胞が出現した正常間質組織でのシンギュラリティ現象
Singularity at emergence of cancer cells in normal stroma
○昆 俊亮（東京理科大学 生命医科学研究所）
Shunsuke Kon (*Tokyo University of Science, Research Institute for Biomedical Sciences*)

2S-7-5　シンギュラリティを捉えるためのダイナミックレンジの広い光音響イメージングの研究開発
Development of photoacoustic imaging to study a singularity in high dynamic range measurement
○石原 美弥（防衛医科大学校）
Miya Ishihara (*National Defense Medical College*)

2S-7-6 りん光寿命イメージング顕微分光法による組織内低酸素細胞の可視化
Visualization of hypoxia cells in tissues by using phosphorescence lifetime imaging microscopy
○吉原 利忠（群馬大・院理工）
Toshitada Yoshihara (*Grad. Sch. Sci. and Tech., Univ. Gunma*)

2S-7-7 動物体内での pH 測定を目指した近赤外レシオ型蛍光プローブの開発
Development of a near-infrared ratiometric fluorescent probe for pH inside the body
○花岡 健二郎（東大院薬）
Kenjiro Hanaoka (*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*)

13:30〜16:00
2S-8 Happy な細胞に聞いた生命のしくみ―井上信也博士に捧げる
Listening to happy cells through the microscope -a tribute to Shinya Inoué

オーガナイザー：谷 知己（産業技術総合研究所），前島 一博（国立遺伝学研究所）
Organizers: Tomomi Tani (AIST), Kazuhiro Maeshima (NIG)

Shinya Inoué had revealed the basic mechanisms of spindles for chromosome segregation through the observation of weak birefringence in living cells. Preparing “Happy Cells” was his central “mantra” for successful imaging and the analysis that lead to fundamental understanding of many biological events. This symposium aims to gather scientists from different research fields with their unique approaches for imaging and the analysis and to share with the audience the excitement to learn the mechanisms of life through the imaging of “Happy Cells”, together with Shinya’s works that he left for us.

2S-8-1 導入；井上信也博士の仕事の紹介
An introduction to the works of Shinya Inoué
○谷 知己（産業技術総合研究所）
Tomomi Tani (*AIST*)

2S-8-2 遠心偏光顕微鏡(CPM)を用いた核を細胞中央へ運ぶ力の測定
Measurement of cellular forces bringing the nucleus to the cell center using the Centrifuge Polarization Microscope (CPM)
○木村 暁 [1,2,3]（[1]遺伝研, [2]ウッズホール海洋生物学研究所, [3]総研大・遺伝学）
Akatsuki Kimura[1,2,3] ([1]*Natl Inst Genet*, [2]*Marine Biological Lab, USA*, [3]*Dept Genet, Sokendai*)

2S-8-3 Cellular machinery for controlling actomyosin contractility in vivo
Asako Shindo (*Grad.Sch.Sci., Univ. Nagoya*)

2S-8-4 植物の紡錘体形成における微小管の起源
Origin of mitotic spindle microtubules in plant cells
○村田 隆 [1,4,5], 大友 康平 [2,3,4], 根本 知己 [2,3,4], 長谷部 光泰 [4,5]（[1]神奈川工科大・応用バイオ, [2]生理研・バイオフォトニクス, [3]自然科学研究機構・生命創成探求セ, [4]総研大・生命科学, [5]基生研・生物進化）
Takashi Murata[1,4,5], Kohei Otomo[2,3,4], Tomomi Nemoto[2,3,4], Mitsuyasu Hasebe[4,5] ([1]*Appl. Biosci., Kanagawa Inst. Tech.*, [2]*Div. Biophoto., NIPS*, [3]*ExCELLS, NINS*, [4]*Sch. Life Sci., Sokendai*, [5]*Div. Evol. Biol., NIBB*)

2S-8-5 植物のスピンドルと染色体の動きについて
Spindle and chromosome motility in plant cells
○五島 剛太 [1,2]（[1]名大・菅島臨海実験所, [2]名大・生命理学）
Gohta Goshima[1,2] ([1]*Sugashima MBL, Nagoya Univ.*, [2]*Div. Bio-Sci, Nagoya Univ.*)

2S-8-6 Toward understanding the real chromatin organization present in the cell
Kazuhiro Maeshima (*National Institute of Genetics*)

13:30〜16:00
2S-9 膜タンパク質を「生きた」状態で再構成・解析・利用するための新しい脂質膜テクノロジー
New lipid membrane technologies for reconstitution, analysis, and utilization of 'living' membrane proteins

オーガナイザー：安原 主馬（奈良先端科学技術大学院大学），森垣 憲一（神戸大学）
Organizers: Kazuma Yasuhara (NAIST), Kenichi Morigaki (Kobe University)

Biomembranes contribute to various essential cellular functions such as signal transduction, material transport, and energy production through the interplay of membrane proteins and lipid bilayers. There is a great need for native-like artificial membranes for reconstituting membrane proteins and their complexes to understand the nature of biomembranes from a biophysical viewpoint. In this symposium, we will focus on novel lipid-based technologies, including artificial lipids, surfactants, micro processing, and advanced measurements that enable the reconstitution and analysis of membrane proteins in a 'living' state.

はじめに
Opening Remarks
安原 主馬（奈良先端科学技術大学院大学）
Kazuma Yasuhara (*NAIST*)

2S-9-1 部分フッ素化リン脂質膜
Partially Fluorinated Phospholipid Membrane
○園山 正史 [1,2,3]（[1]群馬大・院理工, [2]群馬大・未来先端, [3]群馬大・食健康セ）
Masashi Sonoyama[1,2,3] ([1]*Div. Mol. Sci., Gunma Univ.*, [2]*GIAR, Gunma Univ.*, [3]*GUCFW, Gunma Univ.*)

2S-9-2 有機-無機ハイブリッド型メゾ構造を有する脂質キュービック相の構築
Design of lipid cubic phase possessing organic-inorganic hybrid mesostructure
○尾本 賢一郎, 刈谷 未来, 安原 主馬, 林 有吾, 上久保 裕生, ラッペン ゲナエル（奈良先端大・先端科技）
Kenichiro Omoto, Miki Kariya, Kazuma Yasuhara, Yugo Hayashi, Hironari Kamikubo, Gwenael Rapenne (*Grad. Sch. of Sci. and Tech., NAIST*)

2S-9-3 脂質ベシクル系における不均一性と線張力
Heterogeneity and line tension in lipid vesicle system
○瀧上 隆智（九州大学）
Takanori Takiue (*Kyushu University*)

2S-9-4 抗菌ペプチドや細胞透過ペプチドの作用機構を解明するための単一巨大リポソーム法
The Single GUV Method for Revealing Mode of Action of Antimicrobial Peptides (AMPs) and Cell-Penetrating Peptides (CPPs)
○山崎 昌一 [1,2,3]（[1]静大・電研, [2]静大・創造院, [3]静大・院理）
Masahito Yamazaki[1,2,3] ([1]*Res. Inst. Ele., Shizuoka Univ*, [2]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

2S-9-5 LAiR: rapid reconstitution of integral membrane proteins into lipid bilayers
Christoph Gerle[1], Amer Asseri[5], Albert Godoy-Hernandez[3], Aiden Purugganan[3], Chimari Jiko[2], Carol de Ram[3], Holger Lill[5], Martin Pabst[3], Kaoru Mitsuoka[4], Dirk Bald[5], Duncan G.G. McMillan[3] ([1]*Osaka Univ., IPR*, [2]*Kyoto University*, [3]*TU Delft*, [4]*Osaka Univ.*, [5]*VU Amst.*)

2S-9-6 Microsytem for single molecule analysis of membrane proteins
Rikiya Watanabe (*CPR, RIKEN*)

おわりに
Closing Remarks
森垣 憲一（神戸大学）
Kenichi Morigaki (*Kobe University*)

13:30〜16:00
2S-10 Biomolecular Design to Control their Functions

Organizers: Tetsuya Kadonosono (Tokyo Institute of Technology), Duy Phuoc Tran (Tokyo Institute of Technology)

Biomolecular design is among the attractive research themes toward the Sustainable Development Goals of UNESCO. Recent advances in both computational and experimental methods have boosted the theme toward the controlling biomolecular functions after carefully understanding of their activity. In this symposium, we would like to bring to the audience recent advances in: - Application of the machine learning and simulation methods in protein design. - Transmembrane protein design to control the ion pump. - Protein assembly design: toward bio-machinery. - Disease-targeted antibody design. - Peptide design.

2S-10-1 Biomolecular Functional Design: an Introduction to Recent Advances
Duy Phuoc Tran (*TokyoTech, LifeSciTech*)

2S-10-2 配列空間をうまく絞り込むライブラリーデザインサイクル：酵素・抗体の設計アシスト
Library design cycle for efficient exploring in sequence space: design assist for enzyme and antibody
○梅津 光央 [1,2]（[1]東北大学大学院工学研究科, [2]理化学研究所革新知能統合研究センター）
Mitsuo Umetsu[1,2] ([1]*Department of Biomolecular Engineering, Tohoku University*, [2]*Center for Advanced Intelligence Project, RIKEN*)

2S-10-3 微生物ロドプシンの機能と色の制御
Control of functions and colors of microbial rhodopsins
○井上 圭一（東京大学・物性研究所）
Keiichi Inoue (*Inst. Solid State Phys., Univ. Tokyo*)

2S-10-4 機械学習による機能ペプチドの自動設計
Designing functional peptides with machine learning
○津田 宏治（東京大学新領域）
Koji Tsuda (*GSFS, University of Tokyo*)

2S-10-5 ナノ機能化へ向けたタンパク質結晶設計
Protein Crystals for Designing Multiple Nanofunctions
○上野 隆史（東京工業大学　生命理工学院）
Takafumi Ueno (*Tokyo Tech*)

2S-10-6 合理設計による新規タンパク質フォールドの探索
Exploration of novel protein folds by de novo design
○古賀 信康 [1,2,3]（[1]自然科学研究機構・生命創成探究センター, [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）
Nobuyasu Koga[1,2,3] ([1]*NINS, ExCELLS*, [2]*NINS, IMS*, [3]*SOKENDAI*)

2S-10-7 A smart design of target-binding small proteins for molecular target therapy
Tetsuya Kadonosono (*Tokyo Tech*)

13:30〜16:00
2S-11 光生物学研究の多様性〜分子から生物個体まで〜
Diversity of photobiology; from molecules to organisms

オーガナイザー：小島 慧一（岡山大学），山田 大智（兵庫県立大学）
Organizers: Keiichi Kojima (Okayama University), Daichi Yamada (University of Hyogo)

Living organisms utilize light as an energy source and environmental signals. Biological, physical and chemical researches from molecules to organisms have been actively performed to obtain the answer to how organisms rationally utilize light. Recently, understanding of the mechanisms by photobiological researches is accelerating the development of optogenetics and bioimaging technology, and contributed to the field of biophysics. In this symposium, the active (mainly young) researchers from diverse background will present their recent progress and findings in photobiology. We will discuss the future aspect of photobiology.

2S-11-1 赤外分光法を用いた光受容タンパク質の分子機構研究
The molecular mechanism of photoreceptor proteins by infrared spectroscopy
○山田 大智（兵庫県大・院生命理学）
Daichi Yamada (*Grad. Sch. Life Sci., Univ. Hyogo, Japan*)

2S-11-2 Triggers of Primary Protein Dynamics in Photoreceptor Proteins
Shinya Tahara (*Laboratory for Biophysical Chemistry, Osaka University*)

2S-11-3 Analysis of photoinduced reactions in UV-damaged DNA repair of photolyases
Ryuma Sato (*RIKEN*)

2S-11-4　**酵素型ロドプシンの構造基盤**
Structural insights into the mechanism of rhodopsin phosphodiesterase
○志甫谷 渉[1], 生田 達也[1], 杉浦 雅大[2], 吉田 一帆[2], 渡 雅仁[2], 戸叶 貴也[3], 片山 耕大[2], 角田 聡[2], 内橋 貴之[3], 神取 秀樹[2], 濡木 理[1]（[1]東大院理生物, [2]名工大院工生命, [3]名大院理物理）
Wataru Shihoya[1], Tatsuya Ikuta[1], Masahiro Sugiura[2], Kazuho Yoshida[2], Masahito Watari[2], Takaya Tokano[3], Kota Katayama[2], Satoshi Tsunoda[2], Takayuki Uchihashi[3], Hideki Kandori[2], Osamu Nureki[1] ([1]*Dept. of Biol., Grad. Sch. Sci., Univ. of Tokyo*, [2]*Life Sci. Appl. Chem., Grad. Sch. Eng., NIT*, [3]*Dept. of Phys., Grad. Sch. Sci., Nagoya Univ.*)

2S-11-5　**光スイッチの開発を目指したシアノバクテリオクロムの分子基盤**
Molecular basis of cyanobacteriochromes for developing photoswitches
○伏見 圭司, 成川 礼（静大・理学・生物）
Keiji Fushimi, Rei Narikawa (*Biol. Sci., Shizuoka Univ.*)

2S-11-6　**概日時計制御における CRYPTOCHROME の役割**
Function of CRYPTOCHROME in regulation of the circadian clock
○平野 有沙[1,2], 櫻井 武[1,2], Ptacek Louis[3], Fu Ying-Hui[3]（[1]筑波大学医学医療系, [2]筑波大学, WPI-IIIS, [3]カルフォルニア大学サンフランシスコ校）
Arisa Hirano[1,2], Takeshi Sakurai[1,2], Louis Ptacek[3], Ying-Hui Fu[3] ([1]*Faculty of Medicine, University of Tsukuba*, [2]*International Institute for integrative Sleep medicine (WPI-IIIS), University of Tsukuba*, [3]*University of California, San Francisco*)

2S-11-7　**植物の光受容体フォトトロピンのシグナル伝達とモデルケースとしての気孔開口**
Plant photoreceptor phototropin signaling and stomatal opening as a model case
○井上 晋一郎（名古屋大学大学院理学研究科生命理学専攻植物性理学グループ）
Shin-ichiro Inoue (*Division of Biological Science, Graduate School of Science, Nagoya University*)

2S-11-8　**生命機能の理解と制御に向けたロドプシン研究**
Analysis of rhodopsins for a rational understanding and controlling of biological functions
○小島 慧一（岡山大・院・医歯薬(薬)）
Keiichi Kojima (*Grad. Sch. of Med. Dent. Pharm. Sci., Okayama Univ.*)

13:30〜16:00
2S-12　生体分子と薬剤の構造ゆらぎの生命機能科学
Biofunctional Science of the Structural Fluctuations of Biomolecules and Drugs

オーガナイザー：米澤 康滋（近畿大学），宮下 尚之（近畿大学）
Organizers: Yasushige Yonezawa (Kindai University), Naoyuki Miyashita (Kindai University)

Bio-molecules, proteins and drugs, in living cells are thermally fluctuated. It is not surprising that almost all of drugs recognize and bind the fluctuated protein. Many studies showed fluctuation movement of proteins is important for the molecular function. Then, drugs inhibit the functional movement, attract much attention. In this symposium, advanced studies on the interaction mechanism between drugs and proteins, mainly provided by young scientists are widely discussed.

2S-12-1 1分子計測と分子シミュレーションを用いたタンパク質構造ダイナミクスの統合モデリング
Integrative modeling of protein dynamics from single-molecule experiments and molecular dynamics simulations
○松永 康佑 [1,2], 大金 智則 [1,2]（[1]埼玉大学, [2]JST CREST）
Yasuhiro Matsunaga[1,2], Tomonori Ogane[1,2] ([1]*Saitama University*, [2]*JST CREST*)

2S-12-2 新しいペプチド薬と、ターゲットタンパク質と新しい薬の分子動力学シミュレーション
New Peptide Drug and the Molecular Dynamics Simulations of Target Protein and the New Drug
○松倉 里紗 [1], 宮下 尚之 [1,2], 瀧 真清 [2], 渡辺 信一 [2]（[1]近大・生物理工, [2]電通大・情報理工）
Lisa Matsukura[1], Naoyuki Miyashita[1,2], Masumi Taki[2], Shinichi Watanabe[2] ([1]*BOST., KINDAI Univ.*, [2]*Eng. Sci., UEC*)

2S-12-3 アンサンブルドッキングを用いたタンパク質相互作用プロファイル解析
Profile analysis of protein interaction surfaces with ensemble rigid-body docking process
○内古閑 伸之 [1], 松崎 由理 [2]（[1]明治大・総数, [2]東工大・ToTAL）
Nobuyuki Uchikoga[1], Yuri Matsuzaki[2] ([1]*Sch. Interdiscip. Math. Sci., Meiji Univ.*, [2]*ToTAL, Tokyo Tech.*)

2S-12-4 Turn-on / keep-on fluctuated fluorescent molecules as targeted binders
Masumi Taki (*UEC*)

2S-12-5 Analysis of an effect of mutations on the structure of CDR-H3 in the anti-HIV neutralizing antibody PG16
Hiroko X. Kondo[1,2], Ryo Kiribayashi[2], Daisuke Kuroda[3], Kouhei Tsumoto[3,4], Yu Takano[2] ([1]*Fac. Eng., Kitami Inst. Tech.*, [2]*Grad. Sch. Info. Sci., Hiroshima City Univ.*, [3]*Grad. Sch. Eng., Univ. Tokyo*, [4]*IMS, Univ. Tokyo*)

2S-12-6 Autoencoder-based analyses of dynamic allostery on GPCR
Yuko Tsuchiya[1], Kei Taneishi[2], Yasushige Yonezawa[3] ([1]*AIRC, AIST*, [2]*RIKEN*, [3]*KINDAI univ.*)

2S-12-7 タンパク質の熱力学的安定性における主要因子
Dominant factor in thermodynamic stability of protein
○墨 智成 [1], 今村 比呂志 [2]（[1]岡山大・基礎研, [2]立命館大・生命科学）
Tomonari Sumi[1], Hiroshi Imamura[2] ([1]*Res. Inst. Interdiscip. Sci., Okayama Univ.*, [2]*Dep. Appl. Chem., Ritsumeikan Univ.*)

13:30〜16:00
2S-13 核酸が拓く新・生物物理研究
Frontier of Nucleic Acid Biophysics

オーガナイザー：岡部 弘基（東京大学），瀧ノ上 正浩（東京工業大学）
Organizers: Kohki Okabe (The University of Tokyo), Masahiro Takinoue (Tokyo Institute of Technology)

In recent years, it has become clear that DNA and RNA act as the protagonists of intracellular structures and environmental fields in the physicochemical understanding of the intracellular environments, while bioengineering focused on the chemical characteristics of DNA and RNA has also developed innovative nanotechnology. In this symposium, we will take an overview of the latest physics, chemistry, and biology research on nucleic acids, and discuss the future image of biophysics, whose original discipline was to investigate the properties of biopolymers.

2S-13-1　RNA 顆粒内 mRNA の直接観察
Direct observation of mRNA inside of RNA granules
○岡部 弘基（東京大学大学院 薬学系研究科）
Kohki Okabe (*Grad Sch Parm Sci, Univ Tokyo*)

2S-13-2　エピジェネティック修飾がクロマチン転写に及ぼす影響を定量化する
Quantifying the effect of epigenetic modification on chromatin transcription
○梅原 崇史（理化学研究所 生命機能科学研究センター エピジェネティクス制御研究チーム）
Takashi Umehara (*RIKEN BDR*)

2S-13-3　Gene expression and artificial cells: Revisiting the role of active interface
Yusuke T. Maeda (*Department of Physics, Kyushu University*)

2S-13-4　分子の状態と形態を考慮したクロマチン構造の統合的モデリングを目指して
Towards Comprehensive Models of Chromatin Structures Considering the State and Shape of Molecules
○冨樫 祐一 [1,2]（[1]広島大・統合生命, [2]理研・BDR）
Yuichi Togashi[1,2] ([1]*Grad. Sch. Integr. Sci. Life, Hiroshima Univ.*, [2]*RIKEN BDR*)

2S-13-5　合成生命システム創成に向けた RNA-タンパク質複合体の活用
RNA-Protein complexes for synthetic living systems
○齊藤 博英（京都大学 iPS 細胞研究所）
Hirohide Saito (*Center for iPS Cell Research and Application, Kyoto University*)

2S-13-6　相分離とエマルションによる DNA マイクロ液滴の生物物理学
Biophysics on DNA microdroplet technology by phase separation and emulsion
○瀧ノ上 正浩（東京工業大学 情報理工学院）
Masahiro Takinoue (*Department of Computer Science, Tokyo Institute of Technology*)

13:30〜16:00
2S-14　共催：JST さきがけ「生体における微粒子の機能と制御」
多様な細胞外微粒子の生体機能を探る
Open up extracellular nanoparticles! -Their diversity and biodynamics-

オーガナイザー：白崎 善隆（東京大学），田代 陽介（静岡大学）
Organizers: Yoshitaka Shirasaki (The University of Tokyo), Yosuke Tashiro (Shizuoka University)

Various exogenous and endogenous fine particles are commonly found in a living body and those functions gain increasingly attention recent years. The strategic object of the research area is to elucidate biological system of extracellular fine particles. In the research area, we are studying their diversity, dynamics, biological functions, and association with diseases, and developing techniques to observe and measure fine particles. This symposium discusses new cutting edge results regarding extracellular fine particles from the perspective of biophysics.

はじめに
Opening Remarks
中野 明彦（理化学研究所 光量子工学研究センター）
Akihiko Nakano (*RIKEN*)

2S-14-1 Exosome-based therapy and biomarker development for the polyglutamine diseases
Toshihide Takeuchi[1,2] ([1]*Grad Sch Med, Osaka Univ*, [2]*JST-PRESTO*)

2S-14-2 **細菌が形成する細胞外小胞の多様性**
Diversity of bacterial extracellular vesicles
○田代 陽介 [1,2]（[1]静大・院総合科技, [2]JST さきがけ）
Yosuke Tashiro[1,2] ([1]*Grad. Sch. Integr. Sci. Technol., Shizuoka Univ.*, [2]*JST PRESTO*)

2S-14-3 Overlooked redox property of outer membrane vesicle surface
Akihiro Okamoto (*National Institute for Materials Science*)

2S-14-4 Amphipathic helical peptide-based fluorescent probes for exosomes by membrane curvature recognition
Yusuke Sato[1,2] ([1]*Grad. Sch. Sci., Tohoku University*, [2]*JST-PRESTO*)

2S-14-5 **ナノ流体デバイスを用いたエクソソームの簡便単離、1 粒子配列及び統合解析**
Simple isolation and integrated analysis of single exosomes on an aifA chip
○許 岩 [1,2,3]（[1]阪府大・院工, [2]JST さきがけ, [3]阪府大・NanoSquare 研）
Yan Xu[1,2,3] ([1]*Grad. Sch. Eng., Osaka Pref. Univ.*, [2]*PRESTO, JST*, [3]*N2RI, Osaka Pref. Univ.*)

2S-14-6 Collection of Extracellular Vesicles from Single Cell Using Nanopipette
Hiroki Ida[1,2,3,4], Yasufumi Takahashi[5], Akichika Kumatani[3], Yuji Nashimoto[1,6], Hitoshi Shiku[6], Takeshi Yoshida[5], Rikinari Hanayama[5] ([1]*Tohoku Univ., FRIS*, [2]*JST, PRESTO*, [3]*Tohoku Univ., AIMR*, [4]*Tohoku Univ., Grad. Sch. Env. Stu.*, [5]*Kanazawa Univ., WPI-NanoLSI*, [6]*Tohoku Univ., Grad. Sch. Eng.*)

2S-14-7 **細胞外小胞放出の 1 細胞解析**
Single Cell analysis of release dynamics of Extracellular Vesicles
○白崎 善隆（東大・院薬）
Yoshitaka Shirasaki (*Grad. Sch. Pharm. Sci., Univ. Tokyo*)

おわりに
Closing Remarks

16:30〜19:00
2S-15 膜のリモデリングと組織化の分子基盤
Molecular basis for membrane remodeling and organization

オーガナイザー：竹田 哲也（岡山大学），末次 志郎（奈良先端科学技術大学院大学）
Organizers: Tetsuya Takeda (Okayama University), Shiro Suetsugu (NAIST)

Cells and subcellular organelles in living organisms exhibit unique shapes adapted to their respective functions that change dynamically as cells divide, differentiate, migrate and invade. The dynamic morphological changes of cells and organelles require coordinated function of proteins that interact with and remodel (deform or sever) cellular membranes. Dysfunction of the membrane remodeling is tightly linked to pathogenesis of diseases including cancer and developmental defects. In this symposium, we will present and discuss about the latest knowledges on molecular mechanism of membrane remodeling and pathogenesis of diseases caused by its defects.

2S-15-1 Curvature induction and sensing of the F-BAR protein Pacsin1 on lipid membranes via molecular dynamics simulations
Md. Iqbal Mahmood[1], Hiroshi Noguchi[2], **Kei-ichi Okazaki**[1] ([1]*IMS*, [2]*ISSP, Univ. of Tokyo*)

2S-15-2 Molecular mechanisms linking actin cytoskeleton to the plasma membrane
Yosuke Senju (*RIIS, Univ. Okayama*)

2S-15-3 The extracellular vesicle formation by filopodial scission for cell migration
Tamako Nishimura, Takuya Oyama, Hooi Ting Hu, **Shiro Suetsugu** (*Nara Institute of Science and Technology*)

2S-15-4 Molecular mechanisms underlying dynamic behavior of membrane blebbing
Junichi Ikenouchi (*Kyushu Univ., Fac Sci, Dept. of Biol*)

2S-15-5 Proper membrane shaping during autophagosome biogenesis is required for non-selective sequestration of cytoplasmic components
Hitoshi Nakatogawa (*Sch. of Life Sci. & Tech.*)

2S-15-6 Dysregulated membrane remodeling in pathogenesis of congenital diseases
Tetsuya Takeda[1], Kenshiro Fujise[1], Mariko Okubo[2], Tadashi Abe[1], Hiroshi Yamada[1], Ichizo Nishino[2], Satoru Noguchi[2], Kohji Takei[1] ([1]*Okayama Univ. Grad. Sch. Med. Dent. Pharm. Sci.*, [2]*NCNP*)

2S-15-7 The structure-based targeting of alpha-synuclein to mitochondria promotes cellular health
Harvey T. McMahon (*MRC Laboratory of Molecular Biology*)

16:30〜19:00
2S-16 新時代に突入した DNA-タンパク質研究
Beginning of a new era for investigation of DNA-protein systems

オーガナイザー：Vaclav Brazda（ASCR, Czech），鎌形 清人（東北大学）
Organizers: Vaclav Brazda (ASCR, Czech), Kiyoto Kamagata (Tohoku University)

DNA-protein interactions are essential requirements for existence of life. They are involved in basic cellular processes and biological functions. Recent development of analysis and design methods open a new era in investigation of DNA-protein systems. The developed methodology includes crystal structural analysis, dynamics analysis based on single-molecule microscopy in vitro and in vivo or molecular dynamics simulations, and artificial design of DNA origami to study DNA-protein functions. Also, the improvement of genome editing tools is required for medical applications. We will invite specialists for each technique regarding DNA-protein studies and discuss recent hot topics.

2S-16-1 Watching, controlling, and designing of function and phase separation of DNA-binding protein
Kiyoto Kamagata (*IMRAM, Tohoku Univ.*)

2S-16-2 Molecular principles for optimizing protein-DNA interactions
Yaakov Levy (*WIS*)

2S-16-3 CRISPR-Cas 酵素の構造、機能、分子進化
Structure, mechanism and evolution of CRISPR-Cas enzymes
○西増 弘志（東京大学）
Hiroshi Nishimasu (*The University of Tokyo*)

2S-16-4 Construction of DNA nanostructures exhibiting modulated structural transformation
Yuki Suzuki (*FRIS, Tohoku Univ.*)

2S-16-5 RNA 転写/DNA 複製の過程で生じる局所的なクロマチンの運動
Local chromatin motion during RNA transcription/DNA replication
○伊藤 優志, 永島 崚甫, 日比野 佳代, Babokhov Michael, 鐘巻 将人, 前島 一博（遺伝研）
Yuji Itoh, Ryosuke Nagashima, Kayo Hibino, Michael Babokhov, Masato T. Kanemaki, Kazuhiro Maeshima (*NIG*)

2S-16-6 Interactions of local DNA structures and proteins using biophysical and molecular biology approaches
Vaclav Brazda[1,2] ([1]*Institute of Biophysics, Czech Academy of Sciences*, [2]*Brno University of Technology, Faculty of Chemistry*)

16:30〜19:00
2S-17 もっと面白くなる細菌べん毛研究〜残された宿題への挑戦〜
Past, present, and future of the bacterial flagella~ Towards the remaining challenges~

オーガナイザー：中村 修一（東北大学），加藤 貴之（大阪大学）
Organizers: Shuichi Nakamura (Tohoku University), Takayuki kato (Osaka University)

The discovery of the bacterial rotary nanomachine more than 40 years ago has been inspiring researchers to address the well-organized self-assembly, cation-driven high-power rotation, chemically stimulative allosteric reversal, mechanosensitive stator dynamics, and others. These astonishing mechanisms will be an insight into the infection with motile pathogens and are expected to be a significant step forward to the development of artificial micro-/nano machines. However, despite longstanding strenuous studies, there remain abundant mysteries. For discussing what we should do for fully understanding the bacterial flagella, this symposium will provide a historical review of the flagellar studies and talks on recent experimental and theoretical knowledge that has been obtained in terms of structure, single molecule, genetics, physics, and infectious disease by innovative progress.

はじめに
Opening Remarks
中村 修一（東北大学）
Shuichi Nakamura (*Tohoku University*)

2S-17-1 細菌べん毛研究を振り返る：これまでに何がわかったのか？
Historical overview of the bacterial flagellar studies: what do we know about "flagella" so far?
○小嶋 誠司（名古屋大学大学院理学研究科生命理学専攻超分子機能学講座生体膜機能グループ）
Seiji Kojima (*Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

2S-17-2 細菌べん毛モータータンパク質の自然な構造の解析
Structure of the native form of the bacterial flagellar motor component
○加藤 貴之 [1], 牧野 文信 [2], 宮田 知子 [3], 木下 実紀 [3], 南野 徹 [3], 難波 啓一 [3,4,5]（[1]阪大・蛋白研究, [2]日本電子, [3]阪大・生命機能, [4]SPring-8・生命機能, [5]日本電子 YOKOGUSHI 協働研）
Takayuki Kato[1], Fumiaki Makino[2], Tomoko Miyata[3], Miki Kinoshita[3], Tohru Minamino[3], Keiichi Namba[3,4,5] ([1]*IPR/Osaka Univ.*, [2]*JEOL*, [3]*Grad. Front. Biosci./Osaka Univ.*, [4]*BDR / SPring-8 Center*, [5]*JEOL YOKOGUSHI Lab.*)

2S-17-3 バクテリアべん毛蛋白質輸送エンジンのゲート開閉機構
Gating mechanism of the bacterial flagellar protein export engine
○木下 実紀 [1], 宮田 知子 [1], 加藤 貴之 [2], 難波 啓一 [1,3,4,5], 南野 徹 [1]（[1]大阪大・生命機能, [2]大阪大・蛋白研, [3]大阪大・日本電子 YOKOGUSHI, [4]理研・ SPring-8, [5]理研・ 生命機能）
Miki Kinoshita[1], Tomoko Miyata[1], Takayuki Kato[2], Keiichi Namba[1,3,4,5], Tohru Minamino[1] ([1]*Grad. Sch. Frontier Biosci, Osaka Univ.*, [2]*IPR, Osaka Univ.*, [3]*JEOL YOKOGUSHI, Osaka Univ.*, [4]*RIKEN SPring-8*, [5]*RIKEN BDR*)

2S-17-4 Bacterial flagellar rotation at low load
Yoshiyuki Sowa[1,2], Tsubasa Ishida[2] ([1]*Dept. Frontier Biosci., Hosei Univ.*, [2]*Grad. Sch. of Sci. & Eng., Hosei Univ.*)

2S-17-5 Patterns and randomness: Tools for studying bacterial navigation
Erick E. Rodriguez Salas, Emma E. Brock, **Laurence G. Wilson** (*Department of Physics, University of York*)

2S-17-6 数理モデルを用いた細菌の走化性強さの推定
Estimation of the intensity in bacterial Chemotaxis by Using a Mathematical Model
○中井 唱, 後藤 知伸（鳥取大）
Tonau Nakai, Tomonobu Goto (*Tottori Univ.*)

2S-17-7 Studies on bacterial motility as the virulence factor
Jun Xu (*Dept. Bacteriol., Grad. Sch. Med., Univ. Ryukyus.*)

おわりに
Closing Remarks
中村 修一（東北大学）
Shuichi Nakamura (*Tohoku University*)

3 日目（9 月 18 日（金））／Day 3（Sep. 18 Fri.）

9:00〜11:30
3S-1 膜の海を旅するペプチド〜 脂質膜とペプチドの相互作用研究の新展開
New developments in studies on interactions between membranes and peptides

オーガナイザー：川村 出（横浜国立大学），相沢 智康（北海道大学）
Organizers: Izuru Kawamura (Yokohama National University), Tomoyasu Aizawa (Hokkaido University)

Membrane-bound peptides and lipid molecules are involved in crucial biological functions over lipid bilayers, including antimicrobial activity, signaling, and membrane fusion. To under these functions at the molecular level, it is important to elucidate the structure and dynamics of the rational-designed peptides having higher activity. This symposium will cover the current biophysical researches of membrane-bound peptides using the production method of a recombinant peptide, rational design of antimicrobial and nano-pore forming peptides for multi-drug resistance bacteria, and experimental/computational approaches.

はじめに
Opening Remarks

3S-1-1 遺伝子組換え抗菌ペプチドの生産技術の開発と応用
Development and application of novel overexpression systems of antimicrobial peptides
○相沢 智康（北大・先端生命）
Tomoyasu Aizawa (*Fac. Adv. Life Sci., Hokkaido Univ.*)

3S-1-2 ヘリカル構造制御に基づく抗菌ペプチドフォルダマーの開発
Development of helix-stabilized antimicrobial peptide foldamers
○出水 庸介 [1,2]（[1]国立衛研, [2]横市大院・生命医科学）
Yosuke Demizu[1,2] ([1]*NIHS*, [2]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

3S-1-3 Cryptdin-4 conformations and interaction with membrane studied by membrane self-assembly molecular dynamics simulations
Takao Yoda (*Nagahama Institute of Bio-Science and Technology*)

3S-1-4 膜貫通αヘリックスペプチドバレルの理論設計
Rational design of membrane-spanning alpha-helical peptide barrels
○新津 藍 [1], Thomson Andrew R.[2], Scott Alistair J.[2], Sengel Jason T.[3], 杉田 有治 [1], Wallace Mark I.[3], Bayley Hagan[4], Woolfson Derek N.[2]（[1]理研・和光, [2]Bristol 大, [3]ロンドン大キングスカレッジ, [4]Oxford 大）
Ai Niitsu[1], Andrew R. Thomson[2], Alistair J. Scott[2], Jason T. Sengel[3], Yuji Sugita[1], Mark I. Wallace[3], Hagan Bayley[4], Derek N. Woolfson[2] ([1]*Wako Inst., Riken*, [2]*Univ. Bristol*, [3]*KCL*, [4]*Univ. Oxford*)

3S-1-5 Analysis of transmembrane peptides using a lipid bilayer system
Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology (TUAT)*)

3S-1-6 両生類由来カチオン性抗菌ペプチドの生体膜との相互作用
Interaction of amphibian-derived cationic antimicrobial peptides with model membrane
○川村 出（横国大 院理工）
Izuru Kawamura (*Grad. Sch. Eng. Sci., Yokohama Natl. Univ.*)

9:00〜11:30
3S-2 共催：新学術領域研究「発動分子科学：エネルギー変換が拓く自律的機能の設計」 リニアモーターと細胞骨格が生む秩序と制御
Order and control: linear motors and cytoskeleton 2020

オーガナイザー：古田 健也（情報通信研究機構），矢島 潤一郎（東京大学）
Organizers: Ken'ya Furuta (NICT), Junichiro Yajima (The University of Tokyo)

Linear motor proteins and cytoskeleton together generate dynamic processes such as directional transport, contraction and oscillation in living cells. To maintain out-of-equilibrium dynamics, each component continuously converts incoming chemical fuels into mechanical work. This symposium focuses on self-organization, regulatory mechanisms and cooperative phenomena emerged from these systems and will be an opportunity to discuss what is known and what needs to be learned to help improve our understanding of such dynamic motor-driven processes.

3S-2-1 キネシン 1 の運動と細胞骨格が生む無秩序なゆらぎ
Kinesin-1 Movement and Cytoskeletal Disordered Fluctuations
○有賀 隆行（山口大・医）
Takayuki Ariga (*Grad. Sch. Med., Yamaguchi Univ.*)

3S-2-2 紡錘体の形成と機能を支える微小管のメソスケールメカニクス
Mesoscale microtubule mechanics controlling the assembly and function of the chromosome segregation machinery
○島本 勇太 [1,2]（[1]国立遺伝学研究所, [2]総研大）
Yuta Shimamoto[1,2] ([1]*Nat'l Inst Genetics*, [2]*SOKENDAI*)

3S-2-3 繊毛の制御機構
How to control cilia movement
○吉川 雅英（東京大・医・生体構造）
Masahide Kikkawa (*Grad. Schl. of Med. Univ. of Tokyo*)

3S-2-4 ダイニン運動性の制御 -細胞質ダイニンの自己阻害とその調節機構
Regulation of dynein motility -Autoinhibition of cytoplasmic dynein and the regulatory mechanism
○豊島 陽子 [1,2]（[1]東京大学大学院総合文化研究科広域科学専攻生命環境科学系, [2]東京大学大学院総合文化研究科先進科学研究機構）
Yoko Toyoshima[1,2] ([1]*Dept of Life Sciences, Grad Sch of Arts and Sciences, The Univ of Tokyo*, [2]*Komaba Institute for Science, Grad Sch of Arts and Sciences, The Univ of Tokyo*)

3S-2-5 プログラマブルなサルコメア設計から紐解く筋ミオシン集団の協調的な力発生
Coordinated force generation of muscle myosin dissected by a programmable sarcomere design
○岩城 光宏 [1,2], 鷲尾 巧 [3], 柳田 敏雄 [2,4]（[1]理研・生命機能科学研究セ, [2]阪大・院生命機能, [3]東大・新領域, [4]脳情報通信セ）
Mitsuhiro Iwaki[1,2], Takumi Washio[3], Toshio Yanagida[2,4] ([1]*RIKEN, BDR*, [2]*Grad. Sch. Front. Biosci., Osaka Univ.*, [3]*Grad. Sch. Front. Sci., Univ. of Tokyo*, [4]*CiNet*)

3S-2-6 Long range allostery in actin filaments, and its differential requirement in force generation by actomyosin II and V
Taro Uyeda (*Dept Phys, Waseda Univ*)

9:00〜11:30
3S-3 磁覚と磁気応答生体物質の生物物理学
Biophysics of magnetoreception and magnetic responsive biomaterials

オーガナイザー：新井 栄揮（量子科学技術研究開発機構），岡野 俊行（早稲田大学）
Organizers: Shigeki Arai (QST), Toshiyuki Okano (Waseda University)

Many species including birds, mammals, reptiles, amphibians, fish, crustaceans, insects, plants, magnetotactic bacteria, etc. have an ability to detect Earth's magnetic field. This ability is called "magnetoreception". Cryptochrome (Cry) and magnetosome in cells act as receptors of the external magnetic information. Moreover, several biomaterials are known to orientate along the external magnetic force, which might relate to the magnetoreception. In this symposium, we will introduce an overview of the basics and latest findings in this research field. Here we will discuss the quantum and molecular mechanisms of the magnetoreception.

3S-3-1 クリプトクロムを介した光駆動性磁気受容
Light-driven magnetoreception mediated by cryptochromes
○岡野 俊行（早大・先進理工）
Toshiyuki Okano (*Grad. Sch. Adv. Sci. Eng., Waseda University*)

3S-3-2 クリプトクロムタンパク質の光誘起構造変化ダイナミクス
Understanding the photoinduced structural dynamics of cryptochrome proteins
○アンテル ルイス [1,2], 坂田 一郎 [3], 畠山 晋 [3], 前田 公憲 [1]([1]埼玉大学 基礎化学科, [2]科学技術振興機構さきがけ, [3]埼玉大学 生体制御学科)
Lewis M. Antill[1,2], Ichiro Sakata[3], Shin Hatakeyama[3], Kiminori Maeda[1] ([1]*Department of Chemistry, Saitama University*, [2]*PRESTO, Japan Society and Technology Agency (JST)*, [3]*Department of Regulatory Biology, Saitama University*)

3S-3-3 磁場効果から見たタンパク質バインディングポケット中でのラジカル対挙動
Radical pair dynamics in binding pockets of proteins probed by magnetic field effects
岩田 菜々 [1], アンテル ルイス [1,2], ○前田 公憲 [1]([1]埼玉大学理工, [2]JST PRESTO さきがけ)
Nana Iwata[1], Lewis Antill[1,2], **Kiminori Maeda**[1] ([1]*Graduate School of Science and Engineering*, [2]*JST PRESTO*)

3S-3-4 Magnetic field sensitivity of cellular photochemistry
Noboru Ikeya, **Jonathan R. Woodward** (*The University of Tokyo, Graduate School of Arts and Sciences*)

3S-3-5 細菌の磁気コンパス–マグネトソーム形成の生細胞イメージング–
A magnetic compass within a bacterium – Live-cell imaging of magnetosome formation –
○田岡 東 [1,2], 福森 義宏 [2]([1]金沢大・理工, [2]金沢大・ナノ生命)
Azuma Taoka[1,2], Yoshihiro Fukumori[2] ([1]*Inst. Sci. and Eng., Kanazawa Univ.*, [2]*NanoLSI, Kanazawa University*)

3S-3-6 溶液中の超分子の配向挙動：磁場強度，濃度，有効電荷に対する依存性
Orientational behavior of supramolecules in solution depending on magnetic field strength, concentration, and effective charge
○平井 光博（群馬大学大学院理工学府）
Mitsuhiro Hirai (*Graduate School of Science and Technology, Gunma University*)

3S-3-7 磁気受容蛋白質第二候補 ISCA1 の分子挙動
Molecular behavior of the second magnetorecepter candidate protein ISCA1
○新井 栄揮 [1], 清水 瑠美 [1], 安達 基泰 [1], 味戸 聡志 [2,3], 平井 光博 [3]（[1]（国）量研・量子生命科学領域, [2]（国）原子力機構, [3]群馬大・院理工）
Shigeki Arai[1], Rumi Shimizu[1], Motoyasu Adachi[1], Satoshi Ajito[2,3], Mitsuhiro Hirai[3] ([1]*Institute for Quantum Life Science, QST*, [2]*JAEA*, [3]*Department of Physics, Gunma Univ.*)

9:00〜11:30
3S-4 タンパク質の多様な存在形態　―その機能状態、動態から病態まで―
The Multiple Modes of Proteins – From Molecular Dynamics to Pathogenesis -

オーガナイザー：谷中 冴子（分子科学研究所），小川 覚之（東京大学）
Organizers: Saeko Yanaka (Institute for Molecular Science), Tadayuki Ogawa (The University of Tokyo)

Proteins undergo a variety of protein structures such as a monomer, complex, polymer and aggregation, which can display their multiple “modes” of their function in response to the specific contexts throughout their lives. This session focuses on the mechanism of protein functions driven by their multiple modes and discusses about the comprehensive usage of multiple biophysical approaches that can deepen our knowledge of the fundamental protein behavior in molecular dynamics and pathogenesis.

はじめに
Opening Remarks
谷中 冴子（分子科学研究所）
Saeko Yanaka (*Institute for Molecular Science*)

3S-4-1 High-speed atomic force microscopy as a versatile tool to study dynamical and mechanical properties of proteins
Christian Ganser[1], Kimitoshi Takeda[2], Ryota Iino[2], Koichi Kato[1], Takayuki Uchihashi[3] ([1]*NINS, ExCELLS*, [2]*NINS, IMS*, [3]*Grad. Sch. Sci., Nagoya Univ.*)

3S-4-2 Photon Factory における BioSAXS 活用した相関構造解析
Recent hybrid methods approach utilizing Biological Small Angle X-ray Scattering at the Photon Factory
○米澤 健人 [1], 古川 亜矢子 [2], 安達 成彦 [1], 千田 俊哉 [1], 清水 伸隆 [1], 西村 善文 [2,3]（[1]高エネ機構・物構研, [2]横浜市大・生命, [3]広島大・統合生命）
Kento Yonezawa[1], Ayako Furukawa[2], Naruhiko Adachi[1], Toshiya Senda[1], Nobutaka Shimizu[1], Yoshifumi Nishimura[2,3] ([1]*IMSS, KEK*, [2]*Grad. Sch. Med. Life Sci., Yokohama city Univ.*, [3]*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*)

3S-4-3 カルボニルストレスを伴う統合失調症における CRMP2 タンパク質の機能異常解析
Enhanced carbonyl stress induces irreversible multimerization of CRMP2 in schizophrenia pathogenesis
○蒋 緒光 [1], 豊島 学 [2], 小川 覚之 [1], 吉川 武男 [2], 廣川 信隆 [1]（[1]東大・院医, [2]理研 CBS）
Xuguang Jiang[1], Manabu Toyoshima[2], Tadayuki Ogawa[1], Takeo Yoshikawa[2], Nobutaka Hirokawa[1] ([1]*Grad. Sch. Med., Univ. Tokyo*, [2]*Riken CBS*)

3S-4-4 Impacts of the N-glycan variation of antibodies on their dynamic structures of functional relevance
Saeko Yanaka[1,2,3], Rina Yogo[1,2,3], Hirokazu Yagi[3], Koichi Kato[1,2,3] ([1]*ExCELLS, Natl. Inst. Nat. Sci.*, [2]*IMS., Natl. Inst. Nat. Sci.*, [3]*Grad. Sch. Pharma. Sci., Nagoya City Univ.*)

3S-4-5 超遠心分析および光散乱によるタンパク質の溶液挙動の解析
Characterization of Protein Assembly by Analytical Ultracentrifugation and Light Scattering
○有坂 文雄（東工大・生命理工）
Fumio Arisaka (*Grad Sch Biosci Bioeng, Tokyo Tech*)

おわりに
Closing Remarks
小川 覚之（東京大学）
Tadayuki Ogawa (*The University of Tokyo*)

9:00〜11:30
3S-5　共催：新学術領域研究「遺伝子制御の基盤となるクロマチンポテンシャル」
クロマチンの物理生物学
Physical Biology of Chromatin

オーガナイザー：木村 暁（国立遺伝学研究所），坂上 貴洋（青山学院大学）
Organizers: Akatsuki Kimura (NIG), Sakaue Takahiro (Aoyama Gakuin University)

Genomic DNAs in eukaryotes are complexed with various macromolecules and organized into chromatin structures inside the cell nucleus. Chromatin is a long polymer molecule, and its physical properties are closely related to the regulation of gene expression. Currently, there are many interesting attempts to unveil the structure and dynamics of chromatin from the viewpoint of polymer physics. This symposium aims to gather researchers from interdisciplinary fields ranging from molecular and cellular biology, polymer physics to information science, and discuss various aspects of chromatin physics and its implication for biological functions.

3S-5-1　クロマチン濃度により制御されるクロマチン運動
Chromatin mobility controlled by chromatin concentration
○坂上 貴洋（青学大・ 理工）
Takahiro Sakaue (*Aoyama Gakuin Univ.*)

3S-5-2　Measurements of physical properties underlying the chromatin mobility in interphase nuclei
Noritaka Masaki, Akatsuki Kimura (*Cell Arch. Lab., NIG*)

3S-5-3　動的 3 次元ゲノム組織化の物理的理解にむけて
Toward a physical understanding of the dynamic 3D genome organization
○新海 創也 [1], 大浪 修一 [1], 中戸 隆一郎 [2]（[1]理研 BDR, [2]東大 定量研）
Soya Shinkai[1], Shuichi Onami[1], Ryuichiro Nakato[2] ([1]*RIKEN BDR*, [2]*IQB, Univ. Tokyo*)

3S-5-4　1 分子イメージングで迫るヒトゲノムクロマチンの動的組織化
Single nucleosome imaging sheds light on the dynamic organization of the human chromosomes
○日比野 佳代 [1], 境 裕二 [2], 鐘巻 将人 [1], 前島 一博 [1]（[1]遺伝研・総研大, [2]東大）
Kayo Hibino[1], Yuji Sakai[2], Masato Kanemaki[1], Kazuhiro Maeshima[1] ([1]*NIG and SOKENDAI*, [2]*Univ. Tokyo*)

3S-5-5　エントロピー駆動のクロマチン相分離によるゲノム 3D 構造形成
3D genome organization through entropy-driven phase separation of chromatin
藤城 新, ○笹井 理生（名古屋大学工学研究科応用物理学専攻）
Shin Fujishiro, **Masaki Sasai** (*Department of Applied Physics, Nagoya University*)

3S-5-6　DNA contributes to nuclear size control in Xenopus laevis
Shuichi Nakano[1,2], Hiroko Heijo[1], Sora Shimogama[1], Yasuhiro Iwao[2], **Yuki Hara**[1] ([1]*Fac. Sci., Yamaguchi Univ.*, [2]*Grad. Sch. Sci., Yamaguchi Univ.*)

9:00〜11:30
3S-6　共催：新学術領域研究「光圧によるナノ物質操作と秩序の創生」
光圧操作の新展開：生物物理学のための新しいアプローチ
Frontiers in Optical Manipulation: New Approach for Biophysics

オーガナイザー：細川 千絵（大阪市立大学），西山 雅洋（近畿大学）
Organizers: Chie Hosokawa (Osaka City University), Masayoshi Nishiyama (Kindai University)

Since the pioneering works of Nobel laureate Arthur Ashkin in 2018, optical trapping has been widely applied in biophysics for manipulating cells and measuring forces between biomolecules. Recent studies are about to realize optical force technologies for mechanical manipulation such as trapping, transportation, positioning, and aligning of individual nano-materials in a direct and selective way. In this symposium, researchers from various fields related to optical trapping will present the latest results and discuss future prospects of optical manipulation in biophysics.

3S-6-1　異なる圧力下での光操作
Optical Manipulation at Different Pressures
○西山 雅祥（近畿大）
Masayoshi Nishiyama (*Kindai Univ.*)

3S-6-2　May the Red Force be with Educational Unit of Optical Tweezers
Yuichi Inoue (*OptoSigma*)

3S-6-3　3 次元位置検出顕微鏡と光ピンセットを用いた、“繊毛 1 本” のトラッキングとマニピュレーション
Tracking and manipulation of a cilium by the 3-D tracking microscopy and optical tweezers
○加藤 孝信（理化学研究所 生命機能科学研究センター）
Takanobu A Katoh (*BDR, Riken*)

3S-6-4　心筋および骨格筋ミオシンの個性とその機能を探る
Exploring the characteristics of cardiac and skeletal myosins and their functions
○茅 元司（東京大学 院理物理）
Motoshi Kaya (*Dept of Physics, Univ of Tokyo*)

3S-6-5　Nanostructure-assisted optical tweezers for soft matter manipulation
Tatsuya Shoji (*Fac. Sci., Kanagawa Univ.*)

3S-6-6　生化学反応の光誘導加速システムが拓く生物物理の新展開
Prospects of Biophysics Created by Light-induced Acceleration System for Biochemical Reaction
○飯田 琢也 [1,2], 床波 志保 [1,3], 中瀬 生彦 [1,2]（[1]大阪府立大学 理学系研究科, [2]大阪府立大学 LAC-SYS 研究所, [3]大阪府立大学 工学研究科）
Takuya Iida[1,2], Shiho Tokonami[1,3], Ikuhiko Nakase[1,2] ([1]*Grad. Sch. Sci., Osaka Pref. Univ.*, [2]*Res. Inst. for LAC-SYS, Osaka Pref. Univ.*, [3]*Grad. Sch. Eng., Osaka Pref. Univ.*)

3S-6-7　集光レーザービームを用いたタンパク質集合体の作製
Fabrication of Highly Ordered Protein Assembly by Focused Laser Beam
○吉川 洋史（埼玉大院・理工）
Hiroshi Yoshikawa (*Dept. Chem., Saitama Univ.*)

3S-6-8 **光圧による細胞表面分子の直接操作と神経活動制御への応用**

Optical manipulation of cell surface molecules for direct control of neuronal activity

○細川 千絵（大阪市大・院理学）

Chie Hosokawa (*Grad. Sch. Sci., Osaka City Univ.*)

ポスター　Poster

＊ 学生発表賞応募演題
＊ Student Presentation Award Application Poster

A. 蛋白質:機能・構造・物性・計測・工学／A. Protein General

20001A* **全原子分子動力学法による維持メチル化酵素(Dnmt1)とその捕因子の動態解析**
Theoretical Analyses on Dynamic Properties of DNA methyltransferase 1 and its Cofactors Based on All-atom Molecular Dynamics Simulations
Takunori Yasuda[1], Yasuteru Shigeta[2], Ryuhei Harada[2] ([1]*College of Biological Sciences, University of Tsukuba*, [2]*Center for Computational Sciences, University of Tsukuba*, [3]*Center for Computational Sciences, University of Tsukuba*)

20002A **3D−RISM 理論を応用した溶液中におけるペプチドの構造揺らぎの解析**
Analysis of structural fluctuations of a small peptide in the solution phase by means of 3D-RISM theory
Masatake Sugita (*Sch. Computing, Tokyo Tech*)

20003A **細菌べん毛形成開始するために 34 個集まってリングになる 2 回膜貫通タンパク質 FliF の N 末端・C 末端細胞質領域欠損体の解析**
Analysis of the cytoplasmic region-deficient mutants of double-transmembrane protein FliF which forms a MS-ring in flagellar formation
Seiji Kojima[1], Mitsuki Kajino[1], Keiichi Hirano[1], Yuna Inoue[1], Tatsuro Nishikino[2], Hiroyuki Terashima[1], **Michio Homma**[1] ([1]*Nagoya Univ, Sch Sci, Div Biol Sci*, [2]*Osaka Univ, Ins Protein Res*)

20004A **Pin1 の変異体 C113A と C113S の構造解析**
Structural analysis of Pin1 mutants C113A And C113S
Teikichi Ikura, Nobutoshi Ito (*Med. Res. Inst., Tokyo Med. Dent. Univ.*)

20005A* Similarity and difference between substrate analogue-induced and spontaneous folding of staphylococcal nuclease
Yujiro Mori[1], Saho Segawa[2], Kosuke Maki[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Sch. Sci., Nagoya Univ.*)

20006A **タンパク質の複合体の界面の相互作用のデータベース解析**
Database analysis of protein-protein interaction
Wataru Sagawa, George Chikenji (*Dept. Appl. Phys., Nagoya Univ.*)

20007A* Cross-seeding of human and bovine insulin amyloid fibrils induces stepwise conformational transition via intermediate states
Keisuke Yuzu[1], Naoki Yamamoto[2], Masahiro Noji[3], Masatomo So[3], Yuji Goto[3], Tetsushi Iwasaki[1,4], Motonari Tsubaki[1], Eri Chatani[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Fac. Med., Jichi Med. Univ.*, [3]*Inst. Protein Res., Osaka Univ.*, [4]*Biosignal Res. Center, Kobe Univ.*)

20008A **低温電子顕微鏡画像を記述する連続関数の計算法：マニフォールドラーニングによる研究**
A Computational Method for Constructing a Continuous Function Describing Cryo-Electron Microscopy Data: A Study using a Manifold Learning
Ryota Kojima, Takashi Yoshidome (*Dep. of Appl. Phys., Tohoku Univ.*)

20009A Unguided Binding MD of Protein-Protein Complexes by PPI-ColDock
Kazuhiro Takemura, Akio Kitao (*Sch. LST, Tokyo Tech*)

20010A* **tRNA 硫黄修飾酵素における鉄硫黄クラスター構造と酵素活性の相関解析**
Correlation between structures of iron-sulfur clusters and enzymatic activity in tRNA thiolation enzymes
Masato Ishizaka[1], Minghao Chen[2], Shun Narai[1], Masaki Horitani[3], Yoshikazu Tanaka[4], Min Yao[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Facul. Adv. Life Sch., Hokkaido Univ.*, [3]*Facul. Agr., Saga Univ.*, [4]*Grad. Sci. Life Sci., Tohoku Univ.*)

20011A Sampling large-scale motions in proteins using a coarse-grained multi-basin Go model
Ai Shinobu[1], Chigusa Kobayashi[1], Yasuhiro Matsunaga[2], Yuji Sugita[1] ([1]*RIKEN*, [2]*Saitama Univ.*)

20012A Visualization of translational GTPase factor-pool formed on the archaeal ribosomal P-stalk by HS-AFM

Hirotatsu Imai[1], Toshio Uchiumi[2], Noriyuki Kodera[1] ([1]*WPI-NanoLSI, Kanazawa Univ.*, [2]*Faculty of Science, Niigata Univ.*)

20013A NMR 解析によるシニョリンとその変異体の立体構造の決定

Determination of structures of chignolin and its mutant by NMR analysis

Shumpei Koroku[1], Ayori Mitsutake[2], Yutaka Maruyama[3], Koh Takeuchi[4] ([1]*Meiji University*, [2]*Meiji University*, [3]*RIKEN*, [4]*AIST*)

20014A 高速 AFM を用いた磁性細菌の細胞骨格結合タンパク質 MamJ の機能解析

Functional analyses of magnetotactic bacterial cytoskeletal binding protein MamJ using high-speed AFM

Takumi Saito[1], Yosuke Kikuchi[2], Yoshihiro Fukumori[3], Azuma Taoka[2,3] ([1]*Graduate School of Natural Science and Technology, Kanazawa University*, [2]*Institute of Science and Engineering, Kanazawa University*, [3]*Nano Life Science Institute (NanoLSI), Kanazawa University*)

20015A* 18 残基チオエーテル結合環状ペプチド群のシミュレーションデータの解析

Analysis of Molecular Dynamics Simulations of 18-residue Thioether Cyclic Peptides

Daiki Noguchi (*Meiji university graduate school*)

20016A グラフ理論に基づくタンパク質立体構造の位相解析への VOLTES 法の応用

Application of VOLTES to topological analyses of protein structures based on graph theory

Anri Terabayashi, Kyousuke Sakata, Toshitaka Shoji, Masaki Kojima (*Sch. Life Sci., Tokyo Univ. Pharm. Life Sci.*)

20017A The molecular basis for the nucleotide selectivity of the ε subunit from bacterial F-type ATP synthases

Alexander Krah[1,2], Roland G. Huber[1], Duncan G. G. McMillan[3], Peter J. Bond[1,4] ([1]*Bioinformatics Institute (BII)*, [2]*Korea Institute for Advanced Study*, [3]*TU Delft*, [4]*Department of Biological Sciences, National University of Singapore*)

20018A Free Energy Calculations of HIV-1 Protease Binding Indinavir and Its Drug-Resistant Mutant

Masahiko Taguchi[1], Ryo Oyama[2], Masahiro Kaneso[2], Shigehiko Hayashi[2] ([1]*Inst. Quant. Life Sci., QST*, [2]*Grad. Sch. Sci., Kyoto Univ.*)

20019A メタゲノムデータベース由来 PET 加水分解酵素の耐熱性および活性の改良

Improvement of thermostability and catalytic activity of a PET degrading enzyme derived from metagenome database

Akihiko Nakamura[1], Naoya Kobayashi[2], Takahiro Kosugi[2], Rie Koga[2], Nobuyasu Koga[2,3], Ryota Iino[2,3] ([1]*Shizuoka Univ.*, [2]*Inst. Mol. Sci.*, [3]*SOKENDAI*)

20020A 心筋カルシウムチャネル Cav1.2 と薬剤間の結合自由エネルギー計算

Calculation of the binding free energy between the Cav1.2 calcium channel and drugs

Tatsuki Negami, Tohru Terada (*Grad. Sch. Agr. Life Sci., Univ. Tokyo*)

20021A 標的空間を 2,3,4 次元とした Dimensional Scaling 法によるフラグメント間相互作用エネルギー行列解析

Analysis of inter fragment interaction energy by Dimensinal Scaling method in 2,3,4 by Dimensional as the target space

Yuki Abe, Masanori Yamanaka (*Univ.Nihon*)

20022A 蛋白質内部で水素結合を形成する荷電残基が示す強力な安定化効果についての熱力学的評価

The thermodynamic characterization of the strong stabilization effect by a buried and charged residue forming hydrogen bonds

Hiroaki Sato, Akiko Nakazawa, Kohei Yamamoto, **Shun-ichi Kidokoro** (*Dept. Bioeng., Nagaoka Univ. Tech.*)

20023A インスリン受容体全長構造モデリングとその分子動力学研究

Computational modeling of full-length insulin receptor and its molecular dynamics

Yoshiharu Mori (*Grad. Sch. of Sys. Info., Kobe Univ.*)

20024A Size evolution of antibody aggregates by the adsorption of serum albumin
Tomohito Nakayama[1,2], Muneaki Hase[1], Atsushi Hirano[2] ([1]*Grad. Sch. Sci. Tech., Univ. Tsukuba*, [2]*NMRI, AIST*)

20025A Theoretical Study on the Transport Cycle of the Heme ABC Transporter BhuUV-T
Koichi Tamura[1], Yuji Sugita[1,2,3] ([1]*RIKEN R-CCS*, [2]*RIKEN BDR*, [3]*RIKEN CPR*)

20026A ヤエヤマサソリ由来殺虫性毒素 LaIT2 の C 末端ドメインの大腸菌大量発現系構築
Constructon of the *E.coli* ovrexpression system for the C-terminal domain of LaIT2, an insecticidal toxin from *Liocheles australasiae*
Chiharu Tatsushiro[1], Maiki Tamura[2], Shinya Ohki[2], Hayato Morita[1,3] ([1]*Grad.Sch.Sci.,Josai Univ*, [2]*Grad.Sch.Mat Sci.,JAIST*, [3]*Fas Sci.,Josai Univ*)

20027A 高密度マイクロウェルアレイによる酵素関連タンパク質のセレクションを目的とした、ペプチドリガーゼによる遺伝子型-表現型対応付け手法の開発
Peptide ligase display (PL display) for selection of enzyme-related protein by combination with high-density microwell array chip
Shingo Ueno[1,2], Shusuke Sato[1,2], Fumi Toshioka[1], Shoichi Tsuchiya[1], Takanori Ichiki[1,2] ([1]*iCONM, Kawasaki Ins. Ind. Prom.*, [2]*Grad. Sch. Eng., Univ. Tokyo*)

20028A 長時間タンパク質ダイナミクスの拡散マップによる解析
Diffusion map analysis of long time protein dynamics
Hiroshi Fujisaki[1], Hiroto Kikuchi[1], Hiromichi Suetani[2], Ayori Mitsutake[3] ([1]*Nippon Medical School*, [2]*Grad. Sch. Eng., Oita Univ.*, [3]*Grad. Sch. Sci., Meiji Univ.*)

20029A Molecular simulation of pH effect on emission color changes through hydrogen-bond networks in firefly luciferase and its mutants
Kota Nosaka[1], Yuto Kudo[2], Naohisa Wada[1] ([1]*Grad. Sch. Life Sci., Univ.Toyo*, [2]*Fac. Food and Nu. Sci., Univ.Toyo*)

20030A Spectroelectrochemical FTIR studies of an electron-bifurcating [FeFe] hydrogenase
Nipa Chongdar[2], Krzysztof Pawlak[2], Olaf Rudiger[2], Edward Reijerse[2], Patricia Rodriguez-Macia[2], Wolfgang Lubitz[2], James Birrell[2], **Hideaki Ogata**[1,2] ([1]*ILTS, Hokkaido Univ.*, [2]*MPI/CEC*)

20031A 演題取り消し

20032A D313Y 変異をもつノーマル型べん毛繊維を用いた多型変換に関与するアミノ酸相互作用の推測
Prediction of amino acid interactions for polymorphic transformation with normal flagellar filaments with the D313Y curly mutation
Ayano Yanagita[1], Minami Oohata[1], Hikaru Tsufuku[1], Shigeru Yamaguchi[1], Fumio Hayashi[2], Kenji Oosawa[1] ([1]*Dept. Chem. & Chem. Biol., Sch. Sci. Technol., Gunma Univ.*, [2]*Ctr. Instr. Anal. Gunma Univ.*)

20033A* 統計力学モデルの拡張によるタンパク質のフォールディング経路の解析
Protein folding mechanisms predicted by an extended statistical mechanical model
Koji Ooka[1], Munehito Arai[1,2] ([1]*Dept. Phys., Univ. Tokyo*, [2]*Dept. Life Sci., Univ. Tokyo*)

20034A Structural Stability and Unfolding Kinetics of a lytic polysaccharide monooxygenase, CBP21
Yuichi Nakajima, Takeshi Watanabe, Kazushi Suzuki, Hayuki Sugimoto (*Grad. Sch. Sci. & Tech., Niigata Univ.*)

20035A Search for Partial Structural Space of Specific Loop Residues by Hydrogen Bond and Steric Repulsion
Hiroto Murata, George Chikenji (*Dept. Appl. Phys., Nagoya Univ.*)

20036A 機械学習による単粒子 X 線回折像の改善
Improvement for Noisy X-ray Single-Particle Diffraction Pattern using Convolutional Neural Network
Atsushi Tokuhisa[1,2], Yoshinobu Akinaga[1,3], Kei Terayama[1,4], Yasushi Okuno[1,5] ([1]*RIKEN Medical Sciences Innovation Hub Program (MIH)*, [2]*RIKEN Center for Computational Science (R-CCS)*, [3]*VINAS Co.,Ltd.*, [4]*Computational Life Science, Yokohama City Univ.*, [5]*Graduate School of Medicine, Kyoto Univ.*)

20037A* c-Myb-KIX 相互作用を阻害するヘリカルペプチドの合理的設計
Rational design of an α-helical peptide to inhibit c-Myb-KIX interaction
Shunji Suetaka[1], Yoshiki Oka[1], Tomoko Kunihara[1], Yuuki Hayashi[1], Munehito Arai[1,2] ([1]*Dept. Life Sci., Univ. Tokyo.*, [2]*Dept. Phys., Univ. Tokyo*)

20038A Optimized Go-MARTINI coarse-grained force field parameters based on structural flexibility of F-BAR protein Pacsin1 on lipid membrane
Md. Iqbal Mahmood[1], Adolfo Poma[2], Kei-ichi Okazaki[1] ([1]*Institute for Molecular Science*, [2]*Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, poland*)

20039A タンパク質脱イミノ化酵素 PAD3 の構造機能相関解明
Elucidation of the structure-function relationship of peptidyl arginine deiminase type 3
Mizuki Sawata[1], Kazuma Funabashi[1], Tetuya Ohwada[1], Hidenari Takahara[2,3], Masaki Unno[1,3] ([1]*Grad. Sch. Sci. Eng., Univ. Ibaraki*, [2]*Sch. Agr., Univ. Ibaraki*, [3]*Frontier., Univ. Ibaraki*)

20040A トキソプラズマ症を引き起こす病原性原虫トキソプラズマの寄生胞膜破壊に関わる Irgb6 の結晶構造
Crystal structure of Irgb6, which is involved in the destruction of a membrane-bound parasitophorous vacuole of Toxoplasma gondii
Yumiko Saijo-Hamano[1], Naoki Sakai[2], Yoshiaki Sakihama[1], Masahiro Yamamoto[3], Ryo Nitta[1] ([1]*Grad. Sch. Med., Kobe Univ.*, [2]*RIKEN, RCS*, [3]*RIMD, Osaka Univ.*)

20041A 糸状仮足観察のための Cryo-CLEM 法の検討
A study of the Cryo-CLEM method for the observation of filopodia
Miho Nakafukasako, Tomoya Higo, Yusuke V. Morimoto, Takuo Yasunaga (*Grad. Sch. Comp. Sci. Syst. Eng., KIT.*)

20042A ヘリオロドプシンおよびシゾロドプシンの構造から明らかになった微生物型ロドプシンの多様性
Structures of heliorhodopsin and schizorhodopsin elucidate the structural diversity of microbial rhodopsins
Wataru Shihoya[1], Keiichi Inoue[2], Singh Manish[3], Akimitsu Higuchi[1], Masae Konno[2], Rei Yoshizumi[3], Takayuki Uchihashi[4], Hideki Kandori[3], Osamu Nureki[1] ([1]*Dept. of Biol., Grad. Sch. Sci, Univ. of Tokyo*, [2]*ISSP, Univ. of Tokyo*, [3]*Life Sci. Appl. Chem., Grad. Sch. Eng., NIT*, [4]*Dept. of Phys., Grad. Sch. Sci, Nagoya Univ.*)

20043A The relationship between designability of protein and preference of local structures: A lattice model study
Kazuma Toko, George Chikenji (*Dept.Appl.Phys.,Nagoya Univ.*)

20044A βストランドとαヘリックスをつなぐループが特定の主鎖二面角およびアミノ酸を選択する理由
Why loops connecting a β-strand and an α-helix prefer particular dihedral angles and amino acids
Megumi Nakajima, George Chikenji (*Dept.Appl.Phys.,Nagoya Univ.*)

20045A New insight into ion transport mechanism of the Na+/H+ antiporter PaNhaP revealed by transition path shooting and Markov state model
Titouan Jaunet, Kei-ichi Okazaki (*Institute of molecular science (IMS) okazaki, japan*)

20046A Molecular dynamics simulations of the H.pylori FliG N-terminus
Dagnija Tupina[1,2], Alexander Krah[2], Chrystala I. Constantinidou[1], Peter J. Bond[2] ([1]*Univ. of Warwick*, [2]*A*STAR BII*)

20047A A large-scale structural and evolutionary analysis of protein loop regions
Lin Zhang[1], Hafumi Nishi[1,2] ([1]*Tohoku University*, [2]*Ochanomizu University*)

20048A* Ligand Docking Parallel Cascade Selection Molecular Dynamics (ld-PaCS-MD) の開発と応用
A Development of Ligand Docking Parallel Cascade Selection Molecular Dynamics (ld-PaCS MD) and its applications
Hayato Aida[1,2], Yasuteru Shigeta[2], Ryuhei Harada[2] ([1]*Bio., Degree Programs in Life and Earth Sci., Univ. of Tsukuba.*, [2]*CCS, Univ. of Tsukuba.*)

20049A* アスパラギン酸スキャニングを用いた赤外分光法によるタンパク質内局所的環境変化のマッピング解析
Mapping of the local environmental changes in proteins by FTIR spectroscopy with aspartic acid scanning
Masanori Hashimoto, Kota Katayama, Manish Singh, Yuji Furutani, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)

20050A Computational Study of Temperature-Dependent Protein Glass Transition under Varying Solvent Compositions
Michelle Yaochai[1,2], Emmanuella Li[2], Joanna Ng[2], Peter J. Bond[2], Alexander Krah[2] ([1]*NUS High Sch.*, [2]*Bioinformatics Inst., A*STAR*)

20051A 計算モデリングを用いたアブラナ科植物の自家不和合性を制御するタンパク質 SRK/SP11 複合体の包括的理解
Comprehensive understanding of SRK/SP11 protein complexes of Brassicaceae using computational modeling
Yoshitaka Moriwaki[1], Tohru Terada[1], Koji Murase[2], Seiji Takayama[2], Kentaro Shimizu[1] ([1]*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*, [2]*Appl. Biol. Chem., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

20052A Effect of the divalent cation for the activity of alcohol dehydrogenase from *Sulfolobus tokodaii*
Shuichiro Goda[1,2], Sho Takashima[2], Kosei Kajiyama[2], Yuka Nagano[2], Takuro Uchida[2], Hideaki Unno[2], Tomomitsu Hatakeyama[2] ([1]*Fuc. Sci. Eng., Soka Univ.*, [2]*Grad. Sch. Eng., Nagasaki Univ.*)

20053A 細菌機械受容チャネル MscL の G46D 変異体を用いた張力感受活性化機構の考察に関するシミュレーション研究
Computational Study Focusing on the Mechano-Gating in the Bacterial Mechanosensitive Channel MscL Using G46D GOF mutant
Yasuyuki Sawada[1], Ken'ichi Hashimoto[2], Hisashi Kawasaki[2], Masahiro Sokabe[3] ([1]*Dept. Nutrition Nagoya Univ. Economics Fac. Human Life Sci.*, [2]*Biotechnology Res Ctr, Univ Tokyo*, [3]*Mechanobiology Lab. Nagoya Univ. Grad. Sch. Med.*)

20054A* LI-cadherin 遺伝子上の SNP に伴う大腸がん転移リスク上昇の分子メカニズム
Molecular basis of increased risk of colorectal cancer metastasis caused by SNPs in LI-cadherin gene
Anna Yui[1], Chika Kikuchi[2], Shuichiro Goda[3], Takahiro Maruno[4], Susumu Uchiyama[4], Makoto Nakakido[1], Daisuke Kuroda[1,5], Satoru Nagatoishi[6], Osamu Arai[7], Hiroko Iwanari[8], Takao Hamakubo[9], Kouhei Tsumoto[1,2,6] ([1]*Dept. of Bioeng., Sch. of Eng., Univ. of Tokyo*, [2]*Dept. of Chem. Biotech., Sch. of Eng., Univ. of Tokyo*, [3]*Grad. Sch. of Sci. Eng., Soka Univ.*, [4]*Dept. of Biotech., Grad. Sch. of Eng., Osaka Univ.*, [5]*Med. Dev. Dev. Reg. Res. Center, Sch. of Eng., Univ. of Tokyo*, [6]*Inst. of Med. Sci., Univ. of Tokyo*, [7]*RCAST, Univ. of Tokyo*, [8]*Inst. of Immunol. Co., Ltd.*, [9]*Nippon Med. Sch.*)

20055A Aβ 産生抑制タンパク質 ILEI の活性中心の同定
Identification of the active center of the Aβ production suppressor protein ILEI
Emi Hibino[1,2], Masaki Nishimura[2] ([1]*Grad. Sch. Pharm. Sci., Nagoya Univ.*, [2]*Mol. Neuro., Shiga Univ. Med. Sci.*)

20056A GTP-チューブリンはどのようにして微小管の核を生成するか? (1) 直線型オリゴマーの形成
How do GTP-tubulins nucleate microtubules? (1)Formation of straight oligomers
Rie Ayukawa[1], Seigo Iwata[1], Hiroshi Imai[2,5], Shinji Kamimura[2], Masahito Hayashi[1], Kien Ngo[1], Itsushi Minoura[1], Seiichi Uchimura[1], Tsukasa Makino[1], Hideki Shigematsu[6], Ken Sekimoto[3], Benoit Gigant[4], Etsuko Muto[1] ([1]*RIKEN CBS*, [2]*Chuo Univ.*, [3]*Paris Univ.*, [4]*Paris-Saclay Univ.*, [5]*Osaka Univ.*, [6]*RIKEN BDR*)

20057A GTP-チューブリンはどのようにして微小管の核を生成するか? (2) オリゴマーのラテラルな相互作用
How do GTP-tubulins nucleate microtubules? (2)Lateral association of oligomers
Seigo Iwata[1], Rie Ayukawa[1], Hiroshi Imai[2,5], Shinji Kamimura[2], Ken Sekimoto[3], Benoit Gigant[4], Etsuko Muto[1] ([1]*CBS, RIKEN*, [2]*Chuo Univ.*, [3]*Paris Univ.*, [4]*Paris-Saclay Univ.*, [5]*Osaka Univ.*)

20058A クライオ電子顕微鏡を用いたシトクロム酸化酵素とシトクロム c の複合体構造解析
The structural analysis of cytochrome *c* oxidase complexed with cytochrome *c* using cryo-electron microscopy
Atsuhiro Shimada[1], Daisuke Kozai[2], Kouki Nishikawa[3,4], Yoshinori Fujiyoshi[3,4], Gyokucho Sho[1], Takumi Mizutani[1], Kazutoshi Tani[5] ([1]*Dept. Appl. Life Sci., Fac. Appl. Biol. Sci., Gifu Univ.*, [2]*Cell. Struct. Phys. Inst., Nagoya Univ.*, [3]*Adv. Res. Inst., Tokyo Med. Dent. Univ.*, [4]*CeSPIA Inc.*, [5]*Grad. Sch. Med., Mie Univ.*)

20059A 重み付きアンサンブル法による Pin1 異性化のパスサンプリング
Obtaining path ensemble of Pin1-catalyzed cis-trans isomerization by weighted ensemble simulation
Kei Moritsugu[1], Norifumi Yamamoto[2], Yasushige Yonezawa[3], Shin-ichi Tate[4], Hiroshi Fujisaki[5] ([1]*Yokohama City Univ.*, [2]*Chiba Tech.*, [3]*Kindai Univ.*, [4]*Hiroshima Univ.*, [5]*Nippon Med. Sch.*)

20060A 水素結合経由の J 値の定量的解析
Quantitative analysis of J value via hydrogen bonds
Hiroki Nakajima[1], Taiki Koizumi[1], Masaki Uuno[2], Masaki Mishima[1] ([1]*Grad.Sch.Sci., Univ,TokyoMetropolitan*, [2]*Grad.Sch.Sci,. Univ,Ibaraki*)

20061A Design of cyclic and linear peptides interacting with transition metal ions
Rikako Morishita, Atsuo Tamura (*Grad. Sch. Sci., Kobe Univ.*)

20062A 細胞壁を持たない細菌のチューブリンの解析
Analysis of bacterial tubulin in cell wall-less bacterium
Taishi Kasai[1], Yuhei Tahara[2], Makoto Miyata[2], Daisuke Shiomi[1] ([1]*Col. Sci., Rikkyo Univ.*, [2]*Grad. sch. Sci., Osaka City Univ.*)

20063A* コレステロールが膜貫通ペプチドの二量体化に与える影響に関する分子動力学的解析
Effect of cholesterol on the dimerization of transmembrane peptides analyzed by the molecular dynamics simulations
Hayato Itaya[1], Kota Kasahara[2], Yoshiaki Yano[3], Katsumi Matsuzaki[3], Takuya Takahashi[2] ([1]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*, [3]*Grad. Sch. Pharm. Sci., Kyoto Univ.*)

20064A 残基間平均距離統計に基づく方法によるフラボヘモグロビンのフォールディング機構予測
Prediction of folding mechanism of flavohemoglobins using techniques based on inter -residue average residue distance statistics
Maho Osugi, Takeshi Kikuchi (*Dept. Bioinf. Col. Biosci. Ritsumeikan Univ.*)

20065A ドッキングシミュレーションによる Cyclin-dependent kinase-like 5 の基質タンパク質の同定
Identification of Cyclin-dependent kinase-like 5 substrate protein using docking simulation technique
Aya Takahara[1], Shoichi Katayama[2], Takako Kawano[2], Tetsuya Inazu[2], Takeshi Kikuchi[1] ([1]*Dept. Bioinf. Col. Biosci. Ritsumeikan Univ.*, [2]*Col. Pharm.Sci. Ritsumeikan Univ.*)

20066A 構造研究のためのタンパク質連結法の開発
Development of protein ligation techniques for structural studies
Takumi Suzuki (*Grad. Sch. Sci., Univ. TMU*)

20067A* ネガティブ染色電子顕微鏡法により明らかにされた繊毛ダイニンの新規構造
Novel isolated ciliary dynein structure revealed by negative stain EM
Yici Lei[1], Hiroshi Imai[1], Akira Fukunaga[1], Shinji Kamimura[2] ([1]*Dep. Biol. Sci., Grad. Sch. Of Sci., Osaka Univ.*, [2]*Dept. Biol. Sci., Chuo Univ.*, [3]*Dept. Life Sci., Prefect. Univ. Hiroshima*)

20068A カメレオンモデルの二面角ポテンシャルの改良による NtrC の構造転移の解明
Conformational transition of NtrC elucidated by the improvement of dihedral angle potential in chameleon model
Taisei Nagata, Masaki Sasai, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

20069A Expression and Purification of Intact Small Peptides through a Novel Calmodulin-Fusion Protein System
Hao Gu[1], Koki Onuma[1], Takasumi Kato[1], Hiroaki Ishida[2], Yasuhiro Kumaki[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]*Dep. of Biol. Sci., Univ. of Calgary*, [3]*GI-CoRE, Hokkaido univ.*)

20070A RNA 結合タンパク質 FUS の液液相分離を制御するペプチドの探索
Search for peptides to control liquid-liquid phase separation of RNA binding protein FUS
Rika Chiba[1,2], Nanako Iwaki[1,3], Saori Kanbayashi[1], Keisuke Ikeda[4], Tomoshi Kameda[5], Kiyoto Kamagata[1,2,3] ([1]*IMRAM, Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*, [3]*Dep. Chem., Grad. Sch. Sci., Tohoku Univ.*, [4]*Sch. Pharm. Pharm. Sci., Univ. Toyama*, [5]*AIRC, AIST*)

20071A 天然変性タンパク質 LAF-1RGG ドメインの一分子蛍光分光測定による構造特性評価
Conformational properties of the intrinsically-disordered RGG domain of LAF-1 detected by single-molecule fluorescence spectroscopy
Michiko Kimura[1,2], Saya Nakano[1,2], Hiroto Takahashi[1], Hiroyuki Oikawa[1], Satoshi Takahashi[1] ([1]*IMRAM, Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*)

20072A Cryo-EM revealed unique and diverse binding schemes of the microtubule inner proteins at the inner junction region of cilia
Muneyoshi Ichikawa[1], Ahmad Khalifa[2], Daniel Dai[2], Shintaroh Kubo[3], Corbin Black[2], Katya Peri[2], Thomas McAlear[2], Simon Veyron[2], Shun-Kai Yang[2], Javier Vargas[2], Susanne Bechstedt[2], Jean-Francois Trempe[2], Khanh-Huy Bui[2] ([1]*NAIST*, [2]*McGill University*, [3]*Kyoto University*)

20073A 生きた細胞における DXT 法を用いた nAChR のリガンド依存的な分子内部運動の計測
Ligand-dependent intramolecular motion of nAChR in living cells detected by DXT
Koichiro Oishi[1], Yuri Nishino[1], Hiroshi Sekiguchi[2], Yasuhiro Kashino[1], Yuji C. Sasaki[3], Atsuo Miyazawa[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*JASRI*, [3]*Grad. Sch. Sci., The Univ Tokyo*)

20074A Characterization of properties of microtubule inner protein FAP85
Yoshitoki Shibao[1], Corbin Black[2], Muneyoshi Ichikawa[1], Junya Kirima[4], Kazuhiro Oiwa[3], Khanh-Huy Bui[2], Tomoya Tsukazaki[1] ([1]*NAIST*, [2]*McGill University*, [3]*NICT*, [4]*University of Hyogo*)

20075A Binding mode analysis of Hepatitis B virus X protein to DDB1 with Fluorescent based technology detecting Protein-Protein Interactions
Katsumi Omagari (*Department of Virology, Nagoya City University Graduate School of Medical Sciences*)

20076A 大腸菌フェリチン変異体の荷電状態に関する研究
A study on the charge states of Escherichia coli ferritin mutants
Takumi Kuwata, Daisuke Sato, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. of Biosci., Soka Univ*)

20077A* クライオ電子顕微鏡によるヒト PAC1 受容体の構造解析
Cryo-EM structure of the human PAC1 receptor coupled to an engineered heterotrimeric G protein
Kazuhiro Kobayashi[1], Wataru Shihoya[1], Tomohiro Nishizawa[1], Marie Ngako Kadji Francois[2], Junken Aoki[2], Asuka Inoue[2], Osamu Nureki[1] ([1]*Grad. Sch. Sci., Univ. Tokyo*, [2]*Grad. Sch. Pharm. Sci., Univ. Tohoku*)

20078A Cryo-EM structure of *Thermus thermophilus* V/A-ATPase during the rotary catalysis
Atsuko Nakanishi[1,3], Jun-ichi Kishikawa[2,3], Kaoru Mitsuoka[1], Ken Yokoyama[3] ([1]*Res. Ctr. for UHVEM, Osaka Univ.*, [2]*Inst. for Protein Res., Osaka Univ.*, [3]*Faculty of Life Sci., Kyoto Sangyo Univ.*)

20079A タンパク質における連続する 3 つの残基で構成されるユニットの運動学的特性の解析
Analysis of the Kinematic Properties of Units Comprising Three Consecutive Residues in Proteins
Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)

20080A Reconistitution of Cecytb-2 in Phospholipid Bilayer Nanodisc and Meaurments of its Ferric Reductase Activity
Hamed A. Abosharaf[1,2], Yuki Sakamoto[1], Mohammed El behery[1], Thoria Diab[2], Tarek M. Mohamed[2], Tetsunari Kimura[1], Motonari Tsubaki[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Fac. Sci., Tanta Univ.*)

20081A クライオ電子回折法による生体分子微小結晶の高分解能構造解析
High-resolution Structure Determination of Biomolecular Microcrystals by Cryo-Electron Diffraction
Kiyofumi Takaba, Koji Yonekura, Saori Maki-Yonekua (*SPring-8, RIKEN*)

20082A* 液―液相分離によって形成される多相液滴の作成
Multiphase droplet formed by liquid-liquid phase separation
Kanji Tomohara, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

20083A データベースアノテーションに基づく液滴の分析
Analysis of liquid droplets based on database annotations
Mitsuteru Iwatsuka[1], Motonori Ota[1], Satoshi Fukuchi[2], Hiroto Anbo[2] ([1]*Nagoya university*, [2]*Maebashi Institute of Technology university*)

20084A 免疫阻害機能の異なるリッサウイルス P 蛋白質 C 末端ドメインの構造比較
Structural comparison of the C-terminal domain of functionally divergent lyssavirus P proteins
Aoi Sugiyama[1], Tomo Nomai[1], Xinxin Jiang[1], Miku Minami[1], Min Yao[1], Katsumi Maenaka[1], Naoto Ito[2], Paul Gooley[3], Gregory Moseley[4], Toyoyuki Ose[1,5] ([1]*Faculty of Advanced Life Sci., Hokkaido Univ.*, [2]*Faculty of Appl. Biol. Sci., Gifu Univ.*, [3]*School of Bio21 Mol. Sci. and Biotechnol., Univ. of Melbourne*, [4]*School of Biomed. Sci., Monash Univ.*, [5]*PRESTO, Japan Science and Technology Agency*)

20085A High resolution X-ray analysis reveals a stable structure around the catalytic amino acid Asp52 in lysozyme-sugar complex
Ichiro Tanaka[1,2], Ryota Nishinomiya[1] ([1]*Grad. Sch. Sci. & Eng., Ibaraki Univ.*, [2]*Frontier Ctr, Ibaraki Univ.*)

20086A シトクロム *c* が仲介する多段階電子伝達反応における呼吸鎖超複合体形成の機能的意義
Functional significance of formation of respiratory supercomplex for multiple electron transfer reaction mediated by cytochrome *c*
Wataru Sato, Peter Brzezinski (*Stockholm Univ. Fac. of Nat. Sci.*)

20087A* PaCS-MD/MSM を用いたタンパク質複合体の速度定数評価
Kinetic rate evaluation for protein complexes by PaCS-MD/MSM
Yoshiki Miyazawa, Phouc Duy Tran, Kazuhiro Takemura, Akio Kitao (*Grad. Sch. Life Sci Tech., Tokyo Tech*)

20088A How internal cavities destabilize a protein
Ryo Kitahara[1], Mengjun Xue[2], Takuro Wakamoto[3], Frans A.A. Mulder[4] ([1]*Pharm. Sci., Ritsumeikan Univ.*, [2]*Dep. Chem. Univ. Washington*, [3]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [4]*iNANO, Univ. Aarhus*)

20089A クライオ電子線トモグラフィー法からの糸状仮足中のアクチン繊維とファシンのサブトモグラム平均化
Subtomogram Averaging of F-Actin with Fascin in Filopodia by Cryo-Electron Tomography
Atsuko Nakanishi[1], Naoko Kajimura[1], Shun Kurita[2], Takuo Yasunaga[3], **Kaoru Mitsuoka**[1] ([1]*Res. Ctr. UVHEM, Osaka Univ.*, [2]*Grad. Sch. Eng., Osaka Univ.*, [3]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)

20090A Could the biogenic zinc oxide nanoparticles inhibit the ATPase activity of ABC transporters?
Aliaa M. Radwan[1,2], Mai M. El-Keiy[2], Tarek M. Mohamed[2], Tetsunari Kimura[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Fac. Sci., Tanta Univ.*)

20091A Cold adaptation and high thermal stability mechanism of glucokinase from psychrophilic bacteria are revealed by spin-labeling ESR
Akane Yato (*Grad. Sch. Adv Hea Sci., Univ. Saga*)

20092A エネルギー準位統計とペプチドの分子進化
Energy level statistics and molecular evolution of peptide
Masanori Yamanaka (*CST, Nihon Univ.*)

20093A ドーパミン制御タンパク質 MAO-B のミトコンドリア膜中でのダイナミクス
The dynamics of dopamine-regulated protein MAO-B in the mitochondrial membrane
Masaki Ottawa[1], Lisa Matsukura[1], Naoyuki Miyashita[1], Ryuichi Harada[2], Yuichi Kimura[1], Shozo Furumoto[3] ([1]*BOST, KINDAI Univ.*, [2]*Med. Tohoku Univ.*, [3]*CYRIC, Tohoku Univ.*)

20094A* Engineering of genome editing protein Cas9 that slides along DNA faster and might enable efficient target search
Trishit Banerjee[1,2], Dwiky Rendra Graha Subekti[1,2], Hiroto Takahashi[1], Satoshi Takahashi[1], Kiyoto Kamagata[1] ([1]*IMRAM, Tohoku University*, [2]*Grad. Sch. Sci., Tohoku University*)

20095A Influence of disulfide-closed loop structures on the stability of alpha-helix
Yuki Yanagida, Masamichi Ikeguchi, Kiyomi Yoshida, Kazuo Fujiwara (*Dept.of Biosci., Soka Univ.*)

20096A CNT aptamers selection and strucuture study
Ting-Chieh Chu, Huanwen Han, Ichiro Yamashita (*Graduate School of Engineering, Osaka University*)

20097A 逆並行 β-シート中の隣接ストランド間の Cα 距離の解析
Analysis of Cα distances between adjacent strands in anti-parallel β-sheets
Hiromi Suzuki (*Sch. Agri., Meiji Univ.*)

20098A A method for producing recombinant cryptdin by enhancing inclusion body formation
Yuchi Song[1], Weiming Geng[1], Shaonan Yan[1], Wendian Yang[1], Yi Wang[1], Tomoyasu Aizawa[1,2] ([1]*Grad. Sch. of Life Sci, Hokkaido Univ.*, [2]*GI-CoRE, Hokkaido Univ.*)

20099A クライオ電顕データを用いた MD 力場の評価
Assessment of force-field accuracy using data of cryogenic electron microscopy
Tomotaka Oroguchi[1,2], Mao Oide[1,2], Taiki Wakabayashi[1,2], Masayoshi Nakasako[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*)

20100A* TAT ロドプシン変異体に対する陽イオン結合の分光学的研究
Spectroscopic study of cation binding to a TAT rhodopsin mutant
Teppei Sugimoto, Kota Katayama, Hideki Kandori (*Nagoya institute of technology*)

20101A Structural changes of a-synuclein along the lipid-binding and oligomerization revealed by fluorescence lifetime measurements
Ko Sasada, Ryosuke Matsubara, Koichi Fujii, Tetsunari Kimura (*Kobe Univ., Grad. Sch. of Sci.*)

20102A* 単細胞緑藻由来の葉緑体 ATP 合成酵素完全複合体のワンステップ単離と制御機構の解析
One-step purification and functional analysis of the chloroplast ATP synthase complex
Kentaro Akiyama[1,2], Ken-ichi Wakabayashi[1,2], Toru Hisabori[1,2] ([1]*Grad. Sch. Life Science and Technology, Titech*, [2]*CLS, Titech*)

20103A フォトンファクトリーにおける生体高分子の X 線溶液散乱
Current Status of BioSAXS at the Photon Factory
Nobutaka Shimizu, Kento Yonezawa, Masatsuyo Takahashi, Keiko Yatabe, Yasuko Nagatani (*KEK, IMSS, PF*)

20104A 緩和モード解析を用いた NTL9 のシミュレーションデータの解析
Analysis of simulations of NTL9 using relaxation mode analysis
Ayori Mitsutake (*Dept. of Physics, Meiji Univ.*)

20105A Theoretical Studies of Association-Dissociation of Plastocyanin by Coarse Grain Simulation
Dian Fitrasari, M.S. Arwansyah, Helmia Jayyinunnisya, Kazutomo Kawaguchi, Hidemi Nagao (*Kanazawa University*)

20106A 生体分子構造における形状と機能の関係
Shape similarity and functional similarity in biomolecular structures
Hirofumi Suzuki[1], Takeshi Kawabata[2], Kei Yura[1], Genji Kurisu[2] ([1]*Waseda Univ.*, [2]*IPR, Osaka-univ.*)

20107A Pressure-induced acceleration of the cyanobacterial circadian clock
Keita Mitsuhashi[1], Rina Sakurai[2], Soichiro Kitazawa[2], Kazuki Terauchi[1], Ryo Kitahara[2] ([1]*Grad. Sch. Life Sci., Univ. Ritsumeikan*, [2]*Depart. Pharm., Univ. Ritsumeikan*)

20108A In-cell NMR analysis of an anticancer candidate compound against a chemokine-signaling protein FROUNT
Sosuke Yoshinaga[1], Takafumi Sato[1], Airi Higashi[1], Mitsuhiro Takeda[1], Yuya Terashima[2,3], Etsuko Toda[2,3,4], Kouji Matsushima[2,3], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*Grad. Sch. Med., Univ. Tokyo*, [3]*RIBS, Tokyo Univ. Sci.*, [4]*Nippon Med. Sch.*)

20109A Intrinsically Disordered Protein Studied by Multi-scale Divide-and-conquer Molecular Dynamics Simulation
Hiromitsu Shimoyama[1], Yasushige Yonezawa[2] ([1]*Kitasato Univ.*, [2]*Kindai Univ.*)

20110A* Saframycin A 生合成関連蛋白質のクライオ電子顕微鏡単粒子解析
Cryo-EM study on saframycin A biosynthesis related protein
Kiichi Honda[1], Takashi Matsui[2], Ryoko Komatsu[3], Ryo Tanifuji[4], Hiroki Oguri[4], Takeshi Yokoyama[1], Yoshikazu Tanaka[1] ([1]*Laboratory of Applied Biological Molecular Science, Graduate School of Life Sciences, Tohoku University*, [2]*Laboratory of Biophysics, Department of Physics, School of Science, Kitasato University*, [3]*Department of Applied Chemistry, Graduate School of Engineering, Tokyo University of Agriculture*, [4]*Department of Chemistry School of Science The University of Tokyo*)

20111A A Singularity-Free Torsion Angle Potential for Coarse- Grained Molecular Dynamics Simulations
Cheng Tan[1], Jaewoon Jung[1,2], Chigusa Kobayashi[1], Yuji Sugita[1,2,3] ([1]*RIKEN Center for Computational Science*, [2]*RIKEN Cluster for Pioneering Research*, [3]*RIKEN Center for Biosystems Dynamics Research*)

20112A* クライオ電子顕微鏡単粒子解析による百日咳壊死毒の構造解析
Cryo-electron microscopy single particle analysis of pertussis dermonecrotic toxin
Atsushi Tsugita[1], Takashi Matsui[2], Yasuhiko Horiguchi[3], Takeshi Yokoyama[1], Yoshikazu Tanaka[1] ([1]*Laboratory of Applied Biological Molecular Science, Graduate School of Life Sciences, Tohoku University*, [2]*Laboratory of Biophysics, Department of Physics, School of Science, Kitasato University*, [3]*Department of Molecular Bacteriology, Research Institute for Microbial Diseases, Osaka University.*)

20113A Biflavonoids that inhibit ATPase and microtubule-gliding activities of mitotic kinesin Eg5
Tomisin H. Ogunwa[1], Sadakane Kei[1], Maruta Shinsaku[1], Miyanishi Takayuki[2] ([1]*Department of Bioinformatics, Graduate School of Engineering, Soka University, Hachioji, Japan*, [2]*Graduate School of Fisheries and Environmental Sciences, Nagasaki University, Nagasaki, Japan*)

20114A 分子動力学シミュレーションを用いた CDR-Grafting による合成 VHH における分子挙動の解析
Molecular dynamics analysis of structural effects of Grafting CDRs in synthetic VHHs
Seisho Kinoshita[1], Makoto Nakakido[1,2], Daisuke Kuroda[1,2], Jose M.M. Caaveiro[3], Kouhei Tsumoto[1,2,4] ([1]*Dept. of Bioeng., Sch. of Eng., Univ. of Tokyo*, [2]*Dept. of Chem. Biotech., Sch. of Eng., Univ. of Tokyo*, [3]*Grad. Sch. of Pharm. Sci., Kyushu Univ.*, [4]*Inst. of Med. Sci., Univ. of Tokyo*)

20115A* 転写コアクチベータ CBP の KIX ドメインと転写因子の相互作用を標的としたペプチド阻害剤の合理的設計
Rational design of the peptide inhibitor targeting the interaction of the KIX domain of CBP with transcriptional activators
Nao Sato[1], Shunji Suetaka[1], Yuuki Hayashi[1], Munehito Arai[1,2] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Dept. Phys., Univ. Tokyo*)

20116A 分布推定アルゴリズムと勾配降下法最適化アルゴリズムによる単粒子解析初期モデル生成
Initial model generation in single particle analysis using Estimation of Distribution Algorithms and gradient descent optimization
Nobuya Mamizu[1,2], Takuo Yasunaga[1] ([1]*Grad. Sch. Comp. Sci., Kyushu Inst. Tech.*, [2]*SYSTEM IN FRONTIER INC.*)

20117A 粗視化ペプチドの安定構造探索に向けたアミノ酸間相互作用ポテンシャルの開発
Amino-Acid Pair Interaction Potentials for Coarse Grained Peptide Folding
Chieko Terashima, Yoshiaki Tanida, Hiroyuki Sato (*Fujitsu Laboratories Ltd.*)

20118A 環状ペプチド中の隣接プロリンに特徴的な異性化
Characteristic isomerization of two adjacent prolines in a cyclic peptide
Yoshiaki Tanida, Chieko Terashima, Hiroyuki Sato (*Fujitsu Labs.*)

20119A* マイコプラズマ・モービレのモーター構成タンパク質 MMOB1620 の SAXS による構造解析
Structural Analysis of MMOB1620, Component Protein of Mycoplasma mobile's Motor, by SAXS
Hiroki Sato[1], Hisashi Kudo[2,3], Yuuki Hayashi[3], Syunji Suetaka[3], Koji Ooka[4], Munehito Arai[3,4], Makoto Miyata[1,5] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Bioengineering center, Kobe Univ.*, [3]*Dept. Life Sci., Univ. Tokyo.*, [4]*Dept. Phys., Univ. Tokyo.*, [5]*OCARINA, Osaka City Univ.*)

20120A Multiscale Modeling Approach for Conformational Search of Macrocyclic Peptides
Hiroyuki Sato, Chieko Terashima, Yoshiaki Tanida (*Fujitsu Laboratories Ltd.*)

20121A 非リボソーム分子機械によるペプチド合成の静電的ラチェット機構
Electrostatic ratcheting mechanism of peptide synthesis by non-ribosomal molecular machine
Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

20122A Local Structural Similarity of Mononucleotide Binding Sites Around Different Chemical Groups in Ligands
Shota Kawakami[1], Hafumi Nishi[2,3], Kengo Kinoshita[1,2] ([1]*Grad. Sch. Life Sci., Tohoku Univ.*, [2]*Grad. Sch. Info. Sci., Tohoku Univ.*, [3]*Fac. Core. Res., Ochanomizu Univ.*)

20123A* Secondary structure transformation of artificially designed peptide nanofibers
Minami Kurokawa[1], Mika Hirose[2], Akihiro Kawamoto[2], Atsuo Tamura[1] ([1]*Grad. Sch. Sci., Univ. Kobe.*, [2]*IPR,Univ. Osaka.*)

20124A 分子クラウディング環境における光活性化アデニル酸シクラーゼの光反応
Crowding effect on reaction dynamics of photoactivated adenylate cyclase
Hiroto Murakami, Masahide Terazima, Yusuke Nakasone (*Grad. Sch. Sci., Univ. Kyoto*)

20125A 電子伝達系における複数のタンパク質複合体の複合体形成と構造安定性に関する理論的研究
Theoretical study on complex formation and conformational stability of multiple protein complexes in electron transport system
Rena Saito, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Comput. bio., Univ. Kanazawa*)

20126A 高速原子間力顕微鏡を用いたアミロイドβ線維の伸長および抗アミロイドβ抗体による線維伸長阻害の観察
HS-AFM observation of Amyloid β elongation and inhibition by antibodies
Shogo Miyajima[1], Maho Yagi-Utsumi[2], Takayuki Uchihashi[1,2], Koichi Kato[2] ([1]*Dept of Phys, Nagoya univ*, [2]*EXCELLS*)

20127A Bayesian inference and Iterative Boltzmann approach to coarse-grained local potential of disordered proteins
Azuki Mizutani, Shoji Takada, Giovanni B Brandani (*Grad. Sch. Sci, Univ. Kyoto*)

20128A NMR Studies on Cup s 7, an Novel Allergen from Cypress Pollen
Jingkang Zheng[1], Tomona Iizuka[1], Xiaoshaung Lu[1], Tomoyasu Aizawa[1,2] ([1]*Grad. Sci. Life Sci., Hokkaido univ.*, [2]*GI-CoRE Hokkaido univ.*)

20129A* アミノ酸溶媒中における芳香族アミノ酸の溶解度
Solubility of aromatic amino acids in amino acid solutions
Akira Nomoto, Suguru Nishinami, Kentaro Shiraki (*Pure and Appl. Sci, Univ. Tsukuba*)

20130A 経験ベイズ推定を用いた水の効果の最適化によるタンパク質デザイン
Protein design by optimization of role of water using empirical Bayes' estimation
Tomoei Takahashi[1], George Chikenji[2], Kei Tokita[1] ([1]*Grad. Sch. Inform. , Nagoya Univ.*, [2]*Grad. Sch. Eng. , Nagoya Univ.*)

20131A* 脱水に応答して繊維構造を可逆的に形成するクマムシ固有の天然変性タンパク質の解析
Reversible fiber formation of tardigrade-unique intrinsically disordered proteins upon dehydration stress
Akihiro Tanaka, Tomomi Nakano, Takekazu Kunieda (*Dept. of Biol. Sci., Grad. Sch. of Sci., Univ. of Tokyo*)

20132A* スピロプラズマのらせん反転機構
Helical reversal machinery of Spiroplasma
Yuya Sasajima[1], Takayuki Kato[2], Tomoko Miyata[3], Keiichi Namba[3,4,5], Makoto Miyata[1,6] ([1]*Grad. Sch. Sci., Osaka City Univ., Japan*, [2]*IPR., Osaka Univ., Japan*, [3]*Grad. Sch. Front. Biosci., Osaka Univ., Japan*, [4]*BDR & SPring-8 Center, Riken, Japan*, [5]*JEOL Yokogushi Res. Alliance. Lab. Osaka Univ., Japan*, [6]*OCARINA, Osaka City Univ., Japan*)

20133A* 多重平衡状態を持つ光スイッチング蛍光タンパク質「Kohinoor2.0」の開発と、細胞内小器官動態の超解像イメージングへの応用
Photoswitchable fluorescent protein with multiple equilibria states enables super-resolution imaging of intracellular dynamics
Ryohei Noma[1], Tethuichi Wazawa[1], Syusaku Uto[2], Kazunori Sugiura[1], Takeharu Nagai[1] ([1]*Nagai laboratory*, [2]*no affiliation*)

20134A シアノバクテリア由来光受容タンパク質 GAF ドメインの立体構造解析
Structural study of a GAF domain of photosensor protein from Cyanobacteria
Taiki Koizumi[1], Takahiro Aizu[1], Takayuki Nagae[3], Yuu Hirose[2], Masaki Mishima[1] ([1]*Grad. Sch Sci, Tokyo Metropolitan University*, [2]*Department of Environmental and Life Sciences, Toyohashi University of Technology*, [3]*Grad. Sch Eng, Univ.Nagoya*)

B. ヘム蛋白質・膜蛋白質・核酸結合蛋白質／B. Heme-, Membrane- & nucleic acid binding-protein

20135B ウシミトコンドリア呼吸鎖酸素還元酵素の 1.3Å 分解能構造が示唆する二量体化機構
The 1.3 Å resolution structure of bovine mitochondrial respiratory oxygen reductase suggests a dimerization mechanism
Kyoko Shinzawa-Itoh[1], Miki Hatanaka[1], Kazuya Fujita[2], Naomine Yano[1], Yumi Ogasawara[1], Jun Iwata[2], Eiki Yamashita[3], Tomitake Tsukihara[2,3], Shinya Yoshikawa[2], **Kazumasa Muramoto**[1] ([1]*Grad. Sch. Life Sci., Univ. Hyogo*, [2]*Sch. Sci., Univ. Hyogo*, [3]*IPR, Osaka Univ.*)

20136B ゲノム編集酵素の開発に向けたエングレイルドホメオドメインアレイの構造解析
Structural basis for an array of engrailed homeodomains toward the development of genome-editing enzymes
Tomoko Sunami, Yu Hirano, Taro Tamada, Hidetoshi Kono (*iQLS, QST*)

20137B ナノディスクに再構成されたイネキシン 6 ギャップ結合ヘミチャネルの構造
Structures of the Innexin-6 gap junction hemichannels in nanodiscs
Batuujin Burendei[1], Ruriko Shinozaki[2], Masakatsu Watanabe[3], Tohru Terada[4], Kazutoshi Tani[5], Yoshinori Fujiyoshi[6,7], **Atsunori Oshima**[2,8] ([1]*Sch. Sci., Nagoya Univ.*, [2]*Grad. Sch. Pharm. Sci., Nagoya Univ.*, [3]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [4]*III/GSII, Univ. Tokyo*, [5]*Grad. Sch. Med., Mie Univ.*, [6]*Adv. Res., TMDU*, [7]*CeSPIA, Inc.*, [8]*CeSPI, Nagoya Univ.*)

20138B* 分子動力学シミュレーションを用いた、オレキシン 2 受容体の動的性質の研究
Dynamics of Orexin 2 Receptor Using Molecular Dynamics Simulations
Shun Yokoi, Ayori Mitsutake (*Meiji University*)

20139B 酵母の DNA 複製開始機構の一分子観察に向けて
Toward single-molecule observation of yeast pre-replicative complex assembly and firing
Mayu Terakawa S., Tsuyoshi Terakawa (*Dep. Biophys, Grad. Sch. Sci., Kyoto Univ.*)

20140B* β 切断酵素と APP の生体膜中での相互作用と α 切断酵素の構造予測
Interaction Between beta-Secretase and APP in The Biological Membrane, and The Structure Prediction of The TM domain of alpha-Secretase
Kaori Yanagino, Naoyuki Miyashita (*Grad. Sch. BOST, KINDAI Univ.*)

20141B* マラリア原虫のトランスロコンである EXP2 ナノポアのチャネル電流計測
Channel current measurement of EXP2 nanopore as a translocon of the malaria parasite
Mitsuki Miyagi, Sotaro Takiguchi, Kazuaki Hakamada, Masafumi Yoda, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

20142B 四量体と二量体のヘモグロビン平衡混合物の構造の柔らかさの違いによる分離
Separation of tetramer-dimer mixtures mutant hemoglobin by structural flexibility
Shigenori Nagatomo[1], Kitagawa Teizo[2], Nagai Masako[3] ([1]*Dept. Chem., Univ. Tsukuba*, [2]*Grad. Sch.Life Sci., Univ. Hyogo*, [3]*Res. Center Micro-Nano Tech., Hosei Univ.*)

20143B Assembly of a trimeric autotransporter transmembrane domain assisted by BamA embedded into the nanodisc
Eriko Aoki, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. of Biosci., Soka Univ.*)

20144B ナノディスク再構成型ヘム ABC トランスポーターを用いた基質輸送機構の分光学的解析
Spectroscopic analysis of allocrite transport mechanism using nanodisc-reconstituted heme ABC transporter
Takuya Asada[1], Motonari Tsubaki[1], Yoshitsugu Shiro[2], Hiroshi Sugimoto[3], Tetsunari Kimura[1,4] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Grad. Sch. Life Sci. Univ. of Hyogo*, [3]*RIKEN SPring-8*, [4]*K-CONNEX*)

20145B 膜環境の違いがアルカン水酸化酵素の活性に与える影響について
An effect of membrane environment for the activity of alkane hydroxylase
Takaki Okamoto[1], Tomomi Kikuchi[2], Shingo Nagano[1], **Tomoya Hino**[1] ([1]*Grad. Sch. Eng., Tottori Univ.*, [2]*Grad. Sch. Sus. Sci., Tottori Univ.*)

20146B* Investigating the dissociation process of DBD-p53/DNA complex by PaCS-MD and MSM
Mohamed Marzouk Sobeh[1,2], Akio Kitao[1] ([1]*School of Life Science and Technology, Tokyo Institute of Technology, 2-12-1, Ookayama, Meguro-ku, Tokyo, 152-8550, Japan*, [2]*Physics Department, Faculty of Science, Ain Shams University, 11566, Cairo, Egypt*)

20147B Electrochemical studies of human neuroglobin and cytoglobin using nanostructured electrode
Yasuhiro Mie[1], Kyoka Takahashi[1], Itoga Yuka[2], Kenta Sueyoshi[2], Ryo Torii[2], Jingkai Shen[2], Takumi Tanaka[2], Hirofumi Tsujino[2], Taku Yamashita[3] ([1]*Bioproduction Res. Inst., AIST*, [2]*Grad. Sch. Pharm. Sci., Osaka Univ.*, [3]*Sch. Pharm., Mukogawa Women's Univ.*)

20148B スピンラベル ESR 分光法による HP1 の天然変性領域の動的構造解析： DNA 結合とリン酸化の影響
Structural dynamics of IDP region in heterochromatin protein HP1 by spin-labeling ESR: Effects of DNA binding and phosphorylation
Toshiaki Arata[1,5], Kazunobu Sato[4], Ena Hirai[4], Yuichi Mishima[5], Takeji Takui[4], Toru Kawakami[5], Hironobu Hojo[5], Risa Mutoh[6], Toshimichi Fujiwara[5], Makoto Miyata[1], Isao Suetake[2,3,5] ([1]*Dept. Biol., Grad. Sch. Sci., Osaka City Univ.*, [2]*Nakamura Gakuen Univ.*, [3]*Twin Research Center, Osaka Univ.*, [4]*Dept. Chem., Grad. Sch. Sci., Osaka City Univ.*, [5]*IPR, Osaka Univ.*, [6]*Dept. Phys., Fac. Sci.,Fukuoka Univ.*)

20149B Reactive Coarse-Grained Molecular Dynamics Simulation for the Functional Dynamics of Lambda Exonuclease
Toru Niina, Shoji Takada (*Grad. Sch. Sci. Kyoto Univ.*)

20150B マイクロ秒時間領域で形成される一酸化窒素還元酵素反応中間体の分光解析
Characterization of reaction intermediate formed in the microsecond time domain of the catalytic reaction of nitric oxide reductase
Takehiko Tosha[1], Hanae Takeda[1,2], Tetsunari Kimura[3], Masaki Horitani[4], Yoshitsugu Shiro[2] ([1]*RIKEN SPring-8*, [2]*Univ. of Hyogo*, [3]*Kobe Univ.*, [4]*Saga Univ.*)

20151B PyDISH: Database and analysis tools for heme porphyrin distortion in heme proteins
Yu Takano[1], Hiroko X. Kondo[1,2,3], Yusuke Kanematsu[1,4], Gen Masumoto[5] ([1]*Grad. Sch. Info. Sci. Hiroshima City Univ.*, [2]*Faculty of Eng. Kitami Inst. Tech.*, [3]*RIKEN BDR*, [4]*Grad. Sch. Adv. Sci. Eng. Hiroshima Univ.*, [5]*RIKEN ISC*)

20152B Transient binding and non-rotational coupled motion of p53 revealed by sub-millisecond resolved single-molecule fluorescence tracking
Dwiky Rendra Graha Subekti[1,2], Satoshi Takahashi[1,2], Kiyoto Kamagata[1,2] ([1]*IMRAM, Tohoku Univ.*, [2]*Grad. Sch. Sci. Tohoku Univ.*)

20153B リン脂質二重膜ナノディスクへの再構成に伴うヒト Steap3 の三価鉄還元酵素活性の増強
Enhancement of ferric reductase activity of human Steap3 upon reconstitution into phospholipid bilayer nanodisc
Ayane Nishi[1], Akito Nakata[1], Fusako Takeuchi[2], Tetsunari Kimura[1], **Motonari Tsubaki**[1] ([1]*Dept. of Chem., Grad. Sch. Sci., Kobe Univ.*, [2]*IPHE, Kobe Univ.*)

20154B 分子動力学シミュレーションによって明らかになった SLC26A9 の塩素イオン輸送における細胞質ドメインの役割
Role of the cytoplasmic domains of SLC26A9 in chloride ion transport revealed by the molecular dynamics simulations
Satoshi Omori[1], Yuya Hanazono[2], Hafumi Nishi[1,3], Kengo Kinoshita[1,4,5] ([1]*GSIS, Tohoku Univ.*, [2]*Inst. for Quantum Life Sci., QST*, [3]*Faculty of Core Res., Ochanomizu Univ.*, [4]*ToMMo, Tohoku Univ.*, [5]*Inst. of Dev. Aging and Cancer, Tohoku Univ.*)

20155B Time-resolved spectroscopic measurements on the transport dynamics of ABC transporter
Tetsunari Kimura[1,2], Sae Hayashi[1], Yuka Ikemoto[3], Yoshitsugu Shiro[4], Hiroshi Sugimoto[2] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*RIKEN, SPring-8*, [3]*JASRI*, [4]*Grad. Sch. Sci., Univ. Hyogo*)

20156B 大腸菌 UvrD C 末端 40 アミノ酸欠損変異体の DNA 巻き戻しダイナミクス
DNA-unwinding dynamics of *Escherichia coli* UvrD lacking the C-terminal 40 amino acids
Hiroaki Yokota (*Grad. Sch. Creation New Photon. Indust.*)

20157B 高速原子間力顕微鏡によるタンパク質膜輸送装置 Sec の動態観察
Observation of Substrate Binding Sec Translocon and Structural Change of SecA with HS-AFM
Wataru Nagaike[1], Takamitsu Haruyama[2], Tomoya Tsukazaki[2], Takayuki Uchihashi[1,3] ([1]*Dept of phys, Nagoya univ*, [2]*NAIST*, [3]*EXCELLS*)

20158B Structure of the voltage-dependent potassium channel (hERG) using cryo-electron microscopy
Tatsuki Asai[1], Kano Suzuki[1], Naruhiko Adachi[2], Masato Kawasaki[2], Toshio Moriya[2], Toshiya Senda[2], Satoshi Ogasawara[1], Takeshi Murata[1] ([1]*Grad. Sch. Sci., Univ. Chiba*, [2]*KEK, Tsukuba*)

C. 核酸:構造・物性・相互作用・複合体／C. Nucleic acid

20159C 状態遷移機械を実装する多段階 DNA コンピューティング反応の最適化
Optimization of the multi-step DNA computing reaction that implements a state machine
Shuntaro Sato[1], Masayuki Yamamura[2], Ken Komiya[2] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Sch. Comp., Tokyo Inst. Tech.*)

20160C 演題取り消し

20161C* DNA のメチル化パターン依存的な構造動態の解析
Structural Dynamics of DNA Depending on Methylation-Patterns
Takeru Kameda[1,2], Miho M. Suzuki[3], Akinori Awazu[4], Yuichi Togashi[2,4] ([1]*Graduate School of Science, Hiroshima University*, [2]*RIKEN Center for Biosystems Dynamics Research*, [3]*Graduate School of Medicine, Nagoya University*, [4]*Graduate School of Integrated Sciences for Life, Hiroshima University.*)

20162C クロマチンドメインのエントロピー駆動相分離による染色体コンパートメント形成
Entropic phase separation of chromatin domains to form chromosome compartments
Shin Fujishiro, Masaki Sasai (*Grad. Sch. Appl. Phys., Nagoya Univ.*)

20163C* 分子動力学計算による p53-C 末端部位の DNA 結合機構の解明
DNA binding mechanisms of the p53 C-terminal domain elucidated by MD simulation
Yuta Taira, Duy Tran, Akio Kitao (*Titech*)

20164C DNA curtain assay of nucleosome repositioning and collisions induced by translocases
Fritz Nagae, Shoji Takada, Tsuyoshi Terakawa (*Department of Biophysics, Graduate School of Science, Kyoto University*)

20165C 核膜近傍におけるクロマチン構造形成と RNA 輸送モデルの構築
Model construction of chromatin structure formation and RNA transport near the nuclear membrane
Nozomu Imai, Shin Fujishiro, Masaki Sasai (*Dept. Appl. Phys., Nagoya Univ.*)

20166C ArsInsC 配列及び DNA 反復配列の物理的特性・機能性解析
Analysis of physical properties and functionalities of ArsInsC and DNA repeat sequences
Tappei Oda, Masashi Fujii, Naoaki Sakamoto, Akinori Awazu (*Dept. of math. and life sci. Hiroshima Univ.*)

20167C* 並列的な自己集合を基盤とした DNA 演算のナノポアデコーディング
Nanopore decoding for DNA computing based on parallel self-assembly
Sotaro Takiguchi, Ryuji Kawano (*Department of Biotechnology of Life Science, Tokyo University of Agriculture and Technology*)

20168C Local chromatin motion, chromatin quantity and nuclear volume
Shiori Iida[1], Yuji Itoh[2], Kayo Hibino[1,2], Kazuhiro Maeshima[1,2] ([1]*Dept. of Genetics, Sch. of Life Sci., SOKENDAI*, [2]*Genome Dynamics Lab., Natl. Inst. of Genetics*)

20169C* 分子動力学シミュレーションによる転写開始複合体の全原子構造モデリング
Modeling Atomistic Structure of Transcription Initiation Complex with DNA Bubble by Molecular Dynamics Simulation
Genki Shino, Shoji Takada (*Dept. of Biophys., Div. of Bio. Sci., Grad. Sch. of Sci., Kyoto Univ.*)

20170C Toward the construction of artificial organelles with controllability based on liquid-liquid phase separation of DNA nanostructures
Yusuke Sato (*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

20171C* DNA によるミクロ相分離 droplet の安定化と新しい人工細胞系の検討
Stabilization of micro phase-separated droplet and examination of new artificial cell system
Moe Yabuta, Yoshihiro Minagawa, Hiroyuki Noji (*Department of Applied Chemistry, Graduate School of Engineering, University of Tokyo*)

20172C* Large scale simulation of DNA hydrogel
Marcos Masukawa[1], Masahiro Takinoue[1,2] ([1]*Tokyo Inst. of Tech., Dept. of Comp. Sci., Sch. of Artif. Intel.*, [2]*Tokyo Inst. of Tech., Dept. of Comput. Intel. and Syst. Sci.*)

D. 電子状態／D. Electronic state

20173D 銅アミン酸化酵素のプロトン化状態についての QM/MM 解析
QM/MM study for the protonation states of copper amine oxidase
Mitsuo Shoji[1,2], Takeshi Murakawa[3], Yasuteru Shigeta[1], Hideyuki Hayashi[3], Toshihide Okajima[3,4] ([1]*Univ. Tsukuba*, [2]*JST-PRESTO*, [3]*Osaka Medical College*, [4]*Osaka Univ.*)

E. 水・水和・電解質／E. Water, Hydration & Electrolyte

20174E Application of a Deep-Learning Technique to Predict the Hydration Structure around Proteins
Kosuke Kawama[1], Takashi Yoshidome[1], Mitsunori Ikeguchi[2,3], Masateru Ohta[2] ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*RIKEN*, [3]*Grad. Sch. of Med. Life Sci., Yokohama City Univ.*)

20175E リガンド結合サイトにおける水和の包括的解析：3D-RISM 理論アプローチ
Comprehensive Analysis of the Hydration of Small Molecule Binding Sites in Ligand-Free Protein Structures: 3D-RISM Approach
Takashi Yoshidome[1], Mitsunori Ikeguchi[2,3], Masateru Ohta[2] ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*RIKEN*, [3]*Grad. Sch. of Med. Life Sci., Yokohama City Univ.*)

20176E Analysis of urea effect for binding free energy of lysozyme-$(GlcNac)_3$
Simon Hikiri, Nobuyuki Matubayasi (*Grad. Sch. Eng. Sci., Osaka Univ.*)

20177E Simulation-based machine-learning approach for the water dynamics
Taku Muzukami[1], Viet Cuong Nguyen[3], Hieu Chi Dam[2] ([1]*Materials Science, JAIST*, [2]*Knowledge Science, JAIST*, [3]*HPC systems Inc*)

20178E* MED26 による TAF7 と EAF1 認識における多様な結合様式に関する分子動力学研究
Molecular dynamics study on the multiple binding modes of MED26 torecognize EAF1 and TAF7
Satoshi Goto[1], Kota Kasahara[2], Hidehisa Takahashi[3], Hidehisa Takahashi[2] ([1]*Grad. Sch., Life Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*, [3]*Grad. Sch. Med., Yokohama City Univ.*)

20179E ヌクレオチド三リン酸の結合による細胞混雑中の蛋白質間相互作用の減少
Reduced protein-protein interactions in the cellular crowding with binding of nucleoside triphosphates
Isseki Yu[1], Michael Feig[2], Yuji Sugita[3] ([1]*Maebashi Institute of Technology*, [2]*Michigan State University*, [3]*RIKEN Theoretical Molecular Science Lab.*)

20180E 異なる配列と構造のペプチド周囲の水和ダイナミクスを MD シミュレーションで明らかにする
MD simulations reveal hydration dynamics around peptides with different sequences and structures
Takuya Takahashi[1], Shingo Nobunaga[1], Takuya Azami[2], Ryoi Ashida[2], Takuya Fujisawa[2], Kota Kasahara[1] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Grad. Sch., Life Sci., Ritsumeikan Univ.*)

20181E 分子動力学法を用いたポリグルタミン酸周囲の水和ダイナミクス解析
Analysis of hydration dynamics around polyglutamic acid using molecular dynamics method
Takuya Fujisawa[1], Takuya Takahashi[2], Kota Kasahara[2] ([1]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*)

F. 分子遺伝・遺伝情報・制御・発生・分化／F. Molecular genetics & Development

20182F Loop extrusion of chromatin at surfaces modulates the growth dynamics of transcriptional condensates
Tetsuya Yamamoto[1,2], Helmut Schiessel[3] ([1]*Institute for Chemical Reaction Design and Discovery, Hokkaido University*, [2]*PRESTO, JST*, [3]*Instituut-Lorentz for theoretical physics, Universiteit Leiden*)

20183F* 細胞性粘菌の脱分化過程における細胞質 pH の測定
Measurement of cytosolic pH changes during dedifferentiation of *Dictyostelium* cells
Tomomi Usui[1], Yusuke Morimoto[2] ([1]*Dept. Biosci. Bioinfo., Fac. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech.*, [2]*Dept. Phys. and Info. Tech., Fac. Comp. Sci. and Sys. Eng., Kyushu Inst. Tech.*)

20184F 合成遺伝子回路における細胞間相互作用依存的な発現と分化多能性
Cell-cell interaction-dependent expression of a synthetic genetic circuit and its relevance to pluripotency
Kei Ikemori[1], Yuichi Wakamoto[2] ([1]*Col. of Art. & Sci., Univ. Tokyo*, [2]*Grad. Sch. of Arts. & Sci., Univ. Tokyo*)

G. 筋肉・分子モーター／G. Muscle & Molecular motor

20185G 小胞輸送を担う分子モーターの分子数とダイニン阻害剤の影響
Effect of the dynein inhibitor dynarrestin on the number of motor proteins transporting synaptic cargos
Kumiko Hayashi[1,3], Miyamoto Miki[1], Shinsuke Niwa[2] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*FIRS, Tohoku Univ.*, [3]*JST, PRESTO*)

20186G X 線繊維回折解析による真核生物鞭毛軸糸の Ca^{2+}濃度依存的らせん対称性変化
[Ca^{2+}]-dependent changes in the helical symmetry of *Chlamydomonas* and *Ciona* flagellar axonemes revealed by X-ray fiber diffraction
Kazuhiro Oiwa[1], Kenta Ishibashi[1,2], Kogiku Shiba[3], Kazuo Inaba[3], Hiroyuki Iwamoto[4], Hitoshi Sakakibara[1] ([1]*Nat. Inst.Info.Commun.Technol*, [2]*Osaka Univ. CiNet*, [3]*Shimoda Marine Res. Cent. Univ. Tsukuba*, [4]*JASRI, SPring-8*)

20187G KIF1A/UNC-104 によるシナプス小胞前駆体輸送の数理モデル 2
Mathematical modeling of synaptic vesicle precursor transport by KIF1A/UNC- 104 2
Ryo Sasaki[1], Ryota Shinagawa[1], Kimiko Nagino[1], Kazuo Sasaki[1], Shinsuke Niwa[2], Kumiko Hayashi[1,3] ([1]*Dep. Appl. Phys., Grad. Sch. of Eng., Tohoku Univ.*, [2]*FRIS, Tohoku Univ.*, [3]*JST, PRESTO*)

20188G Computer simulation of molecular shuttles driven by biomolecular motors in external force field
Sweet May[1], Takahiro Nitta[1,2] ([1]*Electronic and Information Systems Engineering Division, Faculty of Engineering, Gifu University*, [2]*Applied Physics Course,Faculty of Engineering, Gifu Univerisity*)

20189G The Impact of Defective Motors on Biosensor Integrated with Actin Filaments and Myosin
Samuel Macharia Kang'iri[1], Takahiro Nitta[1,2] ([1]*ELECTRONICS AND INFORMATION SYSTEMS ENGINEERING DIVISION, FACULTY OF ENGINEERING, GIFU UNIVERSITY*, [2]*APPLIED PHYSICS COURSE, FACULTY OF ENGINEERING, GIFU UNIVERSITY*)

20190G* キネシン分子の空間配置が輸送複合体の運動に与える影響の評価
Molecular layout of kinesin affects the collective movement of DNA origami-based transport complex
Kodai Fukumoto[1], Yuya Miyazono[2], Hisashi Tadakuma[3], Yoshie Harada[1] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sch. Front. Sci., Univ. Tokyo*, [3]*SLST, ShanghaiTech Univ.*)

20191G キネシン・ダイニンによる軸索輸送速度の極値統計解析
Extreme value analysis of axonal transport velocity of kinesins and dyneins
Takuma Naoi[1], Kimiko Nagino[1], Kazuo Sasaki[1], Shinsuke Niwa[2], Kumiko Hayashi[1,3] ([1]*Dep. Appl. Phys., Grad. Sch. Eng., Tohoku Univ.*, [2]*FRIS, Tohoku Univ.*, [3]*JST, PRESTO*)

20192G 外眼筋の X 線回折像に対する BDM の効果
Effect of BDM on the structure of extraocular muscle revealed by x-ray diffraction
Maki Yamaguchi[1], Tohru Kurihara[1], Naoya Nakahara[1], Tetsuo Ohno[2], Toshiko Yamazawa[1], Hideki Yamauchi[1], Kazuhiro Hirano[1], Takuhiro Kawahara[1], Shigeru Takemori[1] ([1]*Dept. Mol.Physiol., The Jikei Univ. Sch. Med.*, [2]*Sports Med., Teikyo Heisei Univ.*)

20193G 1 分子・多分子実験から迫る、心機能に特化した心筋ミオシンの性質
Molecular properties of single cardiac myosin adapted for heart functions revealed by single- and multi-molecule approaches
Yongtae Hwang[1], Takumi Washio[2,3], Toshiaki Hisada[2], Hideo Higuchi[1], Motoshi Kaya[1] ([1]*Department of Physics, The University of Tokyo*, [2]*Future Center Initiative, The University of Tokyo*, [3]*UT-Heart Inc.*)

20194G ウシミトコンドリア由来 ATP 合成酵素の内在性阻害因子 IF_1 の 阻害機構解明
Elucidation of inhibition mechanism by IF_1, a natural inhibitor protein for bovine mitochondrial ATP synthase
Ryohei Kobayashi, Sougo Mori, Hiroshi Ueno, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

20195G The N-terminal β-strand of single-headed kinesin-1 is involved in the off-axis force-generation and resultant rotation pitch
Masahiko Yamagishi[1], Shoko Fujimura[2], Mitsuhiro Sugawa[1], Takayuki Nishizaka[2], Junichiro Yajima[1] ([1]*Dept. Life Sci., Grad. Arts & Sci., Univ. Tokyo*, [2]*Dept. Physics, Gakushuin Univ.*)

20196G 心筋サルコメアにおける Fhod3 と cMyBP-C の同定
Identification of Fhod3 and cMyBP-C in cardiac sarcomere
Wataru Kedouin[1], Riho Takiiwa[1], Nao Shimojo[1], Ryu Takeya[2], Takuo Yasunaga[1] ([1]*Kyushu Inst. of Tech.*, [2]*Univ.of Miyazaki*)

20197G キネシンと微小管による印刷可能な人工筋肉のコンピュータシミュレーション
Computer simulation of printable artificial muscles composed of engineered kinesins and microtubules
Yurino Aoyama[1], Yuichi Hiratsuka[2], Takahiro Nitta[3] ([1]*Grad. Sch. Appl. Math. Phys., Gifu Univ.*, [2]*Sch. Materials Sci., JAIST*, [3]*Appl. Phys. Course, Faculty of Eng., Gifu Univ.*)

20198G ウニ胚形態形成の細胞骨格観察に基づくモデル化
Modeling of sea urchin gastrulation based on cytoskeleton imaging
Kaichi Watanabe[1], Yuta Kurose[2], Yuhei Yasui[1], Naoaki Sakamoto[1], Akinori Awazu[1] ([1]*Grad. Sch. of Integrated Sciences for Life, Univ. Hiroshima*, [2]*Grad. Sch. Sci, Univ. Hiroshima*)

20199G ATP 合成酵素の c リングの回転は c サブユニットでのプロトンの受け取りと放出および a サブユニットとの静電相互作用が協調して引き起こされる
Cooperation of proton release/uptake and electrostatic interaction between a subunit and c subunit drive c-ring rotation in ATP synthase
Noriyo Mitome[1,2,3], Shintaroh Kubo[4], Sumie Ohta[2], Hikaru Takashima[3], Yuto Shigefuji[3], Toru Niina[4], Shoji Takada[4] ([1]*Fac. of Educ., Tokoha Univ.*, [2]*Dept. of Chem. and Biochem., Natn. Inst. of Tech., Numazu coll.*, [3]*Dept. of Chem. and Bio. Engin., Natn. Inst. of Tech., Ube coll.*, [4]*Dept. of Biophys., Grad. School of Sci., Kyoto Univ.*)

20200G Performance of step-finding algorithm based on the Schwarz Information Criterion depends on noise and data points per dwell-time

Monique Honsa[1,2], Kimitoshi Takeda[2], Akihiro Otomo[2,3], Hanjin Liu[4], Tomohiro Shima[4], **Ryota Iino**[2,3] ([1]*LMU Munich*, [2]*IMS*, [3]*SOKENDAI*, [4]*U Tokyo*)

20201G 自由エネルギーランドスケープのスイッチングとパワーストロークを考慮した筋収縮の三状態モデル

Three-state model of muscle contraction with switched free energy landscapes and power stroke

Kaima Matsuda, Masaki Sasai, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya. Univ.*)

20202G 体温に温めた心筋細胞に備わる収縮リズム恒常性

Contraction Rhythm Homeostasis in cardiomyocytes warmed to body temperature

Seine A. Shintani (*Dep. of Biomedical Sci., College of Life and Health Sci., Chubu Univ.*)

20203G 電子顕微鏡構造解析により明らかにされた細胞質ダイニンの休止状態の解除メカニズム

Release mechanism of the shutdown state of cytoplasmic dynein revealed by electron microscopy

Kazuki Iwasaki[1], Yui Kurume[1], Hiroshi Imai[1], Shinji Kamimura[2], Rieko Shimo-kon[1], Ryosuke Yamamoto[1], Takahide Kon[1] ([1]*Grad. Sch. Sci., Osaka Univ*, [2]*Dept.Biol.Sci.,huo Univ.*)

20204G 動く幽霊~高度好塩菌ハロフェラックス・ボルカニ~

Motile ghosts of the halophilic archaeon, Haloferax volcanii

Yoshiaki Kinosita[1,2], Richard Berry[2] ([1]*Molecular Physiology Lab., RIKEN*, [2]*Department of Physics, University of Oxford*)

20205G 汎用 3 次元モデリングソフトウェア Blender を利用したタンパク質超分子構造の動的性質の理解

Understanding Supermolecular Structure and Dynamic Property of Proteins using a general purpose 3D Graphics Modeling Software Blender

Yutaka Ueno[1], Kaoru Katou[1], Akira Kakugo[3], Kento Matsuda[3], Akihiko Konagaya[2] ([1]*AIST Tokyo*, [2]*Tokyo Tech., Dept. of Computer Scinence*, [3]*Hokkaido Univ., Graduate School of Chemical Science and Engineering*)

20206G NMR による海洋性ビブリオ菌べん毛モーターの回転方向を制御する回転子タンパク質 FliG の構造変化の解析

NMR analysis of the conformational change in FliG that switches the rotational direction of the flagellar motor in marine bacterium *Vibrio*

Tatsuro Nishikino[1], Seiji Kojima[2], Michio Homma[2], Yohei Miyanoiri[1] ([1]*Inst. for Protein res., Osaka Univ.*, [2]*Div. Biol. Sci. Grad. Sch. Sci., Nagoya Univ.*)

20207G* Multiple step photo regulation of mitotic kinesin Eg5 using a novel photochromic Inhibitor composed of Spiropyran and azobenzene

Islam Md Alrazi, Kei Sadakane, Happy Ogunwa Tomisin, Shinsaku Maruta (*Soka University, Graduate School of Engineering, Department of Bioinformatics*)

20208G Modeling of condensin hinge/DNA structure by molecular dynamics simulations guided by atomic force microscopy

Hiroki Koide[1], Noriyuki Kodera[2], Shveta Bisht[3], Christian Haering[3], Shoji Takada[1], Tsuyoshi Terakawa[1] ([1]*Department of Biophysics, Graduate School of Science, Kyoto University*, [2]*Nano Life Science Institute (WPI-NanoLSI), Kanazawa University*, [3]*Cell Biology and Biophysics Unit, Structural and Computational Biology Unit, European Molecular Biology Laboratory (EMBL)*)

20209G キネシン 1 二量体の前頭部における微小管からの解離抑制の直接観察

Direct observation of the suppression of the leading head of kinesin-1 dimer from detachment from microtubule

Kohei Matsuzaki[1,2], Michio Tomishige[1] ([1]*Dept. Phys., Col. Sci. Eng., Aoyama Gakuin Univ.*,, [2]*Dept. Appl. Phys., Grad. Sch. Eng., Univ.Tokyo*)

20210G ミオシン VI の歩行運動に対するランドスケープ描像

A landscape-based view on the stepping movement of myosin VI

Tomoki P. Terada[1], Qing-Miao Nie[2], Masaki Sasai[1] ([1]*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*, [2]*Dept. Appl. Phys., Zhejiang Univ. Tech.*)

20211G 微小管とキネシンの結合におけるチューブリン C 末端の役割
Role of C-terminal tail of tubulin in microtubule-kinesin binding
Yuta Taguchi, Yukinobu Mizuhara, Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

20212G* べん毛モーター固定子の協働的な集合によるトルクの自律的制御
Cooperative stator assembly of bacterial flagellar motor for autonomous torque regulation
Kenta Ito, Shuichi Nakamura, Shoichi Toyabe (*Grad. Eng., Tohoku Univ.*)

20213G 光てこによる *Volvox*1 個体が生じる推進力の直接測定
Direct force measurement of a swimming *Volvox* spheroid by a high-speed optical lever system
Katsuya Shimabukuro[1], Kosaku Horinaga[1], Kazumo Wakabayashi[1], Hikaru Emoto[1], Noriko Ueki[2], Ken-ichi Wakabayashi[3], Noriyo Mitome[1,4] ([1]*Chem. Bio. Eng., NIT Ube College*, [2]*Sci. Res. Cent., Hosei Univ*, [3]*CLS, Tokyo Tech*, [4]*Tokoha Univ.*)

20214G 高速イメージングで明らかになった遊泳するボルボックスの速度周期性
Periodic fluctuations detected in the swimming velocity of a *Volvox carteri* spheroid by high speed imaging
Naoki Uemura, Tatsuya Suehiro, Midori Nosaka, Katsuya Shimabukuro (*Chem. Bio. Eng., NIT Ube College*)

20215G* 好熱菌由来 F_1-ATPase の完全な化学力学共役は至適生育温度において破れる
The perfect mechanochemical coupling of thermophilic F_1-ATPase breaks at the optimum growth temperature
Tomoaki Okaniwa[1], Yohei Nakayama[1,2], Eiro Muneyuki[1] ([1]*Grad. Sch. Sci. Eng.*, [2]*Grad. Sch. Eng.*)

20216G ATP 加水分解を選択的に抑制する F_1-ATPase の速度論的制御機構
Kinetic ratchet mechanism of F_1-ATPase selectively suppresses hydrolysis of ATP
Yohei Nakayama, Shoichi Toyabe (*Grad. Sch. Eng., Tohoku Univ.*)

20217G Mixed motility assay を用いたフォトクロミック Eg5 阻害剤の Eg5 阻害機構の解析
Analyze inhibitory mechanism of kinesin Eg5 with photochromic Eg5 inhibitor using mixed-motility assay
Kei Sadakane[1], MD Alrazi Islam[2], Happy Ogunwa Tomisin[2], Shinsaku Maruta[1,2] ([1]*Sci. & Eng., Soka Univ.*, [2]*Grad. Sch. Eng., Soka Univ.*)

20218G DNA ナノチューブ上に構築されたダイニン線形アレイの集団運動性
Collective motility of dynein linear arrays built on DNA nanotubes
Ryota Ibusuki[1], Misaki Shiraga[2], Akane Furuta[1], Maki Yoshio[1], Hiroaki Kojima[1], Kazuhiro Oiwa[1,2], Ken'ya Furuta[1] ([1]*Adv. ICR. Res. Ins., NICT. Kobe*, [2]*Grad. Sch. Sci., Univ. Hyogo*)

20219G Increasing speed of single-molecule kinesin movement in vitro
Keitaro Shibata[1], Misaki Sagawa[2], Hiroaki Kojima[1], Ken'ya Furuta[1] ([1]*Adv. ICT. Res. Ins., NICT*, [2]*Grad. Sch. Sci., Univ. Hyogo*)

20220G Single-molecule analysis of artificial kinesin-1 dimers and trimers with different linker lengths
Kimitoshi Takeda[1], Monique Honsa[1,2], Akihiko Nakamura[3], Jun Ando[4], Ryota Iino[1,5] ([1]*Institute for Molecular Science*, [2]*LMU Munich*, [3]*Dep. Appl. Life Sci. Agr. Shizuoka Univ*, [4]*RIKEN*, [5]*SOKENDAI*)

20221G* バーチャル電極上の電場によるキネシンと微小管の駆動システムの制御
Controlling fundamental functions of the kinesin-microtubule by the electrical field on the virtual cathode
Kenta Hatazawa[1], Ryuzo Kawamura[2], Takayuki Hoshino[1] ([1]*Department of Mechanical Science and Engineering, Science and Technology, Hirosaki Univ.*, [2]*Division of Strangic Research and Development, Graduate School of Science and Engineering, Saitama Univ.*)

20222G* ダイナクチンサイドアームのコンフォメーション多様性
Conformational diversity of dynactin sidearm
Kei Saito[1], Takuya Kobayashi[2], Takashi Murayama[2], Yoko Toyoshima[1] ([1]*Grad. Sch. Arts Sci., Univ. Tokyo*, [2]*Dept. of Pharmacology, Juntendo Univ. Sch. of Med.*)

20223G Constructing a simplified axoneme-like system using *Chlamydomonas* outer arm dynein and DNA nanotubes
Akane Furuta[1,2], Yuka Matsuda[3], Ryota Ibusuki[1], Misaki Sagawa[3], Kazuhiro Oiwa[1,3], Hiroaki Kojima[1], Ken'ya Furuta[1] ([1]*NICT*, [2]*JSPS*, [3]*University of Hyogo*)

20224G V/A-ATPase の膜内在性ドメイン V_o のプロトン漏洩防止機構
Mechanical inhibition of isolated Vo from V/A-ATPase for proton conductance
Jun-ichi Kishikawa[1,2], Atsuko Nakanishi[3], Aya Furuta[2], Takayuki Kato[1], Keiichi Namba[4], Masatada Tamakoshi[5], Kaoru Mitsuoka[2], Ken Yokoyama[2] ([1]*Inst. Prot. Res., Osaka Univ.*, [2]*Dept. Mol. Biosci., Kyoto Sangyo Univ.*, [3]*Res. Ctr. UHVEM., Osaka Univ.*, [4]*Grad. Sch. Frontier. Biosci., Osaka Univ.*, [5]*Dept. Mol. Biol., Tokyo Univ. Pharm. Life Sci.*)

20225G* FliL は低負荷条件下で大腸菌べん毛モーターの回転を支援する
FliL assists flagellar motor rotation in *Escherichia coli* under low load condition
Tsubasa Ishida[1], Myu Yoshida[2], Tohru Minamino[3], Yoshiyuki Sowa[1,2,4] ([1]*Grad. Sch. Sci. & Eng., Hosei Univ.*, [2]*Dept. Frontier Biosci., Hosei Univ.*, [3]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [4]*Res. Cent. Micro-Nano Tech., Hosei Univ.*)

20226G *Enterococcus hirae* 由来 V-ATPase のナトリウムイオン濃度に依存した回転運動の 1 分子解析
Single-molecule analysis of rotation of *Enterococcus hirae* V-ATPase depending on sodium ion concentration
Akihiro Otomo[1,2], Tatsuya Iida[1,2], Hiroshi Ueno[3], Takeshi Murata[4], Ryota Iino[1,2] ([1]*Inst. for. Mol. Sci*, [2]*SOKENDAI*, [3]*The Univ. Tokyo*, [4]*Chiba Univ.*)

20227G Autonomous molecular swarm robots realized by sequential transfer of DNA signal
Jakia Jannat Keya[1], Yuta Yamasaki[2], Kazuki Sada[1], Akinori Kuzuya[2], Akira Kakugo[1] ([1]*Hokkaido University*, [2]*Kansai University*)

20228G* 演題取り消し

20229G 鞭毛波形切り替えメカニズムの数理モデル
A mathematical model for mechanism of flagellar waveform change
Kenta Ishibashi[1,2], Hitoshi Sakakibara[3], Kazuhiro Oiwa[2,3,4] ([1]*Osake Univ.*, [2]*NICT-CiNet*, [3]*Advanced ICT Research Institute*, [4]*University of Hyogo*)

20230G The Helical Arrangement of Axonemal Structures Depends on the Region of the Flagellum
Hitoshi Sakakibara[1], Kenta Ishibashi[2], Hiroyuki Iwamoto[3], Hiroaki Kojima[1], Kazuhiro Oiwa[1,4] ([1]*Bio Function PJ, NICT*, [2]*CiNet, Osaka Univ.*, [3]*SPring-8, JASRI*, [4]*Life Sci. Univ. Hyogo*)

20231G ビーズ-DNA 複合体および DNA ナノチューブを利用した人工分子モーターの実現を目指して
Towards the realization of artificial molecular motor using beads-DNA complex and DNA nanotube
Kohei Arai[1], Kenta Ito[1], Yuki Tsushima[2], Yusuke Sato[1,3], Shoichi Toyabe[1] ([1]*Appl. Phys., Grad. sch. eng., Tohoku univ*, [2]*IIS, Tohoku univ.*, [3]*Front. Res. Inst. Interdiscip. Sci., Tohoku Univ*)

20232G 単極毛性細菌 *Vibrio cholerae* におけるべん毛モーター回転切り替えの協同性
Low cooperativity of flagellar motor switching in *Vibrio cholerae* the bacterium of a single polar flagellum
Hirotaka Tajima[1,2], Masatoshi Nishikawa[1], Yuki Miura[3], Yoshiyuki Sowa[1,2,3], Ikuro Kawagishi[1,2,3] ([1]*Dept. Front. Biosci., Hosei Univ.*, [2]*Res. Cent. Micro-Nano Tech., Hosei Univ.*, [3]*Grad. Sch. Eng., Hosei Univ.*)

20233G CbM4 の持つ時計回りの運動活性の解析
Analysis of the clockwise motility of CbM4
Kohei Yoshimura, Takuma Imi, Takeshi Haraguchi, Masanori Tamanaha, Kohji Ito (*Grad. Sch. Sci., Chiba Univ.*)

20234G* 腸管病原性大腸菌が有するⅢ型分泌装置の ATPase の活性特性評価と HS-AFM を用いた構造ダイナミクスに対する考察
Characterization of the enzymatic property and structural dynamics of the T3SS ATPase from Enteropathogenic Escherichia coli
Aya Suzuki[1], Hiroshi Ueno[1], Ryo Kurosaki[2], Takayuki Uchihashi[2], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*Grad. Sch. Sci., Univ. Nagoya*)

20235H 演題取り消し

20236H 演題取り消し

20237H Visualizing of neo-self phenomena in chimeric antigen receptor (CAR)-T cells
Hiroaki Machiyama, Ei Wakamatsu, Tadashi Yokosuka (*Dept. Immunol, Tokyo Med. Univ.*)

20238H ストレスファイバーの張力ホメオスタシスに関する研究
Theoretical consideration of homeostasis in stress fibers
Yuika Ueda, Daiki Matsunaga, Tsubasa Matsui, Shinji Deguchi (*Grad. Eng. Sci., Univ. Osaka*)

20239H 支持脂質二重膜に固定したカドヘリンのモノマー・ダイマー間構造変換の高速 AFM による追跡
Chasing the transformation between monomer and dimer structure of cadherin anchored to supported lipid bilayer by high-speed AFM
Shigetaka Nishiguchi[1], Hiroki Oda[3,4], Takayuki Uchihashi[1,2] ([1]*ExCELLS*, [2]*Nagoya Univ.*, [3]*BRH*, [4]*Osaka Univ.*)

20240H 非接着状態がん細胞の転移能上昇に伴う細胞間接着強度の増加
Increase of intercellular adhesion strength of non-adherent cancer cells associated with the upregulation of their metastatic ability
Kenta Ishibashi[1], Chikashi Nakamura[1,2], **Hyonchol Kim**[1,2] ([1]*Grad. Sch. Eng., Tokyo Univ. Agric. Technol.*, [2]*Cell. Mol. Biotechnol. Res. Inst., AIST*)

20241H* 損傷した細胞における細胞内粘性と生存確率の関係
Cytoplasmic Viscosity and Cellular Viability of the Damaged Cells
Hideaki Ota, Hideo Higuchi (*Department of Physics, School of Science, The University of Tokyo*)

20242H 繊毛への機械刺激依存的な、マウスノードクラウン細胞における mRNA 分解
Mechanical stimuli to a cilium activate mRNA decay in a mouse nodal crown cell
Takanobu A Katoh[1], Katsutoshi Mizuno[1,2], Hiroshi Hamada[1] ([1]*BDR, Riken*, [2]*School of Medical Sciences, University of Fukui*)

20243H* 運動性細胞における Ras の興奮性制御に関わる GEF の同定
Identification of GEFs regulating the excitability of Ras in motile cells
Koji Iwamoto[1], Satomi Matsuoka[1,2,3], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. Sci., Univ. Osaka*, [2]*Grad. Sch. of Front. Biosci., Univ. Osaka*, [3]*BDR, RIKEN*)

20244H クラミドモナス軸糸運動の再活性化イメージング
High hydrostatic pressure induces vigorous flagellar beating in *Chlamydomonas* non-motile mutants lacking the central apparatus
Toshiki Yagi[1], **Masayoshi Nishiyama**[2] ([1]*Pref. Univ. Hiroshima*, [2]*Kindai Univ.*)

20245H 細菌バイオフィルムと骨代謝の ASEM 免疫電顕と cryo-TEM による観察
Observation of biofilm and bone metabolism in aqueous liquid using immuno-labeled ASEM and cryo-TEM
Chikara Sato[1], Shinya Sugimoto[2], Eiko Sakai[3], Mari Sato[1], Naoki Kasahata[1], Masami Naya[1] ([1]*Health & Medical Res.Inst, AIST.*, [2]*Dept. Bacteriol., The Jikei Univ. Sch. Med.*, [3]*Dental Pharmacology,Nagasaki Univ.*)

20246H Tension at adherens junction inhibits proliferation and promotes differentiation of keratinocyte carcinoma cells
Oleg Dobrokhotov, Masahiro Sokabe, Hiroaki Hirata (*Grad. Sch. Med., Nagoya Univ.*)

20247H 細胞質中における p52SHC は GRB2 の細胞膜移行を負に制御する
p52SHC in the cytoplasm negatively regulates GRB2 translocation to the plasma membrane
Ryo Yoshizawa[1,2], Nobuhisa Umeki[2], Masayuki Murata[1], Yasushi Sako[2] ([1]*Grad.sch.arts and ahi., the univ. Tokyo*, [2]*Wako Inst., Riken*)

20248H 細胞内脂肪滴の普遍的相挙動
Liquid-liquid crystal phase transitions in intracellular lipid droplets
Shunsuke F. Shimobayashi[1], Yuki Ohsaki[2] ([1]*Chemical Biological Engineering, Princeton Univ.*, [2]*Grad. Sch. Med., Nagoya Univ.*)

20249H 陰圧条件下における金魚ケラトサイト細胞の移動速度の上昇
Enhanced movement of fish keratocyte cells under negative pressure conditions
Akihiro Yamazaki, Hitoshi Tatsumi (*Kanazawa Inst. of Technology*)

20250H 1 細胞自律的な細胞内温度制御の分子機構
A cell-autonomous control of intracellular temperature by mitochondrial thermogenesis
Akira Murakami[1,2], Kohjiro Nagao[1], Reiko Sakaguchi[1], Kohki Okabe[2], Harada Yoshie[3], Masato Umeda[1] ([1]*Dept. of Synth. Chem. And. Biol. Chem., Grad. Sch. of. Eng., Kyoto Univ.*, [2]*Grad. Sch. of Pharm. Sci., Univ. of Tokyo*, [3]*Inst. for Protein Res., Osaka Univ.*)

20251H 蛍光顕微鏡法による単一デスミンフィラメントの可視化
Visualization of single desmin filaments by fluorescence microscopy in vitro
Masashi Sato, Keigo Murakami, **Kuniyuki Hatori** (*Grad. Sch. Sci. Eng., Yamagata Univ.*)

20252H* 収縮するアクトミオシン構造の綱引きで決まる細胞サイズ液滴内の位置対称性
A tug-of-war between contractile actomyosin structures determines the positioning symmetry in cell-sized droplets
Ryota Sakamoto[1], Tetsuya Hiraiwa[2,3], Masatoshi Tanabe[4], Kazuya Suzuki[4,5], Shin'ich Ishiwata[4], Yusuke Maeda[1], Makito Miyazaki[6,7,8] ([1]*Dept. Phys., Kyushu Univ.*, [2]*Dept. Phys., Tokyo Univ.*, [3]*Mechanobio. Inst., Nat. Univ. Singapore*, [4]*Dept. Phys., Waseda Univ.*, [5]*Cent. Lab., Hamamatsu Photonics K.K*, [6]*Hakubi Cent., Kyoto Univ.*, [7]*Dept. Phys., Kyoto Univ.*, [8]*Curie Inst.*)

20253H* NF-κB mediated transcriptional regulation in B-cell
Johannes Nicolaus Wibisana[1], Takehiko Inaba[2], Yasushi Sako[2], Mariko Okada[1] ([1]*IPR Osaka Univ.*, [2]*RIKEN*)

20254H 神経シナプスでの AMPA 受容体数密度の動的制御：1 分子イメジングによる解明
Dynamic regulation of the AMPA receptor number density in the neuronal synapse as revealed by single-molecule imaging
Yuri L. Nemoto[1], Kazuma Naito[2], Hiroko Hijikata[1], Taka A. Tsunoyama[1], Nao Hiramoto-Yamaki[2], Rinshi S. Kasai[3], Yuki M. Shirai[2], Manami S. Miyahara[2], Takahiro K. Fujiwara[2], Akihiro Kusumi[1,2,3] ([1]*OIST*, [2]*Kyoto University, WPI-iCeMS*, [3]*Kyoto University, Institute for Frontier Life and Medical Sciences*)

20255H γ-tubulin は中心子トリプレット微小管形成に寄与する
γ-tubulin functions in assembling centriolar triplet microtubules
Yuki Nakazawa[1,2], Mao Horii[3], Saki Watanabe[2], Moeko Otsuki[2], Akira Noga[3], Ken-ichi Wakabayashi[4], Masafumi Hirono[2] ([1]*Science and Technology Group, OIST*, [2]*Dept. Frontier Biosci.,Fac. Biosci. Appl. Chem., Hosei Univ.*, [3]*Dept. Biosci., Grad. Sch. Sci., Univ. Tokyo*, [4]*Inst. Innov. Res., Tokyo Inst. Tech.*)

20256H 2 本の内べん毛の同調した回転は細菌の遊泳を制御する
Coordinated rotation of dual endo-flagella controls bacterial swimming
Toshiki Kuribayashi, Shuichi Nakamura (*Grad. Sch. Eng., Tohoku Univ.*)

20257H 細胞の間隙で働く接着性 GPCR の蛍光 1 分子観察
Single molecule observation of adhesion GPCR accumulated at the cell-cell interface
Rinshi Kasai[1], Yuri Nemoto[2] ([1]*Inst. Front. Life. Med. Sci., Kyoto Univ.*, [2]*OIST*)

20258H* マイクロ構造化ハイドロゲル上を移動する細胞の核形態変化の定量解析
Quantitative analysis of dynamic changes in nuclear morphology in cells migrating on microstructured gelatin hydrogel
Ryo Ishida[1], Tomoko Oyama G[2], Kotaro Oyama[2], Mitsumasa Taguchi[2], Hiromi Miyoshi[1] ([1]*Grad. Sch. Syst., Univ. Tokyo. MetroSyst*, [2]*QuBS., QST*)

20259H ADP により調節されるマウス気管繊毛の運動活性
Motility of murine tracheal cilia modulated by ADP
Masashi Iwata[1], Keiju Kawano[1], Masayuki Shiina[1], Toshihito Iwase[1], Nobukiyo Tanaka[1], Koji Ikegami[2], Tomoko Masaike[1] ([1]*Dept. of Appl. Biol. Sci., Tokyo Univ. of Science*, [2]*Grad. Sch. of Biomedical & Health Sci., Hiroshima Univ.*)

20260H 熱量および蛍光滴定により推定されたタウ-DNA 結合熱
Tau-DNA binding heat estimated by calorimetric and fluorescence titrations
Kan Matsuda, Junta Kashima, Hideyuki Komatsu (*Dept. Biosci. Bioinf., Kyushu Inst. Tech.*)

20261H* クラミドモナス繊毛交互打ち変異株の単離と解析
Isolation and analysis of Chlamydomonas mutants showing alternate ciliary beatings
Kazuma Sakamoto[1,2], Toru Hisabori[1,2], Ken-ichi Wakabayashi[1,2] ([1]*CLS, Tokyo Tech.*, [2]*Sch. Life Sci. Tech., Tokyo Tech.*)

20262H Response of plural phagocytosis is regulated by the attached order of antigens as far as macrophages can recognize the time differences
Tomoyasu Sakaguchi[1], Yuya Hurumoto[1], Tosiki Azuma[1], Amane Yosida[1], Kenji Yasuda[1,2,3] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*)

20263H Dominant factor for cease phagocytosis after excess intake of antigens is explained by the volume regulation with 0.62-μm encapsulation
Toshiki Azuma[1], Yuya Furumoto[1], Amane Yoshida[1], Tomoyasu Sakaguchi[1], Kenji Yasuda[1,2,3] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Phys., Sch. Adv. Sci. & Eng., Waseda Univ*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*)

20264H Measurement of the temporal rotation change of individual cells' trajectory in collective cell migration in agarose microchannels
Shun Koide[1], Mitsuru Sentoku[1], Kento Iida[2], Hiromichi Hashimoto[2], Masao Odaka[3], Akihiro Hattori[3], Kenji Yasuda[1,2,3] ([1]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ*, [2]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda U niv.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*)

20265H Maximum limit of phagocytosis is explained by the shortage of consumable cell membrane with 0.9 μm envelope in phagosome
Dan Horonushi[1], Yuya Furumoto[2], Toshiki Azuma[2], Amane Yoshida[2], Tomoyasu Sakaguchi[2], Yumeno Tanaka[1], Kenji Yasuda[1,2,3] ([1]*Dept. 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*)

20266H Velocity split after passing through the wide-narrow-wide capillary tube caused by short-term memory in collective cell migration
Mitsuru Sentoku[1], Hiromichi Hashimoto[2], Kento Iida[2], Kenji Yasuda[1,2,3] ([1]*Dept. 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.*)

20267H PM2.5 antigens maintains efficiency of engulfment ability in serial phagocytosis of single macrophages with on-chip free-flow method
Yuya Furumoto[1], Toshiki Azuma[1], Amane Yoshida[1], Tomoyasu Sakaguchi[1], Yumeno Tanaka[2], Dan Horonushi[2], Kenji Yasuda[1,2,3] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*)

20268H 好気及び嫌気性条件で酸化及び還元型αディフェンシン cryptdin-4 の抗菌メカニズムの検討
Antibacterial mechanism of an α-defensin, cryptdin-4 in redox status under aerobic and anerobic conditions
Yi Wang[1], Weiming Geng[1], Rina Hiramine[1], Chisato Toyokawa[1], Tomoyasu Aizawa[1,2] ([1]*Grad. Sci. Life Sci., Hokkaido Univ.*, [2]*GI-CoRE, Hokkaido Univ.*)

20269H 多電極電位システムを用いたハイスループット心毒性検査法の実用化を目指した少数心筋細胞集団薬剤応答の解析
Analysis of small size of cardiomyocyte population's drug response for high-throughput cardiotoxicity test using multi-electrode system
Kentaro Kito, Naoki Tadokoro, Masahito Hayashi, Tomoyuki Kaneko (*Laboratory for Reconstructive Cell biology, Department of Frontier Bioscience, Hosei University*)

20270H 大腸菌走化性応答適応過程の高い再現性を実現する簡易培養方法の構築
Construction of simple culture method that realizes high reproducibility of Escherichia coli chemotaxis response adaptation process
Hiroto Tanaka, Yasuaki Kazuta, Amina Yano, Hiroaki Kojima (*Adv ICT Res Inst, NICT*)

20271H Hysteresis is not remained in macrophages after engulfment in fluctuation of movement angles with a single-point series phagocytosis assay

Yumeno Tanaka[1], Yuya Furumoto[2], Toshiki Azuma[2], Amane Yoshida[2], Tomoyasu Sakaguchi[2], Dan Horonushi[1], Kenji Yasuda[1,2,3] ([1]*Dept. 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.*)

20272H* アガロース微細加工技術を用いた環状心筋細胞ネットワークによる伝導異常モデルの構築
Construction of conduction abnormality model by circular cardiomyocyte network using agarose microfabrication technology

Koji Emura, Masahito Hayashi, Tomoyuki Kaneko (*LaRC, FB, Grad.Sci&Eng, Hosei Univ.*)

20273H Width-dependent concave velocity distribution in collective migration is explained by two fluid-like behavior rules

Hiromichi Hashimoto[1], Mitsuru Sentoku[2], Syun Koide[2], Kento Iida[1], Kenji Yasuda[1,2,3] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*, [3]*Org. Univ. Res. Initiatives, Waseda Univ.*)

20274H 高静水圧によるウニ精子細胞内カルシウム濃度への影響
Effects of high hydrostatic pressure on intracellular Ca2+ concentration of sea urchin swimming live sperm

Hiroshi Imai[1,2], Masayoshi Nishiyama[3], Yumiko Kaminoe[3], Yoshie Harada[4], Takahide Kon[1], Shinji Kamimura[2] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Dept. Biol. Sci., Chuo Univ.*, [3]*Dep. Phys., Kindai Univ.*, [4]*IPR, Osaka Univ.*)

20275H 生細胞における 1 分子イメージングと超解像顕微鏡法を用いた動態と相互作用の定量解析
Quantification of dynamics and kinetics using single-molecule and super-resolution imaging in living cells

Yuma Ito, **Makio Tokunaga** (*Sch. Life Sci. Tech., Tokyo Tech.*)

20276H 1 分子イメージングで明らかになった糖鎖によるエクソソーム機能制御
Regulation of exosome function by glycans as revealed by single-molecule imaging

Tatsuki Isogai[1], Koichiro M. Hirosawa[2], Yasuhiko Kizuka[2,3], Yasunari Yokota[4], Kenichi G. N. Suzuki[2,3] ([1]*Grad. Sch. Nat Sci Tech.*, [2]*iGCORE, Gifu. Univ.*, [3]*CREST, JST*, [4]*Dept. Eng., Gifu Univ.*)

20277H アクチンの重合と脱重合の熱測定
Calorimetry of actin polymerization and depolymerization

Shouron Kure, Hideyuki Komatsu (*Dept. Biosci. Bioinf., Kyushu Inst. Tech*)

20278H 線虫 MEC-2 および相互作用チャネル蛋白質の構造・生化学的解析
The structural and biochemical analyses of MEC-2 and its partner channel proteins in *C. elegans*

Norihiro Takekawa[1], Maria Uehori[2], Shunji Nakano[3], Ikue Mori[3], Michio Homma[4], Katsumi Imada[1] ([1]*Dept. of Macromol. Sci., Grad. Sch. of Sci., Osaka Univ.*, [2]*Dept. of Chem., Fac. of Sci., Osaka Univ.*, [3]*NSI, Grad. Sch. of Sci., Nagoya Univ.*, [4]*Div. of Biol. Sci., Grad. Sch. of Sci., Nagoya Univ.*)

20279H ヒト iPS 細胞を用いた原腸形成時の自己組織化運動
Self-organizing movement during gastrulation using human iPS cells

Ryo Kobayashi[1], Chihiro Takeuchi[2], Kiyoshi Ohnuma[3] ([1]*Grad. Sch. Eng., Univ. Nagaoka Tech.*, [2]*Eng., Univ. Nagaoka Tech.*, [3]*Inn., Univ. Nagaoka Tech*)

20280H マウス気管の繊毛運動による喘息原因物質キチンの輸送
Observation of ciliary motility of murine trachea and epithelial transport of chitin involved in the development of asthma

Arata Imaizumi[1], Keiju Kawano[1], Nobukiyo Tanaka[1], Susumu Nakae[2], Koji Ikegami[3], Tomoko Masaike[1] ([1]*Dept. Appl. Biol. Sci. Tokyo Univ. Sci.*, [2]*Grad. Sch. of Integrated Sci. for Life, Hiroshima Univ.*, [3]*Grad. Sch. of Biomedical & Health Sci., Hiroshima Univ.*)

20281H リアルタイムフィードバック制御による機械的刺激に影響を受けた心筋細胞の拍動
Beat sequence of cardiomyocytes affected by to mechanical stimulus with real-time feedback control

Shota Nozaki, Kazuki Mammoto, Takashi Miyazawa, Ryuta Watanabe, Yuta Moriyama, Ryu Kidokoro, Toshiyuki Mitsui (*Aoyama Gakuin University*)

20282H 心筋梗塞の治療のための in vitro 移植モデルにおけるペースメーカーの入れ替わり
Pacemaker switching of in vitro transplantation model for heart infarction
Toru Nakamura, Chiho Nihei, Masahito Hayashi, Tomoyuki Kaneko (*Laboratory for Reconstructive Cell biology, Department of Frontier Bioscience, Hosei University, Grad. School of Science and Engineering*)

20283H 圧力がミトコンドリアの機能に及ぼす影響
Effects of pressure on mitochondrial activity
Yoshiki Oie[1], Yoshihiro Ohta[2] ([1]*Grad. Sch. Sci., Tokyo University of Agriculture and Technology*, [2]*Tokyo University of Agriculture and Technology*)

20284H タウ–微小管とタウ–ヘパリン相互作用の等温滴定熱測定の比較
Comparative analysis between isothermal titration calorimetries of tau–microtubule and tau–herparin interactions
Junta Kashima, Rio Okamoto, Hideyuki Komatsu (*Dept. Biosci. Bioinf., Kyushu Inst. Tec*)

20285H ミトコンドリア電子伝達系のプロトンポンプ活性の単一細胞検出
Detection of proton pump activities in mitochondrial electron transfer chain in a single cell level
Yoshiki Suganuma, Masato Miura, Hiroko Kashiwagi, Yoshihiro Ohta (*Tokyo University of Agriculture and Technology, Department of Biotechnology and Life Sciences.*)

20286H 単細胞 FRET とべん毛モーター回転による CheYp 濃度の同時観察による適応系のメカニズム解明
Elucidation of mechanism for adaptation system through the simultaneous observation CheYp by single cell FRET and flagellar motor rotation
Takuma Nakagawa, Tatsuya Yamakoshi, Che Yong-Suk, Hajime Fukuoka, Akihiko Ishijima (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

20287H Simultaneous observation of chemotactic response and intracellular behavior of chemotaxis proteins at single *E. coli* cell
Taro Yuri, Takuma Nakagawa, Keisuke Nishitani, Yong-Suk Che, Yumiko Uchida, Akihiko Ishijima, **Hajime Fukuoka** (*Grad. Sch. Frontier Biosci., Osaka Univ.*)

20288H CheB の細胞内動態とべん毛モーター回転の同時計測
Simultaneous measurement of flagellar motor rotation and Dynamics of CheB localization during chemotactic response
Keisuke Nishitani[1], Tatsuki Hamamoto[2], Yong-Suk Che[1], Akihiko Ishijima[1], Hajime Fukuoka[1] ([1]*Grad. Sch. Frontier Biosci. Osaka Univ.*, [2]*OIST. Grad. Univ.*)

20289H 回転方向に依存したべん毛モーターの回転揺らぎの高時間分解能測定。
High temporal resolution measurement of rotational fluctuation of flagellar motor depending on rotational direction
Koki Murai, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

20290H 心筋細胞における拍動間隔の温度依存性
Temperature dependence of beating rate in cardiomyocytes
Kohei Oyama, Masahito Hayashi, Tomoyuki Kaneko (*Laboratory for Reconstructive Cell Biology, Department of Frontier Bioscience, Hosei University, Grad School of Science and Engineering*)

20291H 走化性タンパク質 CheRCheB の存在と大腸菌スイッチング同調
Requirement for Chemotaxis Protein CheR and CheB for the switching coordination between two flagellar motors on E. coli cell
Tatsuki Hamamoto[2], **Yumiko Uchida**[1], Yong-Suk Che[1], Akihiko Ishijima[1], Hajime Fukuoka[1] ([1]*Grad. Sch. Frontier Biosci. Osaka Univ*, [2]*OIST Grad. Univ*)

20292H* レプトスピラ経皮侵入に関わる運動の重要性
Significance of motility for percutaneous invasion of the spirochete *Leptospira*
Keigo Abe[1], Toshiki Kuribayashi[1], Kyosuke Takabe[2], Shuichi Nakamura[1] ([1]*Department of Applied Physics, Graduate School of Engineering, Tohoku University*, [2]*Faculty of Life and Environmental Sciences, University of Tsukuba*)

20293H* 蛍光および反射干渉顕微鏡による細胞ー基板界面でのがん細胞膜の分子パッキングの評価
Evaluation of molecular packing of cancer cell membrane at cell-substrate interface by fluorescence and interference reflection microscopy
Hayata Noro[1], Mai Fujii[1], Shodai Togo[1], Mami Watanabe[1], Masami Suganuma[2], Naritaka Kobayashi[2], Ryozo Kawamura[1,2], Seiichiro Nakabayashi[1,2], Takahisa Matsuzaki[2], Hiroshi Yoshikawa[1,2] ([1]*Dept. of Chem., Saitama Univ.*, [2]*Div. of Strateg. Res. and Dev., Grad. Sch. of Sci. and Eng., Saitama Univ.*)

20294H* 細胞接着界面の膜分子配列性の評価：がん細胞と正常細胞の比較
Characterization of molecular packing of cell membranes at cell-substrate interface:Comparison between cancer cells and normal cells
Mai Fujii[1], Hayata Noro[1], Syodai Togo[1], Mami Watanabe[1], Masami Suganuma[2], Naritaka Kobayashi[2], Ryuzo Kobayashi[1,2], Seiichiro Nakabayashi[1,2], Takahisa Matsuzaki[2], Hiroshi Y. Yoshikawa[1,2] ([1]*Grad. Chem., Univ. Saitama*, [2]*Division of Strategic Research and Development, Grad. Sci. Eng., Univ. Saitama*)

20295H 人工多細胞型分子ロボットの自動生産に関する研究
Toward Automated Production of Multicellular Molecular Robots
Ryo Shimizu[1], Satoshi Murata[1], Shin-ichiro Nomura[1], Yuki Suzuki[4], Ibuki Kawamata[1], Gen Hayase[3], Taro Toyota[2] ([1]*Murata/Nomura Lab, Univ. Tohoku*, [2]*Toyota Lab, Univ. Tokyo*, [3]*MANA*, [4]*FRIS, Univ. Tohoku*)

20296H 繊毛の初期屈曲形成に重要な根元局在型マイナーダイニン
Requirement of minor-type axonemal dyneins localized to the proximal region for the initial bend formation of cilia
Tomohiro Komatsu, Ayuna Sahara, Yusuke Kondo, **Toshiki Yagi** (*Dept. Life Sci. Prefectural Univ. Hiroshima*)

20297H Formation of actin cortex structure by myosin motor activity
Mitsusuke Tarama, Tatsuo Shibata (*RIKEN BDR*)

I. 生体膜・人工膜／I. Biological & Artificial membrane

20298I* 抗菌ペプチド・マガイニン 2 と脂質膜の相互作用に対する膜電位の効果
Effect of Membrane Potential on Interaction of Antimicrobial Peptide (AMP) Magainin 2 (Mag) with Single GUVs
Or Rashid Md. Mamun[1], Moghal Md. Mizanur[1], Billah Md. Masum[1], Hasan Moynul[1], Yamazaki Masahito[1,2,3] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Res. Inst. Ele., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

20299I* 蛍光プローブでラベルされていない細胞透過ペプチド・トランスポータン 10 の巨大リポソーム内腔への侵入の検出
Detection of the Entry of Nonlabeled Cell-Penetrating Peptide (CPP) Transportan 10 (TP10) into Single Giant Unilamellar Vesicles (GUVs)
Madhabl Lata Shuma[1], Md. Mizanur Moghal[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.*)

20300I* 脂質分子の二分子層膜横断（フリップ・フロップ）に対する浸透圧の効果
The effect of osmotic pressure on the transbilayer movement (flip-flop) of lipid molecules
Samiron Kumar Saha[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.*)

20301I 脂質・コレステロールによって制御される上皮成長因子受容体の膜貫通・膜近傍ドメインの多量体形成機構
Lipid-cholesterol regulation of the oligomerization in transmembrane and juxtamembrane domains of epidermal growth factor receptor
Ryo Maeda[1], Takeshi Sato[2], Yasushi Sako[1] ([1]*Cellular Informatics Lab., RIKEN*, [2]*Kyoto Pharmaceutical Univ.*)

20302I* 抗菌ペプチド・ラクトフェリシン B(4-9)の大腸菌、スフェロプラスト、および巨大リポソームの内腔への侵入に対する膜電位の効果
Effect of Membrane potential on Entry of Antimicrobial Peptide (AMP) LfcinB (4-9) into Single *E. coli* Cells, Spheroplasts, and GUVs
Farzana Hossain[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.*)

20303I* アミロイド線維形成とリン脂質二分子膜破壊との関係性の解明
Investigation of relationships between amyloid fibril formation and phospholipid bilayer destruction
Hiroki Takayama[1], Kaori Mageshi[1], Kenichi Morigaki[2], Eri Chatani[1] ([1]*Graduate School of Science, Kobe University*, [2]*Biosignal research center, Kobe University*, [3]*Graduate School of Agricultural Science, Kobe University*)

20304I Regulation of actin dynamics by phosphoinositides
Yosuke Senju (*RIIS, Univ. Okayama*)

20305I 高速 AFM によるハブ毒液由来脂質分解酵素 PLA2 の膜認識機構の解明
Membrane recognition mechanism of phospholipase A_2 from habu snake venom revealed by high-speed AFM (HS-AFM)
Magoto Kamiya[1], Mikihiro Shibata[2,3], Naoko Oda-Ueda[4], Ayumi Sumino[2,3] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*, [3]*InFiniti, Kanazawa Univ.*, [4]*Dept. Pharm. Sci., Sojo Univ.*)

20306I 2 種類のリン脂質種からなるモデル生体膜の構造に対するコレステロールとラノステロールの影響の比較
Comparative study of the effects of cholesterol and lanosterol on the structure of model biomombrane formed by two phospholipid species
Akira Matsumoto, Hiroshi Takahashi (*Grad. Sch. Sci and Tech., Gunma University*)

20307I* 細胞サイズ閉じ込め中の拡散に対する界面の効果
Effects of membrane interface properties on diffusion in cell-sized confinement
Kanae Harusawa[1,2], Chiho Watanabe[2], Akira Kitamura[3], Masataka Kinjo[3], Miho Yanagisawa[2] ([1]*Grad. Sch. Eng., Tokyo Univ. of Agri. and Technol.*, [2]*Grad. Sch. Arts and Sci., The Univ. of Tokyo*, [3]*Grad. Sch. Life Sci., Hokkaido Univ.*)

20308I 相分離リポソームを用いた膜タンパク質の高濃度再構成
High-density reconstitution of membrane protein into phase-separated liposome
Mizuki Kobayashi[1,2], Kei Fujiwara[3], Chiho Watanabe[2], Miho Yanagisawa[2] ([1]*Grad. Sch. Eng., Tokyo Univ. of Agri. and Tech*, [2]*Grad. Sch. Arts and Sci., The Univ. of Tokyo*, [3]*Sch and Tech.Biosciences and Informatics., Keio Univ*)

20309I 鞭毛で泳ぐ単細胞緑藻クラミドモナスを用いて巨大リポソームを内側から動かす
Driving a giant liposome from inside by a flagellating unicellular green algae *Chlamydomonas*
Shunsuke Shiomi[1], Masahito Hayashi[1], Tomohiro Uemura[2], Tomoyuki Kaneko[1] ([1]*LaRC, FB, Hosei Univ.*, [2]*FB, Hosei Univ.*)

20310I ラベルされていない抗菌ペプチド・PGLa と単一 GUV との相互作用
Interaction of Nonlabeled Antimicrobial Peptide PGLa with Single Giant Unilamellar Vesicles (GUVs)
MD Hazrat Ali[1], Madhabl Lata Shuma[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.*)

20311I Epigallocatechin gallate induces the burst of giant unilamellar vesicles in the tension-dependent manner
Naoya Sugita[1], Mika Terada[1], Yukihiro Tamba[1], Masahito Yamazaki[2] ([1]*Natl. Inst. Tech., Suzuka Coll.*, [2]*Shizuoka Univ.*)

20312I 筋小胞体 Ca ポンプの M2 ヘリックス:膜貫通部分のエネルギー共役における役割
Role of transmembrane portion of M2 helix in energy coupling of sarcoplasmic reticulum Ca pump
Takashi Daiho, Kazuo Yamasaki, Satoshi Yasuda, Jun-ichi Kawabe (*Asahikawa Med. Univ. Biochem.*)

20313I* 脂質分子混み合い効果によるバクテリオロドプシン間実行相互作用の解析
Crowding effects induced by lipid molecules on effective interactions between bacteriorhodopsins
Keiju Suda[1], Ayumi Suematsu[2], Rho Akiyama[1] ([1]*Kyushu University, science faculty, department of chemistry*, [2]*Kyushu sangyo University*)

20314I* ナノサイズリポソームの脂質膜への融合条件の調査
Examination of fusion condition of nano-sized liposome to lipid membrane
Chika Arisaka, Kouki Kamiya (*Grad. Sch. Sci and Tec., Univ. Gunma*)

20315I ハイドロゲル固体試料中で見られた紫膜の特異な積層構造の形成機構
Formation Mechanisms of Anomalous Purple Membrane Stacking in Hydrogels
Yasunori Yokoyama[1], Riku Kurita[1], Shunsuke Yano[1], Koshi Takenaka[1], Hiroshi Takahashi[2], Masashi Sonoyama[2,3,4] ([1]*Grad. Sch. Eng., Nagoya Univ.*, [2]*Grad. Sch. Sci. & Tech., Gunma Univ.*, [3]*GIAR, Gunma Univ.*, [4]*GUCFW, Gunma Univ.*)

20316I ベシクル凝集構造の力学モデル
Mechanical Model of Vesicle Aggregates
Toshikaze Chiba[1], Masayuki Imai[1], Primoz Ziherl[2,3] ([1]*Grad. Sch. Sci., Tohoku Univ*, [2]*Jozef Stefan Inst*, [3]*Ljubljana Univ*)

20317I In vitro selection using cDNA display for liposome binding peptides to generate antibacterial peptides
Takeru Yoshinobu, Naoto Nemoto (*Graduate School of Science & Engineering, Saitama University*)

20318I* Pattern Formation by Mechanochemical Feedback between Membrane Deformation and the Brusselator Model
Naoki Tamemoto, Hiroshi Noguchi (*ISSP, Univ. Tokyo*)

20319I ナノサイズリポソーム融合による細胞サイズ GM1 非対称膜リポソームの構築
Construction of cell-sized GM1 asymmetric vesicles using nano-sized vesicle fusion method
Masato Suzuki[1], Kouki Kamiya[1,2] ([1]*Sci. & Tech., Univ. Gunma*, [2]*Grad. Sci. & Tech., Univ. Gunma*)

20320I 電位依存性プロトンチャネルの細胞内側からの制御
Intracellular regulation of the voltage-gated proton channel
Akira Kawanabe, Yuichiro Fujiwara (*Kagawa Univ.*)

20321I Artificial bilayers on hydrogel for channel current recordings
Toru Ide[1,2], Minako Hirano[2], Daiki Yamamoto[1], Mami Asakura[3], Yuki Kitamura[3] ([1]*Grad Schl Health Systems Okayama Univ*, [2]*GPI*, [3]*Fac Eng Okayama Univ*)

20322I イノシトールリン脂質による KcsA の制御
Functional coupling between phosphoinositides and KcsA studied by lipid-bilayer recording
Takunari Kiya, Akira Kawanabe, Yuichiro Fujiwara (*Kagawa Univ.*)

20323I* 自動顕微鏡計測により見出された，定常流れ場における細胞サイズのリポソームへの分子濃縮
Automated direct observation unveiled hydrodynamic accumulation of molecules into cell-sized liposomes against a concentration gradient
Hironori Sugiyama[1], Toshihisa Osaki[2,3], Shoji Takeuchi[2,4], Taro Toyota[1,5] ([1]*Grad. Sch. Arts and Sci., The University of Tokyo*, [2]*IIS, The University of Tokyo*, [3]*KISTEC*, [4]*Grad. Sch. Info. Sci. Tech., The University of Tokyo*, [5]*UBI, The University of Tokyo*)

20324I 平面脂質膜の組成の違いによる OmpG の膜への挿入の違いについて
Differences of OmpG into the planar lipid membranes with various compositions
Toshiyuki Tosaka[1], Koki Kamiya[2] ([1]*Sci. & Tech., Univ. Gunma*, [2]*Grad. Sci. & Tech., Univ. Gunma*)

20325I 油中水滴エマルションにおけるヒドロキシプロピルセルロースのパターン形成とダイナミクス
Pattern formation and dynamics of hydroxypropyl cellulose in water-in-oil emulsion
Kazunari Yoshida[1], Keitaro Horii[2], Azusa Saito[2], Akito Takashima[2], Izumi Nishio[2] ([1]*Grad. Sch. Sci. Eng., Yamagata Univ.*, [2]*Col. Sci. Eng., Aoyama Gakuin Univ.*)

20326I Effect of lipid quality on the association of membrane bound proteins with phosphoinositide-containing membranes
Eiji Yamamoto[1], Junko Sasaki[2], Takehiko Sasaki[2], Mark S. P. Sansom[3] ([1]*Department of System Design Engineering, Keio University*, [2]*Medical Research Institute and Graduate School of Medical and Dental Sciences, Tokyo Medical and Dental University*, [3]*Department of Biochemistry, University of Oxford*)

20327I 気液界面における人工肺サーファクタント膜へのコレステロールの影響
Effect of cholesterol on a model lung surfactant monolayer at the air-water interface
Masahiro Hibino[1], Saki Izumi[2] ([1]*Div. Sustain. Environ. Eng., Muroran Inst. Tech.*, [2]*Dept. Appl. Sci., Muroran Inst. Tech.*)

20328I 自動生成される人工多細胞体とその電気的活性について
On multicellular lipid compartments and their electrical activity
Shin-ichiro Nomura (*Dep. Robotics, TOHOKU Univ.*)

20329I 分子シミュレーションによるリポソームにおける膜タンパク質拡散解析
Molecular dynamics simulation of the diffusion of membrane proteins on vesicles
Diego Ugarte, Shoji Takada (*Dept. Biol., Sch. Sci., Kyoto Univ., Japan*)

20330I* Observation Protein-Protein Interactions in α-hemolysin
Misa Yamaji, Ryuji Kawano (*Tokyo University of Agriculture and Technology*)

20331I* Outer membrane phospholipaseA (OmpLA)を用いた細胞モデルの構築
Creation of complex-functional cell model using outer membrane phospholipase A
Seren Ohnishi, Koki Kamiya (*Grad. Sci., Univ.Gunma*)

20332I* α-ヘモリシンナノ空間における β ヘアピンペプチドのイオン電流記録
Ion current recording of a β-hairpin peptide in confined α-hemolysin nanospace
Miyu Fukuda, Misa Yamaji, Ryuji Kawano (*Department of biotechnology and life science, Tokyo University of Agriculture and Technology*)

20333I 大腸菌が引き起こすリポソームの形態変化パターン解析
Analysis of morphological change patterns of liposomes driven by encapsulated *E. coli*
Mai Hayakawa, Masahito Hayashi, Tomoyuki Kaneko (*LaRC, FB, Grad. Sch. Sci. & Eng., Hosei Univ.*)

20334I* Construct analysis system between peptide local structure in lipid membrane and membrane deformation
Kayano Izumi, Ryuji Kawano (*Department of Biotechnology and Life science, Tokyo University of Agriculture and Technology*)

20335I サイズ選択性を有する DNA オリガミ人工チャネル
Size-selective molecular transportation by DNA origami channel
Shoji Iwabuchi[1], Ibuki Kawamata[1,2], Satoshi Murata[1], M. Shin-ichiro Nomura[1] ([1]*Rob. Eng., Univ. Tohoku*, [2]*Nat. Sci., Fuc. Core Res., Univ. Ochanomizu*)

20336I* Protein crowder as a modulator of Min wave generation for cell division
Saki Nishikawa, Shunshi Kohyama, Nobuhide Doi, Kei Fujiwara (*Faculty of science and technology, Keio University*)

20337I 脂質二分子膜に働く光捕捉力の検証
Lateral diffusion in lipid bilayers biased by optical forces
Yuto Ishihara[1], Tutsunori Kishimoto[1,2], Fuko Kueda[3,4], Suguru N. Kudoh[2], Kenichi Morigaki[3,4], Chie Hosokawa[1,5] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*Grad. Sch. Sci. Tech., Kwansei Gakuin Univ.*, [3]*Grad. Sch. Agr., Kobe Univ.*, [4]*Biosignal., Kobe Univ.*, [5]*PhotoBIO-OIL, AIST*)

20338I* 細胞膜の物理的状態の制御に向けた生物活性ナノ材料の設計並びに評価
Design and Evaluation of Bioactive Nanomaterials toward Control of Physical Properties of Plasma Membrane
Tomohiro Nobeyama[1], Hyungjin Kim[2], Kazuki Shigyo[3], Hirotaka Nakatsuji[4], Hiroshi Sugiyama[5], Naoko Kawamura[6,7], Hiromune Ando[6,7], Tatsuya Murakami[1,8,9] ([1]*Grad. Sch. of Eng., Toyama Prefectural Univ.*, [2]*Grad. Sch. of Med., Yamaguchi Univ.*, [3]*Grad. Sch. of Integrated Sciences for Life., Hiroshima Univ*, [4]*Grad.Sch. of Eng., Osaka Univ.*, [5]*Grad.Sch.of Sci., Kyoto Univ.*, [6]*G-CHAIN., Gifu Univ*, [7]*iGCORE.,Tokai National Higher Education and Research System*, [8]*Fac.of.Eng., Toyama Prefectural Univ.*, [9]*KUIAS.,Kyoto Univ*)

J. 化学受容・神経／J. Chemoreception,Neuroscience & Sensory systems

20339J* 線虫の低温耐性を制御する新規の GPCR 型温度センサー分子
Novel GPCR-type temperature receptor in cold tolerance of *C. elegans*
Kohei Ohnishi, Toru Miura, Tomoyo Ujisawa, Akane Ohta, Atsushi Kuhara (*Inst. for Integrative Neurobiology, Konan Univ., Japan*)

20340J* ヒトムスカリン性アセチルコリン受容体 (M_2) のリガンド認識機構の理解に向けた赤外分光研究
Infrared spectroscopic study for elucidating ligand recognition mechanism of human M_2 muscarinic acetylcholine receptor
Kohei Suzuki[1], Kota Katayama[1], Ryoji Suno[2], Yuji Sumii[1], Norio Shibata[1], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech*, [2]*Kansai Medical University. Medical.*)

20341J Clostridium 属細菌の走化性アッセイ法の確立
Establishment of Methods for Chemotaxis Assays of *Clostridium* spp.
So-ichiro Nishiyama, Susumu Oogoshi, Hiroshi Urakami (*Fac. App. Life Sci., Niigata Univ. Pharm. App. Life Sci.*)

20342J* 非平衡流動場における脂質膜へのアミロイド β 凝集の単分子観察
Single Molecule Observation of Amyloid β Aggregation to Lipid Membrane under Non-equilibrium Fluidic Condition
Akane Iida[1], Hideki Nabika[2] ([1]*Grad. Sch. of Sci. and Eng., Yamagata Univ.*, [2]*Fac. of Sci., Yamagata Univ.*)

K. 神経回路・脳の情報処理／K. Neuronal circuit & Information processing

20343K 線虫 *C. elegans* を用いた異なる感覚情報の統合に関わる神経回路モデル
The model of neural circuit integrating different sensory information in *C. elegans*
Misaki Okahata[1], Aguan D. Wei[2], Akane Ohta[1], Atsushi Kuhata[1,3] ([1]*Inst. for Integrative Neurobio., Konan Univ.*, [2]*SEA Children's Research Inst.*, [3]*AMED-PRIME*)

20344K 海馬で合成される男性・女性ホルモンやストレスホルモンによる記憶シナプスの早い non-genomic な制御
Rapid non-genomic modulation of synapses by hippocampus-synthesized androgen, estrogen and stress steroid
Suguru Kawato[1,2], Mika Soma[1,2], Mari Ikeda-Ogiue[1,2], Minoru Saito[2] ([1]*Dep. Urology, Grad Sch Medicine, Juntendo Univ.*, [2]*Dep. Life sciences, College Humanities and Sciences, Nihon Univ.*)

20345K 線虫において脂肪酸代謝経路の β 酸化で働く HADH が低温馴化を制御する
HACD-1 that is beta-oxidation of fatty acid metabolism regulates cold acclimation in intestine and sensory neurons in C. elegans
Akihisa Fukumoto[1], Atushi Kuhara[1], Akane Ohta[1], Misaki Okahata[1], Youhei Minakuti[2], Atushi Toyoda[2] ([1]*Inst. for Integrative Neurobio., Konan Univ.*, [2]*NIG, Japan*)

20346K 細胞間の活動同期性に基づく神経クラスタの統計的推測
Statistical inference of neuronal ensembles based on synchronous activity among neurons
Shun Kimura, Koujin Takeda, Yuishi Iwasaki (*Grad. Sch. Sci. Eng., Univ. Ibaraki*)

20347K Integrated signaling from thermosensoryneurons at a tail interneuron regulates cold acclimation
Haruka Motomura, Satoko Fujii, Makoto Ioroi, Atsushi Kuhara, Akane Ohta (*Institute for integrative Neurobiology, Konan Univ.*)

20348K 内因性カンナビノイドによる小脳 GABA シナプス伝達のシナプスタイプ別制御
Endocannabinoids regulate cerebellar GABAergic transmission in a synapse type-dependent manner
Moritoshi Hirono[1,2], Yuchio Yanagawa[3] ([1]*Dep. Physiol., Wakayama Med. Univ. Sch. Med.*, [2]*Grad. Sch. Brain Sci., Doshisha Univ.*, [3]*Dep. Genetic and Behav. Neurosci., Gunma Univ. Grad. Sch. Med.*)

20349K A method to differentiate neurite non-invasively with needle agarose microfabrication technology
Yuhei Tanaka, Haruki Watanabe, Kenji Shimoda, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

20350K 微小多電極解析のための神経細胞の 1 細胞レベル長期培養環境の最適化
Optimization of the long-term cultural environment of isolated single neurons for micro-multielectrode analysis
Kenji Shimoda, Yuhei Tanaka, Haruki Watanabe, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

20351K 1 神経突起の伸長を長期間観察さるための改良された μm 分解能のアガロース微細加工技術の評価
Evaluation of an improved μm resolution agarose microfabrication technology for long-term individual neurite elongation observation
Haruki Watanabe[1], Yuhei Tanaka[1], Kenji Shimoda[1], Kenji Yasuda[1] ([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]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [4]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

20352K マウス海馬の長期増強を膜電位感受色素によるイメージングで観察する
Imaging analysis of the long-term potentiation of the mouse hippocampal activity
Yoko Tominaga, Makiko Taketoshi, **Takashi Tominaga** (*Inst Neurosci Tokushima Bunri Univ.*)

20353K プリオンタンパク質ノックアウトマウスにおける小脳長期抑圧障害
Impairment of cerebellar long-term depression in prion protein-deficient mice ectopically expressing PrPLP/Dpl
Yasushi Kishimoto[1], Moritoshi Hirono[2], Ryuichiro Atarashi[3], Suehiro Sakaguchi[4], Tohru Yoshioka[5], Shigeru Katamine[6], Yutaka Kirino[1] ([1]*Kagawa Sch. Pharm. Sci., Tokushima Bunri Univ.*, [2]*Dep. Physiol., Wakayama Med. Univ. Sch. Med.*, [3]*Fac. Med., Univ. of Miyazaki*, [4]*KOSOKEN, Tokushima Univ.*, [5]*Kaohsiung Medical Univ.*, [6]*CICORN, Nagasaki Univ.*)

20354K ミミズ短期記憶におけるセロトニンの関与
Involvement of serotonin in short-term memory of earthworms
Yoshiichiro Kitamura, Toshiaki Nakahara, Hikaru Takahashi (*Dept Math Sci Phys, Col Sci Eng, KGU*)

L. 行動／L. Behavior

20355L 蟻はピンクノイズで探索する
Ants run on a treadmill with the pink noise
Tomoko Sakiyama[1], Naohisa Nagaya[2], Ryusuke Fujisawa[3] ([1]*Soka University*, [2]*Kyoto Sangyo University*, [3]*Kyushu Institute of Technology*)

20356L* 隠れマルコフモデルと逆強化学習法による生物複数戦略の同定
Identification of multiple strategies by inverse reinforcement learning with hidden-Markov model
Kohei Morimoto[1,2], Muneki Ikeda[3,4], Yuki Tsukada[3], Nakano Shunji[3], Ikue Mori[3,4], Naoki Honda[2,5,6] ([1]*Undergrad. Info. and Math., Kyoto Univ.*, [2]*Grad. Bio., Kyoto Univ.*, [3]*Grad. Sci., Nagoya Univ.*, [4]*CBS., Riken*, [5]*Research Center for Dynamic Living Systems, Kyoto Univ.*, [6]*ExCELLS, NINS.*)

20357L 睡眠の剥奪はショウジョウバエによる食物臭の嗜好性を変化させる
Sleep deprivation alters food odor preference in Drosophila
Fuminori Tanizawa[1,2], Hiroyuki Takemoto[3] ([1]*Kaisei Senior High School*, [2]*Future Scientists' School, Shizuoka University*, [3]*Research Institute of Green Science and Technology, Shizuoka University*)

20358L 壁近くのゾンビ化した単鞭毛クラミドモナスの遊泳
Swimming of zombifield monoflagellated Chlamydomonas near wall
Ken Nagai (*JAIST*)

20359L* 報酬と好奇心によって駆動される行動を表現する意思決定モデル
A decision-making model for reward and curiosity-driven behavior
Yuki Konaka[1,2], Naoki Honda[1,2] ([1]*Graduate School of Biostudies, Kyoto university.*, [2]*Theoretical Biology Research Group, Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences.*)

M. 光生物:視覚・光受容・光合成・光制御／M. Photobiology

20360M マウス桿体視細胞においてロドプシンを介するが光オフで生じるプロテインキナーゼ A の活性化
Rhodopsin-mediated Light-off-induced Protein Kinase A Activation in Mouse Rod Photoreceptor Cells
Shinya Sato[1], Takahiro Yamashita[2], Michyuki Matsuda[1,3] ([1]*Grad. Sch. Biostud., Univ. Kyoto*, [2]*Grad. Sch. Sci., Univ. Kyoto*, [3]*Grad. Sch. Med., Univ. Kyoto*)

20361M 光合成酸素発生系における *g*=5 S_2 状態の分子構造
Molecular Structure of the S_2 State with a *g*=5 Signal in the Oxygen Evolving Complex of Photosystem II
Hiroyuki Mino, Shota Taguchi, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Uni.*)

20362M QM/MM-MD による光回復酵素-紫外線損傷 DNA 複合体の逐次修復反応中における反応中間体の観測に成功
QM/MM-MD approach for photolyase-UV-damaged DNA complex achieved that observe an intermediate in the successive DNA repair reactions
Ryuma Sato[1], Hiroshi Watanabe[2,3], Junpei Yamamoto[4], Makoto Taiji[1] ([1]*RIKEN*, [2]*Keio univ, KQCC*, [3]*PRESTO JST*, [4]*Osaka univ*)

20363M 光化学系Ⅱにおける D1-Asp170 の His 変異体の新規なアミノ酸変換
Novel amino acid conversion of a His mutant of D1-Asp170 in photosystem II
Yuichiro Shimada[1], Tomomi Kitajima-Ihara[1], Ryo Nagao[1,2], Takumi Noguchi[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Res. Inst. Interdiscip. Sci., Okayama Univ.*)

20364M Clarification of proton transfer pathways in water photolysis in photosystem II
Ayane Sugiyama, Yuichiro Shimada, Takumi Noguchi (*Division of Material Science, Graduate School of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan*)

20365M 光化学系Ⅱの第二キノン電子授与体 Q_B の反応における D1-His252 の役割
Role of D1-His252 in the reaction of the secondary quinone electron accepter Q_B in photosystem II
Tomoyuki Kobayashi[1], Yuichiro Shimada[1], Ryo Nagao[2], Takumi Noguchi[1] ([1]*Grad. Sch. Sci, Nagoya Univ.*, [2]*Res. Inst. Interdiscip. Sci., Okayama Univ.*)

20366M 光化学系Ⅱにおけるキノン電子受容体 Q_A・Q_B 間の電子移動の時間分解赤外分光検出
Time-resolved infrared detection of electron transfer between quinone electron acceptors Q_A and Q_B in photosystem II
Honami Ito, Yuki Kato, Takumi Noguchi (*Grad. Sch. Sci, Nagoya Univ.*)

20367M Mutational analysis of the mechanism of an absorption red shift in a marine bacterial Cl^--pumping rhodopsin
Takashi Nagata[1,2], Masayuki Karasuyama[2,3], Ichiro Takeuchi[3,4,5], Yu Nakajima[6], Susumu Yoshizawa[7], Keiichi Inoue[1,4] ([1]*Inst. Solid State Phys., Univ. Tokyo*, [2]*PRESTO, JST*, [3]*Dept. Computer Sci., Nagoya Inst. Tech.*, [4]*RIKEN Center for Advanced Intelligence Project*, [5]*OptoBioTechnology Research Center, Nagoya Inst. Tech.*, [6]*Bioproduction Res. Inst., Nat. Inst. Adv. Indust. Sci. Tech.*, [7]*Atmosphere and Ocean Res. Inst., Univ. Tokyo*)

20368M FTIR spectroelectrochemical study on the mechanism of the pH dependence of the redox potential of the non-heme iron in photosystem II
Yuki Kato, Hiroki Watanabe, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Univ.*)

20369M Spectroscopic properties and energy transfer dynamics of two different forms of acpPC from dinoflagellate *Symbiodinium*

Hayata Yamamoto[1], Keisuke Kawakami[2], Hiroko Uchida[3], Akio Murakami[3], Nobuo Kamiya[4], Daisuke Kosumi[5] ([1]*Dept. of Sci. and Tech., Kumamoto Univ.*, [2]*RIKEN*, [3]*Research Center of Island Seas, Kobe Univ.*, [4]*ReCAP, Osaka City Univ.*, [5]*IINA, Kumamoto Univ.*)

20370M Energy transfers in PSI of cyanobacterium, red alga, and dinoflagellate

Hiroki Serikawa[1], Hayata Yamamoto[1], Keisuke Kawakami[2], Hiroko Uchida[3], Akio Murakami[3], Kimiko Nagayoshi[4], Toshinari Kuroki[4], Susumu Takio[5], Nobuo Kamiya[6], **Daisuke Kosumi**[7] ([1]*Dept. of Sci. and Tech., Kumamoto Univ.*, [2]*RIKEN*, [3]*Research Center of Island Seas, Kobe Univ.*, [4]*Daiichi Seimou Co., Ldt.*, [5]*CWMD, Kumamoto Univ.*, [6]*ReCAP, Osaka City Univ.*, [7]*IINa, Kumamoto Univ.*)

20371M 新しいタイプの光サイクル型動物オプシンの創製

Construction of a novel type of photocycle animal opsin

Kazumi Sakai[1], Yoshinori Shichida[2], Yasushi Imamoto[1], Takahiro Yamashita[1] ([1]*Grad. Sch. Sci., Univ. Kyoto*, [2]*Res. Org. for Sci. and Tech., Univ. Ritsumeikan*)

20372M AUREO1-LOV ドメインの光誘起構造変化

Light-induced conformational switching of the LOV domain in aureochrome-1

Itsuki Kobayashi, Hiroto Nakajima, **Osamu Hisatomi** (*Grad. Sch. Sci., Osaka Univ.*)

20373M* 演題取り消し

20374M* 低温赤外分光測定による(6-4)光回復酵素の修復メカニズム解明

Elucidation of the repair mechanism of (6-4) photolyase by low-temperature FTIR spectroscopy

Katsuya Maeda[1], Mai Kumagai[1], Daichi Yamada[2], Yuma Terai[3], Junpei Yamamoto[3], Hideki Kandori[1] ([1]*Nagoya Inst. Tech*, [2]*Univ. Hyogo.*, [3]*Osaka Univ.*)

20375M* カチオンチャネルロドプシン *Ts*_Rh3 における C 末端領域の重要性

Importance of the C-terminal region in cation channel rhodopsin *Ts*_Rh3

Rintaro Tashiro[1], Kumari Sushmita[2], Suneel Kateriya[2], Hideki Kandori[1], Satoshi Tsunoda[1,3] ([1]*Nagoya Inst. Tech.*, [2]*Jawaharlal Nehru Univ.*, [3]*JST PRESTO*)

20376M 高速 AFM によるロドプシンクラスター上トランスデューシン動的過程の観察

Dynamic process of G protein transducin on rhodopsin cluster observed by high-speed AFM

Kazuhiko Hoshikaya[1], Hayato Yamashita[1], Fumio Hayashi[2], Kenichi Morigaki[3,4], Masashi Fujii[5,6], Akinori Awazu[5,6], Masayuki Abe[1] ([1]*Graduate School of Engineering Science, Osaka University*, [2]*Graduate School of Science, Kobe University*, [3]*Biosignal research center, Kobe University*, [4]*Graduate School of Agricultural Science, Kobe University*, [5]*Graduate School of Science, Hiroshima University*, [6]*Graduate School of Integrated Sciences for Life, Hiroshima University*)

20377M Biophysical characterization of different members of TAT rhodopsins: a new group of microbial rhodopsins

Kentaro Mannen[1], Takashi Nagata[1,2], Oded Béjà[3], Keiichi Inoue[1] ([1]*Inst. Solid State Phys., Univ. Tokyo*, [2]*PRESTO, JST*, [3]*Biol., Israel Inst. Tech.*)

20378M Actinotalea fermentans におけるヘリオロドプシンの発現

Expression of Heliorhodopsin in Actinotalea fermentans

Rei Abe-Yoshizumi, Ai Muto, Hideki Kandori (*Nagoya Inst. Tech.*)

20379M 絶対嫌気性緑色硫黄光合成細菌における Rieske/cyt*b* 複合体と *c* 型シトクロム間の相互作用解析

Studies on interaction between Rieske/cyt*b* complex and *c*-type cytochromes in strictly anaerobic photosynthetic green sulfur bacteria

Hiraku Kishimoto[1], Takahiro Nagaoka[1], Chihiro Azai[2], Risa Mutoh[3], Hideaki Tanaka[4], Yohei Miyanoiri[4], Genji Kurisu[4], Hirozo Oh-oka[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Col. Life Sci., Ritsumeikan Univ.*, [3]*Fac. Sci., Fukuoka Univ.*, [4]*Inst. Protein Res., Osaka Univ.*)

20380M 脊椎動物の非視覚オプシン Opn5 の多様化の起源の探索

Origin of diversification of vertebrate non-visual opsin Opn5

Takahiro Yamashita[1], Kengo Fujii[1], Kazumi Sakai[1], Yasushi Imamoto[1], Hideyo Ohuchi[2], Yoshinori Shichida[3] ([1]*Grad. Sch. of Sci., Kyoto Univ.*, [2]*Grad. Sch. of Med., Dent. and Pharm. Sci., Okayama Univ.*, [3]*Ritsumeikan Univ.*)

20381M* アニオンチャネルロドプシン吸収波長制御機構の解明
Mechanism of absorption wavelength shifts in anion channelrhodopsin mutants
Masaki Tsujimura[1], Tomoyasu Noji[1,2], Keiichi Kojima[3], Yuki Sudo[3], Hiroshi Ishikita[1,2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*RCAST., Univ. Tokyo*, [3]*Grad. Sch. Med. Dent.& Pharm., Okayama Univ.*)

20382M AUREO1-LOV の光誘起構造変化に関与する水素結合
Hydrogen bonds involved in the light-induced conformational switching of AUREO1-LOV
Yumiko Adachi, Hiroto Nakajima, Osamu Hisatomi (*Graduate School of Science, Osaka University*)

20383M* 新たに同定した水素結合ネットワークによる植物由来(6-4)光回復酵素の補因子 FAD の光依存的還元反応の制御
A newly identified hydrogen-bonding network modulates photoreduction of the flavin cofactor in plant (6-4) photolyase
Yuhei Hosokawa[1], Ryuma Sato[2], Martin Saft[3], Pavel Muller[4], Klaus Brettel[4], Lars-Oliver Essen[3], Shigenori Iwai[1], Junpei Yamamoto[1] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Riken*, [3]*Dept. Chem., Philipps Univ.*, [4]*I2BC, CEA, CNRS*)

20384M* 分光学的手法による霊長類青感受性視物質の光反応構造解析
Photochemical dynamics of a primate blue-sensitive pigment by spectroscopic study
Shunpei Hanai[1], Kota Katayama[1], Takuma Sasaki[1], Hiroo Imai[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech*, [2]*Prim. Res. Inst. Kyoto Univ.*)

20385M* Rhodococcus 属細菌が有するヘリオロドプシンの物性および生理機能の探索
Study on physiological functions and physical properties of heliorhodopsin possessed by Rhodococcus bacteria
Ai Muto, Rei Abe-Yoshizumi, Hideki Kandori (*Nagoya Inst. Tech.*)

20386M 光応答転写因子 Photozipper における二量体形成過程の高速 AFM 観察
High-speed AFM observation on dimer formation of a light-sensing transcription factor, Photozipper
Akihiro Tsuji[1], Kento Nomura[1], Hayato Yamashita[1], Osamu Hisatomi[2], Masayuki Abe[1] ([1]*Grad. Sch. of Eng. Sci., Osaka Univ.*, [2]*Grad. Sch. of Sci., Osaka Univ.*)

20387M 光による植物細胞の膜電位制御系の開発
Development of an light regulatory system of membrane potential in plant cell
Masae Konno[1,2], Hiromu Yawo[1], Hideki Kandori[3,4], Keiichi Inoue[1] ([1]*ISSP, Univ. Tokyo*, [2]*JST, PRESTO*, [3]*Life Sci. Appl. Chem., Grad. Sch. Eng., NIT*, [4]*OBTRC, NIT*)

20388M* ビブリオ属のブループロテオロドプシンが示す異常な pH 依存的吸収変化のメカニズム
Mechanism of unusual pH-dependent color change in blue-proteorhodopsin from *Vibrio califitulae*
Mizuki Sumikawa (*Nagoya Inst. Tech*)

20389M* 新規ロドプシンフォスホジエステラーゼ（Rh-PDE）8 種の分子特性
Molecular properties of eight novel rhodopsin phosphodiesterases (Rh-PDEs)
Masahiro Sugiura[1], Satoshi Tsunoda[1], Masahiko Hibi[2], Hideki Kandori[1] ([1]*Nagoya Institute of Technology*, [2]*Graduate School of Science, Nagoya University*)

20390M* 内外の配向でのセンサリーロドプシン II の表面増強赤外分光法
Surface-enhanced infrared spectroscopy on sensory rhodopsin 2 tethered with the inside or outside facing orientation
Jingyi Tang[1], Insyeerah Binti Muhammad Jauhari[1], Yuji Furutani[1,2] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*OptoBioTech. Research Center, Nagoya Inst. Tech.*)

20391M 電子励起状態における、フィコシアノビリンの構造変化に関する理論的研究
Exploring the structural changes of phycocyanobilin in the excited states
Kenji Mishima[1], Mitsuo Shoji[1,2], Yasufumi Umena[3], Yasuteru Shigeta[1] ([1]*CCS. Univ. Tsukuba*, [2]*JST-PRESTO*, [3]*Jichi Medical University*)

20392M 対称 I 型ヘリバクテリア反応中心光捕集過程の理論解析と光化学系 I との比較
Theoretical analysis of light harvesting mechanism of homodimeric type-I Heliobacterial reaction center: comparison to PSI
Akihiro Kimura[1], Hirotaka Kitoh[2,3], Yasuteru Shigeta[3], Shigeru Itoh[1] ([1]*Department of Physics, Graduate School of Science, Nagoya University*, [2]*JST, PRESTO*, [3]*Center for Computational Sciences, University of Tsukuba*)

20393M 錐体・桿体視細胞の外節における脂質環境の解析
Analysis of the lipid environment in outer segment membranes of rod and cone photoreceptor cells
Shuji Tachibanaki[1], Keiji Seno[2], Tateki Matsui[1], Masahiro Ueda[1] ([1]*Grad. Sch. of Frontier Biosci., Osaka Univ.*, [2]*Facultiy of Med., Hamamatsu Univ. Sch. of Med.*)

20394M 固体 NMR による内向きプロトンポンプロドプシン Schizorhodopsin のレチノール発色団の構造解析
Structure of retinal chromophore in Schizorhodopsin as studied by solid-state NMR
Seiya Tajima[1], Hideki Kandori[2], Keiichi Inoue[3], Izuru Kawamura[1] ([1]*Grad. Sch. Eng. Sci, Yokohama Nat. Uni.*, [2]*Nagoya Inst. Tech.*, [3]*Inst. Solid. State. Phys., Univ. Tokyo*)

20395M 共役二重結合系を延長したレチナールアナログによる赤色感受性チャネルロドプシンの更なる長波長シフト
Red-Shift of Red-Activatable Channelrhodopsin Using One-Double-Bond-Inserted Retinal Analogs
Yasushi Imamoto[1], Yi-Chung Shen[1], Toshikazu Sasaki[1], Takahiro Yamashita[1], Takashi Okitsu[2], Yumiko Yamano[2], Akimori Wada[2], Yoshinori Shichida[3] ([1]*Kyoto Univ.*, [2]*Kobe Pharm. Univ.*, [3]*Ritsumeikan Univ.*)

20396M 紅色光合成細菌の LH2 タンパク質の色素改変：色素のサイトエネルギーとタンパク質内励起エネルギー移動への影響
Pigment modification in LH2 proteins from purple photosynthetic bacteria: effects on pigment site-energy and intracomplex energy transfer
Yoshitaka Saga[1], Yuji Otsuka[1], Madoka Yamashita[1], Shiori Nakagawa[1], Yuto Masaoka[2], Tsubasa Hidaka[2], Yutaka Nagasawa[2] ([1]*Fac. Sci. Eng., Kindai Univ.*, [2]*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

20397M* Aureochrome-1 における LOV コアから活性ドメインへの情報伝達機構
Signal transduction from LOV core to effector domain in Aureochrome-1
Hiroto Nakajima, Itsuki Kobayashi, Osamu Hisatomi (*Grad. Sci. Sci., Univ. Osaka*)

20398M 天然アニオンシャネルロドプシン GtACR1 の分子機構に関する理論的研究
Theoretical study on molecular mechanics of natural anion channel rhodopsin GtACR1
Takafumi Shikakura, Cheng Cheng, Shigehiko Hayashi (*Kyoto Univ. Graduate School of Science*)

20399M Theoretical study of electron transport between cytochrome f and plastocyanin by using a coarse-grained simulation
Kazutomo Kawaguchi, Hidemi Nagao (*Inst. Sci. Eng., Kanazawa Univ.*)

20400M 緑色硫黄細菌のルブレドキシン-酸素酸化還元酵素への電子供与系
Electron transfer path to the rubredoxin-oxygen oxidoreductase in green sulfur bacteria
Wanwipa Ittarat[2,4], Takeshi Sato[3], Masaharu Kitashima[2], Hidehiro Sakurai[2,3], Kazuhito Inoue[2,3], **Daisuke Seo**[1] ([1]*Grad Sch Nat Sci&Tec, Kanazawa Univ*, [2]*Dep Biol, Fac Sci, Kanagawa Univ*, [3]*Res Ins Int Sci, Fac Sci, Kanagawa Univ*, [4]*BIOTEC, NSTDA, Thailand*)

20401M *Heliobacterium modesticaldum* 由来反応中心における励起エネルギー移動および初期電荷分離に関する研究
Studies on excitation energy transfer and primary charge separation in the reaction center complex from *Heliobacterium modesticaldum*
Risa Kojima[1], Hayata Yamamoto[2], Chihiro Azai[3], Chiasa Uragami[4], Hideki Hashimoto[4], Daisuke Kosumi[5], Hirozo Oh-oka[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Grad. Sch. Sci & Tech., Kumamoto Univ.*, [3]*Coll. Life Sci., Ritsumeikan Univ.*, [4]*Fac. Sci & Tech., Kwansei Gakuin Univ.*, [5]*IINA, Kumamoto Univ.*)

20402M 光吸収計算によって現れた C-フィコシアニンの 6 量体構造の機能的な意味
Functional meaning of hexamer structure of C-phycocyanin revealed by calculation of absorption wavelength
Hiroto Kikuchi (*Dept. of Phys. Nippon Med. Sch.*)

20403M Connecting the spectral properties to the structure of photosystem I containing Chlorophyll-*f*
Rin Taniguchi[1], **Yutaka Shibata**[1], Toshiyuki Shinoda[2], Tatsuya Tomo[2], Shen Ye[1] ([1]*Tohoku Univ., Grad. Sch. Sci.*, [2]*Tokyo Univ. Sci., Fac. Sci.*)

20404M 海洋性藻類 *Guillardia theta* における微生物ロドプシンの遺伝子発現解析
Gene expression analysis of microbial rhodopsins from marine algae *Guillardia theta*
Yumeka Yamauchi[1], Masae Konno[1,2], Keiichi Inoue[1,2], Hideki Kandori[1,3] ([1]*Life Sci. & Appl. Chem., Nagoya Inst. Tech.*, [2]*ISSP, Univ. Tokyo*, [3]*OBTRC, Nagoya Inst. Tech.*)

20405M Theoretical study on molecular mechanism of a light-driven ion transport of Halorhodopsin
Ryo Oyama, Taisuke Hasegawa, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

20406M Disruption of water-mediated H-bond network in rhodopsin mutations cause night blindness
Kota Katayama[1], Yuri Takeyama[1], Akiko Enomoto[1], Hiroo Imai[2], Hideki Kandori[1] ([1]*Grad.Sch.Eng., Nagoya Inst. Tech*, [2]*Primate Res. Inst. Kyoto Univ*)

20407M クロロフィル *f* をもつ光化学系 I 複合体の構造
Structural of photosystem I complex with chlorophyll *f*
Toshiyuki Shinoda[1], Koji Kato[2], Ryo Nagao[2], Seiji Akimoto[3], Jian-Ren Shen[2], Fusamichi Akita[2,4], Naoyuki Miyazaki[5,6], Tatsuya Tomo[1] ([1]*Fac. Sci., Tokyo Univ. Sci.*, [2]*RIIS., Okayama Univ.*, [3]*Grad. Sch. Sci., Kobe Univ.*, [4]*PRESTO, JST*, [5]*IPR., Osaka Univ.*, [6]*TARA., Tsukuba Univ.*)

20408M* In situ visualization of reversible state transition in live *Chlamydomonas* cells by noninvasive excitation spectral microscopy
Xianjun Zhang[1], Yuki Fujita[1], Ryutaro Tokutsu[2], Jun Minagawa[2], Shen Ye[1], Yutaka Shibata[1] ([1]*Tohoku Univ., Grad. Sch. Sci.*, [2]*NIBB, Div. Environ. Photobiol.*)

20409M Anion binding to mutants of the Schiff base counterion in heliorhodopsin
Anion binding to mutants of the Schiff base counterion in heliorhodopsin
Manish Singh[1], Kota Katayama[1], Oded Beja[2], Hideki Kandori[1] ([1]*Nagoya Inst. Tech*, [2]*Israel Inst. Tech*)

20410M* 光化学系 I 反応中心の電子移動におけるクロロフィルエピマー化の影響
Effect of chlorophyll epimerization on the electron transfer in photosystem I reaction center
Koji Mitsuhashi[1], Keisuke Saito[1,2], Hiroshi Ishikita[1,2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*RCAST, Univ. Tokyo*)

20411M* 光化学系 II 水分解触媒部位の交換カップリングの起源
Origin of exchange couplings of the Mn_4CaO_5 cluster in photosystem II
Shunya Nishio[1], Keisuke Saito[1,2], Hiroshi Ishikita[1,2] ([1]*Fac. Eng., Univ. Tokyo*, [2]*RCAST., Univ. Tokyo*)

20412M Simultaneous Mapping of Fluorescence Spectra and Lifetimes of Chlorophylls Revealed Accumulation of Quenched LHCII
Yuki Fujita, Xianjun Zhang, Touru Kondou, Yutaka Shibata (*Organic Physical Chemistry Lab., Tohoku Univ.*)

20413M アゾベンゼン挿入 DNA と T7RNA ポリメラーゼの光転写制御ダイナミクス
Dynamics of photo-regulated transcription reaction of T7 RNA polymerase and azobenzene-tethered DNA
Gennosuke Takekawa (*Grad. Sch. Sci., Kyoto Univ.*)

20414M 青色光センサータンパク質 VVD の光反応ダイナミクス
Photoreaction dynamics of blue light sensor protein VVD
Takafumi Nakayama, Andrea Mussini, Yusuke Nakasone, Masahide Terajima (*Grad. Sch. Sci., Univ. Kyoto*)

20415M* The gate-keeper role of a highly conserved helix-3 tryptophan for ion transport of the channelrhodopsin chimera, C1C2/ChRWR
Yujiro Nagasaka[1], Shoko Hososhima[2], Keiichi Inoue[1], Hideki Kandori[2,3], Hiromu Yawo[1] ([1]*ISSP., Univ. Tokyo*, [2]*Grad. Sch. Eng., Nagoya Inst. of Tech*, [3]*Optobio., Nagoya Inst. of Tech*)

20416O 演題取り消し

20417O 天然の原核生物由来カルシウムチャネルにおけるイオン透過選択性の進化とその決定残基の同定
The selectivity determinant and evolution of a native prokaryotic voltage-dependent calcium channel
Katsumasa Irie[1], Takushi Shimomura[1,3], Yoshiki Yonekawa[2], Hitoshi Nagura[1], Michihiro Tateyama[3], Yoshinori Fujiyoshi[4] ([1]*CeSPI, Nagoya univ.*, [2]*Grad. Pharm. Med. Sci., Nagoya univ.*, [3]*Div. Biophys. Neurobio., NIPS*, [4]*CeSPL,TMDU*)

20418O* Effects of Oligopeptides on Growth of Primitive Vesicles
Akiko Baba[1], Kazuki Yokoyama[1], Ulf Olsson[2], Masayuki Imai[1] ([1]*Department of Physics, Faculty of Science, Tohoku University*, [2]*Department of Chemistry, Faculty of Science, Lund University*)

20419O* ベシクル表面上での情報分子成長
Growth of Information Molecules on Vesicle Surface
Yuto Hachiya[1], Hikaru Hatori[1], Syoichi Toyabe[2], Steen Rasmussen[3], Masayuki Imai[1] ([1]*Phys, Tohoku Univ.*, [2]*Appl. Phys., Grad. Sch. Eng., Tohoku Univ.*, [3]*Phys, Chem Pharm, Univ. Southern Denmark*)

20420O 膜のないドロップレット内での RNA ゲノムの自己複製
Translation-coupled RNA replication in membrane-free droplets
Ryo Mizuuchi[1,2], Norikazu Ichihashi[1] ([1]*Komaba Institute for Science, Univ. Tokyo*, [2]*JST PRESTO*)

20421O Study on evolutionary fluctuation-response relationship in multicellular development
Chikara Furusawa[1,2] ([1]*BDR, RIKEN*, [2]*UBI, Graduate School of Science, The University of Tokyo*)

20422O* 膜面上の高分子合成と連携した持続的なベシクルの自己生産
Sustainable Reproduction of Vesicles coupled with a Surface-Confined Template Polymerization
Minoru Kurisu[1], Harutaka Aoki[1], Takehiro Jimbo[1], Yuka Sakuma[1], Sandra Luginbuhl[2], Peter Walde[2], Masayuki Imai[1] ([1]*Dept. of Phys., Tohoku Univ.*, [2]*Dept. of Mater., ETH*)

20423O How combination of DNA recombination and translation error allows efficient evolution?
Kenta Mitsutomi, **Daisuke Kiga** (*Waseda Univ, Dept Electrical Eng and Biosci*)

20424O* 進化実験による最も単純な等温条件下 DNA 複製機構の探索
Minimization of Elements for Isothermal DNA Replication by an Evolutionary Approach
Hiroki Okauchi[1], Yoshihiro Sakatani[2], Kensuke Otuka[2], Norikazu Ichihashi[1,2] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Dept. Bioinfo. Eng., Univ. Osaka*)

20425O ホストパラサイト相互作用による表現型可塑性の進化
Evolution of Phenotypic Plasticity in Host-Parasite Interactions
Naoto Nishiura, Kunihiko Kaneko (*The University of Tokyo Graduate School of Arts and Sciences*)

20426O* 高分子混雑環境下でのミクロ相分離が創成する細胞様構造体
Emergence of cell-like structure through micro phase separation in a crowding macromolecular solution
Fumika Fujita[1], Hiroki Sakuta[1], Kanta Tsumoto[2], Takahiro Kenmotsu[1], Kenichi Yoshikawa[1] ([1]*Facul. Life Med. Sci., Doshisha Univ.*, [2]*Facul. Eng., Mie Univ.*)

20427O* 人工膜小胞内リン脂質合成による自律的細胞分裂機構の構築
Development of a self-reproducing vesicular system driven by internal phospholipid synthesis
Kota Nakajima[1], Shunsuke Okada[2], Hiroshi Ueno[1], Naoki Soga[1], Takahiro Muraoka[2], Hiroyuki Noji[1] ([1]*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*, [2]*Dept. Appl. Chem., Grad. Sch. Eng., Tokyo Univ. Agri. Tech.*)

20428O* 細菌アクチン MreB からスピロプラズマ遊泳モーターへの進化
Development of *Spiroplasma* swimming motor from bacterial actin, MreB
Daichi Takahashi[1], Ikuko Fujiwara[1,2], Makoto Miyata[1,2] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*OCARINA, Osaka City Univ.*)

20429O 遺伝暗号における適応度地形の解析
Analysis of the fitness landscape of the genetic code
Yuji Omachi[1], Nen Saito[1], Chikara Furusawa[1,2] ([1]*Grad. Sch. Sci. UTokyo*, [2]*RikenBDR*)

20430O ~Parasite による Host 多様化の促進~ 原始的な多様性は如何にして生まれたか？
Host diversification promoted by parasites: prebiotic diversity in evolution
Rikuto Kamiura[1,2], Norikazu Ichihashi[1,2] ([1]*Graduate School of Arts and Science, The University of Tokyo*, [2]*Komaba Institute of Science, The University of Tokyo*)

P .ゲノム生物学・生命情報科学: ゲノミクス・分子進化／P. Genome biology & Bioinformatics

20431P Selection originating from protein stability/foldability: Relationships between protein folding free energy, sequence ensemble and fitness
Sanzo Miyazawa

20432P 自己集合ペプチドのオリゴマー形成に関する分子動力学的解析
Capturing oligomerization process of self-assembly peptides by using molecular dynamics simulations
Kota Kasahara[1,3], Junya Okigawa[1], Hiroki Terazawa[2], Qilin Xie[3], Satoshi Goto[2], Hayato Itaya[2], Katsufumi Nakayama[3], Takuya Takahashi[1] ([1]*Coll. Life. Sci., Ristumeikan Univ.*, [2]*Grad. Sch. Life Sci, Ritsumeikan Univ.*, [3]*Coll. Pharm. Sci., Ritsumeikan Univ.*)

20433P* Protein Data Bank に基づくタンパク質-ペプチド結合予測のための相互作用パターンの網羅的な分類と分析
Comprehensive classification and analysis of interaction patterns for protein-peptide binding prediction based on the Protein Data Bank
Keiichiro Sato[1], Kota Kasahara[1,2], Takuya Takahashi[1,2] ([1]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*)

20434P 演題取り消し

20435P* 荷電性残基の分布がタンパク質の液-液相分離に与える影響の解明に向けた分子動力学シミュレーション
Molecular dynamics simulations to dissect effects of charge distributions in protein sequence on the liquid-liquid phase separation
Hiroki Terazawa[1], Junya Okigawa[2], Kota Kasahara[2], Hiroshi Imamura[2], Minoru Kato[2], Takuya Takahashi[2] ([1]*Grad. Sch. Life Sci, Ritsumeikan Univ.*, [2]*Coll. Life Sci, Ritsumeikan Univ.*)

20436P 分子動力学シミュレーションによるアクチン構造ゆらぎの解析
Structural flexibility of actin studied by molecular dynamics simulation
Ryotaro Koike, Motonori Ota (*Grad. Sch. Info., Nagoya Univ.*)

20437P* PC4 天然変性領域の VP16 結合の制御メカニズムの解明
Simulation study of the mechanism of PC4 unstructured region which regulates binding with VP16
Qilin Xie[1], Kota Kasahara[2], Masafumi Nakayama[1], Takuya Takahashi[2] ([1]*Coll. Pha Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*)

20438P ウニ初期胚の核及び核内動態の蛍光イメージング観察・解析
Imaging analysis of inter- and intra-nuclear dynamics of sea urchin embryo
Miko Imada[1], Ayaka Sugiyama[2], Sayaka Hayashi[2], Kaichi Watanabe[1], Yuhei Yasui[1], Naoaki Sakamoto[1], **Akinori Awazu**[1] ([1]*Dept. Math and Life Sciences*, [2]*Dept. Math and Life Sciences*)

20439P 不凍タンパク質の予測及び解析
Prediction and analysis of antifreeze protein
Ryosuke Miyata, Kentaro Shimizu, Tohru Terada, Yoshitaka Moriwaki (*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

20440P 酵母の胞子形成の時系列マイクロアレイデータに対する効果的な非階層的クラスタリング手法開発の検討
Consideration of efficient non-hierarchical clustering method for time series microarray data of sporulation of S. cerevisiae
Aoi Tani[1], Masahiro Sugimoto[2], Takanori Sasaki[1] ([1]*Fac. Adv. Math. Sci., Meiji Univ.*, [2]*RDCMIT, Tokyo Med. Univ.*)

20441P DTX: 新規ヒト創薬ターゲット探索のための統合化ウェブツールの開発
DTX: An integrative web tool for exploring new potential drug targets in humans
Atsushi Hijikata, Masafumi Shionyu, Tsuyoshi Shirai (*Facult. Biosci, Nagahama Inst. Bio-Sci. Tech.*)

20442P DR-SIP: Predicting the Quaternary Structures of Homo-oligomeric Transmembrane Proteins
Wai Soon Chan[1,2,3], Jinhao Zhou[2,4], Christopher Llynard Ortiz[2], Chi-Hong Chang Chien[2], Rong-Long Pan[2], Lee-Wei Yang[2,3,5] ([1]*BioMol. Sim. Grp., Kansai Photon Sci. Inst., QST, Japan*, [2]*Inst. of BioInfo. and Struct. Bio., Nat. Tsing Hua Uni., Taiwan*, [3]*BioInfo., TIGP, Inst. of Info. Sci., Academia Sinica, Taiwan*, [4]*UTHealth Grad. Sch. of Biomed. Sci., Uni. of Texas, USA*, [5]*Phys. Div., Nat. Center for Theoretical Sci., Nat. Tsing Hua Uni., Taiwan*)

20443P 機械学習を利用した scRNAseq からの空間的遺伝子発現パターンの再構成
Prediction of spatial gene expressions from scRNAseq data by machine learning
Yasushi Okochi[1,2], Shunta Sakaguchi[3], Ken Nakae[4], Takefumi Kondo[3,5], Naoki Honda[1,6,7] ([1]*Laboratory for Theoretical Biology, Graduate School of Biostudies, Kyoto University*, [2]*Faculty of Medicine, Kyoto University*, [3]*Laboratory for Cell Recognition and Pattern Formation, Graduate School of Biostudies, Kyoto University*, [4]*Graduate School of Informatics, Kyoto University*, [5]*K-CONNEX*, [6]*Research Center for Dynamic Living Systems, Kyoto University*, [7]*Theoretical Biology Research Group, ExCELLS*)

20444P 蛍光増強 RNA アプタマーと cDNA ディスプレイを用いた高感度抗原検出法の開発
Development of a highly sensitive antigen detection method using fluorescence-enhanced RNA aptamer and cDNA display
So Higashide, Naoto Nemoto (*Graduate School of Science & Engineering, Saitama-University*)

20445P 機械学習を用いた PLP 結合タンパク質の予測
Prediction of PLP-binding proteins by using machine learning-based methods
Masafumi Shionyu, Tomohiro Hatta, Atsushi Hijikata (*Fac. Biosci., Nagahama Inst. Bio-Sci. Tech.*)

20446P Formation of chromatin remodeler Chd1-ADP-Pi analogues ternary complexes which mimic transient states in ATPase cycle
MD Noor A Alam, Sadakane Kei, Maruta Shinsaku (*SOKA UNIVERSITY*)

20447P 細胞イメージングへの応用のための蛍光増強アプタマーの開発
Development of fluorescence enhancement aptamers of dye for cell imaging applications
Tomoyuki Koike[1], Takashi Kubo[1], Kenjiro Hanaoka[2], Mitsuyoshi Ueda[3], Koichi Kuroda[3], Naoto Nemoto[1] ([1]*Graduate School of Science and Engineering, Saitama University.*, [2]*Graduate School of Pharmaceutical Sciences, The University of Tokyo.*, [3]*Graduate School of Agriculture, Kyoto University.*)

20448P* マルチタスク学習を用いたタンパク質-リガンド結合部位の統合的な予測
Integrated prediction of protein-ligand binding sites using multi-task learning
Haruka Nakashima, Yoshitaka Moriwaki, Tohru Terada, Kentaro Shinizu (*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

20449P 電顕フィッティング計算のための高速な原子モデルの GMM への変換：PCA ボックスダウンサンプル法
Fast calculation of Gaussian mixture models for atomic models to fit them on electron microscopy map: PCA-box down-sampling method
Takeshi Kawabata, Haruki Nakamura, Genji Kurisu (*IPR, Osaka U.*)

20450P* GPCR オリゴマーに影響を及ぼすがん関連ホットスポット変異の予測
Prediction of cancer associated hotspot mutations that affect GPCR oligomerization
Sakie Shimamura[1], Vachiranee Limviphuvadh[2], Hiroyuki Toh[3], Wataru Nemoto[1] ([1]*Dept. Sch. & Tech., Tokyo Denki Univ.*, [2]*A*STAR, BII.*, [3]*Sch. of Sci. & Tech., Kwansei Gakuin Univ.*)

20451P Remodelers exploit spontaneous nucleosome fluctuations to reorganize chromatin
Giovanni Brandani, Shoji Takada (*Kyoto University, School of Science*)

20452P 電顕画像と立体構造情報との照合による膜タンパク質ファミリーの判別技術開発
Development of membrane protein family identifier by collating EM images and atomic coordinate data
Ryuji Shinozaki[1], Masami Ikeda[2], Chikara Sato[3], **Makiko Suwa**[1] ([1]*College of Sci. and Eng., Aoyamagakuin Univ.*, [2]*AIRC, AIST*, [3]*Health med., AIST*)

20453P Analysis of Genetic Variants Through Protein and Residue Sociability
Hafumi Nishi[1,2], Yuki Kagaya[1], Matsuyuki Shirota[3], Kengo Kinoshita[1] ([1]*Grad. Sch. Info. Sci., Tohoku Univ.*, [2]*Faculty Core Res., Ochanomizu Univ.*, [3]*Sch. Med., Tohoku Univ.*)

20454P* タンパク質機能部位予測に適切な相同配列群選択手法の構築
Construction of a set of appropriate homologous sequences to predict functional regions of a protein
Yuto Takahashi[1], Shoichiro Kato[1], Hiroyuki Toh[2], Wataru Nemoto[1] ([1]*Dept. Sch. & Tech., Tokyo Denki Univ.*, [2]*Sch. of Sci. & Tech., Kwansei Gakuin Univ.*)

20455P* 転写翻訳系とゲノムが同種の無細胞ゲノム転写翻訳系の確立
In vitro genome transcription-translation system using Escherichia coli systems
Yukino Matsui, Tatsuki Deyama, Nobuhide Doi, Kei Fujiwara (*Dept. Biosci. Info., Keio univ.*)

20456P A comparative study of external morphology and phylogeny in the two species of earthworms
Hayato Endou (*Oyama Highschool*)

20457P Protein-Protein interaction patterns distinguish the hearing-loss phenotype between syndromic and non-syndromic types
Thi Thu Ha Duong[1,2], Kei Yura[1,3,4] ([1]*Graduate School of Humanities and Sciences, Ochanomizu University, 2-1-1 Otsuka, Bunkyo, Tokyo 112-8610, Japan*, [2]*nstitute of Genome Research, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet, Cau Giay, Ha Noi, Vietnam*, [3]*Center for Interdisciplinary AI and Data Science, Ochanomizu University, 2-1-1 Otsuka, Bunkyo, Tokyo 112-8610, Japan*, [4]*Graduate School of Advanced Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku, Tokyo 169-8555, Japan*)

20458P* PLA2 産生に関与する遺伝子と経路の同定
Identification of the genes and pathways responsible for PLA2 production
Eri Hayashi[1], Yuto Kimura[1], Shuichi Hirose[2], Satoko Nakamura[3], Norimasa Kashiwagi[3], Chiaki Ogino[3,4], Wataru Nemoto[1] ([1]*Dept. Sch. & Tech., Tokyo Denki Univ.*, [2]*NAGASE R&D Center*, [3]*hem Sci. & Eng., Grad. Sch. of Eng., Kobe Univ.*, [4]*Org. of Adv Sci & Tec., Kobe Univ.*)

Q. 生態・環境／Q. Ecology & Environment

20459Q 栄養構造を持つ 12 種微生物の人工生態系における確率現象
Stochastic phenomena in synthetic ecosystems of 12 microbial species with a trophic structure
Kazufumi Hosoda[1], Naomi Murakami[1], Shigeto Seno[2], Yutaka Osada[3], Hideo Matsuda[2], Chikara Furusawa[4], Michio Kondoh[5] ([1]*ITGP, Osaka univ.*, [2]*IST, Osaka univ.*, [3]*FRA*, [4]*Sci, Univ. Tokyo / BDR, Riken*, [5]*Life sci, Tohoku univ.*)

20460Q 蝶の模様の多様性と複雑性は、やわらかい要素やかたい要素を組み合わせて進化してきた
Combinations of flexible and fixed components facilitate colorful divergence and complexity in butterflies
Takao Suzuki (*Grad. Sch. Sci., Univ. Tokyo*)

20461Q 大阪府の石川における外来のアメリカツノウズムシの繁殖生態
The breeding ecology of the invasive alien Planaria, Girardia dorotocephala, in the middle reaches of the Isikawa river in Osaka Pref
Sakura Takahashi (*Osaka Pref. Tondabayashi H.S.*)

20462Q マミズクラゲの無性世代の 2 つの芽体を決める生息条件について
The habitat conditions determined two types of sprout formation of the asexual generation of Freshwater jellyfish, Craspedacusta sowerbii
Yuki Tanino, Yuta Hirayama, Sota Moriyama (*Osaka Pref.Tondabayashi H.S.*)

20463Q 金剛山地(大阪府)におけるヨツワクガビルの生息環境について
The Habitat of the Orobdella whitmani Oka in the Kongo Mountains (Osaka pref.)
Yuya Uenishi (*Osaka pref. Tondabayshi H.S.*)

20464Q 大阪府で初めて繁殖を確認したイワナ Salvelinus leucomaenis の生態とその由来の研究
The study of the ecology and origin of Salvelinus leucomaenis that has been confirmed to breed for the first time in Osaka prefecture
Kanato Nakamura, **Kaito Oana** (*Osaka pref. Tondabayashi H.S.*)

20465Q 三面コンクリート張り水路でゲンジボタルが生息できる理由
Reasons why Japanese Firefly, Luciola cruciate, can inhabit in a three-sided concrete channel
Takumi Matsuo, Tomoki Ikegawa (*Osaka Pref. Tondabayashi H.S.*)

20466Q 海浜植物のハマヒルガオが浜辺で生育できる理由
Reasons why the beach plant, Calystegia Soldanella, can grow on the beach
Kei Yanazawa (*Osaka Pref. Todabayashi H.S.*)

20467Q ドジョウの繁殖行動を誘発するトリガーについて
Triggers that trigger breeding behavior in loaches, Misgurnus anguillicaudatus,
Yohei Okugawa (*Osaka Pref. Tondabayashi H.S.*)

R. 数理生物学・非平衡・生体リズム／R. Mathematical biology, Nonequilibrium state & Biological rhythm

20468R Fisher 情報量による ERK リン酸化ダイナミクスの熱力学的性質の解明
The Fisher information of time reveals the thermodynamic property of ERK phosphorylation dynamics
Keita Ashida[1], Yohei Kondo[2,3,4], Kazuhiro Aoki[2,3,4], Sosuke Ito[1,5] ([1]*Universal Biology Institute, The University of Tokyo*, [2]*Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Science*, [3]*National Institute for Basic Biology, National Institutes of Natural Sciences*, [4]*Department of Basic Biology, School of Life Science, SOKENDAI*, [5]*JST, PRESTO*)

20469R Life-logger, 1000 匹の線虫の寿命時間スケールでの行動動態を計測するためのビデオ撮影装置の開発
Life-logger, a video-recorder of crawling motion of 1,000 *C. elegans* individuals during their lifespan
Yukinobu Arata, Peter Jurica, Yasishi Sako (*Cellular Informatics Laboratory, Riken*)

20470R 度数情報だけで再訪性を判断するエージェントのネットワーク探索
A Random walk model on the Scale-Free Network with the Cognitive Biases
Koji Takashima, Tomoko Sakiyama (*Soka University*)

20471R* 遺伝子発現レベルの情報から ErbB シグナルの動態を予測する数理モデリング基盤の開発
Model-based prediction of ErbB signaling dynamics solely from the information about gene expression levels
Hiroaki Imoto, Marie Maeda, Suxiang Zhang, Mariko Okada (*IPR, Osaka Univ.*)

20472R Approximation of transition density of the conductance based neuronal model with noise
Takanobu Yamanobe (*Sch. Med., Hokkaido Univ.*)

20473R 人工トリペプチドからなる自己集合性ナノファイバーの進行波による力発生
Force generation by a propagating wave of artificial tripeptide-based fibrous assemblies
Ryou Kubota[1], Masahiro Makuta[2], Ryo Suzuki[3], Masatoshi Ichikawa[2], Motomu Tanaka[3], Itaru Hamachi[1,4] ([1]*Grad. Eng., Kyoto Univ.*, [2]*Grad. Sci., Kyoto Univ.*, [3]*Inst. Adv. Stud., Kyoto Univ.*, [4]*JST ERATO*)

20474R Quantifying expressive power of gene regulatory systems
Yohei Kondo[1,2], Kazuhiro Aoki[1,2,3] ([1]*ExCELLS*, [2]*SOKENDAI*, [3]*NIBB*)

20475R 質量保存を満たす反応拡散系にみられる相分離的な挙動
Phase-separation like behavior in mass-conserved reaction diffusion systems
Michio Tateno, Shuji Ishihara (*Shuji Ishihara Lab., Graduate School of Arts and Sciences, The University of Tokyo*)

20476R Investigation of related genes in the development of atopic dermatitis by geometric feature extraction from gene expression patterns
Takuya Hasebe[1], Masahiro Sugimoto[2], Takanori Sasaki[1] ([1]*Grad. Sch. Adv. Math. Sci., Meiji Univ*, [2]*RDCMIT, Tokyo Med. Univ*)

20477R 脳神経系の可塑的結合力学系モデルにおける自己組織的ネットワーク
Self-organized network structures in coupled dynamical system with connection plasticity inspired by cerebral nervous system
Amika Ohara, Masashi Fujii, Akinori Awazu (*Dept. of math. and life sci. Hiroshima univ.*)

20478R ディープラーニング及びオートエンコーダーを用いた乳癌組織中の DEGs からの特徴抽出と予後予測
Feature extraction and prognosis prediction from DEGs in breast cancer tissue using Deep learning and Autoencoder
Yusuke Mizukoshi[1], Masahiro Sugimoto[2], Takanori Sasaki[1] ([1]*Fac. Adv. Math. Sci., Meiji Univ.*, [2]*RDCMIT, Tokyo Med. Univ.*)

20479R Determination of the interacting time between KaiA and KaiB during clock oscillation
Risa Mutoh[1], Takahiro Iida[1], Mino Hiroyuki[2] ([1]*Faculty of Sci. Fukuoka Univ.*, [2]*Grad. Sch. of Sci., Nagoya Univ.*)

20480R オンチップ単一細胞培養システムによる 3 細胞系心筋ネットワークの拍動同期過程の観察
Observation of synchronized beating cycles of cardiomyocytes during three cell network formation in on-chip single cell measurement assay
Yoshitsune Hondo[1], Kazufumi Sakamoto[1], Rikuto Sekine[2], Yuhei Tanaka[1], Haruki Watanabe[1], Kenji Shimoda[1], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*)

20481R Active Inference of Gradient in Reward-oriented Behavior
WeiQing Chen[1], Naoki Honda[1,2] ([1]*Grad. Sch. Bio., Univ. Kyoto*, [2]*Theoretical Biology Research Group, Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences, Okazaki, Aichi, Japan.*)

20482R 膜タンパク質のクラスター形成機構の数理的研究
A Mathematical study on the mechanism of cluster formation of membrane proteins
Hiroaki Takagi (*Sch. Med., Nara Med. Univ.*)

20483R ES 細胞分化初期における染色体動態
The dynamics of chromosomes on early differentiation stage from ES cell
Tetsushi Komoto, Masashi Fujii, Akinori Awazu (*Hiroshima univ. Grad. Sch. Integrated Sciences for Life*)

20484R* Inferring domain of Interactions among Dictyostelium discoideum colony from the Ensemble of Trajectories of cells
Udoy S. Basak[1,2], Sulimon Sattari[1], Md. Motaleb Hossain[1], Kazuki Horikawa[3], Tamkiki Komatsuzaki[1] ([1]*Hokkaido University*, [2]*Pabna University of Science and Technology*, [3]*Tokushima University*)

20485R 栄養の枯渇が引き起こす酵母の解糖系振動現象
Glycolytic Oscillation in Yeast Induced by Nutrient Depletion
Seiji Hatano[1], Noboru Nagata[1], Yutetsu Kuruma[2], Toshihiro Kawakatsu[1], Masayuki Imai[1] ([1]*Grad. Sch. Sci., Tohoku Univ.*, [2]*ELSI, Tokyo Inst. Tech.*)

20486R ミトコンドリア呼吸鎖エナジェティクスの速度論的解析
Kinetic analysis of energetics in mitochondrial respiratory chain
Ikuo Kujiraoka[1], Kotaro Takeyasu[2,3], Junji Nakamura[2,3] ([1]*Graduate school of science and technology, Univ. Tsukuba*, [2]*Faculty of pure and applied sciences, Univ. Tsukuba*, [3]*Tsukuba research center for energy materials science, Univ. Tsukuba*)

20487R Chromatin dynamics in Hox-mediated animal body development
Yoshifumi Asakura[1], Naoki Honda[1,2] ([1]*Grad. Sch. Biostudies, Univ. Kyoto*, [2]*ExCELLS, NINS*)

20488R エピジェネティック修飾の変化の影響を考慮した EM 遷移のシミュレーション
A model on the effects of epigenetic modification on epithelial-mesenchymal transitions (EMT)
Kenichi Hagiwara, Masaki Sasai (*Dept.Appl.phys.,Nagoya Univ.*)

20489R Length scale-dependent relaxation in chromatin with and without the transcription factory
Ashwin S. S[1], Yuji Itoh[2], Kazuhiro Maeshima[2], Masaki Sasai[1] ([1]*Department of Applied Physics, Nagoya University, Nagoya, JAPAN*, [2]*Structural Biology Center, National Institute of Genetics, Mishima, JAPAN*)

20490R 出芽酵母の DNA 二本鎖切断時における染色体動態の数理モデル
A mathmatical model of chromosomal dynamics in budding yeast during DNA double strand break
Shinjiro Nakahata, Akinori Awazu, Masashi Fujii (*Hiroshima univ. Grad. Sch. Integrated Sciences for Life*)

20491R Quantifying the length- and time-scales of influence of cells in collective motion
Sulimon Sattari[1], Udoy Basak[1], Md. Hossain Motaleb[1], Kazuki Horikawa[2], Tamiki Komatsuzaki[1] ([1]*Hokkaido University Research Institute for Electronic Science*, [2]*Tokushima Unviersity, Institute of Biomedical Sciences*)

20492R Circular probability currents and correlation functions for gene switching coupled with epigenetic dynamics
Bhaswati Bhattacharyya, Masaki Sasai (*Department of Applied Physics, Graduate School of Engineering, Nagoya University*)

20493R 植物のストレス応答を担う植物ホルモン時空間動態の数理モデル
Mathematical model of spatiotemporal dynamics of plant hormones responsible for plant stress response
Mariko Arimoto, Akinori Awazu, Masashi Fujii (*Grad. Sch. Sci., Univ. Hiroshima*)

20494R 協同的に振る舞う遺伝子発現制御ネットワークの定量的解析
Quantitative analysis of cooperative network from sloppy gene expression dynamics
Masayo Inoue[1], Kunihiko Kaneko[2] ([1]*IMS, Meiji Univ.*, [2]*Univ. of Tokyo*)

20495R ヒトゲノム中の 3 塩基リピート配列周辺エピゲノムとクロマチン構造のゲノムワイドな解析
Genome-wide analysis of epigenetic and chromatin-structural features around triplet repeat sequences in human genome
Kenji Ojima[1], Yuudai Hirose[2], Masashi Fujii[1], Akinori Awazu[1] ([1]*Department of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University*, [2]*Department of Mathematical and Life Sciences, Graduate School of Science, Hiroshima University*)

20496R バクテリアの集団運動による走性の変化
Enhanced bacterial taxis by collective movement
Tatsuro Kai, Takahiro Abe, Shuichi Nakamura, Seishi Kudo, Shoichi Toyabe (*Department of Applied Physics, Graduate School of Engineering, Tohoku University*)

20497R Fluctuation distribution of propagation time was conserved during excitation conduction in lined-up cardiomyocyte networks
Kazufumi Sakamoto[1], Yoshitsune Hondo[1], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*)

20498R Vector analysis of amoeba motion with respect to the propagation of chemoattractant cyclic-AMP
Vector analysis of amoeba motion with respect to the propagation of chemoattractant cyclic-AMP
Md. Motaleb Hossain[1,2], Sulimon Sattari[1], Udoy S Basak[1], Kazuki Horikawa[3], Tamiki Komatsuzaki[1] ([1]*Hokkaido University*, [2]*University of Dhaka*, [3]*Tokushima University*)

20499R* 免疫系の記憶ダイナミクスにおける適応的な抗原の有害・無害識別
Adaptive Discrimination of Risk of Antigens in Immune Memory Dynamics
Kana Yoshido[1], Naoki Honda[1,2] ([1]*Grad. Sch. Biostudies, Univ. Kyoto*, [2]*ExCELLS, NINS*)

20500R* ERK シグナル伝達系の進化生化学
Evolutionary biochemistry of ERK signaling network
Masaya Mukai[1,2,3], Yohei Kondo[2,3], Kazuhiro Aoki[1,2,3] ([1]*Division of Quantitative Biol., NIBB*, [2]*Quantitative Biol. Group, ExCELLS*, [3]*Dept. of Basic Biol., Sch. of Life Sci., SOKENDAI*)

20501S BSA における AQDS 結合サイトの光誘起電子電子二重共鳴(DEER)計測
Light-induced DEER measurement on the AQDS-binding site in Bovine Serum Albumin
Hiroki Nagashima, Lewis Antill, Kiminori Maeda (*Dep. Chem., Grad. Sch. Sci., Saitama University*)

20502S ヒト皮膚または培養皮膚に貼付したセラミド含有粘着性ゲルシートからのセラミド放出のマイクロ FT-IR 分光法による計測
Micro FT-IR Spectroscopic Study on Ceramide-release from Ceramide-Containing Adhesive Gel Sheet Affixed to Human Skin or Cultured Skin
Hiroshi Takahashi[1], Ryota Watanabe[2], Kenichi Nishimura[2], Taro Moriwaki[3] ([1]*Grad Sci Sci.&Tech., Gunma Univ.*, [2]*ALCARE Co., Ltd.*, [3]*JASRI/SPring-8*)

20503S ウニの発生初期における核内染色体構造の動的および細胞特異的変化
Dynamic and cell specific changes in intranuclear chromosomal structures during early development of sea urchin
Yuhei Yasui, Ayaka Sugiyama, Naoaki Sakamoto, Akinori Awazu (*Integrated science for life, Hiroshima University*)

20504S 伝導度計測を用いたペプチドのリン酸化の単一分子検出
Single-molecule detection of peptide phosphorylation using electrical conductance measurement
Takanori Harashima[1], Yoshiyuki Egami[2], Tomoya Ono[3], Tomoaki Nishino[1] ([1]*School of Science, Tokyo Institute of Technology*, [2]*Faculty of Engineering, Hokkaido University*, [3]*Department of Electrical and Electronic Engineering, Kobe University*)

20505S* イオン液体-スピン乾燥法で走査型電子顕微鏡の試料作製を容易にする
A simple and quick method to prepare biological specimens for scanning electron microscopy by an ionic liquid
Tatsuya Suehiro, Naoki Uemura, Saki Taguchi, Katsuya Shimabukuro (*Chem. Bio. Eng., NIT Ube College*)

20506S 短波赤外光を発する量子ドットによる無侵襲マウス脳表血管造影とその焦点合わせについて
Novel angiography for mouse cerebral vasculature using short-wave infrared light emitting quantum dots and its focusing
Tatsuto Iida[1], Hiro Yamato[1], Takashi Jin[2], **Yasutomo Nomura**[1,2] ([1]*Department of Systems Life Engineering, Maebashi Institute of Technology*, [2]*RIKEN Center for Biosystems Dynamics Research*)

20507S Variogram/Correlogram 法を使った生物対流解析
Variogram and correlogram assay of cell motility: Bioconvection in harmful algae *Chattonella*
Mina Nakahara, Atsuto Kobayashi, **Shinji Kamimura** (*Dept. Biol. Sci., Fac. Sci. & Eng., Chuo Univ.*)

20508S 分裂期の染色体の 3D-AFM 像の理論予測と実測との比較
A theoretical prediction of 3D atomic force microscopy image of chromosomes in mitotic phase and its comparison with experiments
Takashi Sumikama[1], Keisuke Miyazawa[1,2], Makiko Meguro-Horike[3], Ryohei Kojima[2], Naoko Okano[2], Shin-ichi Horike[3], Adam S. Foster[1,4], Takeshi Fukuma[1,2] ([1]*Nano Life Sci. Inst. (WPI-NanoLSI), Kanazawa Univ.*, [2]*Grad. Sch. of Nat. Sci. and Tech., Kanazawa Univ.*, [3]*Div. of Func. Gen., Adv. Sci. Res. Center, Kanazawa Univ.*, [4]*Dept. of Appl. Phys., Aalto Univ.*)

20509S 原子間力顕微鏡の位相イメージングを用いた *Paracoccus denitrificans* 細胞に結合した膜小胞の解析
Analysis of bacterial extracellular membrane vesicles bound to *Paracoccus denitrificans* cell by atomic force microscopy phase imaging
Yousuke Kikuchi[1], Yuuki Ichinaka[1], Masanori Toyofuku[2,3], Nozomu Obana[3,4], Nobuhiko Nomura[2,3], Azuma Taoka[1,5] ([1]*Col. of Sci. and Eng., Kanazawa Univ.*, [2]*Life and Env. Sci., Tsukuba Univ.*, [3]*MiCS, Tsukuba Univ.*, [4]*Trans. Med. Res., Tsukuba Univ.*, [5]*WPI-NanoLSI, Kanazawa Univ.*)

20510S 神経細胞分化における細胞内温度の関与
Involvement of intracellular temperature in neuronal differentiation
Shunsuke Chuma[1], Kohki Okabe[2,3], Yoshie Harada[1,4] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sch. Pharm. Sci., The Univ. Tokyo*, [3]*PRESTO, JST*, [4]*QIQB, OTRI, Osaka Univ.*)

20511S 原子間力顕微鏡と多孔窒化シリコン薄膜を用いた生きた細胞表面の高分解能観察方法の開発
Development of high-resolution observation method of living cell surface in atomic force microscope using porous silicon nitride membrane
Takehiko Ichikawa[1], Taiki Kitamura[2], Dong Wang[1,3], Hiroko Oshima[3], Masanobu Oshima[1,3], Takeshi Fukuma[1,2] ([1]*NanoLSI, Kanazawa Univ.*, [2]*College of Science and Engineering, Kanazawa Univ.*, [3]*Cancer Research Institute, Kanazawa Univ.*)

20512S 自動イオンチャネル電流測定装置の開発
Development of a system for automated ionic current measurement
Minako Hirano[1], Masahisa Tomita[2], Chikako Takahashi[1], Nobuyuki Kawashima[2], Toru Ide[3] ([1]*Grad. Sch. Creation Photon Indust.*, [2]*SYSTEC Corporation*, [3]*Okayama Univ.*)

20513S 上皮成長因子受容体癌変異への自動化 1 分子解析の薬理学的応用
Pharmacological application of automated single-molecule analysis for EGFR cancerous mutants
Michio Hiroshima[1,2], Daisuke Watanabe[3], Masahiro Ueda[1,3] ([1]*RIKEN BDR*, [2]*RIKEN CPR*, [3]*FBS, Osaka Univ.*)

20514S 生細胞 1 分子超解像イメージングによるヒストンバリアントのナノスケール局在解析
Nano-scale localization analysis of histone variants in living cells using single-molecule super-resolution imaging
Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

20515S サブミリ秒光波面シェイピングシステムによる厚さ 2mm の鶏肉を通した光集束及び蛍光イメージング
Optical focusing and fluorescence imaging through a 2mm thick chicken tissue slice by submillisecond wavefront shaping system
Atsushi Shibukawa, Keiichi Kojima, Yuki Sudo (*Grad. Sch. of Med. Dent. Pharm. Sci., Okayama Univ.*)

20516S Development of continuous non-clogging cell fractionation technique using pillar arrangement and AC electric field
Kaito Asahi[1], Moe Iwamura[2], Masao Odaka[3,4], Akihiro Hattori[3,4], Kenji Yasuda[1,2,3,4] ([1]*Dept. 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*)

20517S Interaction of nicked-DNA with solid state nanopores
Shimba Ichino, Kento Lloyd, Takumi Yoshikawa, Ryoma Omori, Yuuta Moriyama, Toshiyuki Mitsui (*Aogaku Univ.*)

20518S Simple precise flow speed measurement in an on-chip flow cytometer with simultaneous two-wavelength differential image analysis
Toshinosuke Akimoto[1], Shuya Sawa[1], Masao Odaka[3], Akihiro Hattori[3], Mitsuru Sentoku[1], Hiromiti Hasimoto[2], Kaito Asahi[1], Kenji Yasuda[1,2,3] ([1]*Dept. 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.*)

20519S 多次元デジタルバイオアッセイで明らかになった、インフルエンザウイルスにおける粒子ごとの薬剤応答の多様性
Multi-Dimensional (MD) Digital Bioassay unveils heterogeneous drug-susceptibility of influenza A virus in a single-virus resolution
Shingo Honda[1], Kazuhito V. Tabata[2], Yoshihiro Minagawa[2], Hiroyuki Noji[1,2] ([1]*Dept. Bioeng., Grad. Sch. Eng., Univ. Tokyo*, [2]*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

20520S Ligand is not necessary for progress of engulfment in IgG-coated and non-coated mixture of antigen cluster
Amane Yoshida[1], Yuya Furumoto[1], Toshiki Azuma[1], Tomoyasu Sakaguchi[1], Kenji Yasuda[1,2,3] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Org. Univ. Res. Initiatives, Waseda Univ.*, [3]*WASEDA Biosci. Res. Ins. in Singapore (WABIOS)*)

20521S 光ファイバー型蛍光相関分光装置を用いたエクソソームの同定
Identification of exosome by using optical fiber based fluorescence correlation spectroscopy
Misato Osaka[1], Johtaro Yamamoto[2,3], Masataka Kinjo[3] ([1]*Grad. Sch. of Life Sci., Hokkaido Univ.*, [2]*Health & Med. Res. Inst., AIST*, [3]*Fac. of Adv. Life Sci., Hokkaido Univ.*)

20522S 最大エントロピー法と変分ベイズクラスタリングを用いた 1 分子 FRET データ解析による細胞質中 RAF のダイマー化状態の検出
Dimer formation of cytosolic RAF detected by single-molecule FRET analysis based on maximum entropy and variational Bayes-culstering
Kenji Okamoto, Yasushi Sako (*RIKEN CPR*)

20523S Investigation of automatic single-molecule tracking method for large-scale single-molecule imaging analysis
Sotaro Mori[1], Masato Yasui[4], Satomi Matsuoka[1,2,3,5], Masahiro Ueda[1,2,3] ([1]*Grad. Sch. Sci., Univ. Osaka*, [2]*Grad. Sch. Sci. of Front. Biosci., Univ. Osaka*, [3]*BDR, RIKEN*, [4]*ZIDO Corp.*, [5]*PRESTO, JST*)

20524S* ヨーロッパモノアラガイの咀嚼神経系の蛍光 NO イメージング ー味覚嫌悪学習前後の NO 放出の比較
Fluorescence NO imaging for feeding nervous system of the pond snail-Comparison of NO release before and after taste-aversive conditioning
Ayaka Itoh[1], Yoshimasa Komatsuzaki[2], Minoru Saito[1] ([1]*Grad. Sch. of Int. Bas. Sci., Nihon Univ.*, [2]*Coll. Sci. Tech., Nihon Univ.*)

20525S DNA ナノデバイスを用いた細胞の機械シグナルイメージング技術開発
Development of mechanical signal imaging technique using DNA nano-device
Hiroki Fukunaga[1], Takahiro Saito[1], Satiko Onishi[2], Mitsuhiro Iwaki[1,2] ([1]*FBS, Univ. Osaka*, [2]*BDR, Riken*)

20526S クロモセンター領域内外におけるヘテロクロマチンタンパク質 HP1α 動態の生細胞 1 分子イメージング定量解析
Dynamics of Heterochromatin protein 1α inside and outside chromocenter domain in living cells using single-molecule imaging
Masanori Nakano[1], Yuma Ito[1], Takahiro Maeda[1], Chikashi Obuse[2], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Biosci. Grad Sch Sci., Osaka Univ*)

20527S 補償光学系を用いた 1 分子イメージングにおける収差補正のシミュレーション
Light field simulation of single-molecule imaging for aberration correction using adaptive optics
Xiang Zhou, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech.*)

20528S 核小体タンパク質の多色超解像 1 分子イメージング解析
Multicolor single-molecule imaging analysis of the nucleolar proteins
Supanut Sirisukhodom[1], Yuma Ito[1], Noriko Saitoh[2], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Tech.*, [2]*Div. of Cancer Biol., The Cancer Inst. JFCR.*)

20529S Development of an enzyme-coupled fluorometric digital bioassay for ATPase
Hiroshi Ueno, Mayu Hara, Mio Sano, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

20530S 2 光子生体イメージングでみるインフルエンザウイルス感染肺
In vivo imaging of the cellular pathophysiology in influenza virus-infected mouse lung
Hiroshi Ueki[1], Yoshihiro Kawaoka[1,2,3] ([1]*Division of Virology, Department of Microbiology and Immunology, Institute of Medical Science, University of Tokyo*, [2]*Department of Special Pathogens, International Research Center for Infectious Diseases, Institute of Medical Science, University of Tokyo*, [3]*Department of Pathobiological Sciences, School of Veterinary Medicine, University of Wisconsin-Madison*)

20531S Direct observation of force-induced release of SecM translation arrest
Zhuohao Yang[1], Ryo Iizuka[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., The Univ. Tokyo.*, [2]*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

20532S パッチクランプ AFM の開発に向けて
Toward the development of Patch Clamp Atomic Force Microscopy
Takeru Matsubara[1], Shinji Watanabe[2], Toshio Ando[2], Noriyuki Kodera[2] ([1]*Grad. Sch. NanoLS., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*)

20533S* Biophysical analysis of pH-dependent conformational change of LDLR family members in ligand capture and release

Aki Shiozawa[1], Noriyuki Kodera[2], Terukazu Nogi[1] ([1]*Grad. Sch. of Med. Lif. Sci., Yokohama City Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*)

20534S* 客観的な生物物理学データ解析に向けた初期パラメータ設定を必要としない隠 れマルコフモデルフィッティング手法の開発

Development of a new hidden Markov model fitting algorithm without predefinition of parameters for objective biophysical data analysis

Hanjin Liu, Tomohiro Shima, Sotaro Uemura (*Sch. Sci., Univ. Tokyo*)

20535S DNA motions near geometrically anisotropic nanopores

Takumi Yoshikawa, Ryoma Omori, Shimba Ichino, Yuuta Moriyama, Toshiyuki Mitsui (*Aogaku Univ.*)

20536S* 統計的蛍光画像解析による濃度分布イメージング

Fluorescence Imaging for Concentration Based on Statistical Analysis

Ryosuke Fukushima[1], Johtaro Yamamoto[2,3], Masataka Kinjo[3] ([1]*Grad. Sch. of Life Sci., Hokkaido Univ.*, [2]*Health & Med. Res. Inst., AIST*, [3]*Fac. of Adv. Life Sci., Hokkaido Univ.*)

20537S* Hybrid Photon Counting (HPC)検出器の microED 法への応用

Hybrid Photon Counting (HPC) detector application for microED method

Keigo Takahira[1,2], Kotaro Tanaka[1], Takeyoshi Taguchi[2], Hiroyuki Kanda[2], Akihito Yamano[2], Takuo Yasunaga[1] ([1]*Grad.Sch.Comp.Sci.Syst.Eng.,KIT,Fukuoka,Japan*, [2]*Rigaku Corporation,Tokyo,Japan*)

20538S* 環境の温度変化に対する RNA の状態変化を介した細胞応答の解明

Investigating cell response to environmental temperature change via RNA state changes

Hiroki Shibata[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. of Pharm. Sci., The Univ of Tokyo*, [2]*PRESTO, JST*)

20539S* 繊毛虫 *Tetrahymena* による遊泳軌跡の三次元定量

Three-dimensional analysis of the swimming trajectories of *Tetrahymena*

Akisato Marumo, Kyohei Matsuda, Masahiko Yamagishi, Mitsuhiro Sugawa, Junichiro Yajima (*Dept. Life Sci., Grad. Arts & Sci., Univ. Tokyo*)

20540S 相関顕微鏡法（CLEM）による同一試料観察に向けた相関・位置合わせ精度の改善

Improvement of correlation and alignment accuracy toward the same sample observation by CLEM

Yuki Gomibuchi[1], Risa Ezoe[2], Hiroko Takazaki[1,3], Yasuhisa Honda[2], Yusuke V. Morimoto[1], Takuo Yasunaga[1] ([1]*Dept. of Phys. Info. Tech., Kyushu Inst. Tech*, [2]*Dept. of Biosci. Bioinfo., Kyushu Inst. Tech.*, [3]*IPR. Osaka Univ.*)

20541S 画像解析システム Eos の次世代開発に向けて

Approach to the next generation of our developing image processing system, Eos

Takuo Yasunaga (*Comp. Sci and Sys. Eng., Kyutech*)

20542S 高速原子間力顕微鏡データと分子シミュレーションのデータ同化によるミオシン V の動的構造解析

Dynamic structure analysis of myosin V by data assimilation combining HS-AFM data and molecular simulations

Sotaro Fuchigami[1], Rie Koga[2], Shoji Takada[1] ([1]*Grad. Sch. of Science, Kyoto Univ.*, [2]*ExCELLS, NINS*)

20543S 水素化アモルファスシリコンと有機半導体で増強された分子薄膜を用いた揮発性 化合物のセンサシステム

A sensor system for volatile organic compound using molecular film enhanced by hydrogenated amorphous silicon and organic semiconductor

Hikaru Hatakeyama[1], Kisiro Seino[1], Shu Mugita[1], Kairi Shimazaki[1], Hiroshi Masumoto[2], Yutaka Tsujiuchi[1] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary, Tohoku University*)

20544S 水素化アモルファスシリコンの上に積層したバクテリオロドプシンの分子間相互作用と構造変化
Inter molecular interaction and structural change of bacteriorhodopsin film laminated on hydrogenated amorphous silicon film
Yutaka Tsujiuchi[1], Hikaru Hatakeyama[1], Koki Shimanaka[1], Hiroshi Masumoto[2] ([1]*Mat.Sci.AkitaUNIV*, [2]*Fris.TohokuUNIV*)

20545S 粒子フィルター MD シミュレーションによる高速 AFM の非斉時ビデオのデータ同化
Particle-filter MD simulations to assimilate asynchronous video data of high-speed AFM
Suguru Kato, Sotaro Fuchigami, Shoji Takada (*Kyoto University*)

20546S HPD を用いた広視野蛍光 1 分子検出による局所環境変化のモニタリング
Local ambient condition monitoring by hybrid photo-detector (HPD)-based wide-field single-molecule fluorescence detection
Atsuhito Fukasawa[1], Gaku Nakano[1], Takayasu Nagasawa[1], Minako Hirano[2], Toru Ide[3], Hiroaki Yokota[2] ([1]*Hamamatsu Photonics K.K.*, [2]*Grad. Sch. Creation Photon Indust.*, [3]*Grad. Sch. Interdiscip. Sci. Eng. Health Sys.*)

20547S 多様な構造をもつタンパク質複合体の単粒子解析を改善する方法の調査研究
A survey and investigation on methods to improve single particle analysis of heterogeneous protein complexes
Kotaro Tanaka, Takuo Yasunaga (*Grad. Sch. Comp. Sci. Syst. Eng., Kyutech*)

20548S 生物発光共鳴エネルギー移動による発光バクテリアルシフェラーゼの高輝度化
Enhanced brightness of bacterial luciferase by bioluminescence resonance energy transfer
Tomomi Kaku, Megumi Iwano, Tetsuyuki Entani, Kenji Osabe, Takeharu Nagai (*The Institute of Scientific and Industrial Reseach, Osaka University*)

20549S* Wash-free デジタルバイオ計測のための split enzyme の開発
Development of a split enzyme for wash-free digital bioassay
Yanbo Ma, Hiroshi Ueno, Hiroyuki Noji (*Department of Applied Chemistry, Graduate School of Engineering, University of Tokyo*)

20550S Raman imaging for cancer diagnosis
Clement Jean-Emmanuel[1], Mochizuki Kenntaro[2], Fujita Katsumasa[3], Komatsuzaki Tamiki[1] ([1]*RIES Hokkaido University*, [2]*Kyoto University*, [3]*Osaka University*)

T .バイオエンジニアリング・結晶成長・結晶化技術／T. Bioengineering, Crystal growth & Crystallization technique

20551T FRAP 法と遺伝子組換えを併用した反応拡散分子の細胞内動態解析
FRAP combined with genetic manipulation reveals the kinetics of actin-binding proteins in cells
Takumi Saito[1,2], Daiki Matsunaga[1], Tsubasa Matsui[1], Kentaro Noi[1], Shinji Deguchi[1] ([1]*Grad. Sch. Eng. Sci., Osaka uni.*, [2]*JSPS Research Fellow*)

20552T 高汎用性を目指した改良凝固ゲル中結晶化法の開発と評価
Development and evaluation of the high-strength hydrogel method for high versatility
Taichi Naruse[1], Mihoka Amano[1], Noriaki Kunimune[2], Tsuguo Nagasawa[2], Hiroaki Adachi[3], Yusuke Mori[4], Shigeru Sugiyama[5] ([1]*Grad. Sch. Sci., Kochi Univ.*, [2]*KUNIMUNE Inc.*, [3]*SOSHO Inc.*, [4]*Grad. Sch. Eng., Osaka Univ.*, [5]*Fac. Sci. & Tec., Kochi Univ.*)

20553T DNA オリガミによる人工 γ-TuRC
Artificial γ-TuRC made by DNA origami
Daisuke Inoue (*Kyushu University*)

20554T 集光レーザービームによる動的微小管ネットワークの形成
Formation of dynamic microtubule networks by focused laser beam
Kei Takano[1], Takuya Takeshige[1], Humika Kiryu[1], Ryuzo Kawamura[1], Chi-shiun Wu[2], Shih Yang-Hshin[2], Seiichiro Nakabayashi[1], Teruki Sugiyama[2,3], Hiroshi Yoshikawa[1] ([1]*Grad. Chem., Saitama Univ.*, [2]*App. Chem., National Chiao Tung Univ.*, [3]*Mate. Sci., Nara Inst. Sci. Tech. Univ.*)

20555T Combination approach for identification of highly-active mutant of processive chitinase
Akasit Visootsat[1,2], Akihiko Nakamura[3], Tak-Wai Wang[4], Ryota Iino[1,2] ([1]*Department of Functional Molecular Science, School of Physical Sciences, The Graduate University for Advanced Studies*, [2]*Institute for Molecular Science*, [3]*Department of Applied Life Sciences, Faculty of Agriculture, Shizuoka University*, [4]*Chimie ParisTech*)

20556T Culture-independent method for screening macromolecule-degrading microbes using deformability-based microfluidic microdroplet sorting
Mikihisa Muta[1], Kai Saito[1], Ryo Iizuka[1], Wataru Kawakubo[2], Hyun Yoon Dong[3], Tetsushi Sekiguchi[3], Shuichi Shoji[2], Mei Ito[4], 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.*, [4]*Dept. of Life Sci. and Green Chem., Saitama Inst. of Technol.*)

20557T 方向性を持った運動をするアメーバ型分子ロボットの開発
Toward vector motion of the cell-sized motorized molecular
Noriki Fukami[1], Yuichi Hiratsuka[2], Ibuki Kawamata[1], Yuki Suzuki[1,3], Satoshi Murata[1], Shin-ichiro Nomura[1] ([1]*Department of Robotics, Graduate School of Engineering, Tohoku University, Sendai 980-8579, Japan.*, [2]*Japan Advanced Institute of Science and Technology*, [3]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

U. その他／U. Other topics

20558U Topological Data Analysis of Large-scale Multicellular Networks
Suguru Shimomura[1], Satoru Iwasaki[1], Tadashi Nakano[2] ([1]*Graduate School of Information Science and Technology, Osaka University*, [2]*Institute for Datability Science, Osaka University*)

20559U Observation of floating phenomenon of *Cyclotella meneghiniana* by direct microscope: Temperature dependence analysis using a heater
Yuki Ide[1], Yuji Matsukawa[1], Daisuke Miyashiro[1], Shigeki Mayama[2], Matthew L. Julius[3], Kazuo Umemura[1] ([1]*Tokyo Univ. Sci.*, [2]*Tokyo Gakugei Univ.*, [3]*St. Cloud State Univ.*)

20560U 矢が優れた飛び道具である理由ー自作風洞実験装置を用いた飛行する矢に働く力の分析ー
The reason why the arrow is superior flying tool - Analysis of forces acting on flying arrows by using a home-made wind tunnel device -
Haruto Tgawa, Akito Wada, Hinata Furuya, Ayumu Yamamori (*Osaka Pref. Tondabayashi H.S.*)

20561U 一本鎖 DNA を被覆した単層カーボンナノチューブと細胞膜間の力学的相互作用
Mechanical interaction between single-strand DNA wrapped single-walled carbon nanotubes and cell membrane
Daisuke Miyashiro[1,2], Ryo Hamano[1], Kazuo Umemura[1] ([1]*Tokyo University of Science*, [2]*ESTECH CORP.*)

20562U 二本鎖 DNA とカルボキシメチルセルロースで分散した単層カーボンナノチューブの吸光度特性
Absorption properties of single-walled carbon nanotubes dispersed with double-stranded DNA and carboxymethylcellulose
Ryo Hamano[1], Daisuke Miyashiro[1,2], Kazuo Umemura[1] ([1]*Tokyo Univ. Sci.*, [2]*ESTEC CORP.*)

20563U 空気の抵抗が雷の発生と発光に及ぼす影響
Effect of air resistance on the generation and lightning of thunderbolt
Shingo Iwasaki (*HatusibaTondabayasi H.S.*)

20564U 基準振動解析を用いたロドプシンの動態予測と機能の連関
Relationship between function and dynamics of rhodopsin using normal mode analysis
Yukito Kaneshige[1], **Masashi Fujii**[1,2], Fumio Hayashi[3], Kenichi Morigaki[4], Hayato Yamashita[5], Akinori Awazu[1,2] ([1]*Dept. Math. Sci., Grad. Sch. Sci., Hiroshima Univ.*, [2]*Dept. Math. Sci., Grad. Integ. Sci. Life, Hiroshima Univ.*, [3]*Grad. Sch. Sci., Kobe Univ.*, [4]*Biosignal Research Center, Kobe Univ.*, [5]*Grad. Sch. Eng. Sci., Osaka Univ.*)

20565U Attempts at CA-type formal analysis of fibrous assembly of particles
Takashi Konno (*Math. Biol. Med. Univ. Fukui*)

20566U Formation of small G-protein Ras multimer induced by chemical modification of HVR domain
Rufiat Nahar[1], Maruta Shinsaku[2] ([1]*NAHAR RUFIAT*, [2]*SHINSAKU MARUTA*)

20567U 模型飛行機の主翼長が滑空性能に与える影響
The Effect of Wing Length on Gliding Performance of Model Airplanes
Fumiya Yamanaka (*Osaka Pref. Tondabayashi H.S.*)

20568U 円環気流接合殺菌法によるウイルス感染ルートの遮断
Blocking virus infection routes by CARS-sterilizattion
Kuniaki Nagayama[1], Ryoichi Matsuda[2] ([1]*N-EM Labs.*, [2]*Grad. Sch. Sci., Tokyo Univ. Sci.*)

20569U* Self-Assembly of Flexible DNA Ring Motif
Shiyun Liu[1], Ibuki Kawamata[1,2], Satoshi Murata[1] ([1]*Grad. Sch. Eng., Univ. Tohoku*, [2]*Div. Natural Sci. Fac. Core Research, Univ. Ochanomuzu*)

20570U 分子スウォームの自動制御のための DNA 反応回路の最適化
Optimization of the molecular circuit for automatic controlling movement of microtubules
Daiki Matsumoto[1], Ibuki Kawamata[1], Yuki Suzuki[1,2], Satoshi Murata[1], Jakia Jannat Keya[3], Akira Kakugo[3], Shin-ichiro Nomura[1] ([1]*Department of Robotics, Graduate School of Engineering, Tohoku University, Japan*, [2]*Creative Interdisciplinary Research Division,Frontier Research Institute for Interdisciplinary Sciences,Tohoku University*, [3]*Department of Chemistry, Faculty of Science, Hokkaio University*)

20571U 機械学習を用いた生物形態の定量化とその応用
Characterization of biological morphology by using machine learning
Masato Tsutsumi[1], Nen Saito[1,2], Chikara Furusawa[1,2,3] ([1]*Dept. of Physics,Grad School of Science, The Univ. of Tokyo*, [2]*Universal Biology Institute, The Univ. of Tokyo*, [3]*Center for Biosystems Dynamics Research, RIKEN*)

20572U Circularization in coding regions of Flaviviruses are crucial for viral fitness
Roland G. Huber (*A*STAR BII*)

1S-P-1 ソフトマター物理と大沢
Contribution of Fumio Oosawa to Soft Matter Physics

Kazue Kurihara (*NICHe, Tohoku Univ.*)

When Fumio Oosawa completed his Ph.D. under Masao Kotani, he hoped to do non-orthodox physics, and studied the sedimentation of soil dispersions at Nagoya University with Naomi Miyabe, who was a student of Torahiko Terada. This paper reviews his major early achievements including “depletion force” (A-O) theory (J. Chem. Phys., 1954) which treats the attraction between particles dispersed in a polymer solution due to lower osmotic pressure between them than in bulk; and a counterion condensation model summarized in his famous monograph “Polyelectrolytes” (Marcel Dekker, 1971). The first, one page, paper on the depletion theory was not noticed for 30 years after published, but now has the record of more than 2000 citations. We appreciate his contributions to soft matter physics based on his deep understanding of statistical mechanics and broad interests in nature (a detailed abstract is in news of my homepage).

1S-P-2 Asakura-Oosawa 理論とその広がり
Variations on a Theory by Asakura and Oosawa

Ryo Akiyama (*Department of Chemistry, Kyushu University*)

Depletion interactions between colloidal particles are well known in various fields, such as soft matter. The effective interaction was proposed by Asakura and Oosawa in 1954. I met their theory in a lecture given by Prof. Lekkerkerker at Cornell University. It was March 2001. So, my first acquaintance with the theory was very late. However, it was impressive because the freshness was kept in the theory. The sense of theory is fascinating still now. The secret of the freshness lies in the simple logic with the surprising conclusion. According to the theory the “ordered” structure appears due to the entropy increase. The grasp of this paradoxical conclusion is not easy intuitively. Thus it has made interesting variations. We will discuss them in the presentation.

1S-P-3 生物運動の仕組みを解く：大沢さんから学んだもの
Unraveling the Mechanism of Biological Movement: What I Learned from Oosawa-san

Shin'ichi Ishiwata (*Waseda University, Faculty of Science and Engineering, Department of Physics*)

I will discuss what I learned from Oosawa-san, especially the mechanism of actin polymerization (Kondo & Ishiwata, 1976) and the flexibility of F-actin (Ishiwata & Fujime, 1972). Later, we demonstrated the treadmill process of actin polymerization by single-molecule imaging, and succeeded in selective reconstruction of thin (actin) filaments in striated muscle (Funatsu et al., 1994; Fujita et al., 1996). Moreover, I will introduce the model for regulatory mechanism of muscle (Ishiwata & Oosawa, 1974), spontaneous oscillatory contraction (SPOC) of muscle (Ishiwata et al., 2017), supercoiling of F-actin, and the formation of contractile rings (Miyazaki et al., 2015) and the positioning of the actin ring in artificial cell systems (Sakamoto et al., 2020) and so forth.

1S-P-4 アクチン ATP 加水分解反応のメカニズム：ATPase 蛋白質の共通性と独自性
Reaction mechanism of actin ATP hydrolysis: as compared with other ATP hydrolysis proteins

Yuichiro Maeda (*Nagoya University, Graduate School of Informatics*)

We have obtained crystal structures of F-form actin in AMPPNP- ADP-Pi- and ADP-bound forms, all at 1.15A resolutions. Based on these structures, the reaction path of actin ATP hydrolysis has been identified, which is identical to those of P-loop motor proteins like myosin. On the other hand, the active site protein structure of actin is distinct to those of P-loop proteins: in actin, the nucleotides are stabilized by P1- and P2-loop, instead of P-loop, while Sw-1 and -2 are missing. The simplified structure of actin likely represents the common hydrolysis mechanism, and reflects the lack of conformational change upon Pi-release. In the P-loop ATPase protein, Sw-1 and -2 perform protein-specific mechanism driving the Pi-release with protein conformational changes.

1S-P-5 筋収縮とイオン能動輸送
Muscle contraction and ion active transport

Tsutomu Kouyama (*Nagoya Univ. Graduate School of Science*)

How high is the energy conversion efficiency of muscle contraction? Is it higher than the energy conversion efficiency of a car engine? Similar questions also arise when discussing active ion transport at the cell membrane. These bioenergy conversion systems have a common feature in that unidirectional movements of substances are coupled with cyclic chemical reactions. Comparison of these systems will uncover the fundamental characteristics of biomolecular machines. After investigating these systems, F. Oosawa proposed a loose-coupling theory in which the ratio between input and output is supposed to vary depending on the environmental condition. To deal with this theory, we will investigate structural data of reaction states of ion-pumping rhodopsins.

1S-P-6 揺らぎと生命機能
Fluctuation and the function of life

Toshio Yanagida[1,2] ([1]*Osaka University Graduate school of Frontier Biosciences*, [2]*NICT CiNet*)

In recent years, single molecule imaging and nano-technologies have rapidly been expanding to include a wide range of life science applications. The dynamic properties of biomolecules and the unique operations of molecular machines, which were previously hidden in averaged ensemble measurements, are now being unveiled. The aim of our research is to approach the engineering principle of adaptive biological systems by uncovering the unique operation of biological molecular machines. Here, I review our single molecule experiments designed to investigate molecular motors and discuss how thermal fluctuations (noise) play a positive role in the unique operation of biological molecular machines allowing for flexible and adaptive biological systems including cell and brain.

1S-P-7 アクチン重合の熱力学測定～ギブスの平行論に沿って～
Thermodynamic quantities of actin polymerization ~along Gibbs' equilibrium theory~

Mahito Kikumoto[1], Fumio Oosawa[2,3] ([1]*NaritaG, Bio., Sci., Nagoya-u.*, [2]*Prof.Emertis,Nagoya/Osaka-u.*, [3]*Deceised*)

We estimated thermodynamic quantities of actin polymerization to measure the critical concentration polymerized by different cation.

1S-P-8 筋収縮とその制御におけるアクチン繊維の構造と役割
Actin filament in muscle contraction and regulation

Keiichi Namba[1,2,3] ([1]*Graduate School of Frontier Biosciences, Osaka University*, [2]*RIKEN Center for Biosystems Dynamics Research and Spring-8 Center*, [3]*JEOL YOKOGUSHI Research Alliance Laboratories, Osaka University*)

Actin is ubiquitous in all eukaryotic cells and is one of the major components of cytoskeleton. It forms a highly well-conserved double-stranded helical polymer called actin filament, which plays a major role in muscle contraction by cyclic interaction with myosin driven by its ATP hydrolysis and also in the Ca2+ regulation of striated muscle contraction together with troponin and tropomyosin bound on the surface of the filament. Actin was the first biological system Prof. Oosawa started working on after studying colloids and polyelectrolytes for some years in his early scientific career. I was introduced to the system by his stimulating lecture series for an undergraduate class at Osaka University and have been studying the structure and dynamics since then.

1S-1-1 Protein dynamics structures revealed by time-resolved serial femtosecond crystallography

Eriko Nango[1,2] ([1]*IMRAM, Tohoku Univ.*, [2]*RIKEN RSC*)

Serial femtosecond crystallography (SFX) is a technique for the determination of a room-temperature protein structure by collecting diffraction images from randomly oriented microcrystals using X-ray free electron lasers. The combination of SFX and the pump-probe method using a visible light pulse laser enables the visualization of structural dynamics and reactions in light-sensitive proteins as a molecular movie with a high spatial and temporal resolution. Furthermore, mix-and-inject SFX allows for the capture of enzymatic reactions via the rapid mixing of protein crystals with a substrate solution. Thus, we have developed techniques and devices for time-resolved SFX. In this symposium, our latest results will be presented.

1S-1-2 分子動画に基づく量子分子動力学シミュレーションによるバクテリオロドプシンにおけるプロトン移動の微視的機構の解明
Microscopic mechanisms of proton transfers in bacteriorhodopsin revealed by quantum molecular dynamics method based on molecular movies

Junichi Ono[1,2] ([1]*C-PIER, Kyoto Univ.*, [2]*WISE, Waseda Univ.*)

Bacteriorhodopsin (BR) is a prototype of light-driven proton pumps, in which the vectorial proton translocation across the membrane achieved by five proton transfer reactions results in light-energy conversion. Although a great deal of effort has been devoted, the microscopic mechanisms of the proton transfers in BR have not been completely understood. In this study, large-scale quantum molecular dynamics simulations combined with the enhanced sampling method, in which the system including BR, lipid membranes, and water solvent is treated quantum-mechanically, were performed with the aid of the molecular movie of BR captured by X-ray free electron laser (XFEL). Here, the detailed analyses for the primary, secondary, and tertiary proton transfers in BR will be discussed.

1S-1-3 分子シミュレーションによるタンパク質の機能活性化過程の原子論的解明
Atomistically Deciphering Functional Activation Processes of Proteins with Molecular Simulations

Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

Functional processes of proteins are often fulfilled by their dynamic molecular conformational changes which correlate with local chemical events at reaction centers. In this talk, I will present our recent studies on photo-activation processes of channelrhodopsin and redox processes of photosystem II by a hybrid QM/MM free energy geometry optimization technique, which combines ab initio QM calculations for the chemical reaction at the active sites with long-time MD simulations for the protein global dynamics. I will also present an atomistic MD study of alternating access of mitochondria ADP/ATP transporter with a linear response path following method, which has been shown to successfully predict at atomic resolution an X-ray crystallographic one reported later.

1S-1-4 Observation of protein dynamics with solution scattering

Masaaki Sugiyama, Rintaro Inoue (*Kyoto University*)

Multi-domain protein has an inter-domain dynamics, meaning that the inter-domain configuration is fluctuating. Time scale of this dynamics is supposed to be in nano-micro second. Therefore, to observe this slow dynamics is rather difficult because the required energy resolution is relatively high. The, we adopted two strategies to observe the slow dynamics: one is to derive information of domain dynamics from SAXS and SANS data by using computer simulation techniques and the other is directly to observe such dynamics with high resolution neutron scattering method, named Neutron Spin Echo (NSE). In this presentation, we will show our typical results concerned about two approaches.

1S-1-5 SPring-8 におけるシリアル放射光結晶解析法の開発
Develpment of serial synchrotron crystallography at SPring-8

Takashi Kumasaka (*Prot. Cryst. Anal. Div., Jpn. Sync. Rad. Res. Inst.*)

The serial femtosecond crystallography (SFX) developed at XFELs opened a new paradigm for MX data collection and successfully applied to the time-resolved (TR) analysis. Its success has led to establish synchrotron serial crystallography (SSX) by combining a high-flux microbeam and a fast-readout detector. And then SSX is going to evolve to TR-SSX. At SPring-8, we are also developing an room-temperature SSX combined with our original sample ambient control method, HAG. We hope this development will finally expand crystallographic TR method to analyze longer time-course systems over milliseconds and it will totally achieve wide-range time resolutions in TR serial crystallography at SPring-8 and SACLA. In this presentation we will show its current status.

1S-1-6 SACLA を用いたチャネルロドプシンの時分割構造解析によって明らかになったイオン透過経路形成の初期構造変化
Time-resolved serial femtosecond crystallography reveals early structural changes in channelrhodopsin

Tomohiro Nishizawa (*The Univ. of Tokyo*)

Channelrhodopsins (ChRs) are microbial light-gated ion channels utilized in optogenetics to control neural activity by light illumination. Light absorption causes retinal chromophore isomerization and subsequent protein conformational changes visualized as optically distinguished intermediates, coupled to channel opening and closing. However, the detailed molecular events underlying channel gating remain unknown. We performed time-resolved serial-femtosecond crystallographic analyses of channelrhodopsin by using an X-ray free electron laser and revealed early conformational changes around the chromophore retinal, which are likely to be triggers that lead to the ion pore opening.

1S-2-1 Native mass spectrometry for Bio-Metal Science

Satoko Akashi (*Grad. Sch. Med. Life Science, Yokohama City Univ.*)

Native mass spectrometry (Native MS) enables accurate determination of the binding state of metals to biomolecules, because the samples can be mildly ionized and detected without dissociation even in the gas phase. With these characteristics, Native MS has been utilized to determine the molecular mass of intact metal-bound proteins and to analyze their biophysical properties. In this paper, recent advancement of application of Native MS to protein complexes will be demonstrated and discussed.

1S-2-2 X-ray Crystallography and EPR Spectroscopy Reveal Active Site Rearrangement of Cold-Adapted Inorganic Pyrophosphatase

Masaki Horitani[1], Hiroshi Sugimoto[2], Keiichi Watanabe[1] ([1]*Saga Univ., Dept of Appl Biochem & Food Sci*, [2]*RIKEN, SPring-8 Center*)

Inorganic pyrophosphatase (PPase) catalyses the hydrolysis reaction of inorganic pyrophosphate to phosphates. Our previous studies showed that manganese activated PPase from the psychrophilic bacterium *Shewanella* sp. AS-11 (Sh-PPase) has a characteristic temperature dependence of the activity with an optimum at 5℃. Its molecular mechanism, however, has not been elucidated due to lack of structural information. Here we report the structural analyses of Sh-PPase with and without substrate by X-ray crystallography and EPR spectroscopy combined with rapid freeze-quench. The results demonstrated that Sh-PPase has the ability of unique active site rearrangement by bound of substrate. Thus, we propose that this ability plays an important role in the cold adaptation mechanism.

1S-2-3 Exploiting paramagnetic metal ions for protein structural study in solution

Tomohide Saio, Koichiro Ishimori (*Faculty of Science, Hokkaido University*)

Paramagnetic metal ions can be exploited in protein structural study by solution NMR. Long-reach (< ~40 Å) paramagnetic effects provide location information of the observed nuclei with respect to the paramagnetic center. We here demonstrate structural study of a multi-domain protein enzyme in solution by paramagnetic NMR. We show that paramagnetic lanthanide ion fixed in one of the domains induces significant paramagnetic effects that provide detailed view of the conformational states of the protein and detect conformational changes induced by the ligand binding. In addition to NMR, our recent approaches exploiting EPR with the paramagnetic lanthanide ion will also be discussed.

1S-2-4 複数の異なる NMR データの統合解析によるタンパク質 multi-state 立体構造解析
Multi-state protein structure determination by integrated analysis of several NMR data sets

Teppei Ikeya, Yutaka Ito (*Graduate School of Science, Tokyo Metropolitan University*)

Considering that protein dynamics is substantially sensitive against surrounding environments, it is indispensable to study their 3D structures near-physiological conditions. Solution NMR is currently only the technique to investigate the dynamics and conformations of biomacromolecules in the natural condition or even in living cells. To date, various NMR measurements using paramagnetic effects and magnetic anisotropy have been developed, allowing to extract more accurate structural ensemble information. We recently developed a method to determine multi-conformations of proteins by integrating these NMR data. Here, we show the multi-state structure determinations with model proteins and discuss further applications such as protein structure determination in cells.

1S-2-5 核共鳴振動分光法による鉄含有酵素の元素選択的測定 -世界最強強度の放射光源を利用した最近の進展-
Atom-selective measurement of iron enzymes by nuclear resonance vibrational spectroscopy

Yoshitaka Yoda (*Japan Synchrotron Radiation Research Institute*)

Nuclear resonance vibrational spectroscopy, which is called NRVS, is a novel technique using synchrotron radiation to investigate the atomic vibration in molecules. Vibration modes of the specific atom can be selectively excited via the nuclear level. It gives quite different and complementary information from that taken by Raman or IR spectroscopy. Therefore it has been intensively used to see the active center of the metalloenzyme by Prof. Cramer and other research groups. I will introduce the recent progress and activities using the long undulator beamline BL19LXU at SPring-8 that produce the world's highest intensity X-ray.

1S-2-6 量子ビームによる細胞内生命金属動態
Application of quantum beam elemental analyses for dynamics of cellular distribution of bio-metals

Shino Homma-Takeda (*National Institutes for Quantum and Radiological Sciences*)

A tactics for analyzing elemental distribution, localization, and chemical state without destroying tissue structure or cell arrangement is required for understanding cellular dynamics of bio-metals. In the present symposium, the studies for the elemental characteristics and formation mechanism of localized and concentrated bio-metals in tissues by combination of pathological observation and in situ elemental analyses, such as PIXE (particle induced X-ray emission), SR- XRF (X-ray fluorescence spectrometry using high energy synchrotron radiation) or XAFS (X-ray absorption fine structure) will be introduced.

2S-1-1 Thermodynamic inequalities and applications to biological systems

Andreas Dechant, Shin-ichi Sasa (*Grad. Sch. Sci., Kyoto U.*)

This talk gives an introduction to and overview of thermodynamic inequalities. These inequalities are universal relations between different physical observables. On the one hand, they provide constraints that every physical system must obey, limiting for example the power output of molecular motors. On the other hand, thermodynamic inequalties can offer a way to estimate quantities like entropy production, which are often difficult to measure directly, by using measurable quantities. We will illustrate how such inequalities arise from information-theoretic bounds and provide some suggestions how they might be applied to biological systems.

2S-1-2 ERK MAPK 活性化の熱力学コストを定量化する情報幾何学的手法
Information-geometric method to quantify the thermodynamic cost of ERK MAPK activation

Keita Ashida[1], Kazuhiro Aoki[2], **Sosuke Ito**[1,3] ([1]*Universal Biology Institute, the University of Tokyo*, [2]*Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences*, [3]*JST PRESTO*)

The relationships between information theory and thermodynamics have been intensively studied over the past few years, and their relationships would provide promising methods to analyze biological systems. In our recent study, we propose an information-geometric method to quantify thermodynamic cost of the speed and the fluctuation in the biochemical reactions. We here focus on an excitable system, i.e., the ERK MAPK pathway in mammalian cells. We have previously shown that ERK exhibits stochastic and pulsatile activation dynamics, and that an increase in the frequency of ERK activation pulse leads to the increase in cell proliferation rate. In this symposium, we will discuss an application of our information-geometric method to the dynamics of ERK activity.

2S-1-3 高密度バクテリア集団研究のための広域マイクロ灌流系と、それによる細胞集団の統計物理学・情報物理学実験の試み
Extensive microperfusion system for dense bacterial populations and its applications for statistical physics of cells with information

Kazumasa A. Takeuchi (*Dept. Physics, Univ. Tokyo*)

To explore information physics of cell populations, it is useful to have an experimental device that can culture dense cell populations under uniform and controlled conditions. Here we develop such a microfluidic device, named the extensive microperfusion system (EMPS), in which cells can be confined in a large region and uniformly supplied with fresh medium through a porous membrane. In the talk, I will first show the outline of EMPS and results of performance evaluation, then present a few attempts we undertake to seek for statistical physics and information physics of bacterial populations. The latter include scaling properties of cell size fluctuations and crowding of motile bacterial populations.

2S-1-4 バクテリア走化性の情報物理学
Information Physics of Bacterial Chemotaxis

Tetsuya Kobayashi[1,2], Kento Nakamura[2] ([1]*Institute of Industrial Science, the University of Tokyo*, [2]*Department of Mathematical Informatics, Graduate School of Information Science and Technology, the University of Tokyo*)

Chemotaxis of bacteria is the simplest biological information processing system. The chemotactic network has been intensively studied both biophysical and information-theoretically. Even with the accumulation of research on two aspects, a link between these two aspects of chemotaxis, in other words, the information physics of chemotaxis, has not yet been established. In this work, we link these two approaches by showing that a standard biochemical model of the chemotactic network is mathematically identical to an information-theoretically optimal dynamics and reproduces experimental response relation. These results suggest that the biochemical network of bacterial chemotaxis has been designed, in the process of evolution, so as to optimally obtain gradient information.

2S-1-5 アクティブマター系でのレヴィ・フライトのミクロ導出
Microscopic theory for Levy flights in active suspension

Kiyoshi Kanazawa (*Faculty of Engineering, Information and Systems, University of Tsukuba*)

The Levy flights model is one of the most important classes for anomalous diffusion in nonequilibrium statistical physics. In this presentation, we will report a microscopic theory to derive the Levy-flights dynamics in an active matter system by extending the kinetic theory based on our recent article (K. Kanazawa et al. Nature 579, 364 (2020)). We start from a microscopic setup composed of a tracer particle and active swimmers (such as Chlamydomonas). The tracer dynamics is shown to obey the colored Poisson process, by studying the swimmer-tracer interactions. This model finally exhibits the Levy flights at a longer timescale. This work provides the first theoretical derivation of the Levy flights from microscopic physical dynamics by appropriate coarse-graining.

2S-1-6 Condensed matter concepts in collective cell dynamics

Kyogo Kawaguchi[1,2,3] ([1]*RIKEN CPR*, [2]*RIKEN BDR*, [3]*UBI, Univ. Tokyo*)

Collective dynamics of molecular motors, bacteria, and mammalian cells have been studied under the name of active matter physics. Recent progress both in theory and experiments have further clarified how concepts of nonequilibrium many-body physics can emerge from biological examples. Here we introduce several examples of these developments, such as active topological nematics and quantum active matter, through experiments using cells and theory involving non-Hermitian physics.

2S-2-1 Optogenetic control of intracellulary expressed functional antibodies

Fuun Kawano[1,2] ([1]*The University of Tokyo*, [2]*JST PRESTO*)

Optogenetics is a useful technology for controlling the activity and localization of proteins of interest with high spatiotemporal accuracy. However, optogenetic control of endogenous proteins remains unsolved so far, because existing tools require direct fusion of photoreceptors to the target protein. Here we develop photoactivatable antibodies based on the modifications of the dimer interface between the heavy and light chains and effective fusing with a LOV domain. By using a translocation assay, we found that the antibodies can quickly and reversibly recover the antigen-binding ability in a light-dependent manner. This technology will facilitate optogenetic applications for targeting not only endogenous proteins but also nucleic acids and lipids in living cells.

2S-2-2 オプトメカニカル画像走査による高速ライトシート顕微鏡
High-speed light-sheet microscopy using optomechanical image scanning

Hideharu Mikami[1,2,3] ([1]*RIES, Hokkaido Univ.*, [2]*Sc. Sci., UTokyo*, [3]*PRESTO, JST*)

We propose and demonstrate light-sheet microscopy using optomechanical image scanning that enables volumetric imaging at unprecedentedly high volume rates of >1,000 volumes/sec. In our method, multiple 2D images at different depth positions are simultaneously captured by a single-frame readout of a CMOS camera, allowing for volumetric image acquisition by a single-frame 2D image. As a proof-of-concept demonstration, we obtained volumetric images of neurons of Caenorhabditis elegans that express Yellow Cameleon 2.60 at a volume rate of 60 volumes/sec, demonstrating the increase of the volume rate by a factor of ~10.

2S-2-3 フェムト秒レーザー誘起衝撃力による細胞操作とその物理
Single cell manipulations utilizing femtosecond laser impulse and the physics

Yoichiroh Hosokawa (*Divison of Materials Science, Nara Institute of Science and Technology*)

The 2018 Nobel Prize in Physics recognized wide applications of femtosecond laser amplifier that have been made to cell and tissue manipulations. Nowadays, the femtosecond laser amplifier is one of key tool in ophthalmology, biology, and basic medicine. We have developed several kinds of cell manipulation methodologies utilizing the femtosecond laser amplifier and optical microscope. In this presentation, we introduce single cell manipulations utilizing impulse phenomena occurring with the intense pulse irradiation and the underlying physics. [Ref] Y. Hosokawa "(Invited Review) Applications of the femtosecond laser-induced impulse to cell research," Jpn. J. Appl. Phys. 58, 110102 (2019).

2S-2-4 Optogenetic control of phospholipids flipping and related biomembrane functions in budding yeast

Tomomi Suzuki[1,2], Tetsuo Mioka[3], Kazuma Tanaka[3], Akira Nagatani[1] ([1]*Grad. Sch. Sci, Kyoto Univ.*, [2]*JST, PRESTO*, [3]*Genetic Medicine Inst., Hokkaido Univ.*)

Lipid asymmetry across membranes play a crucial role in many cell functions, such as vesicular transport, cell signaling and the immune response. Asymmetry of phospholipids in membranes is established and maintained by lipid translocase. We therefore focused on the optical manipulation of the lipid asymmetry, choosing lipid translocase, flippase, as an optogenetic target. Flippase is widely conserved in eukaryotes. We investigated whether the activity of flippase in budding yeast could be photoregulated using the *Chlamydomonas* blue-light receptor, phototropin. As a result, we succeeded in photo-controlling lipids uptake and related biomembrane functions. At the symposium, we will present these results in detail and discuss the usefulness of this system.

2S-2-5 植物の高速シグナル伝達を視る
Shining light on rapid signal transduction in plants

Masatsugu Toyota (*Dept. Biochem. & Mol. Biol., Saitama Univ.*)

Plants do not possess the nerves and muscles that make rapid movements in most animals. However, several plant species such as Mimosa pudica can fold and move their leaves quickly in response to various mechanical stimuli. Here, by using a highly-sensitive simultaneous recording system of cytosolic calcium and electrical signals, we show that long-distance calcium transmission coupled with the action potential triggers rapid movements in Mimosa. Furthermore, pharmacological manipulation of the cytosolic calcium dynamics and CRISPR-Cas9 genome editing technology revealed that an immotile Mimosa is more susceptible to insect attacks. Our findings provide an evidence that calcium-based electrical movements protect the plants from herbivory.

2S-2-6 光による不随意運動疾患根治法
Optogenetic neuromodulation for movement disorders

Fumiaki Yoshida (*Saga Univ.Med.Sch.*)

Pathological brain oscillatory activity has been found in movement disorders such as Parkinson disease. Clinical evidence coupled with experimental work, has led to the hypothesis that pathological oscillation may have a causal role, by dynamically disrupting the transmission of information through the brain. Deep brain stimulation is an effective treatment for these diseases, but can be made more effective by using optogenetic techniques. Optogenetics allows for cell-type specific manipulation which can avoid causing side effects through unwanted propagation of the stimulation. In this talk I will propose the use of the pathological oscillation as a biomarker and optogenetics as a neuromodulation method, with the aim of translating insights to neuropsychiatric therapy.

2S-3-1 角化細胞の増殖の接触阻害には接着結合の引張力が必須である
Tensile force at adherens junctions is responsible for contact inhibition of keratinocyte proliferation

Hiroaki Hirata, Oleg Dobrokhotov, Masahiro Sokabe (*Grad. Sch. Med., Nagoya Univ.*)

Confluence-dependent inhibition of cell proliferation, termed 'contact inhibition', is crucial for tissue homeostasis; loss of contact inhibition is a hallmark of cancer cells. While the actomyosin cable is connected to the cell-cell adhesion structure, adherens junction (AJ), we have found that actomyosin-based tensile force at AJs is required for inhibition of cell proliferation in confluent keratinocytes. Compared with normal keratinocytes, keratinocyte carcinoma cells have much lower actomyosin activity. Applying exogenous tensile force to AJs of keratinocyte carcinoma cells can attenuate their proliferation. Our results show that tensile force at AJs acts as an anti-proliferative factor and may provide a novel therapeutic target for keratinocyte carcinoma.

2S-3-2 細胞間シグナル–上皮リモデリングのフィードバックループが制御する神経管閉鎖ジッパリング
Dynamic integration of signaling, force generation and tissue remodeling control zippering and neural tube closure

Hidehiko Hashimoto[1], Francois Robin[2], Kristin Sherrard[1], Edwin Munro[1] ([1]*University of Chicago*, [2]*Sorbonne University*)

We use zippering during neural tube closure in the simple chordate Ciona robusta to study how dynamic coupling of signaling and force generation patterns collective cell movements. Combining quantitative microscopy, biophysical manipulations and modeling, we show that two overlapping patterns of actomyosin contractility underlie zipper progression; Sequential and rapid contractions just ahead of the zipper provide the "powerstroke", while tissue level contractile asymmetry converts this symmetrical powerstroke into unidirectional zipper progression. Both patterns are controlled by local signaling across cell-cell contacts. Local signals and dynamic remodeling of tissue contacts are coupled through tissue-level feedback loops to drive unidirectional zipper progression.

2S-3-3 Strain-triggered mechanical feedback in self-organizing epithelial morphogenesis

Satoru Okuda (*Nano Life Science Institute, Kanazawa University*)

Organogenesis is a self-organizing process of multiple cells in three-dimensional (3D) space. While the robust regulation of multicellular dynamics requires feedback from tissue deformations to cellular force generations, however, it is still unclear how individual cells sense 3D tissue deformations during morphogenesis. To address this issue, we carried out computational simulations using a 3D vertex model as well as mechanical and biochemical assays of stem cell-derived optic cup organoids. As a results, we revealed the crucial role of mechanical force in signaling between distant cells to trigger their next-step behaviors in the sequential tissue deformations.

2S-3-4 Cell dynamics under high hydrostatic pressure conditions

Masatoshi Morimatsu[1], Masayoshi Nishiyama[2], Keiji Naruse[1] ([1]*Grad. Sch. of Med., Dent. and Pharma. Sci., Okayama Univ.*, [2]*Department of Physics, Kindai Univ.*)

Periodontal ligament (PDL) and articular cartilage are always exposed to mechanical stress such as occlusion and walking. However, the effect of pressure on cells at a molecular level is poorly understood due to the lack of methods that directly observe cell motility under high pressure condition. Here we used hydrostatic pressure system to apply mechanical stress to cells in vitro and investigated cell morphology, molecules, and gene expression levels under mechanical stress conditions. We observe some transcription factors translocate to nucleus from cytosol under the high pressure condition. Our systems directly show translocation of transcription factor and give us new pressure-sensing mechanism.

2S-3-5 Mechanical stress by extracellular confinement trigger a mode transition of neuronal migration

Naotaka Nakazawa[1], Gianluca Grenci[2], Mineko Kengaku[1,3] ([1]*iCeMS, Kyoto University*, [2]*Mechanobiology Institute, National University of Singapore*, [3]*Graduate School of Biostudies, Kyoto University*)

The migration of newly born neurons in the crowded neural tissue is a critical step during brain development. In the cerebellar granule cells on a flat surface, F-actin and Myosin II localize at the nuclear front and generate traction force for nuclear translocation during their migration. In contrast, previous studies using other neurons have shown the accumulation of F-actin and Myosin II at the nuclear rear during migration in 3D environment. Unlike the previous view that the distinct cell types adopt differential mechanisms of nuclear translocation, our preliminary data suggest that cerebellar granule cells switch nuclear translocation modes by activating actomyosin in distinct subcellular compartments in response to mechanical stress in opened and confined spaces.

2S-3-6 リンパ管の弁の形成における Piezo1 を介した空間的に規定されたメカノトランスダクション
Spatially defined mechanotransduction via Piezo1 involved in lymphatic valve formation

Keiko Nonomura[1], Hiroki Katsuta[2], Akemi Kanie[1], Ardem Patapoutian[3], Toshihiko Fujimori[1] ([1]*National Institute for Basic Biology*, [2]*Nagoya Univ. Grad. Sch. Med.*, [3]*The Scripps Institute*)

Our team has been studying contribution of mechanotransduction to tissue formation and/or function, by focusing on Piezo1/2 mechanosensor channels and analyzing KO mouse lines. When Piezo1 was deleted in endothelial cells, it resulted in reduction of lymphatic/venous valves, the essential structure for proper circulation of lymph/blood. In order to further investigate Piezo1-mediated mechanotransduction during valve formation, we have conducted live imaging analysis of intracellular Ca2+ in the lymphatic vessels, as Piezo1 activation results in its upregulation. In this talk, I would like to introduce our latest data about spatially defined mechanotransduction via Piezo1 connecting mechanical force and tissue morphogenesis.

2S-4-1 Molecular mechanisms that regulate secretion of sonic hedgehog

Yusong Guo (*Division of Life Science, Hong Kong University of Science and Technology*)

Sonic Hedgehog (Shh) is an important signaling molecule that regulates various developmental processes in metazoan. Although significant progress has been achieved in understanding the signal transduction pathways activated by Shh, it remains largely unclear how newly synthesized Shh is secreted from the Shh-producing cells. We identified specific cellular factors that recognize a specific sorting motif in Shh to regulate export of Shh out of the endoplasmic reticulum (ER) and out of the trans Golgi network (TGN) in the secretory transport pathway. Our results reveal clear mechanistic insight into the trafficking machinery that regulates secretion of Shh. The novel protein interactions that are critical for secretion of Shh will provide new drug targets to downregulate the Hedgehog signaling transduction pathway.

2S-4-2 自己組織化による細胞極性形成の 1 分子粒度シミュレーション
Self-organization in cellular polarity signaling reconstituted by single-molecule-imaging based single-particle simulation

Satomi Matsuoka[1,2,3], Masahiro Ueda[1,2] ([1]*Grad. Sch. Frontier Biosciences, Osaka Univ.*, [2]*BDR, RIKEN*, [3]*PRESTO, JST*)

Cell membrane provides a milieu where signaling molecules generate spatial asymmetry to polarize eukaryotic motile cells. A domain spontaneously arises on the membrane where the active Ras level is elevated due to an excitability and leads to an elevation of the PtdIns(3,4,5)P_3 level though PI3K, which is counteracted by PTEN. Single-molecule imaging reveals stochastic behavior of these molecules, and statistical analysis offers an estimation of the reaction rates and diffusion coefficients. Using these parameters, we have succeeded in reconstituting the self-organization dynamics *in silico* by single-particle simulation, illustrating that feedback regulation of these enzymes by membrane lipids underlies the cooperativity among the stochastically operating molecules.

2S-4-3 Towards the mechanism of mitochondrial outer membrane fusion

Song Gao (*Sun Yat-sen University Cancer Center*)

Mitochondria are double-membrane organelles that constantly undergo fusion and fission. Fusion is pivotal to the health and functioning of mitochondria, and defects in fusion cause several human diseases. In mammals, mitochondrial outer membrane fusion is mediated by MFN1 and MFN2, which belong to the dynamin superfamily of large GTPases. We determined crystal structures of truncated MFN1 and MFN2, and elucidated their features in oligomerization and conformational changes at different stages of GTP hydrolysis. These data allow us to analyze the difference and cooperation between MFN1 and MFN2, and pave the way for the understanding the biological process of mitochondrial fusion.

2S-4-4 1分子イメージングによる生細胞膜中のGPCRシグナロソーム計測
Single-molecule imaging of GPCR signalosome in living cell membrane

Masataka Yanagawa (*Cellular Informatics Lab., Riken*)

G protein-coupled receptors (GPCRs) act as a signaling hub through G proteins and arrestins upon ligand binding. Biased ligands with pathway-selective activity have attracted much attention as drugs with lower side effects. However, it is yet to be clear how the multiple signaling pathways of GPCR are spatial-temporally regulated in living cell membrane. Here, we show a novel signalosome that regulates the signal-bias of the angiotensin signaling by AT1R, a class A GPCR. The NanoBiT assays and BRET imaging revealed the AT1R/G protein/GRK preassembly complex in living cell membrane. The dual color single-molecule imaging analysis suggested that the preassembly complex regulates the signal bias in a confined region of the plasma membrane.

2S-4-5 A proximity labeling method to resolve membrane protein interaction networks

Min Zhuang (*School of Life Science and Technology, ShanghaiTech University*)

The communication between cells and the communication between cellular organelles are often controlled by the interaction of membrane proteins. Despite of many methods to identify protein-protein interactions (PPIs), there are still challenges in detecting membrane PPIs. We have developed a proximity tagging method to facilitate the identification of weak and transient membrane protein-protein interactions in living cells. In general, a fused ligase catalyzes the covalent linkage between the tag and target proteins, thus the tagged proteins can be enriched for mass spectrometry-based identification. This approach has been applied to several plasma membrane proteins as well as organelle membrane proteins to map the interaction networks.

2S-4-6 1分子イメージングで明らかになったラフト組織化と機能
Raft organization and function as revealed by single-molecule imaging

Kenichi Suzuki[1,2] ([1]*G-CHAIN, Gifu Univ.*, [2]*Tokai National Higher Education System, iGCORE*)

Raft domains have been drawing extensive attention as signaling platforms. However, raft structure and function are still enigmatic. Here, we developed fluorescent probes of representative raft lipids, sphingomyelin, ceramide and 32 kinds of glycosphingolipids, which behave like the parental molecules. Single-molecule imaging showed that all of the observed ganglioside probes continually formed transient homodimers based on glycan-glycan interactions, which were stabilized by raft-lipid interactions. Furthermore, we found that GM3 homodimers interacted with EGFRs, which resulted in inhibition of EGFR activation. The transient ganglioside homodimers are likely one of the basic units for the organization and function of rafts.

2S-4-7 Fusion of the inner mitochondrial membrane

Junjie Hu (*Institute of Biophysics, CAS*)

The fusion of inner mitochondrial membranes is mediated by dynamin-like GTPases OPA1/Mgm1. Here, we determined the crystal structure of the short form Mgm1 (s-Mgm1) in complex with GDP. The structure reveals an N-terminal GTPase (G) domain followed by two sets of helix bundle (HB) and a unique C-terminal lipid-interacting stalk (LIS). The G engages the HB2 and LIS of the neighboring molecule, resulting a head-to-tail trimer. Mgm1 interacts with negatively charged lipids using both the G and LIS. Biochemical and physiological analyses confirm structural observation of s-Mgm1. These results lead to a novel mode of homotypic membrane fusion, in which Mgm1 assembles in cis, potentially generating a highly curved membrane tip to allow inner membrane fusion.

2S-5-1 ビリン結合光受容体の多様な吸収波長の分子基盤
Molecular basis of spectral tuning of the bilin-based photosensors

Yuu Hirose (*Toyohashi Univ. of Tech.*)

Phytochromes and cyanobacteriochromes are photosensors that covalently bind a linear tetrapyrrole (bilin) chromophore within their GAF domain and regulate diverse photoresponses in plant, algae, fungi and bacteria. These photosensors photoconvert between two light-absorbing forms, which is triggered by the 15Z/15E photoisomerization of the bilin. Substantial variation in their absorbing wavelength, spanning near-UV to far-red parts of the spectrum, has been discovered. However, molecular mechanisms underlying the spectral diversity are not yet fully understood. Here, we summarize current researches of these photosensors and introduce our biochemical, spectroscopic, and structural approaches to reveal the spectral sensitivity the bilin-based photosensors.

2S-5-2 GAF ドメインの結晶構造解析と NMR 解析
Crystallography and NMR Studies of GAF domain

Masaki Mishima (*Grad. Sch. Sci., Tokyo Metro. Univ.*)

The GAF domain of the Cyanobacterial photosensor binds a phycocyanobilin, one of the tetrapyrrole chromophores. To elucidate the molecular mechanism of the light absorption, we performed X-ray crystallography and NMR spectroscopies of the red light absorbing form and the green light absorbing form. We have succeeded in obtaining well dispersed NMR spectra of the GAF-domain for both red light absorption and green light absorption form, which provide information of the structure change and protonation states. We also succeeded in determining the structure of Pr state. In this presentation, we will report the progress and discuss the light absorption mechanism deduced from the crystallographic and NMR studies

2S-5-3 フラッシュフォトリシス法を用いた微生物ロドプシンの光反応解析
Photoreaction analysis of microbial rhodopsin by flash photolysis techniques

Takashi Kikukawa[1,2] ([1]*Fac. Adv. Life Sci., Hokkaido Univ.*, [2]*GI-CoRE, Hokkaido Univ.*)

In the field of photoreceptor protein research, flash photolysis is a conventional technique, in which a protein is activated by a short light pulse to enable the time-resolved detection of the subsequent reaction. This transient change is typically followed by an absorption change, which is useful to know the overall reaction but not so powerful to probe the events occurring inside the protein. Here, we will show our research on ion-pump rhodopsins, where we detected the flash-induced absorption changes under varying conditions and the flash-induced electrochemical signals reflecting the ion uptake and release reactions. The comparison of these data enabled us to identify the intermediates for these elementary reactions and thus to discuss the ion-pump processes.

2S-5-4 ラマン光学活性を利用したプロトンポンプ型ロドプシンにおける発色団の立体構造解析
Three-dimensional chromophore structures in proton-pumping microbial rhodopsins from Raman optical activity

Tomotsumi Fujisawa (*Fac. Sci. Eng., Saga Univ.*)

Microbial rhodopsins are the seven-transmembrane photoreceptor proteins which are widespread over micro-organisms. They contain the retinal chromophore to catch the photon energy, and the most representative function is the light-driven proton pump that transports H+ across cell membrane. The function of microbial rhodopsin is closely related to the conformation of retinal chromophore in the active site. In order to capture this chromophore conformation, we utilize the capability of Raman optical activity (ROA) spectroscopy to sensitively probe the three-dimensional molecular structures. We present the detailed chromophore conformations in the mirobial rhodopsins known as outward and inward proton-pumps on the basis of their ROA spectra.

2S-5-5 FTIR 分光法で示されたフラビン結合光受容体における特異的な水素結合の形成
Unique hydrogen-bonding formation in Flavin-binding photoreceptors revealed by FTIR spectroscopy

Tatsuya Iwata (*Phar. Sci. Toho Univ.*)

Fourier transform infrared (FTIR) spectroscopy can detect chemical bonds according to their hydrogen-bonding strength. We have been applied FTIR spectroscopy to flavin-binding photoreceptors. Especially, light-induced difference FTIR spectroscopy can extract information on chemical bonds whose environments have changed upon the photoreaction. We found that the formation of unusually strongly hydrogen-bonded N-H or O-H group in flavin-binding photoreceptors, LOV and BLUF domains. The origin of the chemical groups was identified by isotope labeling. Their unique environments in proteins were partially supported by quantum mechanics/molecular mechanics calculations. Unique environments in proteins where strong hydrogen bonds are formed will be discussed.

2S-5-6 分光学による光受容体の構造・機能解析：将来展望
Future perspective of spectroscopic study on structure and function of photoreceptor proteins

Jun Tamogami (*College Pharm. Sci., Univ. Matsuyama*)

Photoreceptor protein family is one of the most advantageous target proteins because we can apply varying spectroscopic approaches to analysis of these proteins, which are activated by light stimulus. A variety of spectroscopic methods including conventional static and time-resolved visible absorption spectroscopy, NMR, FTIR, and resonance Raman spectroscopy presented in this symposium enable insight from various perspectives, leading to deep understanding protein structure and function. In this talk, future prospect of spectroscopic study on various photoreceptor proteins such as cyanobacteriochrome, microbial rhodopsin, and flavin-binding photoreceptor, will be discussed.

2S-6-1 デング・エンベロープ蛋白質第 3 ドメインのミスフォールディングと凝集
Misfolding and aggregation of the dengue envelop protein domain 3

Yutaka Kuroda, Tomonori Saotome (*Tokyo Univ Agr and Tech*)

Most proteins can function only when they are natively folded. Protein aggregation and misfolding are thus deeply associated with the biochemical and biological functions of a protein. Here, we will discuss the misfolding and aggregation of the dengue envelop protein domain 3 (ED3) from a biophysical, conformational, and structural viewpoint and their consequences on its biological/physiological function.

2S-6-2 再構築型無細胞タンパク質合成系を用いたタンパク質凝集の網羅解析
Comprehensive analysis of protein aggregation by using a reconstituted cell-free translation system

Tatsuya Niwa, Hideki Taguchi (*Institute of Innovative Research, Tokyo Institute of Technology*)

Protein folding is highly complicated process and hence the nature of the protein folding remains largely unknown. To gain insight, we conducted a large-scale analysis of the tendency to make amorphous aggregates in vitro. By using a reconstituted cell-free translation system, we evaluated the aggregation propensity, which is assumed to reflect the ability of spontaneous folding, for thousands of bacterial proteins and hundreds of yeast proteins one-by-one under the chaperone-free condition. The results showed several properties relate to the aggregation propensity. The analysis for yeast proteins also showed that intrinsically disordered regions (IDRs) might relate to the aggregation propensity, although the IDRs themselves were not a main cause of forming aggregation.

2S-6-3 Molecular basis for diversification of amyloid conformation

Yumiko Ohhashi[1], Motomasa Tanaka[2] ([1]*Grad.Sch.Sci., Kobe Univ.*, [2]*CBS, RIKEN*)

Formation of protein aggregates including amyloid fibers is often associated with human diseases. Amyloidogenic proteins frequently misfold into distinct amyloid conformations, and the conformational differences are closely related to the pathology of amyloid diseases. However, the mechanism that determines the amyloid conformation remains unclear. In this study, we suggest that altered conformational equilibrium of amyloidogenic monomer protein affect the amyloid conformation. High-resolution nuclear magnetic resonance analysis revealed the presence of a local compact structure in the Sup35 intrinsically disordered domain and suggested the destabilization of local structure in Sup35 mutant that induces distinct amyloid conformation.

2S-6-4 6 M 塩化グアニジニウム中で変性したユビキチンの DMSO-停止 2D NMR 法による H/D 交換反応解析
The H/D-Exchange Kinetics of Unfolded Ubiquitin in 6 M Guanidinium Chloride Studied by the DMSO-Quenched 2D NMR Techniques

Kunihiro Kuwajima[1,2], Maho Yagi-Utsumi[3,4], Saeko Yanaka[3,4], Koichi Kato[3,4] ([1]*Univ. Tokyo*, [2]*KIAS*, [3]*IMS*, [4]*ExCELLS*)

The presence or absence of any residual structures in a protein unfolded in a concentrated denaturant is an important issue for elucidating molecular mechanisms of protein folding. The use of spin desalting columns in the DMSO-quenched H/D-exchange NMR experiments has made it possible to monitor the H/D-exchange behavior of a fully unfolded protein in a concentrated denaturant. Here, we applied the techniques to unfolded ubiquitin in 6 M GdmCl. We successfully identified all peptide NH signals in the 1H 800-MHz 1H-15N HSQC spectrum of the protein dissolved in the DMSO quenching solution, and monitored the H/D-exchange kinetics of the protein in 6 M GdmCl at pD 3.7 and 15ºC. Implications of the results in understanding folding mechanisms of ubiquitin will be discussed.

2S-6-5 タンパク質のフォールディングとデザインへの理論的アプローチ
Theoretical approaches to protein folding and design

Munehito Arai[1,2] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Dept. Phys., Univ. Tokyo*)

Solving the protein folding problem has been one of the most important issues in biophysics. However, since the problem has been unsolved, computational protein design has been a great challenge. Here, I will present our recent theoretical studies on protein folding and design. By introducing a new Hamiltonian to the statistical mechanical model of protein folding, which can predict folding pathways of small, single-domain proteins, we succeeded in predicting folding pathways of large, multi-domain proteins, including α-lactalbumin and lysozyme. We also succeeded in computationally designing the mutants of an enzyme that have four-fold higher activity than the wild type. Our approaches will be useful for advancing the protein folding and design studies.

2S-7-1 Singularity in Immunity: Immune-aging associates with a defect in Chromatin Regulation on Immune Cells

Shunsuke Chikuma (*Microbiology and Immunology, Keio University School of Medicine*)

Immune reaction is initiated by a few antigen-specific T lymphocytes, which provides life-long protection against same antigen. We aim to detect singularity events in many phases of immune reactions. As an example, aging causes immunodeficiency, inflammation, and autoimmune diseases. The changes in aged immune cells that leads to immune-aging is not understood. TRIM28, a nuclear protein, crucial for heterochromatin-mediated gene silencing, was found to be defective in aged immune cells. Mice lacking TRIM28 on immune cells showed many aspects of immune-aging. We hypothesize that the eventual loss of precise chromatin regulation on immune cells during life-course may cause expression of unwanted genes and contribute to age-related defects of immune system.

2S-7-2 Which cells initiate lymph node formation?

Shinichiro Sawa (*Medical Institute of Bioregulation, Kyushu University*)

Lymph node (LN) is a highly organized immune tissue that initiates acquired immune response against pathogens drained from peripheral tissues. LN development is currently described as a programmed process governed through stepwise activation of three types of cells; lymphatic endothelial cell, hematopoietic lymphoid tissue inducer (LTi) cell and mesenchymal cell. However, it is still unknown which type of cells initiate complex LN formation process. Recently, we identified particular mesenchymal cells indispensable for LN formation. In this presentation, we would like to propose novel model; particular mesenchymal cells appear prior to LTi cell colonization, eventually activate neighboring mesenchymal cells and finally build up complex stromal network in the LN.

2S-7-3 Live imaging of epidermal sensory nerves and keratinocyte tight junctions

Takaharu Okada[1,2] ([1]*RIKEN IMS*, [2]*Grad School of Med Life Sci, Yokohama City Univ*)

The epidermal barrier is thought to protect sensory nerves from overexposure to environmental stimuli, and barrier impairment leads to pathological conditions associated with itch, such as atopic dermatitis. However, it is not known how the epidermal barrier continuously protects nerves for the sensory homeostasis during turnover of the epidermis. By using multidimensional imaging techniques, we have found that epidermal sensory nerves are contained underneath the keratinocyte tight junction barrier in the normal skin, due to nerve pruning at newly forming tight junctions. Our imaging data also suggest that during the itch development caused by epidermal barrier impairment, the nerve pruning process is disrupted and epidermal nerves are aberrantly activated.

2S-7-4 がん細胞が出現した正常間質組織でのシンギュラリティ現象
Singularity at emergence of cancer cells in normal stroma

Shunsuke Kon (*Tokyo University of Science, Research Institute for Biomedical Sciences*)

Tumor microenvironment (TME) is a specialized, complex compartment comprising of tumor-educated stromal cells, which promotes both survival and proliferation of cancer cells. However, it remains enigmatic what happens at emergence of cancer cells in stroma, where normal stromal cells firstly face to cancer cells. Our preliminary results suggest that normal stroma countervails the expansion of low-grade cancer cells, while high-grade cancer cells transform normal stroma into TME. These results suggest that the high-grade cancer cells behave as 'singularity cells' to induce robust stromal cancerization. In this study, we aimed to reveal the nature of singularity at the initial stage of TME formation through combined in vitro experiments and ex vivo imaging.

2S-7-5 シンギュラリティを捉えるためのダイナミックレンジの広い光音響イメージングの研究開発
Development of photoacoustic imaging to study a singularity in high dynamic range measurement

Miya Ishihara (*National Defense Medical College*)

How to visualize a singularity in immunity and cancer? How to set the scale and/or observation condition? Photoacoustic (PA) imaging (also called optoacoustic imaging), which visualizes the distribution of optical absorption molecules with noninvasively, is based on optical excitation and ultrasound detection. The technical feature is combination of optical and ultrasound resolution. We developed an original photoacoustic imaging system with a large dynamic range, and will be applicable to both in vitro and in vivo studies. The system has a fluorescent imaging mode with the same field of view. In the talk, I would like to present the various data acquired thus far, and discuss the role of PA imaging to study a singularity.

2S-7-6 りん光寿命イメージング顕微分光法による組織内低酸素細胞の可視化
Visualization of hypoxia cells in tissues by using phosphorescence lifetime imaging microscopy

Toshitada Yoshihara (*Grad. Sch. Sci. and Tech., Univ. Gunma*)

Detection and visualization of molecular oxygen in cells and tissues are becoming increasingly important in cell biology and pathophysiology of various hypoxia-related diseases such as cancer. In this study, we demonstrate a method to visualize in vivo oxygen tension with spatial resolution at a cellular level using a cell-penetrating phosphorescent probe based on cationic iridium complex and a confocal phosphorescence lifetime imaging microscope (PLIM) to precisely assess tumor hypoxia. Imaging with our phosphorescent probe and PLIM system revealed that oxygen tension of tumor cells decreased gradually with an increase of the distance from blood vessels. We also determined absolute oxygen tensions in cells and capillary vessels in tumor tissues.

2S-7-7 動物体内での pH 測定を目指した近赤外レシオ型蛍光プローブの開発
Development of a near-infrared ratiometric fluorescent probe for pH inside the body

Kenjiro Hanaoka (*Grad. Sch. of Pharm. Sci., The Univ. of Tokyo*)

In biological systems, the pH in tissues is strictly regulated, and differences of pH are deeply related to key biological events such as cancer. Ratiometric fluorescence imaging is useful for determination of precise pH values, but existing fluorescence probes have substantial limitations, such as inappropriate pKa, inadequate photobleaching resistance, and insufficiently long excitation and emission wavelengths. We developed a near-infrared ratiometric fluorescent probe for pH measurement inside the body, Me-pEPPR. In biological applications, by using dextrin tagged with Me-pEPPR, we were able to image extracellular pH of tumors in situ. This chemical tool should be useful for studying the influence of extracellular pH on biological processes.

2S-8-1 導入；井上信也博士の仕事の紹介
An introduction to the works of Shinya Inoué

Tomomi Tani (*AIST*)

This is a short introduction of the life and times of Dr. Shinya Inoué.

2S-8-2 遠心偏光顕微鏡(CPM)を用いた核を細胞中央へ運ぶ力の測定
Measurement of cellular forces bringing the nucleus to the cell center using the Centrifuge Polarization Microscope (CPM)

Akatsuki Kimura[1,2,3] ([1]*Natl Inst Genet*, [2]*Marine Biological Lab, USA*, [3]*Dept Genet, Sokendai*)

In the summer of 2014, Dr. Goshima introduced me the Centrifuge Polarization Microscope (CPM). The microscope was invented and built by the late Dr. Inoué and his collaborators, which can apply high-power centrifugal forces while capturing high-resolution images of living samples (*J Microscopy* 2001). At first sight, I conceived a research to quantify the force bringing the nucleus to the cell center using the CPM. With the help of Dr. Goda, I was able to characterize the forces acting on the nucleus during the centration in the *C. elegans* embryo. Importantly, the embryos developed into an adult worm after recovering from the sample chamber. Therefore, we are able to characterize the forces acting inside the 'happy' cell by using the CPM.

2S-8-3 Cellular machinery for controlling actomyosin contractility in vivo

Asako Shindo (*Grad.Sch.Sci., Univ. Nagoya*)

Actomyosin contractility is a major force to drive tissue formation during animal development. However, its regulatory molecules in vivo are not fully understood. We established a chemical screening assay system using Xenopus embryos to identify actomyosin regulators in developing epidermis. The screening results gave several unexpected candidates, including the adrenergic receptor (AR), a receptor of adult's autonomic nervous system. We found that AR is expressed in the epidermis before embryos develop nervous systems. Live imaging revealed that the AR knockdown disturbed cell shape with frequent cell contraction and abnormal morphogenesis. I will discuss the possible mechanisms for balancing actomyosin contractility during tissue formation.

2S-8-4 植物の紡錘体形成における微小管の起源
Origin of mitotic spindle microtubules in plant cells

Takashi Murata[1,4,5], Kohei Otomo[2,3,4], Tomomi Nemoto[2,3,4], Mitsuyasu Hasebe[4,5] ([1]*Appl. Biosci., Kanagawa Inst. Tech.*, [2]*Div. Biophoto., NIPS*, [3]*ExCELLS, NINS*, [4]*Sch. Life Sci., Sokendai*, [5]*Div. Evol. Biol., NIBB*)

In plant cells, the mitotic spindle is formed in the absence of the centrosome. The mechanism of acentrosomal spindle formation has been studied from 1950s (Inoue 1953). The cytoplasmic microtubular structure around the prophase nucleus, called as a polar cap or a prospindle (Inoue and Bajer 1961, Vos et al. 2008), is regarded as a cytoplasmic microtubule organizing center (Kosetsu et al. 2017). However, whether the prospindle microtubules are the origin of spindle microtubules or the spindle microtubules are formed by other mechanisms is unknown. In this symposium, we demonstrate the origin of the spindle microtubules by 2-photon spinning disk microscopy and photobleaching technique with 2-color labelled microtubules.

2S-8-5 植物のスピンドルと染色体の動きについて
Spindle and chromosome motility in plant cells

Gohta Goshima[1,2] ([1]*Sugashima MBL, Nagoya Univ.*, [2]*Div. Bio-Sci, Nagoya Univ.*)

Force generation by microtubule assembly/disassembly in mitosis was originally proposed by Shinya Inoué over 50 years ago. Since then, numerous studies using animal cells have confirmed his model and uncovered the mechanism by which microtubule-based force is generated in the spindle to move chromosomes and the spindle itself. In contrast, our knowledge on plant spindles is still limited. The mechanism employed in animal cells might not operate in plant cells, as plants lack centrosomes and astral microtubules, which are key elements of the animal spindle. I will discuss two recent observations on mitotic motility in plant cells: 1) chromatid segregation assisted by a kinesin motor, and 2) spindle motility involving a microtubule-associated protein and actin.

2S-8-6 Toward understanding the real chromatin organization present in the cell

Kazuhiro Maeshima (*National Institute of Genetics*)

How is chromatin organized in the living cell? Over the past ten years, newly developed technologies have drastically shifted our view on chromatin from a static regular structure to a more irregular and dynamic one. Using single nucleosome imaging, we have revealed that chromatin is highly dynamic and locally similar to a fluid in living human cells. Many factors including chromatin binding proteins, the transcriptional state, and cations, can greatly influence chromatin organization and dynamics in living cells. Toward understanding the real chromatin organization present in the cell, 'imaging with happy living cells' by Inoue-sensei is a really golden saying.

2S-9-1 部分フッ素化リン脂質膜
Partially Fluorinated Phospholipid Membrane

Masashi Sonoyama[1,2,3] ([1]*Div. Mol. Sci., Gunma Univ.*, [2]*GIAR, Gunma Univ.*, [3]*GUCFW, Gunma Univ.*)

Fluorinated amphiphilic molecules exhibit remarkable surface and interfacial properties. We have developed a series of novel partially fluorinated analogs of dimyristoylphosphatidylcholine and dipalmitoylphosphatidylcholine with different perfluoroalkyl (Rf) chain lengths (PF-PCs) as possible materials for biophysical and biochemical studies of membrane proteins. Significant Rf-chain length-dependent thermotropic behaviors of PF-PC membranes and very high thermal stability of bacteriorhodopsin molecular assembly in PF-PC vesicles comparable to the native purple membrane will be discussed.

2S-9-2 有機-無機ハイブリッド型メゾ構造を有する脂質キュービック相の構築
Design of lipid cubic phase possessing organic-inorganic hybrid mesostructure

Kenichiro Omoto, Miki Kariya, Kazuma Yasuhara, Yugo Hayashi, Hironari Kamikubo, Gwenael Rapenne (*Grad. Sch. of Sci. and Tech., NAIST*)

Lipid cubic phase (LCP) is a kind of liquid crystal composed of continuous lipid bilayers and water nano-channels. Owing to its cell membrane mimetic mesostructure, LPC has been recognized as a promising material that realizes reconstitution, analysis, and utilization of membrane proteins. However, as the mesostructure of LCP is generally unstable, its available condition (temperature and concentration etc.) is limited. We have recently developed "cerasome", a morphologically stable vesicle with a ceramic coated lipid bilayer. Utilization of such an organic-inorganic hybrid mesostructure would overcome insintric structural instability of LCP. Herein, we report a strategy to prepare organic-inorganic hybrid LCPs via sol-gel condensation of organosilicon lipids.

2S-9-3 脂質ベシクル系における不均一性と線張力
Heterogeneity and line tension in lipid vesicle system

Takanori Takiue (*Kyushu University*)

The vesicles composed of phospholipid and cholesterol show lateral phase separation into liquid-ordered (Lo) and liquid-disorderd (Ld) phases. This heterogeneity is regarded as a simple model of biological membrane raft and the morphology of domain is controlled mainly by line tension, as excess energy at domain boundary. In this study, we focus on Lo/Ld coexisting in mixed DPPC/DOPC/cholesterol vesicle and examined the effect of hybrid phospholipid, POPC on the domain morphology by quantifying line tension. The line tension decreases from 1.0 pN in ternary system to less than 0.3 pN by adding POPC to the system. The domain morphology changes from circular at high to mosaic at low line tension, and finally domains are disappeared within a resolution of microscope.

2S-9-4 抗菌ペプチドや細胞透過ペプチドの作用機構を解明するための単一巨大リポソーム法
The Single GUV Method for Revealing Mode of Action of Antimicrobial Peptides (AMPs) and Cell-Penetrating Peptides (CPPs)

Masahito Yamazaki[1,2,3] ([1]*Res. Inst. Ele., Shizuoka Univ*, [2]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

For AMPs with bactericidal activity and CPPs with activity of translocation across plasma membranes, their interactions with lipid bilayers play important roles in the functions of these peptides. However, the elementary processes and mechanisms of the actions of AMPs and CPPs have not been clearly revealed. We have developed the single giant unilamellar vesicle (GUV) method for investigation on the interaction of peptides/proteins with lipid bilayers (1), which provides the details of elementary processes of action of AMPs and CPPs such as their kinetic constants. The role of membrane tension (2) and membrane potential (3) on their actions have been revealed.
(1) *Phys. Chem. Chem. Phys.* 16, 15752, 2014, (2) *Biophys. Rev*. 11, 431, 2019, (3) *Biophys. J.* 118, 57, 2020.

2S-9-5 LAiR: rapid reconstitution of integral membrane proteins into lipid bilayers

Christoph Gerle[1], Amer Asseri[5], Albert Godoy-Hernandez[3], Aiden Purugganan[3], Chimari Jiko[2], Carol de Ram[3], Holger Lill[5], Martin Pabst[3], Kaoru Mitsuoka[4], Dirk Bald[5], Duncan G.G. McMillan[3] ([1]*Osaka Univ., IPR*, [2]*Kyoto University*, [3]*TU Delft*, [4]*Osaka Univ.*, [5]*VU Amst.*)

We report reintegration of IMPs into a lipid environment an order of magnitude faster than currently used standard techniques by a new method termed LAiR. LAiR displays superior performance to standard methods in terms of protein activity, long-term stability and proton tightness of proteoliposomes. Our method is suitable for reintegration into liposomes as well as into surface-tethered membrane bilayers. We anticipate it to become a popular tool in basic research, pharmaceutical applications, and biotechnology.

2S-9-6 Microsytem for single molecule analysis of membrane proteins

Rikiya Watanabe (*CPR, RIKEN*)

Micro-chamber arrays enable highly sensitive and quantitative bioassays at the single-molecule level. Accordingly, they are widely used for ultra-sensitive biomedical applications; however, the versatility is generally limited to reactions in aqueous solutions, although various functions of membrane proteins are extremely important. To address this issue, microsystems using arrayed micro-sized chambers sealed with lipid bilayers, referred to here as biomembrane microsystems, have been developed for the analysis of membrane proteins. Here, I would like to introduce recent progress on the single molecule analysis of membrane proteins using a biomembrane microsystem, and discuss the future prospects for its use in analytical and pharmacological applications.

2S-10-1 Biomolecular Functional Design: an Introduction to Recent Advances

Duy Phuoc Tran (*TokyoTech, LifeSciTech*)

Biomolecular design is among the attractive research themes toward the Sustainable Development Goals of UNESCO. Recent advances in both computational and experimental methods have boosted the theme toward the controlling biomolecular functions after carefully understanding of their activity. This presentation gives a short introduction to recent advances in biomolecular design followed by the expert presentations in the symposium "Biomolecular Design to Control their Functions".

2S-10-2 配列空間をうまく絞り込むライブラリーデザインサイクル：酵素・抗体の設計アシスト
Library design cycle for efficient exploring in sequence space: design assist for enzyme and antibody

Mitsuo Umetsu[1,2] ([1]*Department of Biomolecular Engineering, Tohoku University*, [2]*Center for Advanced Intelligence Project, RIKEN*)

Molecular evolution techniques have been widely used for alteration, maturation, and enhancement of protein function: principal methods are two approaches of Iterative saturation mutagenesis (ISM) and library approach. However, Both the approaches have several serious problems; so that appropriate variants are not always generated by means of the Molecular evolution techniques. Here, we propose the combination of library approach with several techniques to design small-scale library. The information obtained from the combined techniques is utilized for designing the small-scale library, and the small-scale of library enable us to iterate the library approach for efficiently exploring a huge sequence space.

2S-10-3 微生物ロドプシンの機能と色の制御
Control of functions and colors of microbial rhodopsins

Keiichi Inoue (*Inst. Solid State Phys., Univ. Tokyo*)

Microbial rhodopsin is heptahelical transmembrane protein with a retinal chromophore, and most of them transport various ions in a light-dependent manner. We reported the first light-driven Na^+ pump rhodopsin in 2013. The ion-transport pathway and mechanism were revealed by spectroscopic and structural studies. Based on these insights, we designed artificial K^+ and Cs^+ pumps. Also, functional conversions among H^+, Cl^- and Na^+ pumps were achieved by rational mutations. The absorption wavelength of retinal determines which color of light rhodopsin uses. We found that optimization of the positions of residues bearing -OH group around retinal induces red-shift of absorption wavelength. Also, a new approach of color tuning based on machine learning method will be presented.

2S-10-4 機械学習による機能ペプチドの自動設計
Designing functional peptides with machine learning

Koji Tsuda (*GSFS, University of Tokyo*)

Antimicrobial peptides are a potential solution to the threat of multidrug-resistant bacterial pathogens. Recently, deep generative models including generative adversarial networks (GANs) have been shown to be capable of designing new antimicrobial peptides. Intuitively, a GAN controls the probability distribution of generated sequences to cover active peptides as much as possible. We present a peptide-specialized model called PepGAN that takes the balance between covering active peptides and dodging non-active peptides. As a result, PepGAN has superior statistical fidelity with respect to physicochemical descriptors including charge, hydrophobicity and weight. Top six peptides were synthesized and one of them was confirmed to be highly antimicrobial.

2S-10-5 ナノ機能化へ向けたタンパク質結晶設計
Protein Crystals for Designing Multiple Nanofunctions

Takafumi Ueno (*Tokyo Tech*)

Protein crystals have recently become known as potential molecular scaffolds for various applications. Efforts to design protein crystals for the construction of protein-based hybrid materials with metal complexes or nanomaterials now represent a growing field to provide novel or mimicking natural functions. However, the crucial functions of protein crystals have not been systematically investigated and characterized. We are now focusing on protein crystals as molecular scaffolds providing unique chemical environments and have found that they are suitable for designing various reactions that can be applied in living cells.

2S-10-6 合理設計による新規タンパク質フォールドの探索
Exploration of novel protein folds by de novo design

Nobuyasu Koga[1,2,3] ([1]*NINS, ExCELLS*, [2]*NINS, IMS*, [3]*SOKENDAI*)

Naturally occurring protein folds are only an infinitesimal subset of the considerable protein fold patterns. There is a vast protein fold space that has not yet been explored in nature. Here, we attempted to explore the fold space to identify novel protein topologies and create them by de novo design. We discovered novel folds including a knot topology, and computationally designed the structures. The designs expressed in E. coli and purified are found to be stable monomer in solution. The NMR structures of the designs show close agreement to the design models. Our study indicates that thousands of designable folds exist outside the biological evolution.

2S-10-7 A smart design of target-binding small proteins for molecular target therapy

Tetsuya Kadonosono (*Tokyo Tech*)

Small proteins that have high affinity for target proteins can be promising cheap alternatives for antibody drugs. We have proposed “smart design strategy”, a semi-rational design strategy for creating target-binding small proteins. In the smart design, first, a relatively small number of target-binding small protein candidates is designed by structural calculation or machine learning. Next, candidate molecules are comprehensively evaluated by various protein display or protein expression systems to identify target-binding small proteins. As a result, it becomes possible to efficiently search a vast molecular space. In this symposium, our recent successes in the development of HER2-binding small proteins will be introduced.

2S-11-1 赤外分光法を用いた光受容タンパク質の分子機構研究
The molecular mechanism of photoreceptor proteins by infrared spectroscopy

Daichi Yamada (*Grad. Sch. Life Sci., Univ. Hyogo, Japan*)

Living organisms use light as information and energy as represented by vision and photosynthesis. Photoreceptor proteins are responsible for the first reaction that captures light in such life activities. We study the structural changes in the function of photoreceptor proteins at the atomic level by using infrared spectroscopy which can detect molecular vibrations, and attempt to clarify the molecular mechanism of light conversion of information and energy. In this presentation, we would like to discuss the molecular mechanism in the photoreceptor proteins, especially about enzymes such as "DNA photolyase" that repairs specifically UV-damaged DNA and "photoactive adenylate cyclase" that synthesizes cAMP, the intracellular second messenger.

2S-11-2 Triggers of Primary Protein Dynamics in Photoreceptor Proteins

Shinya Tahara (*Laboratory for Biophysical Chemistry, Osaka University*)

Photoreceptor proteins are essential for converting light to the chemical energy to initiate biological functions. Upon photoexcitation, the chromophore of photoreceptor proteins undergoes structural changes. It has been widely accepted that these chromophore structural changes are transmitted to the protein part through covalent bonds, salt bridges and hydrogen bonds. We recently studied primary structural changes of the protein moiety for microbial rhodopsins and myoglobin by means of time-resolved UV resonance Raman techniques. In this talk, we discuss primary structural changes of these proteins and show that nonbonded atomic contacts and the chromophore dipole moment also play a pivotal role in driving primary structural changes of the protein moiety.

2S-11-3 Analysis of photoinduced reactions in UV-damaged DNA repair of photolyases

Ryuma Sato (*RIKEN*)

Photolyases (PLs) have been known as UV-damaged DNA repair enzymes and are a flavoprotein including flavin adenine dinucleotide (FAD). PLs often utilize several efficient light-harvesting antenna chromophores. In DNA repair reaction of PLs, FAD is activated by the direct photoexcitation or the excitation energy transfer from antenna pigments and an electron transfers from FAD to UV-damaged DNA. We theoretically investigated the electron transfer reaction and the excitation energy transfer in PLs. We found several electron transfer pathways from FAD to UV-damaged DNA and indicated that an artificial light-harvesting antenna affects DNA repair quantum yield using molecular dynamics simulations and quantum chemical calculations.

2S-11-4 酵素型ロドプシンの構造基盤
Structural insights into the mechanism of rhodopsin phosphodiesterase

Wataru Shihoya[1], Tatsuya Ikuta[1], Masahiro Sugiura[2], Kazuho Yoshida[2], Masahito Watari[2], Takaya Tokano[3], Kota Katayama[2], Satoshi Tsunoda[2], Takayuki Uchihashi[3], Hideki Kandori[2], Osamu Nureki[1] ([1]*Dept. of Biol., Grad. Sch. Sci., Univ. of Tokyo*, [2]*Life Sci. Appl. Chem., Grad. Sch. Eng., NIT*, [3]*Dept. of Phys., Grad. Sch. Sci., Nagoya Univ.*)

Rhodopsin phosphodiesterase (Rh-PDE) is an enzyme rhodopsin belonging to a recently discovered class of microbial rhodopsins. Rh-PDE consists of the N-terminal rhodopsin domain and C-terminal phosphodiesterase (PDE) domain, connected by 76-residue linker, and hydrolyzes both cAMP and cGMP in a light-dependent manner. Here we present structural and functional analyses of the Rh-PDE derived from Salpingoeca rosetta. The crystal structure of the transmembrane domain revealed a new topology of rhodopsin, with 8 TMs including the N-terminal extra TM, TM0. We further solved the crystal structures of the transmembrane and PDE domain with their connecting linkers. Integrating these structures, we proposed a model of full-length Rh-PDE.

2S-11-5 光スイッチの開発を目指したシアノバクテリオクロムの分子基盤
Molecular basis of cyanobacteriochromes for developing photoswitches

Keiji Fushimi, Rei Narikawa (*Biol. Sci., Shizuoka Univ.*)

We can manipulate light quality and intensity with high spatiotemporal resolution. Thus, “photoswitches” regulating various biological functions by light exposure have been developed in the "optogenetics" field. Cyanobacteriochrome photoreceptors can sense various light qualities covering UV-to-visible wavelength area in a small soluble unit, and thus promising platforms to develop state-of-the-art photoswitches. We focus on development of two kinds of photoswitches; One is advantageous for in vivo optogenetics by far-red light illumination based on the AnPixJg2 scaffold, while another for multiband optogenetics by various light illumination based on the AM1_1499g1 scaffold. Here, we describe engineering details of these two photoswitches in the structural context.

2S-11-6 概日時計制御における CRYPTOCHROME の役割
Function of CRYPTOCHROME in regulation of the circadian clock

Arisa Hirano[1,2], Takeshi Sakurai[1,2], Louis Ptacek[3], Ying-Hui Fu[3] ([1]*Faculty of Medicine, University of Tsukuba*, [2]*International Institute for integrative Sleep medicine (WPI-IIIS), University of Tsukuba*, [3]*University of California, San Francisco*)

The circadian clocks are driven by a transcription-translation based negative feedback loop. CRYPTOCHROME (CRY) is a principal clock component in the molecular feedback loop of the mammalian clock system, while CRY acts as a photoreceptor in fly and plants. We have shown regulatory mechanism of CRY by using forward-genetics approach in humans. A missense mutation in the hCRY2 FAD binding loop causes Familial Advanced Sleep Phase, which is a heritable sleep phenotype characterized by very early sleep and wake time. The mutation alters its accessibility and affinity for FBXL3 (an E3 ubiquitin ligase), thus promoting its degradation. We demonstrated novel function of chromophore binding to CRY in mammals, which is competing with FBXL3 and protecting CRY from degradation.

2S-11-7 植物の光受容体フォトトロピンのシグナル伝達とモデルケースとしての気孔開口
Plant photoreceptor phototropin signaling and stomatal opening as a model case

Shin-ichiro Inoue (*Division of Biological Science, Graduate School of Science, Nagoya University*)

Stomatal pores in the plant epidermis open in response to blue light and affect photosynthesis and plant growth by regulating CO2 uptake and transpiration. In stomatal guard cells under blue light, plasma membrane (PM) H+-ATPase is phosphorylated and activated via blue light-receptor phototropins, and the H+-ATPase then activates K+ channles via PM hyperpolarization. K+ uptake into guard cells via K+ channels finally induces stomatal opening. However, details of the signaling for H+-ATPase and K+ channel activation remain largely unknown. Recently, through a protein-protein interaction screening, we obtained two protein kinases as phototropin interactors. In the presentation, I will talk about functions of these kinases in phototropin signaling for stomatal opening.

2S-11-8 生命機能の理解と制御に向けたロドプシン研究
Analysis of rhodopsins for a rational understanding and controlling of biological functions

Keiichi Kojima (*Grad. Sch. of Med. Dent. Pharm. Sci., Okayama Univ.*)

Rhodopsins, a photoreceptive membrane protein family, are seven-transmembrane protein containing retinal as a chromophore and distributed in numerous organisms including humans. Rhodopsin molecules inherently play important roles in various biological functions, such as vision, energy production, phototactic response. Furthermore, they recently serve as fundamental tools of optogenetics, a technology to regulate biological functions with light by their heterologous expression. We characterized the molecular properties of animal and microbial rhodopsins for a rational understanding and controlling of biological functions. We will discuss the recent progress and future prospects of photobiology as a closing remark of this symposium.

2S-12-1 1 分子計測と分子シミュレーションを用いたタンパク質構造ダイナミクスの統合モデリング
Integrative modeling of protein dynamics from single-molecule experiments and molecular dynamics simulations

Yasuhiro Matsunaga[1,2], Tomonori Ogane[1,2] ([1]*Saitama University*, [2]*JST CREST*)

Combining experimental measurements with molecular simulations often significantly improves the description of conformational dynamics. Ensemble refinements, where the simulations are utilized to refine ensemble averaged data in NMR or SAXS are a popular approach in integrative structural biology. On the other hand, there are few studies on using time-series data measured by single-molecule experiments despite their rich temporal information. So far, we have developed data-assimilation approaches for combining molecular simulations with single-molecule fluorescence microscopy data. Here, we show our recent efforts on the use of high-speed atomic force microscopy for integrative modeling.

2S-12-2 新しいペプチド薬と、ターゲットタンパク質と新しい薬の分子動力学シミュレーション
New Peptide Drug and the Molecular Dynamics Simulations of Target Protein and the New Drug

Lisa Matsukura[1], Naoyuki Miyashita[1,2], Masumi Taki[2], Shinichi Watanabe[2] ([1]*BOST., KINDAI Univ.*, [2]*Eng. Sci., UEC*)

Heat Shock Protein (HSP) 90 is known as one of the targets for anticancer drugs. Many of HSP90 inhibitors that have been developed so far were compound drugs and these bind to ATP binding site on HSP90 N-Terminal Domain to inhibit the activation by ATP. Recently new peptide drug inhibitor which does not bind to ATP binding site has been developed by our collaborators. However, the binding site of the new drug and the inhibition mechanism of the HSP90 NTD by the peptide drug has not been clear yet. Therefore, to understand the binding mechanism, we performed several molecular dynamics simulations and the docking simulations of HSP90 and peptide drugs. Our results suggested that the peptide drug inhibits the HSP90 dimer formation mechanically.

2S-12-3 アンサンブルドッキングを用いたタンパク質相互作用プロファイル解析
Profile analysis of protein interaction surfaces with ensemble rigid-body docking process

Nobuyuki Uchikoga[1], Yuri Matsuzaki[2] ([1]*Sch. Interdiscip. Math. Sci., Meiji Univ.*, [2]*ToTAL, Tokyo Tech.*)

Most proteins work with their conformation changes. For understanding protein functions, it is necessary to know their protein interaction mechanisms with their conformations. We then used a profile method for analysis of protein-protein interactions, which involved with amino acid sequences of target proteins, and then, is independent of their conformations. In single target protein analysis, this method can compare protein interaction surfaces of various conformations using an identical amino acid sequence.After generating various conformations by MD, we could perform a rigid-body docking for each conformation, so-called ensemble docking. In this work, we will show some results from this profile method with ensemble rigid-body docking.

2S-12-4 Turn-on / keep-on fluctuated fluorescent molecules as targeted binders

Masumi Taki (*UEC*)

We have obtained peptide-conjugated solvatochromic probes by using an extended phage-display system; a conjugation of an optimized peptide to a fluorophore strengthened both specificity and affinity to the target along with the solvatochromism, and consequently created protein-specific turn-on binders [Anal. Chem., 2016]. Alternatively, a low-molecular-weight pharmacophore, as a targeted fluoroprobe, was selected from a dynamic combinatorial library of Schiff bases. The identified pharmacophore retained its fluorescence when bound to the hydrophobic site of the target, whereas it lost because of hydrolysis when unbound. We defined it as keep-on type fluorescence probe because the fluorescent pharmacophore is only kept intact when bound to the target [ABC, 2018].

2S-12-5 Analysis of an effect of mutations on the structure of CDR-H3 in the anti-HIV neutralizing antibody PG16

Hiroko X. Kondo[1,2], Ryo Kiribayashi[2], Daisuke Kuroda[3], Kouhei Tsumoto[3,4], Yu Takano[2] ([1]*Fac. Eng., Kitami Inst. Tech.*, [2]*Grad. Sch. Info. Sci., Hiroshima City Univ.*, [3]*Grad. Sch. Eng., Univ. Tokyo*, [4]*IMS, Univ. Tokyo*)

PG16 is a broadly neutralizing antibody to the HIV. A previous experimental assay showed that the mutation of Tyr-H100Q to Ala, which is remote from the paratope, decreased the neutralization ability of PG16. However, the molecular mechanism by which this mutation affects the neutralization potency has remained unclear. Here, we performed molecular dynamics simulations of the wild-type and 2 mutants (Tyr-H100Q to Ala, and Tyr-H100Q to Phe) of PG16, to clarify the effects of these mutations on the dynamics of complementarity determining region (CDR) H3. Our simulations revealed that the structural rigidity of the CDR-H3 in PG16 attribute to the hydrogen bond interaction between Tyr-H100Q and Pro-H99, as well as the steric support by Tyr-H100Q.

2S-12-6 Autoencoder-based analyses of dynamic allostery on GPCR

Yuko Tsuchiya[1], Kei Taneishi[2], Yasushige Yonezawa[3] ([1]*AIRC, AIST*, [2]*RIKEN*, [3]*KINDAI univ.*)

Analyses of subtle changes in side-chain dynamic motion, and not large rigid conformational changes, are essential to understand the regulation of protein functions. We applied our autoencoder-based method that can detect dynamic allostery, to the analysis of the signal transduction by ligand in GPCR. The method detected a pattern of fluctuations that was led by several ligand residues, and the N-terminus and the turn between TM5 and TM6 helices in GPCR. The ligand binding is known to lead to the conformational change of TM5 and TM6. The TM5-TM6 turn is located in a cell, which is distant from the ligand and the N-terminus of GPCR involved in the ligand binding. They suggest that the pattern of fluctuations is essential to the GPCR signaling.

2S-12-7 タンパク質の熱力学的安定性における主要因子
Dominant factor in thermodynamic stability of protein

Tomonari Sumi[1], Hiroshi Imamura[2] ([1]*Res. Inst. Interdiscip. Sci., Okayama Univ.*, [2]*Dep. Appl. Chem., Ritsumeikan Univ.*)

Kauzmann's hydrophobic interaction hypothesis on thermodynamic stability of protein has been widely accepted for about sixty years and attracted many scientists. The hypothesis, however, has not been both theoretically and experimentally verified or disproved. Here, we examined solvation free-energy change upon leucine zipper formation in a coiled-coil protein GCN4-p1, a typical model for the hydrophobic interaction. The water-mediated interactions were unfavorable for the association of the nonpolar groups in the native state, while the direct dispersion forces were responsible for the association. This result poses the critical question as to a classical view that an energetic cost of hydration of nonpolar groups of proteins drives the folding.

2S-13-1 RNA 顆粒内 mRNA の直接観察
Direct observation of mRNA inside of RNA granules

Kohki Okabe (*Grad Sch Parm Sci, Univ Tokyo*)

Besides undergoing translation, mRNAs spend most of their time being packaged into ribonucleoproteins referred as RNA granules. Although it has been revealed that RNA granules are in the state of liquid-liquid phase separation (LLPS), the mechanism of directly initiating RNA granule formation and the behavior of mRNA inside of these granules are elusive. We developed a method for the direct observation of endogenous mRNA in living cells using fluorescently labeled linear antisense 2'O-methyl RNA oligonucleotides. Here we investigated the single particle tracking of mRNA in RNA granules and furthermore in the initiation process of granule formation. Our result indicated unique behaviors of mRNA which facilitate the characteristic molecular communication such as LLPS.

2S-13-2 エピジェネティック修飾がクロマチン転写に及ぼす影響を定量化する
Quantifying the effect of epigenetic modification on chromatin transcription

Takashi Umehara (*RIKEN BDR*)

Eukaryotic transcription is epigenetically regulated by chromatin structure and post-translational modifications. However, quantitative understanding of the contribution of a particular post-translational modification to eukaryotic transcription is limited because reconstitution of a chromatin template with a designed modification is difficult. Here, we reconstituted a chromatin template with a site-specific histone acetylation, which contained a gene with a unique sequence detectable by hybridization-assisted fluorescence correlation spectroscopy. Along with detection and mathematical analysis of nascent transcripts generated on the chromatin template, we provide a kinetic model to quantify the contribution of an epigenetic modification to chromatin transcription.

2S-13-3 Gene expression and artificial cells: Revisiting the role of active interface

Yusuke T. Maeda (*Department of Physics, Kyushu University*)

Artificial cells made of molecular components and lipid membrane are emerging platforms to characterize living systems properties. In this talk, we revisit the physical role of compartments involved in gene expression. Cell-free transcription-translation (TXTL) offers advantages for the bottom-up synthesis of cellular reactors in order to examine how its active surface alters gene expression of DNA in bulk. We find that the amount of synthesized proteins in artificial cells of radius R shows an anomalous geometric scaling different from qubic. In small artificial cells where surface effects are large, a physical process alters gene expression activity in bulk, suggesting that an active cell-sized interface can be a regulatory factor for TXTL.

2S-13-4 分子の状態と形態を考慮したクロマチン構造の統合的モデリングを目指して
Towards Comprehensive Models of Chromatin Structures Considering the State and Shape of Molecules

Yuichi Togashi[1,2] ([1]*Grad. Sch. Integr. Sci. Life, Hiroshima Univ.*, [2]*RIKEN BDR*)

In contrast to classical view of DNA as a "data tape", structural changes of chromatin are now known to be crucial for the function, showing that DNA is a part of the information processing device, or "computer" itself. Hence, the structure has been intensively studied using a variety of experimental methods. However, it is still difficult to make a comprehensive model, particularly at the meso-scale, which can combine such experimental results to reproduce dynamic motions and functions. In this presentation, I will introduce our modeling efforts at DNA strands to single nucleosome level, and also at the level of abstract polymer models, and discuss possible strategies to fill the gap between them.

2S-13-5 合成生命システム創成に向けた RNA-タンパク質複合体の活用
RNA-Protein complexes for synthetic living systems

Hirohide Saito (*Center for iPS Cell Research and Application, Kyoto University*)

RNA and RNA-protein (RNP) complexes play important roles in the regulation of gene expressions and cellular functions. It functions as both as an informational carrier and a nanomachine due to its complementary base-pairing ability and complexed three-dimensional structure. Several nanostructures have been designed and constructed by exploiting these natural RNA properties. In this talk, I will introduce the design principles of RNA and RNP nanostructures and their biotechnology applications. For example, synthetic RNA/RNP-based genetic switches and circuits have attracted attention for future therapeutic applications because of their safety and functional diversity. Future perspectives of RNA and RNP systems for synthetic living systems will also be addressed.

2S-13-6 相分離とエマルションによる DNA マイクロ液滴の生物物理学
Biophysics on DNA microdroplet technology by phase separation and emulsion

Masahiro Takinoue (*Department of Computer Science, Tokyo Institute of Technology*)

DNA nanotechnology is an interdisciplinary research field that aims at nano/micrometer-sized sophisticated structures and dynamical reaction systems that achieve molecular sensing, molecular computation, and molecular robotic actuation. In this field, we have to understand soft matter physics of DNA not only in natural use in living systems but also artificial situations, so, ‘new’ biophysics on DNA is actively explored now. In this presentation, I will show aqueous phase-separated droplet and Pickering emulsion-like microcapsules made of DNA nanostructures in a physical point of view. The DNA microdroplet technology will be applied to artificial organelles, artificial nuclei, and artificial cells constructed and functionalized in a programmable manner.

2S-14-1 Exosome-based therapy and biomarker development for the polyglutamine diseases

Toshihide Takeuchi[1,2] ([1]*Grad Sch Med, Osaka Univ*, [2]*JST-PRESTO*)

The polyglutamine diseases including Huntington’s disease are a group of inherited neurodegenerative diseases with no effective therapies developed to date. In this talk, we will show our exosome-based studies on therapeutic development for the polyglutamine diseases. We found that exosome-mediated intercellular transmission of molecular chaperones such as Hsp70 and Hsp40 suppress aberrant aggregation of the disease-causative proteins in a non-cell autonomous manner and exert therapeutic effects on the animal models of the polyglutamine diseases. We will also discuss our recent findings on blood exosome-based biomarkers using the non-human primate model and human patient samples.

2S-14-2 細菌が形成する細胞外小胞の多様性
Diversity of bacterial extracellular vesicles

Yosuke Tashiro[1,2] ([1]*Grad. Sch. Integr. Sci. Technol., Shizuoka Univ.*, [2]*JST PRESTO*)

Membrane vesicle (MV) formation has been recognized as a common mechanism in prokaryotes, and MVs play critical roles in intercellular interaction. However, a broad range of MV types and their multiple production processes make it difficult to gain a comprehensive understanding of MVs. In this work, we demonstrated morphological heterogeneity of MVs using an engineered strain, *Buttiauxella agrestis* 1090^T Δ*tolB* mutant. We also discovered a previously undiscovered type of vesicles, multilamellar outer membrane vesicles (M-OMVs), which were released in an unconventional process from this mutant. These findings have enabled considerable progress in understanding MV biogenesis and characteristics.

2S-14-3 Overlooked redox property of outer membrane vesicle surface

Akihiro Okamoto (*National Institute for Materials Science*)

Membrane vesicles (MVs) produced by bacteria carry various biological molecules inside, but we recently found ones with surface redox property. We here study the electrochemical interaction between the redox-active MVs and their host of pathogenic bacteria. Various pathogens were recently identified as electrochemically active bacteria that transport electrons to the electrode surface associated with biofilm formation. The microbial current producing capability enables to directly track the biofilm metabolic activity by electrochemical methods. Upon the addition of MVs, the current production was highly enhanced. The current enhancement mechanism and biochemical analysis of MVs will be presented.

2S-14-4 Amphipathic helical peptide-based fluorescent probes for exosomes by membrane curvature recognition

Yusuke Sato[1,2] ([1]*Grad. Sch. Sci., Tohoku University*, [2]*JST-PRESTO*)

With increasing knowledge about the diverse roles of exosomes, much attention has been paid to chemical tools for analyzing the biological functions of exosomes. Recently, we developed new class of exosome-binding fluorescent probes based on amphipathic helical peptides with membrane curvature sensing abilities. These probes facilitate the fluorescent detection and quantification of exosomes without the use of the protein markers on the exosomal membranes, which stands in sharp contrast to traditional immunoassays. I will present the details on the probe design and its binding and fluorescence signaling ability with a view toward the practical application to exosome analysis.

2S-14-5 ナノ流体デバイスを用いたエクソソームの簡便単離、1粒子配列及び統合解析
Simple isolation and integrated analysis of single exosomes on an aifA chip

Yan Xu[1,2,3] ([1]*Grad. Sch. Eng., Osaka Pref. Univ.*, [2]*PRESTO, JST*, [3]*N2RI, Osaka Pref. Univ.*)

The current greatest challenge in the elucidation of the biological significance of exosomes and the development of clinical technology targeted at exosomes is the difficulty of isolation, detection and analysis of exosomes due to their small particle sizes. In this study, we developed an integrated technology allowing simple one-step isolation/arraying, rapid high-throughput detection, and high-precision analysis of single exosomes by using our original nanofluidic device technology, which is called aL-in-fL Array (aifA). The aifA would be a powerful tool for studies and applications of exosomes because it provides a simple and efficient way to isolate, manipulate, detect and characterize single exosomes from cell culture supernatants or body fluids.

2S-14-6 Collection of Extracellular Vesicles from Single Cell Using Nanopipette

Hiroki Ida[1,2,3,4], Yasufumi Takahashi[5], Akichika Kumatani[3], Yuji Nashimoto[1,6], Hitoshi Shiku[6], Takeshi Yoshida[5], Rikinari Hanayama[5] ([1]*Tohoku Univ., FRIS*, [2]*JST, PRESTO*, [3]*Tohoku Univ., AIMR*, [4]*Tohoku Univ., Grad. Sch. Env. Stu.*, [5]*Kanazawa Univ., WPI-NanoLSI*, [6]*Tohoku Univ., Grad. Sch. Eng.*)

Extracellular vesicles (EVs) are expected to play various roles in intercellular communications. However, their characters are still not clear in detail due to the identification of different types of EVs in cell culture or body fluids. Therefore, a variety of techniques have been developed to isolate EVs released from cells with high throughput and high quality. As a complementary approach, we have established a unique approach by using a nanopipette to collect EVs directly from a cell before their release. This technique has some advantages such as isolation of high-quality EVs with spatio-temporal information. Recently, we have challenged to evaluate the collected EVs for further understanding of their characters.

2S-14-7 細胞外小胞放出の 1 細胞解析
Single Cell analysis of release dynamics of Extracellular Vesicles

Yoshitaka Shirasaki (*Grad. Sch. Pharm. Sci., Univ. Tokyo*)

Extracellular vesicles（EVs) possess intracellular molecular information on the surface or inside of the supplying cell, which is then transplanted to the receiving cell. Traditionally, such actions have been known as those of EVs derived from a multi-vesicular body called an exosome. However, in recent years, various types of EVs of similar size to exosomes have been found, and it has become necessary to investigate the action of EVs in detail. Our study attempts to explain the classification of EVs by linking the state of the supplied cells to the type of EVs that are released. In this presentation, I will present the latest data on EV production dynamics and discuss the mechanism of this process.

2S-15-1 Curvature induction and sensing of the F-BAR protein Pacsin1 on lipid membranes via molecular dynamics simulations

Md. Iqbal Mahmood[1], Hiroshi Noguchi[2], **Kei-ichi Okazaki**[1] ([1]*IMS*, [2]*ISSP, Univ. of Tokyo*)

F-BAR proteins play essential roles in biological processes that involve membrane remodelling, such as endocytosis and exocytosis. Notably, Pacsin1 from the Pacsin/Syndapin subfamily has the ability to transform the membrane into various morphologies: striated tubes, featureless wide and thin tubes, and pearling vesicles. The molecular mechanism of this interesting ability remains elusive. In coarse-grained (CG) simulations with parameters tuned from the all-atom (AA) simulations, we show that the regularly assembled Pacsin1 dimers bend a tensionless membrane. We also show that a single Pacsin1 dimer senses the membrane curvature, binding to a buckled membrane with a preferred curvature. These results provide molecular insights into polymorphic membrane remodelling.

2S-15-2 Molecular mechanisms linking actin cytoskeleton to the plasma membrane

Yosuke Senju (*RIIS, Univ. Okayama*)

The generation of membrane curvature is crucial for the formation of plasma membrane protrusions and invaginations during cell migration, morphogenesis, and endocytosis. Bin/Amphiphysin/Rvs (BAR) domain proteins bind to phosphoinositides, sense/generate membrane curvatures, and deform the plasma membrane into protrusions or invaginations during these processes. To elucidate the molecular mechanisms by which BAR domain proteins generate membrane curvatures, we reconstituted membrane protrusions generated by BAR domain protein and actin filaments on giant unilamellar vesicles (GUVs). We are now examining physiological relevancies of this reconstitution study to reveal how BAR domain proteins coordinate actin cytoskeleton and plasma membrane dynamics.

2S-15-3 The extracellular vesicle formation by filopodial scission for cell migration

Tamako Nishimura, Takuya Oyama, Hooi Ting Hu, **Shiro Suetsugu** (*Nara Institute of Science and Technology*)

Extracellular vesicles are classified into microvesicles and exosomes. Exosomes are generated from endosomes dependently on the ESCRT protein complex, including ALIX. However, mechanisms of microvesicle generation have not been identified. Membrane curvatures are generated by BAR domains, of which the inverse BAR (I-BAR) proteins are involved in filopodia. Here, we show that the I-BAR protein, Missing-in-metastasis (MIM), generates microvesicles by scission of filopodia. The amount of MIM-containing microvesicles increased by external forces equivalent to those in vivo and by the suppression of ALIX. The MIM-dependent microvesicles contained cell-surface proteins for stimulation of cell migration through lamellipodia formation.

2S-15-4 Molecular mechanisms underlying dynamic behavior of membrane blebbing

Junichi Ikenouchi (*Kyushu Univ., Fac Sci, Dept. of Biol*)

Amoeboid cell movement is a universal mode of cell migration. Amoeba-like cell movement is driven by the formation of membrane blebs. Membrane blebs are spherical protrusions of the plasma membrane that detach from the underlying actin filaments. In blebs, the plasma membrane protrudes by the rapid influx of the cytoplasm to the actin cortex-free membrane region. Therefore, it is necessary to compartmentalize the cytoplasm into regions of high fluidity and low fluidity in order to restrict the region where intracellular pressure is relieved and to produce cytoplasmic flow towards the protrusion at once. In my talk, I will introduce our recent findings about how heterogenization of cytoplasm is associated with the changes of plasma membrane.

2S-15-5 Proper membrane shaping during autophagosome biogenesis is required for non-selective sequestration of cytoplasmic components

Hitoshi Nakatogawa (*Sch. of Life Sci. & Tech.*)

In the intracellular degradation system autophagy, a small membrane cisterna called the isolation membrane forms in the cytoplasm, expands, bends into spherical shape and finally closes to generate a double-membrane vesicle called the autophagosome, which encloses various cellular components and transports them into lysosomes or vacuoles for degradation. Previous studies have revealed molecular mechanisms underlying autophagosome biogenesis, but those for membrane shaping during this process still remain elusive. In this symposium, based on our recent results, I will discuss a mechanism that expands the opening of the growing isolation membrane, which is required for the non-selective sequestration of cytoplasmic material into the autophagosome.

2S-15-6 Dysregulated membrane remodeling in pathogenesis of congenital diseases

Tetsuya Takeda[1], Kenshiro Fujise[1], Mariko Okubo[2], Tadashi Abe[1], Hiroshi Yamada[1], Ichizo Nishino[2], Satoru Noguchi[2], Kohji Takei[1] ([1]*Okayama Univ. Grad. Sch. Med. Dent. Pharm. Sci.*, [2]*NCNP*)

BAR domain proteins and dynamins are key molecules in membrane remodeling and they work together on membrane deformation and fission. Mutations in genes encoding a BAR domain protein BIN1 and the ubiquitous isoform dynamin 2 have been reported to be causative of centronuclear myopathy. However, precise pathogenic mechanisms of centronuclear myopathy by defective membrane remodeling remained unclear. In this study, we provides molecular insights into dysregulated membrane remodeling triggering the pathogenesis of DNM2-related centronuclear myopathy.

2S-15-7 The structure-based targeting of alpha-synuclein to mitochondria promotes cellular health

Harvey T. McMahon (*MRC Laboratory of Molecular Biology*)

Parkinson's Disease is a common neurodegenerative disorder. Mutations or increased copy numbers of the α-synuclein gene, SNCA, cause Parkinsonism. Fibrillar α-synuclein protein aggregates, called Lewy bodies, are found in neurons in both genetic and idiopathic forms of the disease. While aggregates are thought to be a central driver of disease, the function of α-synuclein is undefined. We examine the membrane binding properties of α-synuclein in cells and in vitro. We identify the compartment in cells targeted by α-synuclein and examine its function and how disruption of this function may give rise to disease states. Our work shows how one can go from the biophysical of a protein to a functional understanding.

2S-16-1 Watching, controlling, and designing of function and phase separation of DNA-binding protein

Kiyoto Kamagata (*IMRAM, Tohoku Univ.*)

DNA-binding proteins are involved in the regulation of various cell functions and many diseases, and used as a genome editing tool. First, we developed single-molecule fluorescence microscopy coupled with DNA garden to visualize the movements of proteins on DNA. We identified various target search mechanisms of a tumor suppressor p53 including sliding along DNA and transfer between DNAs. Also, p53 can induce liquid-liquid phase separation (LLPS). Second, we developed a rational design method of the peptide targeting an intrinsically disordered region using only sequence information. The designed peptide suppressed binding to DNA and sliding along DNA by p53. Furthermore, I will present the current trials for controlling LLPS and designing of a genome editing protein.

2S-16-2 Molecular principles for optimizing protein-DNA interactions

Yaakov Levy (*WIS*)

The remarkable efficiency and specificity of protein-DNA recognition presents a major theoretical puzzle given the size of the genome and the large number of molecular species in vivo at a given time. The fast association between proteins and DNA is governed by electrostatic interactions that allow protein to perform a helical motion when it is placed in the major groove. Proteins that interact with DNA share unique properties than proteins that interact with other negatively charged biopolymers such as microtubules or single-stranded DNA. In my presentation, I will discuss the molecular design principles adopted by nature that allow fast dynamics and high affinity binding and thus optimized search for function.

2S-16-3 CRISPR-Cas 酵素の構造、機能、分子進化
Structure, mechanism and evolution of CRISPR-Cas enzymes

Hiroshi Nishimasu (*The University of Tokyo*)

RNA-guided DNA cleaving enzymes derived from the microbial CRISPR-Cas adaptive immune systems are widely used as genome-engineering tools. Among diverse CRISPR-Cas effector nucleases, the type V-F Cas12f proteins are exceptionally compact, and associate with a guide RNA to cleave double-stranded DNA targets. Here, we determine the structure of Cas12f in complex with a guide RNA and its target DNA, explaining the action mechanism of the compact Cas12f enzyme. A structural comparison of Cas12f with other Cas12 enzymes provided insights into the molecular evolution of type V Cas12 enzymes. Collectively, our findings improve mechanistic understanding of diverse CRISPR-Cas nucleases, and provide a framework for the development of compact genome-engineering tools.

2S-16-4 Construction of DNA nanostructures exhibiting modulated structural transformation

Yuki Suzuki (*FRIS, Tohoku Univ.*)

Making use of the programmability and structural flexibility of the DNA molecule, we designed DNA origami nanostructures capable of exhibiting modulated structural transformation. Our DNA origami nanostructure comprised serially repeated tension-adjustable modules, the cumulative actuation of which resulted in a large deformation of the structure, which transformed from a linear shape into a curved shape. We demonstrate that the degree of deformation can be systematically controlled by merely replacing a set of strands that is required for the actuation of the module. Moreover, by employing tetraplex-forming sequences for the actuation, we could achieve reversible stimuli-induced contraction and relaxation of the nanostructure.

2S-16-5 RNA 転写/DNA 複製の過程で生じる局所的なクロマチンの運動
Local chromatin motion during RNA transcription/DNA replication

Yuji Itoh, Ryosuke Nagashima, Kayo Hibino, Michael Babokhov, Masato T. Kanemaki, Kazuhiro Maeshima (*NIG*)

Chromatin organization and dynamics play a critical role in gene transcription and DNA replication, but how they interplay remains unclear. To approach this issue, we investigated genome-wide chromatin behavior in living human cells using single-nucleosome imaging. We revealed that inhibition of transcription by drug treatment and rapid degradation of RNA polymerase II (RNAPII) increased chromatin motion. Based on these data, we propose RNAP II and other transcription factors form loose genome chromatin networks, which is consistent with recent reports on liquid droplets of transcription factors. By contrast, inhibition of DNA replication did not affect chromatin motion, implying that DNA replication machinery has a distinct mechanism from transcription one.

2S-16-6 Interactions of local DNA structures and proteins using biophysical and molecular biology approaches

Vaclav Brazda[1,2] ([1]*Institute of Biophysics, Czech Academy of Sciences*, [2]*Brno University of Technology, Faculty of Chemistry*)

Local alternative DNA structures, such as cruciforms (CF), left-handed DNA, triplex and quadruplex (G4) structures, are known to exist in all organisms. Many proteins have been shown to exhibit CF-specific binding properties or G4-binding properties. We have developed easy accessible web tools for analyses of CF and G4 and analyzed their presence in various genomic datasets including human genome. Using various biophysical and molecular biological methods including AFM, EMSA, fluorescent anisotropy, CD, yeast isogenic transactivation assay as well by DNA garden single-stranded DNA analyses we have evaluated DNA-protein binding properties. A deeper understanding of DNA-protein interactions is an important component to consider in the post-genomic era.

2S-17-1 細菌べん毛研究を振り返る：これまでに何がわかったのか？
Historical overview of the bacterial flagellar studies: what do we know about "flagella" so far?

Seiji Kojima (*Div. Biol. Sci., Grad. Sch. Sci., Nagoya Univ.*)

I became enthusiastic about bacterial flagella when I was a second year of undergraduate student in 1991 (30 years ago). At that time, the EM picture of flagellar basal body (1971) and free swimming cell movie (1991) grasped my heart. The discovery of flagellar motor is 1974, and then three years later in 1977, proton motive force was reported as the energy source of motor rotation. Now we are in 21th century, facing the burst of technology development, for examples, cryo-EM/tomography for supramolecular structure analysis, and single molecule analysis for high-resolution motor behavior. I will overview historical breakthrough moments, and then uncover the questions what we need to know in the near future to fully understand the mechanism of flagellar function.

2S-17-2 細菌べん毛モータータンパク質の自然な構造の解析
Structure of the native form of the bacterial flagellar motor component

Takayuki Kato[1], Fumiaki Makino[2], Tomoko Miyata[3], Miki Kinoshita[3], Tohru Minamino[3], Keiichi Namba[3,4,5] ([1]*IPR/Osaka Univ.*, [2]*JEOL*, [3]*Grad. Front. Biosci./Osaka Univ.*, [4]*BDR / SPring-8 Center*, [5]*JEOL YOKOGUSHI Lab.*)

Structural analysis by cryo-EM has become a major trend in structural biology. It has the advantage of analyzing native structures of biomolecular complexes. The flagellum is composed of about 30 different proteins and can be roughly divided into three parts: the basal body, the hook, and the filament. The hook is a relatively short axial segment working as a universal joint connecting the basal body and the filament for smooth transmission of motor torque to the filament. The native supercoiled hook structure was solved at 3.6 Å resolution by cryoEM single particle analysis. We clarified the mechanisms of its bending flexibility and rotation stability as a universal joint. We will also talk about other flagella components in the native structure.

2S-17-3 バクテリアべん毛蛋白質輸送エンジンのゲート開閉機構
Gating mechanism of the bacterial flagellar protein export engine

Miki Kinoshita[1], Tomoko Miyata[1], Takayuki Kato[2], Keiichi Namba[1,3,4,5], Tohru Minamino[1] ([1]*Grad. Sch. Frontier Biosci, Osaka Univ.*, [2]*IPR, Osaka Univ.*, [3]*JEOL YOKOGUSHI, Osaka Univ.*, [4]*RIKEN SPring-8*, [5]*RIKEN BDR*)

The bacterial flagellar protein export machinery utilizes ATP and proton motive force to translocate polypeptides across the cell membrane. The export machinery regulates its gating function because an increase in the probability of gate opening could be deleterious to cells due to leakage of small solutes. The transmembrane export engine acts as a proton-protein antiporter to couple the proton flow through a proton channel with protein translocation through a polypeptide channel to construct flagella in the cell exterior, but it remains unknown how the export engine opens its proton and polypeptide channels in a coupled manner. In this symposium, we will discuss our current understanding of the well-coordinated gating mechanism of the flagellar export engine.

2S-17-4 Bacterial flagellar rotation at low load

Yoshiyuki Sowa[1,2], Tsubasa Ishida[2] ([1]*Dept. Frontier Biosci., Hosei Univ.*, [2]*Grad. Sch. of Sci. & Eng., Hosei Univ.*)

The bacterial flagellar motor is a rotary nano-machine powered by the ion flux across the cytoplasmic membrane. Multiple torque-generating stator units can simultaneously interact with a rotor. To reveal how the motor works, we've developed single motor assays to measure its rotation over a wide range of loads to motors. In this talk, in particular, we focus on the motor behavior at low load. The motor rotation near zero load showed distinct levels, corresponding to the number of stator units interacting with a rotor. This indicates the motor working at low load has a low duty ratio.

2S-17-5 Patterns and randomness: Tools for studying bacterial navigation

Erick E. Rodriguez Salas, Emma E. Brock, **Laurence G. Wilson** (*Department of Physics, University of York*)

The randomising influence of Brownian motion dominates life on the micrometre scale and confounds microorganisms' attempts to navigate. Bacterial strategies for overcoming this phenomenon vary depending on the morphology of cells and the nature of the environment in which they swim. We have developed a high-throughput holographic microscope system for tracking several hundreds of cells simultaneously. We image sample volumes up to a cubic millimetre, at capture rates up to 500 Hz. I will discuss how the system operates and outline key results from tracking experiments and the numerical models they inform, in bulk fluids and complex media such as agar.

2S-17-6 数理モデルを用いた細菌の走化性強さの推定
Estimation of the intensity in bacterial Chemotaxis by Using a Mathematical Model

Tonau Nakai, Tomonobu Goto (*Tottori Univ.*)

Peritrichous bacteria repeat a straight swimming (run) and an abrupt change of the swimming direction (tumble). Cells exhibit chemotaxis by decreasing the frequency of the tumbles if they have swum toward the favorable direction. A mathematical model has been proposed where the probability of tumbling is correlated with the chemotaxis intensity. In this study, we observe the chemotactic behaviors of bacterial cells and compare the measurement with the mathematical model. Salmonella typhimurium SJW1103 cells swimming in the concentration gradient of a chemoattractant (L-serine) were observed. The duration of runs is longer for "up the gradient"(2.0 s) than "down" (1.3 s) and then the chemotaxis intensity (takes the value from 0 to 1) is estimated to be 0.35.

2S-17-7 Studies on bacterial motility as the virulence factor

Jun Xu (*Dept. Bacteriol., Grad. Sch. Med., Univ. Ryukyus.*)

Motility is crucial for many bacteria in the process of invasion and/or dissemination. Our studies focus on the flagellated pathogenic bacteria with motility that is necessary during the infection. We investigated the unknown motility-dependent pathogenicity of Leptospira spp., which can swim in the liquid and crawl on the solid surface. Crawling motility on the kidney cell surface was observed and analyzed and related to the host-pathogen relation during the actual infection. The results associate the kinetics and kinematic features of the spirochetal pathogens with their virulence. On the other hand, we searched on the biochemical compounds that potentially compromise the physiological activities such as bacterial motility then leads to the attenuation of virulence.

3S-1-1 遺伝子組換え抗菌ペプチドの生産技術の開発と応用
Development and application of novel overexpression systems of antimicrobial peptides

Tomoyasu Aizawa (*Fac. Adv. Life Sci., Hokkaido Univ.*)

The production of large numbers of targets is a key step in studies on antimicrobial peptides. For example, NMR studies using stable isotope-labeled recombinant peptides are among the most powerful means of studying the structures and interaction. Many protein expression systems have been established to produce recombinant proteins. Moreover, a wide variety of strategies have been developed to improve the yield of recombinant proteins. However, it is very difficult to produce small target peptides that are lethal to host cells and/or are easily degraded in soluble form. In this talk, some methods of facilitating the expression level of recombinant peptides that are difficult to express in conventional production systems will be discussed.

3S-1-2 ヘリカル構造制御に基づく抗菌ペプチドフォルダマーの開発
Development of helix-stabilized antimicrobial peptide foldamers

Yosuke Demizu[1,2] ([1]*NIHS*, [2]*Grad. Sch. Med. Life Sci., Yokohama City Univ.*)

Antimicrobial peptides (AMPs) have been paid much attention as the next-generation drugs against multidrug-resistant bacteria. One of the most studied of the amphipathic helical AMPs is Magainin 2 (Mag 2), which is composed of 23 amino acid residues, and its helical structure and amphipathic property play a pivotal role to exert the potent antimicrobial activity. However, the large molecular weight and the chemical stability of the peptide backbone against digestive enzymes could be a barrier for clinical use of the AMPs. In this study, we aimed to develop the novel Mag 2-based AMPs with potent antimicrobial activity and chemical stability by the enhancement of the helicity and the amphipathicity of Mag 2 sequence utilizing non-proteinogenic amino acids.

3S-1-3 Cryptdin-4 conformations and interaction with membrane studied by membrane self-assembly molecular dynamics simulations

Takao Yoda (*Nagahama Institute of Bio-Science and Technology*)

Cryptdin-4 (Crp4) is an antimicrobial peptide of mice. It permeabilizes negatively charged membrane. It also translocates across the membrane. A kinetic study of the translocation using vesicles suggested that Crp4 oligomerization takes place just before the translocation. However, the role of the translocation and the possible oligomerization for the permeabilization activity is not known. To address this issue, we performed a molecular dynamics simulation study. Since the time scale of Crp4 bactericidal action is ~100 seconds, we cannot observe the translocation process straightforwardly by a molecular simulation. Thus, we tried to observe Crp4 interacting with other molecules and the oligomer conformations by use of membrane self-assembly simulations.

3S-1-4 膜貫通αヘリックスペプチドバレルの理論設計
Rational design of membrane-spanning alpha-helical peptide barrels

Ai Niitsu[1], Andrew R. Thomson[2], Alistair J. Scott[2], Jason T. Sengel[3], Yuji Sugita[1], Mark I. Wallace[3], Hagan Bayley[4], Derek N. Woolfson[2] ([1]*Wako Inst., Riken*, [2]*Univ. Bristol*, [3]*KCL*, [4]*Univ. Oxford*)

Rational design of membrane proteins tests our knowledge of membrane protein folding while delivering novel protein structures which do not exist in nature. However, membrane protein design is still in its infancy due to the limited number of high-resolution structures. To advance the research field, we design, synthesize and characterize membrane-spanning alpha-helical peptide barrels by combining computational peptide design, molecular dynamics simulation, and experimental biophysics. In this presentation, we demonstrate new de novo designs of coiled-coil peptide-based ion channels, which could further our understanding of fundamental helix-helix interaction competing with lipid-peptide interaction in lipid bilayers.

3S-1-5 Analysis of transmembrane peptides using a lipid bilayer system

Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology (TUAT)*)

We have developed the molecular basis of the structure of the transmembrane peptide in a bilayer lipid membrane. The channel current signals measured in our lipid bilayer system reflect the assembling structure such as the pore formation of the transmembrane peptides. We assigned the current signal against the transmembrane model of peptides: the barrel-stave, toroidal pore, and penetration models that have previously proposed. Besides, we analyzed the spike signals to estimate the membrane penetration of model cell-penetration peptides (CPPs). Based on our method, I will share our recent progress on the molecular basis of the pore formation of antimicrobial peptides and the cell penetration behavior of CPPs.

3S-1-6 両生類由来カチオン性抗菌ペプチドの生体膜との相互作用
Interaction of amphibian-derived cationic antimicrobial peptides with model membrane

Izuru Kawamura (*Grad. Sch. Eng. Sci., Yokohama Natl. Univ.*)

Hymenochirin-1Pa (H-1Pa) is a cationic antimicrobial peptide (+7) isolated from the frog *P. merlini*. H-1Pa in a family of hymenochirins is the most active against *S. aureus* (MIC = 2.5 microM). However, the atomic-level membrane-bound structure has not been clarified. In this study, we investigated the behavior of the conformations and interactions of H-1Pa with the *S. aureus* mimetic membrane using solid-state NMR and MD simulations. ^{13}C NMR signals of isotope-labeled H-1Pa showed the transition of secondary structure from random coil in a solution to amphiphilic alpha-helix in the membrane. MD simulations showed that Lys residues in the helical H-1Pa interact with anionic lipid head groups in the membrane to disturb the structure of the lipid bilayer.

3S-2-1 キネシン 1 の運動と細胞骨格が生む無秩序なゆらぎ
Kinesin-1 Movement and Cytoskeletal Disordered Fluctuations

Takayuki Ariga (*Grad. Sch. Med., Yamaguchi Univ.*)

Kinesin 1 is a biomolecular motor that transports cargo in cells. We have measured the dissipation of the walking kinesin in vitro, and found that almost 80% of the input free energy change from the ATP hydrolysis was dissipated without being transmitted to the probe particles [Ariga PRL 2018]. On the other hand, the intracellular environment in which kinesin actually acts is actively (nonthermally) fluctuating maybe due to the cytoskeletal networks [Nishizawa Sci. Adv. 2017], indicating a critical difference from the in vitro environment. In this symposium, we will briefly introduce these previous findings and report our current results on the kinesin movement in vitro artificially mimicking the cell, comparing with the mathematical model simulation of kinesin.

3S-2-2 紡錘体の形成と機能を支える微小管のメソスケールメカニクス
Mesoscale microtubule mechanics controlling the assembly and function of the chromosome segregation machinery

Yuta Shimamoto[1,2] ([1]*Nat'l Inst Genetics*, [2]*SOKENDAI*)

Spindles are bipolar arrays of microtubules whose mechanism of self-organization for proper cell division remains a mystery. Recently, we have established an assay in which the motility and force responses of individual spindle microtubules could be systematically analyzed using force-calibrated microneedles, confocal live imaging, Xenopus egg extract, and microrheology. This led us to discover the local mechanical heterogeneity of the spindle and how microtubules slide apart in response to a force that alters spindle length. Molecular perturbation assay suggested that the mechanical heterogeneity depends on kinesin-5 and dynein, two key microtubule motors. Our data propose how the collection of microtubules gives rise to the robust and adaptable nature of the spindle.

3S-2-3 繊毛の制御機構
How to control cilia movement

Masahide Kikkawa (*Grad. Schl. of Med. Univ. of Tokyo*)

Eukaryotic cilia are complex cell organelles and play important roles in various cells. They consist of hundreds of different proteins that are precisely organized. In addition, the movement of cilia in higher organism have various modes, such as symmetric, asymmetric. and rotational movement. To understand how those movement are controlled, we combine genetics and cryo-electron microscopy. For example, we knocked-out efcab1 in zebrafish, which encode calaxin, and found that the mutant zebrafish have situs inversus due to the irregular ciliary beating of Kuppfer's vesicle cilia. We also analyzed olfactory cilia (asymmetric) and sperm flagella (symmetric) of zebrafish using cryo-electron tomography to elucidate the mechanism of cilia beating mode.

3S-2-4 ダイニン運動性の制御 -細胞質ダイニンの自己阻害とその調節機構
Regulation of dynein motility -Autoinhibition of cytoplasmic dynein and the regulatory mechanism

Yoko Toyoshima[1,2] ([1]*Dept of Life Sciences, Grad Sch of Arts and Sciences, The Univ of Tokyo*, [2]*Komaba Institute for Science, Grad Sch of Arts and Sciences, The Univ of Tokyo*)

Dynein is a microtubule (MT) minus end-directed molecular motor. The purified dynein moves MTs in motility assay, however, single molecules of mammalian dynein did not move unidirectionally, but moved diffusively along a MT. The two heads of dynein molecule were stacked and dynein molecules are autoinhibited (Torisawa et al. 2014). This autoinhibition was removed when a small force was loaded on dynein by tethering to a bead via dynein tail or linking multiple dynein molecules. The ability is consistent with the dynein behavior in the cell, that is, free dynein molecules without the cargo cannot move on MTs, but they switch to active or produce the force when necessary. Other regulatory mechanism by dynein binding proteins, such as dynactin, will be also discussed.

3S-2-5 プログラマブルなサルコメア設計から紐解く筋ミオシン集団の協調的な力発生
Coordinated force generation of muscle myosin dissected by a programmable sarcomere design

Mitsuhiro Iwaki[1,2], Takumi Washio[3], Toshio Yanagida[2,4] ([1]*RIKEN, BDR*, [2]*Grad. Sch. Front. Biosci., Osaka Univ.*, [3]*Grad. Sch. Front. Sci., Univ. of Tokyo*, [4]*CiNet*)

Muscle is a highly sophisticated mechanical system that functions as a universal natural actuator in animals. To achieve the mechanical performance, muscle myosin IIs should well coordinate together in the highly-structured sarcomere, the minimal mechanical unit of muscle, which is composed of rigorously arranged myosin II-based thick filaments and actin-based thin filaments. Although extensive studies have revealed the single myosin mechanics, the coordinated mechanism remains elusive. Here we designed the sarcomere composed of DNA origami scaffold and recombinant human muscle myosin II. The design is tunable and enabled us to directly and simultaneously visualize individual myosin dynamics by high-speed AFM. We'll discuss the cooperative phenomena.

3S-2-6 Long range allostery in actin filaments, and its differential requirement in force generation by actomyosin II and V

Taro Uyeda (*Dept Phys, Waseda Univ*)

Chemical crosslinking and two actin mutations that likely perturb conformational dynamics of actin filaments (AF) inhibit actomyosin II movements in vitro. However, they do not affect the ATPase activity and rigor binding, arguing against the idea that the roles of AF are only to stimulate Pi release from M-ADP-Pi and to provide foothold to maintain tension. Moreover, sparse binding of Rng2CHD (actin binding domain of an IQGAP) and G680V S1 to AF inhibit and accelerate the movements, respectively, implicating long range allostery along AF in the movements. Intriguingly, the mutant actins and Rng2CHD do not inhibit actomyosin V. Thus the conformational dynamics and long-range allostery of AF appear essential for the force generation by actomyosin II but not by myosin V.

3S-3-1 クリプトクロムを介した光駆動性磁気受容
Light-driven magnetoreception mediated by cryptochromes

Toshiyuki Okano (*Grad. Sch. Adv. Sci. Eng., Waseda University*)

Cryptochromes (CRYs) are multifunctional photoreceptive proteins found in a wide variety of living organisms. In animals, CRYs play roles in a core circadian transcriptional repression, a circadian photoreception, a blue light sensing, and a light-driven magnetoreceptor. Especially in aves, photosensitive CRYs are shown to reside in the retina and suggested to operate as a magnetoreceptor. Although the molecular mechanism for the CRY-mediated magnetoreception is uncovered yet, a radical pair model (RPM) has been proposed as the most plausible mechanism. In this presentation, I will briefly introduce the animal magnetoreception and theoretical aspect of RPM and review relevant studies including our recent data.

3S-3-2 クリプトクロムタンパク質の光誘起構造変化ダイナミクス
Understanding the photoinduced structural dynamics of cryptochrome proteins

Lewis M. Antill[1,2], Ichiro Sakata[3], Shin Hatakeyama[3], Kiminori Maeda[1] ([1]*Department of Chemistry, Saitama University*, [2]*PRESTO, Japan Society and Technology Agency (JST)*, [3]*Department of Regulatory Biology, Saitama University*)

A magnetic field effect (MFE) on a photochemical reaction is believed to be responsible for the magnetic compass sense of migratory birds. Previous research focussed on the primary light-induced magnetic field sensitive processes, yet the CRY photoreaction comprises four key steps, (i) photoexcitation of the chromophore, flavin adenine dinucleotide (FAD), (ii) intermolecular electron and/or proton transfer, (iii) the conformational change in the protein, and (iv) signal transduction and functional expression. Steps (iii) and (iv) remain elusive. To address these steps, we propose to study the propagation of the signal produced from the second radical pair, by focussing on the relationship between inherent CRY oligomerisation and magnetic field sensitivity.

3S-3-3 磁場効果から見たタンパク質バインディングポケット中でのラジカル対挙動
Radical pair dynamics in binding pockets of proteins probed by magnetic field effects

Nana Iwata[1], Lewis Antill[1,2], **Kiminori Maeda**[1] ([1]*Graduate School of Science and Engineering*, [2]*JST PRESTO*)

A drug binding protein, BSA (bovine serum albumin), reacts with a photo-excited triplet state of 2,6-AQDS (2,6-anthraquinone disulfonate) and produce radical pairs (RPs) of Trp(H+) and AQDS3- radicals. BSA has a few binding pockets and 2,6-AQDS is bound in a pocket. Here, we study the RP dynamics of BSA/2,6-AQDS system by static and pulsed MFE (magnetic field effect) techniques precisely. The results can be modelled by two site RP system. In that, one RP is reactive, and the other RP works as a reservoir. This kinetic feature is similar to the cryptochrome, which is the most likely candidate of the magnetic sensor for animal navigation. The further dynamical feature and assignment of the second binding pocket can be discussed with the molecular dynamics simulation.

3S-3-4 Magnetic field sensitivity of cellular photochemistry

Noboru Ikeya, **Jonathan R. Woodward** (*The University of Tokyo, Graduate School of Arts and Sciences*)

The radical pair mechanism is the favoured hypothesis for explaining biological effects of weak magnetic fields. To date, however, there is no direct experimental evidence for magnetic effects on photochemical processes in living cells. In this study, using a custom-built microscope, we demonstrate that flavin based autofluorescence in native, untreated HeLa cells is magnetic field sensitive, due to the formation and electron spin-selective recombination of spin-correlated radical pairs. In addition, we discuss our recently developed techniques for investigating the magnetic field sensitivity of photochemical reactions at the cellular level.

3S-3-5 細菌の磁気コンパス–マグネトソーム形成の生細胞イメージング–
A magnetic compass within a bacterium – Live-cell imaging of magnetosome formation –

Azuma Taoka[1,2], Yoshihiro Fukumori[2] ([1]*Inst. Sci. and Eng., Kanazawa Univ.*, [2]*NanoLSI, Kanazawa University*)

Magnetotactic bacteria (MTB) possess a unique bacterial organelle, termed the magnetosome, which functions as a magnetic sensor. The integration of this magnetic sensor into their motility process allows MTB to swim along the geomagnetic field in order to find a favorable microaerobic habitat. Although the magnetosome is organized by magnetosome associated proteins (Mam proteins), the molecular mechanism of magnetosome synthesis is still unknown. We developed the microscopic techniques for imaging magnetosomes in a living bacterial cell and analyzed functions of the Mam proteins in magnetosome formation. We will discuss how MTB organize the nano-meter sized magnetic sensor organelle.

3S-3-6 溶液中の超分子の配向挙動：磁場強度，濃度，有効電荷に対する依存性
Orientational behavior of supramolecules in solution depending on magnetic field strength, concentration, and effective charge

Mitsuhiro Hirai (*Graduate School of Science and Technology, Gunma University*)

The mechanism of the biomagnetic effect is an old and new issue. The recent report of a multimeric magnetosensing protein complex has refocused this issue. By using X-ray solution scattering, we reported previously on the dependence of the orientational behavior of supramolecules (rod-like viruses: TMV and CGMMV) in solution on magnetic field strength and gradient, concentration, and effective charge. Although TMV and CGMMV have an isomorphic structure, those responses to the magnetic field were quite different owing to the difference in the effective surface charge between those constituents. The application of the magnetic field caused the phase transition and the cooperative orientation of the molecules due to the clustering and/or growth of the nematic domain.

3S-3-7 磁気受容蛋白質第二候補 ISCA1 の分子挙動
Molecular behavior of the second magnetorecepter candidate protein ISCA1

Shigeki Arai[1], Rumi Shimizu[1], Motoyasu Adachi[1], Satoshi Ajito[2,3], Mitsuhiro Hirai[3] ([1]*Institute for Quantum Life Science, QST*, [2]*JAEA*, [3]*Department of Physics, Gunma Univ.*)

Cryptochromes (Crys) in some species like clCry4 of Columba livia act as the quantum magnetic sensors. However, it is unclear where and how the clCry4 receives the magnetic information and transmits it to perception. The Fe-S cluster assembly 1 homolog clISCA1, which interacts with clCry4, is one of the candidates that may assist the magnetic response and/or the signal transduction of clCry4. By SAXS analysis, we revealed that the native structure of clISCA1 is changeable between the globular and the rod-like shapes. This structural change affects the affinity of clISCA1 for Fe-S cluster, and consequently the magnetoreception reaction of the clCry4/clISCA1 complex might be controlled. In this symposium, we introduce our research including the overview and future plans.

3S-4-1 High-speed atomic force microscopy as a versatile tool to study dynamical and mechanical properties of proteins

Christian Ganser[1], Kimitoshi Takeda[2], Ryota Iino[2], Koichi Kato[1], Takayuki Uchihashi[3] ([1]*NINS, ExCELLS*, [2]*NINS, IMS*, [3]*Grad. Sch. Sci., Nagoya Univ.*)

High-speed atomic force microscopy (HS-AFM) has proven to be an invaluable tool to characterize dynamical behavior of proteins on the sub-second time scale. While the most used HS-AFM mode is topography imaging of proteins in real-space and real-time, newer developments extend this functionality. First, an example of topographical imaging of kinesin walking on microtubules will be presented and - by keeping microtubules in the focus - advanced methodology for mechanical characterization will be introduced. The extended functionalities are in-line single point probing of mechanical properties without interrupting scanning and full force mapping where hundreds of force curves are recorded within two seconds to create a map of mechanical properties.

3S-4-2 Photon Factory における BioSAXS 活用した相関構造解析
Recent hybrid methods approach utilizing Biological Small Angle X-ray Scattering at the Photon Factory

Kento Yonezawa[1], Ayako Furukawa[2], Naruhiko Adachi[1], Toshiya Senda[1], Nobutaka Shimizu[1], Yoshifumi Nishimura[2,3] ([1]*IMSS, KEK*, [2]*Grad. Sch. Med. Life Sci., Yokohama city Univ.*, [3]*Grad. Sch. Integ. Sci. Life, Hiroshima Univ.*)

Biological small-angle X-ray scattering (BioSAXS) enables us not only to evaluate the solution structural information of a biological macromolecule but also to analyze the structural transition of the target sample during the chemical reactions and oligomerizations. The hybrid approaches combined with BioSAXS are expected to supply a more reliable explanation of phenomena in various molecular complex systems. We, Photon Factory (PF), have updated the software and the hardware for the analysis of highly accurate SAXS data attributed to these phenomena. In this presentation, we will introduce the recent progress of BioSAXS measurement systems at the PF, and the current hybrid approach analysis concerned with the heterochromatin protein as an example of its application.

3S-4-3 カルボニルストレスを伴う統合失調症における CRMP2 タンパク質の機能異常解析
Enhanced carbonyl stress induces irreversible multimerization of CRMP2 in schizophrenia pathogenesis

Xuguang Jiang[1], Manabu Toyoshima[2], Tadayuki Ogawa[1], Takeo Yoshikawa[2], Nobutaka Hirokawa[1] ([1]*Grad. Sch. Med., Univ. Tokyo*, [2]*Riken CBS*)

Enhanced carbonyl stress is a critical pathophysiology for multiple diseases, including schizophrenia, but little is known about the molecular pathogenesis. CRMP2, a crucial multifunctional regulatory protein that is highly expressed in human brain, was identified as a major target of hyper-carbonyl modification (AGE modification) in schizophrenia patient-derived iPS cells. Using a multimodal combination of iPS technology, cell biology, biochemistry, mass spectrometry and structural biology, we found that carbonylated CRMP2 is stacked in irreversible cross-linked multimer states via AGE modification and thereby results in neurodevelopmental deficits, which underlies the major pathogenic pathway of schizophrenia under carbonyl stress.

3S-4-4 Impacts of the N-glycan variation of antibodies on their dynamic structures of functional relevance

Saeko Yanaka[1,2,3], Rina Yogo[1,2,3], Hirokazu Yagi[3], Koichi Kato[1,2,3] ([1]*ExCELLS, Natl. Inst. Nat. Sci.*, [2]*IMS., Natl. Inst. Nat. Sci.*, [3]*Grad. Sch. Pharma. Sci., Nagoya City Univ.*)

The Fc region of immunoglobulin G (IgG) harbors a pair of N-glycans with microheterogenieties depending on physiological and pathological states. IgG exerts versatile immune function through its interactions with effector molecules such as Fcγ receptor, which depend on the N-glycan structures. However, the molecular mechanisms linking the N-glycan diversity and the functional interactions of IgG remain largely unknown. We address this issue from a structural point of view. The IgG structure is characterized by quaternary conformational plasticity coupled with conformational flexibility of the N-glycans. Here we present our latest findings obtained by experimental and computational approaches, revealing dynamic structures of a panel of IgG-Fc glycoforms.

3S-4-5 超遠心分析および光散乱によるタンパク質の溶液挙動の解析
Characterization of Protein Assembly by Analytical Ultracentrifugation and Light Scattering

Fumio Arisaka (*Grad Sch Biosci Bioeng, Tokyo Tech*)

Analytical Ultracentrifugation and Light Scattering are methods for determination of molecular weight and Stokes radius or radius of gyration based on the first principle, which nowadays are experiencing tremendous developments in both instrumentation and methodology. Analytical ultracentrifugation itself can do both separation and analysis, but light scattering does not have the ability for separation. It, therefore, utilizes SEC(size exclusion chromatography) or FFF(field-flow fractionation) which is connected in series to separate the solutes and are analyzed by the former. The systems are called SEC-MALS and FFF-MALS, respectively. In this talk, we introduce a number of protein assembly systems which have been analyzed by the two methods.

3S-5-1 クロマチン濃度により制御されるクロマチン運動
Chromatin mobility controlled by chromatin concentration

Takahiro Sakaue (*Aoyama Gakuin Univ.*)

Recent experiment has reported that the chromatin mobility in C.elegans embryos decreases with the cell stage. During the embryogenesis, the nucleus becomes smaller, and the resultant increase of the chromatin concentration in nucleoplasm is expected to be a primal source for the mobility reduction. To assess such a view quantitatively, we propose a physical model, in which the chromatin mobility is dictated by the topological constraint (i.e., polymers can not pass through each other freely). This framework, with its ability to naturally explain the observed cell-stage dependent chromatin mobility through the concentration dependent topological length and time scales, suggests an importance of generic physical mechanics at play in the regulation of gene expression.

3S-5-2 Measurements of physical properties underlying the chromatin mobility in interphase nuclei

Noritaka Masaki, Akatsuki Kimura (*Cell Arch. Lab., NIG*)

Motion of chromatin loci observed in interphase nuclei correlates with various DNA metabolism including transcription and recombination. P hysical bases of the motility, such as driving force and viscoelastic environment, are remained unclear. Our group has revealed the reduction in the chromatin mobility during early embryogenesis of *C. elegans* [1]. Interestingly, the mobility is not simply scaled against cleavage division but seems to reflect alteration in friction or viscosity. Therefore, we are attempting to characterize the physical properties in the nucleus. Our experimental measurements of the dynamics and physical properties of the nuclei in early embryogenesis of *C. elegans* are presented and discussed. [1] Arai *et al*. *Sci. Rep.* 7, 3631- (2017)

3S-5-3 動的 3 次元ゲノム組織化の物理的理解にむけて
Toward a physical understanding of the dynamic 3D genome organization

Soya Shinkai[1], Shuichi Onami[1], Ryuichiro Nakato[2] ([1]*RIKEN BDR*, [2]*IQB, Univ. Tokyo*)

The three-dimensional (3D) genome architecture plays a crucial role in diverse biological activities intricately cooperating in the genome. Recent genome-wide chromosome conformation capture (Hi-C) experiments have uncovered the 3D genome organization and revealed multiscale chromatin domains. Although thermal fluctuations inevitably drive the genome molecules' movements in the microscale cell environment, there is no way to understand such a dynamic 3D genome organization of hierarchical and structural chromatin units. We will highlight our recent works for deciphering Hi-C data into polymer dynamics toward a physical understanding of the dynamic 3D genome organization.

3S-5-4 1 分子イメージングで迫るヒトゲノムクロマチンの動的組織化
Single nucleosome imaging sheds light on the dynamic organization of the human chromosomes

Kayo Hibino[1], Yuji Sakai[2], Masato Kanemaki[1], Kazuhiro Maeshima[1] ([1]*NIG and SOKENDAI*, [2]*Univ. Tokyo*)

The chromosome condensation during cell division is a dramatic reorganization of the long thin genome chromatin polymers (several centimeters) into compact short chromosomes (several micrometers). While this process requires some large proteins including condensins and topoisomerase IIα. the underlying mechanism remains unclear. Here, we measured local nucleosome dynamics during the condensation process by single nucleosome imaging in living human cells. Using rapid depletion of target proteins by auxin-inducible degron (AID) system, we investigated possible roles of condensins and other factors in the process in terms of local nucleosome behavior. Combining with simulation studies, we discuss the physical aspect of the mitotic chromosome condensation.

3S-5-5 エントロピー駆動のクロマチン相分離によるゲノム 3D 構造形成
3D genome organization through entropy-driven phase separation of chromatin

Shin Fujishiro, **Masaki Sasai** (*Department of Applied Physics, Nagoya University*)

We simulated the G1 nuclei of human cells to show that phase separation driven by the difference in the way of chromatin movement is the key mechanism. Starting from the initial condensed chains representing the late M phase, the simulated chains were expanded by the heterogeneous repulsive interactions among chromatin to form the nuclear envelope and nucleoli. Chromosome territories and A/B compartments were formed and the calculated genome structure reproduced the observed inter- and intra-chain Hi-C data, and LAD and NAD distributions. The method predicted formation of chromatin domains of movement and active regions of transcription, thus provides a platform to examine the relations among genome structures, dynamics, and functions.

3S-5-6 DNA contributes to nuclear size control in Xenopus laevis

Shuichi Nakano[1,2], Hiroko Heijo[1], Sora Shimogama[1], Yasuhiro Iwao[2], **Yuki Hara**[1] ([1]*Fac. Sci., Yamaguchi Univ.*, [2]*Grad. Sch. Sci., Yamaguchi Univ.*)

Cells adapt to drastic changes in genome during evolution and cell cycle by adjusting the nuclear size to exert genomic functions. However, the mechanism by which DNA content and chromatin structure within the nucleus contribute to controlling the nuclear size, remains unclear. Here, we experimentally evaluated the effects of DNA content and chromatin structure by utilizing cell-free Xenopus egg extracts. Upon manipulation of DNA properties, expansion dynamics and structure of the nucleus correlated with DNA physical properties. These results demonstrate a novel model in which the physical properties of the chromatin, rather than the coding sequences themselves, contribute to nuclear size determination by generating forces.

3S-6-1 異なる圧力下での光操作
Optical Manipulation at Different Pressures

Masayoshi Nishiyama (*Kindai Univ.*)

Optical tweezers technique is one of the powerful methods that manipulate microscopic objects under microscope. By using this technique, the mechanical properties of many molecular machines have been investigated. However, it is not technically easy to apply forces to a lot of research targets under the microscope. On the other hand, high-pressure technique has an advantage that an isotropic and uniform force could be applied to the system. Here, we report a novel technique that combines optical forces and high-pressure techniques. The developed system could be used for studying the mechanical properties of molecular machines.

3S-6-2 May the Red Force be with Educational Unit of Optical Tweezers

Yuichi Inoue (*OptoSigma*)

Light source of optical tweezers, typically ~1000 mW and ~1064 nm, has been changed into a weak red laser (4.5 mW, 635 nm) for educational unit of optical tweezers. The new unit can be used with not only professional microscopes but also educational microscopes for easy and low-priced start of optical tweezers as well as new applications as local activation of biomolecules on single carbon nanotube (Inoue et al., 2015). The new unit is also compatible to future upgrades of the laser power and/or the optional kit for nanometer measurement. Although the trapping stiffness of ~0.008 pN/nm (1 μm bead, 4.5 mW) is not enough to measure stall force of motor proteins, we hope beginners in the various field enjoy to make the first step of optical tweezers and future upgrades.

3S-6-3 3 次元位置検出顕微鏡と光ピンセットを用いた、“繊毛 1 本” のトラッキングとマニピュレーション
Tracking and manipulation of a cilium by the 3-D tracking microscopy and optical tweezers

Takanobu A Katoh (*BDR, Riken*)

Cilium, a hair-like protrusion on the surface of cells, is one of nature's elaborate structures. Motile type of cilium shows self-organized beating driven by thousands of axonemal dyneins. Here, we achieved the manipulation of mouse tracheal cilium with nanometer accuracy by the optical tweezers, revealing that cilium changes their beating-mode under auxotonic loading condition (Katoh *et al., Sci Rep*., 2018).
Currently, I focus on the immotile primary cilium, another type of cilium which senses flow-dependent signal as the cell's antenna. By manipulating the nodal immotile cilium, we demonstrated that mechanical stimuli activate mRNA degradation *in situ*, suggesting that nodal immotile cilium functions as a mechano-sensor.

3S-6-4 心筋および骨格筋ミオシンの個性とその機能を探る
Exploring the characteristics of cardiac and skeletal myosins and their functions

Motoshi Kaya (*Dept of Physics, Univ of Tokyo*)

Skeletal and cardiac myosins have been assumed to be similar in molecular function because of high amino-acid identity between these proteins. By using optical-tweezer-based microscopy, we revealed that dynamic responses of these myosins are distinctively different in response to loads and these molecular properties strongly influence on their ensemble behaviors. Our simulation model further suggested that these molecular properties are prerequisite for skeletal muscle and heart contractions, respectively. In this symposium, our recent findings obtained from the comprehensive approach based on optical-tweezer-based force measurements on single cardiac and skeletal myosins / myofilaments combined with simulations will be discussed.

3S-6-5 Nanostructure-assisted optical tweezers for soft matter manipulation

Tatsuya Shoji (*Fac. Sci., Kanagawa Univ.*)

Since the pioneering work of Arthur Ashkin in 1970, there has been the significant development in optical tweezers (OT) for the manipulation of microparticles such as living cells, bacteria, and so on. Such trapping techniques will become an indispensable tool for the manipulation of soft matters such as DNA and proteins. For such motivation, we have recently developed novel optical tweezers by using nanostructured silicon surfaces. We named it NASSCA (nanostructured semiconductor-assisted) OT. Such nanostructured-assisted OT allows us to trap numerous nanoparticles in a wide area, being capable of optically separating and aligning them on the basis of chemical composition, shape and size of nanoparticles.

3S-6-6 生化学反応の光誘導加速システムが拓く生物物理の新展開
Prospects of Biophysics Created by Light-induced Acceleration System for Biochemical Reaction

Takuya Iida[1,2], Shiho Tokonami[1,3], Ikuhiko Nakase[1,2] ([1]*Grad. Sch. Sci., Osaka Pref. Univ.*, [2]*Res. Inst. for LAC-SYS, Osaka Pref. Univ.*, [3]*Grad. Sch. Eng., Osaka Pref. Univ.*)

A biomolecular recognition (DNA double strand formation, antigen-antibody reaction etc.) is crucial for the high selectivity in the specific detection used in medical care and food inspection. In this talk, I would like to introduce our recent development on "light-induced acceleration system (LAC-SYS)" focusing on three topics as follows: (A) Rapid formation of submillimeter structure triggered by light-induced hybridization of zmol-level DNA, (B) Detection of a small amount of protein (pg-level to fg-level), and (C) Light-induced assembly of microbes with bio-mimetic optical substrate. Based on these achievements, I will show our challenge in LAC-SYS for various biochemical reactions and prospects toward the next generation biophysics.

3S-6-7 集光レーザービームを用いたタンパク質集合体の作製
Fabrication of Highly Ordered Protein Assembly by Focused Laser Beam

Hiroshi Yoshikawa (*Dept. Chem., Saitama Univ.*)

Protein forms assemblies with various ordered structures such as crystals and fibers. The control of formation of such assemblies is one of the keys to understand protein machinery and its application. However, self-organization of protein is usually driven with weak interactions, and thus it is often very challenging to obtain assemblies with desired size, shape, and structures even with systematic optimization of key parameters. In this talk, I introduce the spatiotemporal control of formation of protein assemblies by focused laser beams, laser ablation and laser trapping. These laser techniques enable us to obtain protein assemblies with unique properties that are not formed by spontaneous methods alone.

3S-6-8 光圧による細胞表面分子の直接操作と神経活動制御への応用
Optical manipulation of cell surface molecules for direct control of neuronal activity

Chie Hosokawa (*Grad. Sch. Sci., Osaka City Univ.*)

Neurons in a complex network communicate with each other through synaptic connections. Molecular dynamics of neurotransmitter receptors is essential to regulate synaptic transmission. Novel approaches using reversible perturbation on neurons with high spatial and temporal resolutions hold promise for direct control of neuronal activity. Here, we demonstrate optical manipulation of glutamate receptors on neuronal cells using a focused laser beam. Simultaneous measurements that combine optical trapping and fluorescence imaging with patch-clamp recordings to monitor the electrical activity of target neuron are performed to reveal the relationship between optical manipulation and neuronal activity.

20001A* 全原子分子動力学法による維持メチル化酵素(Dnmt1)とその捕因子の動態解析
Theoretical Analyses on Dynamic Properties of DNA methyltransferase 1 and its Cofactors Based on All-atom Molecular Dynamics Simulations

Takunori Yasuda[1], Yasuteru Shigeta[2], Ryuhei Harada[2] ([1]*College of Biological Sciences, University of Tsukuba*, [2]*Center for Computational Sciences, University of Tsukuba*, [3]*Center for Computational Sciences, University of Tsukuba*)

DNA methylation is an important epigenetic mechanism for determining the character of cells. DNA methylation is divided into de novo methylation and maintenance methylation. Dnmt1 mainly works in maintenance methylation and play an important role of cell memory. In the preceding studies, several X-ray structures have been experimentally determined. Structurally, Dnmt1 shows large-amplitude conformational transitions are induced during its activation. However, there is still unclear for the dynamic transitions of Dnmt1 and its cofactors.Therefore, we traced the dynamics of Dnmt1 and its cofactor based on μs-order molecular dynamics (MD) simulations.

20002A 3D−RISM 理論を応用した溶液中におけるペプチドの構造揺らぎの解析
Analysis of structural fluctuations of a small peptide in the solution phase by means of 3D-RISM theory

Masatake Sugita (*Sch. Computing, Tokyo Tech*)

Recently, B. Kim and F. Hirata derived a new statistical mechanics formulation of characterizing the structural fluctuation of a complicated solute correlated with the molecular solvents based on the Generalized Langevin Equation and 3D-RISM theory. This formulation suggests that the Hessian matrix of the free energy corresponds to the inverse of the variance covariance matrix of the solute molecule in the solution phase. In this study, we analyze structural fluctuation of a Small peptide immersed in water by calculating the second order derivative, Hessian, of the free energy and diagonalizing the hessian matrix. We propose two protocols for estimating the Hessian. After that comparing the results with those from the Normal Mode analysis and MD simulation.

20003A 細菌べん毛形成開始するために 34 個集まってリングになる 2 回膜貫通タンパク質 FliF の N 末端・C 末端細胞質領域欠損体の解析
Analysis of the cytoplasmic region-deficient mutants of double-transmembrane protein FliF which forms a MS-ring in flagellar formation

Seiji Kojima[1], Mitsuki Kajino[1], Keiichi Hirano[1], Yuna Inoue[1], Tatsuro Nishikino[2], Hiroyuki Terashima[1], **Michio Homma**[1] ([1]*Nagoya Univ, Sch Sci, Div Biol Sci*, [2]*Osaka Univ, Ins Protein Res*)

The MS ring is flagellar basal body parts and formed by about 30 FliFs, which are 2-transmembrane protein. We made the FliF mutants which lucked the N- or C-terminal cytoplasmic regions. The N-terminal deletions were functional, but the C-terminal ones were not. When expressing N-terminal deletions, there were fewer MS rings. In a C-terminal deletion, MS ring was similarly observed to wild-type. However, no MS ring was observed with C-terminal region with the second transmembrane region. These results suggest that the N-terminal region is not indispensable, but affects the ring stability, whereas the C-terminal cytoplasmic region is essential for the function but unnecessary for MS ring formation but the second transmembrane region is indispensable to form MS ring.

20004A Pin1 の変異体 C113A と C113S の構造解析
Structural analysis of Pin1 mutants C113A And C113S

Teikichi Ikura, Nobutoshi Ito (*Med. Res. Inst., Tokyo Med. Dent. Univ.*)

Pin1 is a PPIase which catalyzes cis/trans isomerization of pS/pT-P bond. Its activity is related to various cellular functions including suppression of Alzheimer's disease. A cysteine residue C113 is known to be important for its PPIase activity; mutation of C113A or C113S resulted in a 123-fold or 20-fold decrease in kcat/Km, respectively. So far, various nuclear magnetic resonance experiments were performed for these mutants of C113, but only for their PPIase domains. It was still unclear how these mutations affected the overall structure of Pin1. In the present study, we determined crystal structures of full-length Pin1 mutants C113A and C113S at high resolutions. The effects of the mutations on full-length Pin1 will be discussed on the basis of these structures.

20005A* Similarity and difference between substrate analogue-induced and spontaneous folding of staphylococcal nuclease

Yujiro Mori[1], Saho Segawa[2], Kosuke Maki[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Sch. Sci., Nagoya Univ.*)

Although many proteins spontaneously fold into the native state, some proteins are folded coupled with binding to partner proteins or ligands even under physiological conditions. Previous study suggested that the initiation site of folding is different between spontaneous and ligand-induced folding of staphylococcal nuclease (SNase). In fact, it is located within the β-barrel domain in the spontaneous folding whereas it is around the ligand-binding site bridging the two domains of this protein in the ligand-induced folding. Here we aim at characterizing the difference and similarity in the two types of folding of SNase. We will discuss the physical chemical mechanisms of the folding/binding behavior.

20006A タンパク質の複合体の界面の相互作用のデータベース解析
Database analysis of protein-protein interaction

Wataru Sagawa, George Chikenji (*Dept. Appl. Phys., Nagoya Univ.*)

Protein-Protein Interaction (PPI) is important for molecular functions in biology. Understanding its mechanism is needed to design proteins that interact with other proteins. To gain deeper understanding of PPI, we performed a database analysis of PPI. In particular, unlike many researches of database analysis of PPI, which focus on prefferd contact pairs, we focused on the composition of PPI members. We performed hierarchical clustering for interfaces of protein complexes and found that these are classified into only a limited number of patterns. The composition of amino acid constituting the interface largely differs depending on the pattern. In the presentation, we will provide detail data and discuss how our results are useful for designing protein binder.

20007A* Cross-seeding of human and bovine insulin amyloid fibrils induces stepwise conformational transition via intermediate states

Keisuke Yuzu[1], Naoki Yamamoto[2], Masahiro Noji[3], Masatomo So[3], Yuji Goto[3], Tetsushi Iwasaki[1,4], Motonari Tsubaki[1], Eri Chatani[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Fac. Med., Jichi Med. Univ.*, [3]*Inst. Protein Res., Osaka Univ.*, [4]*Biosignal Res. Center, Kobe Univ.*)

It has recently been recognized that amyloid fibrils, aberrant protein aggregates associated with many serious diseases, exhibit structural diversity leading to a variety of physiological phenotypes. The diverse structures propagate by a seed-dependent growth, although much remains unknown regarding their propagation manners. Here, we investigated structures and cross-seeding behaviors of human and bovine insulin amyloid fibrils by iodine staining. We demonstrated that cross-seeding between heterologous proteins induces multi-step conformational changes via intermediate metastable states, in contrast to robust propagation in self-seeding. Notably, when human insulin was cross-seeded with bovine insulin seeds, a new fibril structure with distinct cytotoxicity was formed.

20008A 低温電子顕微鏡画像を記述する連続関数の計算法：マニフォールドラーニングによる研究
A Computational Method for Constructing a Continuous Function Describing Cryo-Electron Microscopy Data: A Study using a Manifold Learning

Ryota Kojima, Takashi Yoshidome (*Dep. of Appl. Phys., Tohoku Univ.*)

We investigated a computational method for constructing a continuous function that describes two-dimensional electron density maps of a protein as a function of projection direction (polar angle). If the function is obtained using experimentally obtained maps, the maps that are failed to sample can be computed using the function, providing applications such as an improvement of the resolution of the three-dimensional electron density map of the protein. In the computational method, the generative topographic mapping method that is a manifold-learning technique is employed. To investigate the method, we performed a simulation for a cryo-electron microscopy experiment. We successfully reproduced the electron density maps from the continuous function.

20009A Unguided Binding MD of Protein-Protein Complexes by PPI-ColDock

Kazuhiro Takemura, Akio Kitao (*Sch. LST, Tokyo Tech*)

Accurately predicting complex structures of proteins is vital to understand their functions. Recently, we proposed a simple but efficient and accurate method, ColDock (Concentrated ligand Docking), to predict protein-ligand complex structures using MD simulation at high ligand concentration. In ColDock, many ligands are randomly distributed around a target protein to induce spontaneous binding of the ligand to the correct binding site. To apply ColDock to protein-protein interactions (PPI), multiple molecules of two kinds of proteins that make complex are distributed to increase the number of encounter events. PPI-ColDock is applied to few protein complexes, and binding events to reproduce near-native complexes are successfully observed.

20010A* tRNA 硫黄修飾酵素における鉄硫黄クラスター構造と酵素活性の相関解析
Correlation between structures of iron-sulfur clusters and enzymatic activity in tRNA thiolation enzymes

Masato Ishizaka[1], Minghao Chen[2], Shun Narai[1], Masaki Horitani[3], Yoshikazu Tanaka[4], Min Yao[1,2] ([1]*Grad. Sch. Life Sci., Hokkaido Univ.*, [2]*Facul. Adv. Life Sch., Hokkaido Univ.*, [3]*Facul. Agr., Saga Univ.*, [4]*Grad. Sci. Life Sci., Tohoku Univ.*)

tRNA thiolation is one of the post-transcriptional modifications required for all organisms for the biological function of tRNA. Abnormal tRNA thiolation induces mitochondrial disease and cancer. Our target, 2-thiouridine synthase (TtuA) catalyzes tRNA thiolation with sulfur donor TtuB. Recently, we have successfully determined the structure of the TtuA-TtuB complex, showing that TtuA has an oxygen-sensitive co-factor, [4Fe-4S] cluster. Interestingly, one of the Fe (the unique Fe) coordinated to C-terminus of TtuB. However, the detailed function of the unique Fe is still unclear. In this study, we analyzed the structural changes of iron-sulfur clusters and the effect of enzymatic activity of TtuA. Based on the results, we proposed the detailed tRNA thiolation mechanism.

20011A Sampling large-scale motions in proteins using a coarse-grained multi-basin Go model

Ai Shinobu[1], Chigusa Kobayashi[1], Yasuhiro Matsunaga[2], Yuji Sugita[1] ([1]*RIKEN*, [2]*Saitama Univ.*)

Large-scale motions in multi-domain proteins are essential for their function. Coarse-grained (CG) molecular dynamics (MD) simulations are an inexpensive and useful tool for studying large-scale motions in proteins, however, they sometime miss possible transitions paths and intermediate structures. We developed a multi-basin (MB) structure-based Go model for describing conformational motions in proteins with more than two labile domains and implemented it in the GENESIS MD program. We applied the scheme to the enzyme Adenylate Kinase and sampled multiple conformational transitions between its open and closed states. Moreover, by altering the model parameters we successfully sampled different transition pathways and characterized the structures of intermediate states.

20012A Visualization of translational GTPase factor-pool formed on the archaeal ribosomal P-stalk by HS-AFM

Hirotatsu Imai[1], Toshio Uchiumi[2], Noriyuki Kodera[1] ([1]*WPI-NanoLSI, Kanazawa Univ.*, [2]*Faculty of Science, Niigata Univ.*)

The ribosomal stalk protein plays an essential role in the recruitment of translational GTPase factors EF1A and EF2 to the ribosome and their GTP hydrolysis for efficient translation elongation. However, due to the flexible nature of the ribosomal stalk, its structural dynamics and mechanism of action remain unclear. Here, we applied HS-AFM to directly visualize the action of the archaeal ribosomal P-stalk. HS-AFM movies clearly demonstrated that archaeal aEF1A and aEF2 spontaneously assembled around the ribosomal P-stalk. Our results provide the first visual evidence for the factor-pooling mechanism and reveal that the ribosomal P-stalk promotes translation elongation by increasing the local concentration of translational GTPase factors.

20013A NMR 解析によるシニョリンとその変異体の立体構造の決定
Determination of structures of chignolin and its mutant by NMR analysis

Shumpei Koroku[1], Ayori Mitsutake[2], Yutaka Maruyama[3], Koh Takeuchi[4] ([1]*Meiji University*, [2]*Meiji University*, [3]*RIKEN*, [4]*AIST*)

Chignolin, which was designed by Honda et al., is an artificial mini-p rotein consisting of 10 amino acids: GYDPETGTWG. Its atomic coordinate s were determined by NMR. It is widely used to test new simulation al gorithm and analysis methods. Chignolin is characterized by two stable states in molecular dynamics (MD) simulations: a native state and a m isfolded state. In our previous works, we proposed several mutations o f Thr8 to stabilize the misfolded structure rather than the native str ucture. Here, we show the results of determination of structures of super-chignolin, chignolin and its mutant by NMR analysis.

20014A 高速 AFM を用いた磁性細菌の細胞骨格結合タンパク質 MamJ の機能解析
Functional analyses of magnetotactic bacterial cytoskeletal binding protein MamJ using high-speed AFM

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Magnetosomes are positioned in a chain-like arrangement along long axis of a magnetotactic bacteria cell. Although two magnetosome-associated proteins, MamK and MamJ, are essential for the magnetosome arrangement has not been clarified. Here, we purified both of monomeric MamK and MamJ. We analyzed effects of MamJ on structure of MamK filament. We compared structures of MamK filaments polymerized with and without MamJ using fluorescence microscopy and High-speed AFM. The microscopic observations indicated that MamJ prevents forming large bundles of MamK filaments and promotes forming short MamK filament. These results suggested that MamJ might effect on the property of MamK polymerization and regulate MamK filament structure.

20015A* 18 残基チオエーテル結合環状ペプチド群のシミュレーションデータの解析
Analysis of Molecular Dynamics Simulations of 18-residue Thioether Cyclic Peptides

Daiki Noguchi (*Meiji university graduate school*)

In recent years, peptide drugs, which are created by applying a compound “peptide” consisting of several amino acids. It acts specifically on the target protein and can reduce the development cost. The thioether bond cyclic peptides have a thioether bond in which the carbon atom of the N-terminal cap and the sulfur atom of the cysteine at the 15th or 16th residue are bonded. In addition, experimental results have been reported that each peptide has a different affinity for human plexin B1. To elucidate the mechanism of different compatibility between these peptides, we performed molecular dynamics simulations. Then, we examined the stability of these peptides using methods such as principal component analysis and relaxation mode analysis.

20016A グラフ理論に基づくタンパク質立体構造の位相解析への VOLTES 法の応用
Application of VOLTES to topological analyses of protein structures based on graph theory

Anri Terabayashi, Kyousuke Sakata, Toshitaka Shoji, Masaki Kojima (*Sch. Life Sci., Tokyo Univ. Pharm. Life Sci.*)

We have developed a series of program package VOLTES (Virtual Optimization of Local TErtiary Structures), to analyze protein structures based on not the physicochemical but the geometric context. In our program, all the protein structures are expressed as torsion angles of rotatable bonds, and the torsion-angle values are arranged into 'trees' having the same topologies as the proteins’ structures. In addition, each torsion angle is discretized into 6 classes to reduce the number of conformations to be considered. We applied VOLTES to proteins with convergent evolution by comparing their trees based on the homeomorphism of graph theory. We aimed to elucidate the correlation between converged structures and their topologies with geometrical constraints.

20017A The molecular basis for the nucleotide selectivity of the ε subunit from bacterial F-type ATP synthases

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The ε subunit of bacterial ATP synthases binds ATP with high affinity and selectivity, which then undergoes a large conformational change from an ATP hydrolysis inhibitory up- to a non-inhibitory down-state. The isolated ε subunit has been engineered to develop novel sensors to measuring the ATP concentration in real-time in cells. This approach could potentially be extended other nucleotides if the ε subunit selectivity could be rationally tuned. Here, we demonstrate how this might be achieved, via molecular dynamics simulations and free energy calculations. We are able to reproduce the experimentally observed ATP vs. GTP selectivity, and subsequently predict differences in binding free energies for CTP and UTP.

20018A Free Energy Calculations of HIV-1 Protease Binding Indinavir and Its Drug-Resistant Mutant

Masahiko Taguchi[1], Ryo Oyama[2], Masahiro Kaneso[2], Shigehiko Hayashi[2] ([1]*Inst. Quant. Life Sci., QST*, [2]*Grad. Sch. Sci., Kyoto Univ.*)

HIV-1 protease is a target of drug development and various inhibitors binding to two Asps in the catalytic site were developed. However, it has a serious drug-resistance, that is, some mutations cause existing inhibitors ineffective, even though hydrolysis reaction of substrate proceeds. To resolve the drug-resistance problem, it is important to clarify difference of recognition mechanism of the protease for inhibitors in the case of native and drug resistance mutational structures, respectively. For indinavir, it is known that mutation (V82T/I84V) greatly affects its binding free energy to HIV-1 protease. We performed QM/MM free energy calculations, and succeeded to determine the protonated states of catalytic Asps and the relative binding free energy.

20019A メタゲノムデータベース由来 PET 加水分解酵素の耐熱性および活性の改良
Improvement of thermostability and catalytic activity of a PET degrading enzyme derived from metagenome database

Akihiko Nakamura[1], Naoya Kobayashi[2], Takahiro Kosugi[2], Rie Koga[2], Nobuyasu Koga[2,3], Ryota Iino[2,3] ([1]*Shizuoka Univ.*, [2]*Inst. Mol. Sci.*, [3]*SOKENDAI*)

Recently, environmental pollution by synthetic polymers has been concerned. Polyethylene terephthalate (PET) is one of the most produced synthetic polymers in the world and commonly used for consumable products such as beverage bottles. After the discovery of PET hydrolase (PETase) from a bacterium Ideonella sakaiensis, a new thermostable PETase, PET2 was found in a metagenome database. Here we engineered PET2 by computational design and structure-guided mutagenesis to improve its thermostability and catalytic activity. We found a mutant F105R-E110K-S156P-T297P-G180A is stable at 65℃, and shows 3.4 times higher PET hydrolysis rate than the wild-type. We are currently trying to further increase thermostability over 70℃, which is the grass transition temperature of PET.

20020A 心筋カルシウムチャネル Cav1.2 と薬剤間の結合自由エネルギー計算
Calculation of the binding free energy between the Cav1.2 calcium channel and drugs

Tatsuki Negami, Tohru Terada (*Grad. Sch. Agr. Life Sci., Univ. Tokyo*)

All drug candidates are tested for cardiotoxicity. Predicting interactions between drugs and cardiac channels, hERG, Nav1.5, and Cav1.2, is important for the proarrhythmia assessment. We are developing a method to predict the channel-drug binding affinity based on the ligand docking simulation and the MP-CAFEE method. Previously, we have shown that the calculated binding free energies of drugs were correlated with experimental data for the hERG channel and the Nav1.5 channel. In this study, we applied the method to the Cav1.2 channel. We generated structural models based on the experimental structures of the Cav1.1 channel and then performed ligand docking simulations and free energy calculations. We will discuss the accuracy of the calculated binding free energies.

20021A 標的空間を 2,3,4 次元とした Dimensional Scaling 法によるフラグメント間相互作用エネルギー行列解析
Analysis of inter fragment interaction energy by Dimensinal Scaling method in 2,3,4 by Dimensional as the target space

Yuki Abe, Masanori Yamanaka (*Univ.Nihon*)

Fragment molecular orbital (FMO) method is a method of calculating the enregy and the electron density by dividing a molecular system into fragments, calculating the electronic states of fragments and fragment pairs, and gathering them. In this work, we investigate the inter fragment interaction energy (IFIE) matrix by non metric multidimensional scaling (MDS) method and perform a cluster analysis for the aminos acids and the ligand. The non metric MDS is a method of enbedding an object under conditions that preserve the distance relationship between elements in a certain space, which is one of the multivariate analysis. The method is essentially non linear analysis, which will be compensate for linear analysis such as the principal component analysis.

20022A 蛋白質内部で水素結合を形成する荷電残基が示す強力な安定化効果についての熱力学的評価
The thermodynamic characterization of the strong stabilization effect by a buried and charged residue forming hydrogen bonds

Hiroaki Sato, Akiko Nakazawa, Kohei Yamamoto, **Shun-ichi Kidokoro** (*Dept. Bioeng., Nagaoka Univ. Tech.*)

The 45th aspartic acid of a cold shock protein(CSP) derived from *Thermus thermophilus* HB8 is buried and forms two hydrogen bonds. In order to evaluate the denaturation thermodynamics precisely, the mutation D45N is introduced into the 2SS-CSP mutant whose thermal stability was increased by about 30 K by introducing two disulfide bonds on the surface. The heat capacity with thermal denaturation of 2SS-CSP and D45N-2SS-CSP between pH 2.5 to 4.5 was measured by a high precision DSC. All data were well fitted by a global two-state model. The pH dependence of $\Delta\Delta G$ by the mutation indicated the stabilization effect by Asn to Asp replacement is about -11 kJ/mol and mainly due to enthalpic stabilization.

20023A インスリン受容体全長構造モデリングとその分子動力学研究
Computational modeling of full-length insulin receptor and its molecular dynamics

Yoshiharu Mori (*Grad. Sch. of Sys. Info., Kobe Univ.*)

Insulin receptor is one of the receptor tyrosine kinases, which is responsible for many signal transductions among cells. Structure models of the extracellular domain, transmembrane domain, and intracellular kinase domain of the receptor have been determined experimentally. However, the structure of full-length insulin receptor is still unknown.
We modeled the full-length insulin receptor with insulin molecules or without any insulins using computational modeling algorithms and coarse-grained molecular dynamics simulations. The transmembrane domain and kinase domain of the receptor were largely fluctuated during the simulations, which could play an important role in the function of insulin receptor.

20024A Size evolution of antibody aggregates by the adsorption of serum albumin

Tomohito Nakayama[1,2], Muneaki Hase[1], Atsushi Hirano[2] ([1]*Grad. Sch. Sci. Tech., Univ. Tsukuba*, [2]*NMRI, AIST*)

Despite recent antibody drug development, there are concerns about undesired immune response caused by antibody aggregates. The level of immune response was reported to depend on the aggregate size. To date, the sizes of the aggregates generated in pharmaceutical processes have been well characterized, whereas those in blood remain to be done. The aggregate size is possibly increased by adsorption of serum proteins. Here we observed size evolution of the aggregates in the presence of human serum albumin (HSA). The aggregate diameter was found to increase to 20 times. Importantly, this size evolution was suppressed by the addition of salts. It was thus suggested that antibody aggregate size is increased even in blood by the adsorption of HSA via electrostatic attraction.

20025A Theoretical Study on the Transport Cycle of the Heme ABC Transporter BhuUV-T

Koichi Tamura[1], Yuji Sugita[1,2,3] ([1]*RIKEN R-CCS*, [2]*RIKEN BDR*, [3]*RIKEN CPR*)

Heme ATP-binding cassette (ABC) transporter BhuUV-T mediates transport of heme across the inner membrane. In this presentation, we present our recent computational studies on the transporter. First, we construct atomistic models of the experimentally unknown conformations of BhuUV-T by means of homology modeling and molecular dynamics (MD) simulation. Further, we performed the string method calculation and umbrella sampling to reveal the free energy associated with the ATP-induced conformational transition. The free energy simulation validates the predicted model of the occluded conformation. Lastly, we describe a pitfall one can encounter on the string calculation and how to overcome the problem by a simple annealing procedure.

20026A ヤエヤマサソリ由来殺虫性毒素 LaIT2 の C 末端ドメインの大腸菌大量発現系構築
Constructon of the *E.coli* ovrexpression system for the C-terminal domain of LaIT2, an insecticidal toxin from *Liocheles australasiae*

Chiharu Tatsushiro[1], Maiki Tamura[2], Shinya Ohki[2], Hayato Morita[1,3] ([1]*Grad.Sch.Sci.,Josai Univ*, [2]*Grad.Sch.Mat Sci.,JAIST*, [3]*Fas Sci.,Josai Univ*)

L. australasiae is one of the scorpions that inhabit Japan and is known to secrete venom being specifically toxic to insect. LaIT2, which is one of the toxins in this venom, exhibits not only insecticidal, but also antibacterial activities, and is thought to be a member of two domain toxins. From amino acid sequence, C-terminal region (C-LaIT2) may have rigid structure based on several Cys-Cys bridges, and N-terminal region may be flexible. To identify this structural speculation, we have constructed the *E. coli* overexpression system for C-LaIT2 with pGEX-6P-2 vector. With this system, we have succeeded to obtain ~0.5mg/L LaIT2 as soluble protein. We now evaluate the heat stability of this C-LaIT2 with UV-CD measurements and the results will be reported.

20027A 高密度マイクロウェルアレイによる酵素関連タンパク質のセレクションを目的とした、ペプチドリガーゼによる遺伝子型-表現型対応付け手法の開発
Peptide ligase display (PL display) for selection of enzyme-related protein by combination with high-density microwell array chip

Shingo Ueno[1,2], Shusuke Sato[1,2], Fumi Toshioka[1], Shoichi Tsuchiya[1], Takanori Ichiki[1,2] ([1]*iCONM, Kawasaki Ins. Ind. Prom.*, [2]*Grad. Sch. Eng., Univ. Tokyo*)

A novel protein display method using a peptide ligase has been developed. This method enables us to link the DNA and its encoding protein via covalent bonding during cell-free translation reaction. A protein-coding DNA is modified with a substrate peptide of transpeptidase sortase A (srtA), and a protein of interest (POI) fused with srtA and its alternative substrate peptide is cell-free expressed from the DNA. The substrate peptides are ligated by the srtA and the srtA is released from POI. As a result, POI is linked with its coding DNA via only short peptide sequence. As a demonstration, kinase and kinase-inhibiting peptide was displayed on these DNA, which immobilized on microbeads, and the protein activity was measured using high-density microwell array chip.

20028A 長時間タンパク質ダイナミクスの拡散マップによる解析
Diffusion map analysis of long time protein dynamics

Hiroshi Fujisaki[1], Hiroto Kikuchi[1], Hiromichi Suetani[2], Ayori Mitsutake[3] ([1]*Nippon Medical School*, [2]*Grad. Sch. Eng., Oita Univ.*, [3]*Grad. Sch. Sci., Meiji Univ.*)

Due to rapid progress in computing power and sophisticated algorithms for molecular dynamics simulations, it is common to generate huge trajectory data from protein dynamics simulation. Hence it is desirable to extract the essential features of the dynamics from such huge data and some statistical methods such as principal component analysis or relaxation mode analysis have been often employed. Here we employ the diffusion map method, which is known to be related to the relaxation mode analysis, and try to apply the landmark diffusion map or time-coupled diffusion map methods to very long time trajectories of protein-G.

20029A Molecular simulation of pH effect on emission color changes through hydrogen-bond networks in firefly luciferase and its mutants

Kota Nosaka[1], Yuto Kudo[2], Naohisa Wada[1] ([1]*Grad. Sch. Life Sci., Univ.Toyo*, [2]*Fac. Food and Nu. Sci., Univ.Toyo*)

In the bioluminescence of firefly Luciola cruciate luciferase(Luc), red and yellow-green lights are emitted in vitro under acidic and basic conditions, respectively. Mutations of Luc also produce emission color-changes. Investigating what causes emission color changes, we calculated the pK values of some amino acid residues around the Luc's catalytic center using a DS2019 in MM level. As a result, we could clarify the emission color changes might be caused by such complicated factors as the hydrogen-bond network differences between heterogeneous microenvironments around the catalytic centers of Luc and its mutants. The structures thus obtained can be applied to calculating these absorption spectra to examine whether or not is reasonable our conclusion.

20030A Spectroelectrochemical FTIR studies of an electron-bifurcating [FeFe] hydrogenase

Nipa Chongdar[2], Krzysztof Pawlak[2], Olaf Rudiger[2], Edward Reijerse[2], Patricia Rodriguez-Macia[2], Wolfgang Lubitz[2], James Birrell[2], **Hideaki Ogata**[1,2] ([1]*ILTS, Hokkaido Univ.*, [2]*MPI/CEC*)

The [FeFe] hydrogenases are well-known for their high turnover frequencies for H_2 production. In this work we have attempted to characterize the electron-bifurcating [FeFe] hydrogenase from *Thermotoga maritima* (TmHydABC). Using FTIR and EPR spectroscopy the three typical states present in all [FeFe] hydrogenases, i.e. H_{ox}, $H_{red}H^+$, and H_{ox}-CO could be identified in TmHydABC. The unprotonated singly reduced state H_{red} as well as the doubly reduced state $H_{sred}H^+$ (both with a reduced [4Fe-4S]) were not observed under any condition. The H_{ox} state undergoes proton coupled one electron reduction to form the $H_{red}H^+$ state where the bridging CO becomes terminal, as observed in other [FeFe] hydrogenases.

20031A 演題取り消し

20032A D313Y 変異をもつノーマル型べん毛繊維を用いた多型変換に関与するアミノ酸相互作用の推測
Prediction of amino acid interactions for polymorphic transformation with normal flagellar filaments with the D313Y curly mutation

Ayano Yanagita[1], Minami Oohata[1], Hikaru Tsufuku[1], Shigeru Yamaguchi[1], Fumio Hayashi[2], Kenji Oosawa[1] ([1]*Dept. Chem. & Chem. Biol., Sch. Sci. Technol., Gunma Univ.*, [2]*Ctr. Instr. Anal. Gunma Univ.*)

Salmonella cells have several helical flagellar filaments and swim by rotating them. Flagellar filaments are a huge protein aggregate consisting of about 30,000 molecules of protein, flagellin. The flagellar filaments change their shape among different helical structures upon changing their rotational direction. It is called polymorphic transformation. We analyzed polymorphic transformation of filaments from 16 pseudorevertants derived from SJW2875 (D313Y) under various pH and salt concentrations. From the results, we will discuss the effects of the second mutations on the conversion from R-type to L-type protofilaments and the amino acid interactions involved in the conversion.

20033A* 統計力学モデルの拡張によるタンパク質のフォールディング経路の解析
Protein folding mechanisms predicted by an extended statistical mechanical model

Koji Ooka[1], Munehito Arai[1,2] ([1]*Dept. Phys., Univ. Tokyo*, [2]*Dept. Life Sci., Univ. Tokyo*)

Wako-Saitô-Muñoz-Eaton (WSME) model can calculate free energy landscapes of protein folding using a native structure. The model has successfully predicted experimentally observed folding mechanisms of small proteins. However, the WSME model cannot be applied to large proteins that have specific non-local interactions formed early in the folding process. To overcome this problem, here we extended the WSME model by introducing extra energy terms in the Hamiltonian. We applied our extended WSME model to the folding of lysozyme, α-lactalbumin and apomyoglobin and succeeded in deriving the free energy landscapes consistent with experimentally observed folding pathways. Development of a general method for applying our extended model to various proteins is now under way.

20034A Structural Stability and Unfolding Kinetics of a lytic polysaccharide monooxygenase, CBP21

Yuichi Nakajima, Takeshi Watanabe, Kazushi Suzuki, Hayuki Sugimoto (*Grad. Sch. Sci. & Tech., Niigata Univ.*)

Chitin-binding protein 21 (CBP21) from *Serratia marcescens* is a chitin-active lytic polysaccharide mono-oxygenase and contains a copper ion as a cofactor. We analyzed the effects of Cu^{2+} on its structural stability and unfolding kinetics to elucidate the unfolding mechanism of apo- and holoCBP21. Denaturant-induced equilibrium unfolding analysis showed that the unfolding of apo- and holo-CBP21 are reversible. The midpoint concentration of guanidium chloride for unfolding was 1.0 and 1.7 M for apo- and holoCBP21, respectively. Furthermore, copper binding decreased the apparent rate of unfolding: the value for holoCBP21 was one fifth of that for apoCBP21. These results suggest that copper binding is a key for both the structural stability and the folding process.

20035A Search for Partial Structural Space of Specific Loop Residues by Hydrogen Bond and Steric Repulsion

Hiroto Murata, George Chikenji (*Dept. Appl. Phys., Nagoya Univ.*)

Understanding the structure space of the protein is one of the most important aspects of protein structure analysis and design.Since proteins are composed of chains of hundreds of amino acids, it is not practical to explore the entire structure space of the protein.Here, we propose a theory that explains the reason of the limited number of protein folds by physical factors.The theory is based on a statistical analysis of the protein structure database and computer simulation.The database analysis revealed that some loop structures connecting the secondary structures are limited to several patterns.The origin of the limited variety of the loop structures was explored by the computer simulation, and was found to be the consequence of physical factors.

20036A 機械学習による単粒子 X 線回折像の改善
Improvement for Noisy X-ray Single-Particle Diffraction Pattern using Convolutional Neural Network

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Biomolecular imaging using X-ray free-electron lasers has been successfully applied to not only serial femtosecond crystallography but also single-particle analysis(SPA) of viruses. However, the application of SPA with -100 nm molecules has two practical problems: the noisy incomplete datasets and the heterogeneous conformational states. Here, we propose a single image super-resolution to improve diffraction images using convolutional neural network. The method is proposed that achieves high generalization performance, which is effective for improving the images in incident X-ray fluctuations, structural fluctuations, and different orientations. It was succeeded in improving the images corresponding to the observed one using 3-7 times stronger incident X-ray intensity.

20037A* c-Myb-KIX 相互作用を阻害するヘリカルペプチドの合理的設計
Rational design of an α-helical peptide to inhibit c-Myb-KIX interaction

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The transcriptional activator c-Myb interacts with the KIX domain of CBP and regulates hematopoiesis. However, its aberrant expression causes leukemia. Here, we rationally designed α-helical peptides as inhibitors of the c-Myb-KIX interaction by introducing mutations into the transactivation domain of c-Myb (c-Myb32). Although c-Myb32 is intrinsically disordered, it has high helical propensity and binds KIX by the conformation selection mechanism. Therefore, to increase the affinity to KIX, we introduced mutations that stabilize their helices using theoretical helicity predictions. As a result, we succeeded in designing the peptide that binds KIX ~3-fold more tightly than the wild type. We are currently working on studying its ability as an inhibitor.

20038A Optimized Go-MARTINI coarse-grained force field parameters based on structural flexibility of F-BAR protein Pacsin1 on lipid membrane

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Coarse-grained (CG) molecular dynamics (MD) simulations allow us to access much larger length and time scales compared to atomistic MD. Recently developed Go-MARTINI CG force field (FF) for proteins based on the well-known MARTINI CG FF adopts Lennard-Jones (LJ) interactions. We conducted Go-MARTINI MD of the F-BAR Pacsin1 on lipid bilayer and observed that protein structural changes were largely dependent on the FF. To address this issue, we have tuned the cutoff distance of native contacts and the interaction strength of LJ. Then structural fluctuation of the protein is close to the one from atomistic MD and assembly of the protein dimers through lateral interaction was observed. Our results provide a strong motivation for refining the FF parameters in Go-MARTINI.

20039A タンパク質脱イミノ化酵素 PAD3 の構造機能相関解明
Elucidation of the structure-function relationship of peptidyl arginine deiminase type 3

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Peptidyl arginine deiminase (PAD) is a Ca2+-dependent enzyme that catalyzes the conversion of protein arginine residues to citrulline. PAD3 in hair follicle has been reported to citrullinates Arg51 of a Ca2+-binding protein S100A3, selectively. This substrate selectivity of PAD3 is different from PAD1 and PAD2 those citrullinate all arginine residues of S100A3. In this study, structure analysis of PAD3 in complex with Ca2+ and structural comparisons with PAD isozymes were conducted. The results obtained here will be useful for drug discovery of PAD3-specific inhibitor. Then we analyzed whether PAD3 citrullinated itself as seen in PAD4. In this study, we confirmed that auto-citrullination of PAD3 were occurred in dependent to Ca2+ concentration by Western blotting.

20040A トキソプラズマ症を引き起こす病原性原虫トキソプラズマの寄生胞膜破壊に関わる Irgb6 の結晶構造
Crystal structure of Irgb6, which is involved in the destruction of a membrane-bound parasitophorous vacuole of Toxoplasma gondii

Yumiko Saijo-Hamano[1], Naoki Sakai[2], Yoshiaki Sakihama[1], Masahiro Yamamoto[3], Ryo Nitta[1] ([1]*Grad. Sch. Med., Kobe Univ.*, [2]*RIKEN, RCS*, [3]*RIMD, Osaka Univ.*)

Toxoplasma gondii is a protozoan parasite that infects most species of warm-blooded animals, including human, and causes the disease toxoplasmosis. T. gondii enters host cells and resides in the cytoplasm in a membrane-bound parasitophorous vacuole (PV). Inducing an interferon response enables IFN-γ-inducible immunity-related GTPase (IRG protein) to accumulate on the PV and to restrict parasite growth. However, little is known about the mechanisms by which IRG proteins recognize and destroy the PV. Irgb6 is strongly suggested to act as a pioneer in the process by which multiple IRG proteins access the PV. Here we show the crystal structures of Irgb6 in its nucleotide-free and GTP-bound form, and discuss the function of Irgb6 from the structures and published data.

20041A 糸状仮足観察のための Cryo-CLEM 法の検討
A study of the Cryo-CLEM method for the observation of filopodia

Miho Nakafukasako, Tomoya Higo, Yusuke V. Morimoto, Takuo Yasunaga (*Grad. Sch. Comp. Sci. Syst. Eng., KIT.*)

Cells move using the filopodia as an antenna. We found that there are two types of the filopodial structure during cell move, i.e. “Round structure” with a rounded tip and “Sharp structure” with formed up by F-actin bundles to the tip. Thus, we have investigated dynamical changes in conformation by cryo-CLEM methods, but it is challenging to take a good aim of elongating/regressing filopodia before photoing by cryo-EM. Here we tried to develop suitable grids for cryo-EM, which attach fluorescent beads. Three types of fluorescent beads, which are different in size, were scattered on the grids for NG108-15 cell observation, and we will report our current development of cryo-EM grids and the LM and EM views to propose how to create EM-grids suitable for cryo-CLEM.

20042A ヘリオロドプシンおよびシゾロドプシンの構造から明らかになった微生物型ロドプシンの多様性
Structures of heliorhodopsin and schizorhodopsin elucidate the structural diversity of microbial rhodopsins

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Heliorhodopsins (HeRs) are a distinct abundant group of microbial rhodopsins, whose function remains unknown. Schizorhodopsins (SzRs) is a family of rhodopsins from Asgard archaea that function as light-driven inward H+ pumps. Owing to the lack of structural information, little is known about the overall fold and the photoactivation mechanism of HeRs and SzRs. Here we present the crystal structures of HeR and SzR. A Structural and biophysical analyses reveal the similarities and differences between HeRs, SzRs, and type-1 rhodopsins. Our study increases the understanding of the functions of HeRs and SzRs, and the structural similarity and diversity among the microbial rhodopsins.

20043A The relationship between designability of protein and preference of local structures: A lattice model study

Kazuma Toko, George Chikenji (*Dept.Appl.Phys.,Nagoya Univ.*)

Designability of protein structure is the number of sequences that can design the structure. What features determine the designability of structures? Here, we hypothesize that local rules of real protein determine designability. We use the HP lattice protein model in order to verify this hypothesis. We found that the relationship between sequences and structures of HP model with penalty on local structure is consistent with that of observed in the database of real proteins: The local structure with penalty does not appear in highly designable structures, and it appears in some of the poorly designable structures. These results suggest that local rules of protein are the determinant of the designability of protein structures.

20044A βストランドとαヘリックスをつなぐループが特定の主鎖二面角およびアミノ酸を選択する理由
Why loops connecting a β-strand and an α-helix prefer particular dihedral angles and amino acids

Megumi Nakajima, George Chikenji (*Dept.Appl.Phys.,Nagoya Univ.*)

A β-α loop is a local protein structure that connects a β-strand and an α-helix in this order. When the loop is composed of 2-residue amino acids, its main chain tends to have the dihedral angle of the particular combination “A” and “B”, where A and B are dihedral angle classes of ABEGO representation of main chains. In addition, there is a clear trend in the types of amino acids favored by the two residues in the AB loops. Here, we show that this tendency is the result of physical factors rather than the chance product of evolution. We performed computer simulations(exhaustive conformational sampling and energy calculation) and confirmed that low energy structures are well consistent with the database statistics.

20045A New insight into ion transport mechanism of the Na+/H+ antiporter PaNhaP revealed by transition path shooting and Markov state model

Titouan Jaunet, Kei-ichi Okazaki (*Institute of molecular science (IMS) okazaki, japan*)

The electroneutral Na+/H+ antiporter NhaP from archaea Pyrococcus abyssi (PaNhaP) is a functional homolog of the human Na+/H+ exchanger NHE1, which is an important drug target. In this study, we performed a Markov state modelling based on trajectory data from transition path shooting between the inward/outward-open states of PaNhaP. It has been recently highlighted that this conformational transition is accompanied by a hydrophobic gate formed by a key residue-pair interaction and its mutation modulates the ion transport speed. The Markov state modelling identifies the presence of metastable states during the conformational transition, the most important pathway based on the transition path theory and kinetic properties that can be compared to the experimental values.

20046A Molecular dynamics simulations of the H.pylori FliG N-terminus

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Bacteria are propelled through their environment by the flagellum, a complex multi-protein complex consisting of a molecular motor, a joint and a propeller. FliG is a key component of the C-ring one of the motor building blocks. FliG is involved in the early steps of motor assembly through its interaction with FliF and in the torque generation that rotates the flagellum. Crystal structures of the FliG N-terminus show different conformations of the helices that join the N-terminus and middle domains of FliG and both have been argued to be biologically relevant. Molecular dynamics simulations show that one of the known conformations of the FliG N-terminus in complex with C-terminal helices of FliG is induced by crystal contacts and might not be biologically relevant.

20047A A large-scale structural and evolutionary analysis of protein loop regions

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Protein loop regions often play important roles in function. Here we study the structural and evolutionary aspects of protein loops on a large-scale. We prepared three loop sets from whole PDB, human, and E.coli proteins. The numbers of loop regions were 556,404, 121,052, and 33,594, respectively. We found that the human set showed the abundance of Lys, Ser, and Cys compared to the E.coli. The CATH classification revealed that loops that linked diverse superfamilies showed biases on amino acids (Leu, Pro, Val) and loop length. Additionally, more than one superfamily context of a loop was found, and that heterogeneity was not observed in Topology/Homologous level. For the evolution, conserved loops between human and E.coli were found to be overrepresented in proteins.

20048A* Ligand Docking Parallel Cascade Selection Molecular Dynamics (ld-PaCS-MD) の開発と応用
A Development of Ligand Docking Parallel Cascade Selection Molecular Dynamics (ld-PaCS MD) and its applications

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Ligand-docking processes are important to understand the functions of proteins controlled by the binding of ligands. We here propose a ligand-docking parallel cascade selection molecular dynamics (ld-PaCS-MD), which is an extension of the original PaCS-MD specialized for detecting ligand binding pathways. The original PaCS-MD has been developed as a bias-free sampling method to detect rare events related to the biological functions. As this extension, in ld-PaCS-MD, we placed multiple ligands around a target protein and always treating all the ligands as binding candidates. In the present study, we confirmed that ld-PaCS-MD efficiently elucidated the ligand-binding processes and was applied it to more complicated proteins.

20049A* アスパラギン酸スキャニングを用いた赤外分光法によるタンパク質内局所的環境変化のマッピング解析
Mapping of the local environmental changes in proteins by FTIR spectroscopy with aspartic acid scanning

Masanori Hashimoto, Kota Katayama, Manish Singh, Yuji Furutani, Hideki Kandori (*Grad. Sch. Eng., Nagoya Inst. Tech.*)

Stimulus-induced difference FTIR spectroscopy is a powerful method to probe protein structural changes, but detected vibrations have to be assigned by isotope-labeling. On the other hand, carboxylic C=O stretch (1800-1700 cm^{-1}) is well isolated from other vibrations, and if there are no spectral changes for intact protein in this frequency region, introduction of carboxylate by mutation may be a good tool to probe local protein structural changes. This method can also evaluate hydrophobicity of the local environment by monitoring the protonation state of the incorporated carboxylic acid. We will show systematic aspartate mapping applied to heliorhodopsin, where light-induced difference FTIR spectra were measured by the ATR technique.

20050A Computational Study of Temperature-Dependent Protein Glass Transition under Varying Solvent Compositions

Michelle Yaochai[1,2], Emmanuella Li[2], Joanna Ng[2], Peter J. Bond[2], Alexander Krah[2] ([1]*NUS High Sch.*, [2]*Bioinformatics Inst., A*STAR*)

At the glass transition temperature, biological functions of proteins are believed to be activated by a dynamical transition into a glassy state. To characterize the role of protein-solvent interactions in the protein glass transition phenomenon, we simulated lysozyme at different temperatures in these three solvents: water, sucrose/water and trehalose/water. Disaccharide molecules take a longer time to reorient than water molecules due to their large size, thus we equilibrated and conducted Molecular Dynamics(MD) simulations over time scales of hundreds of nanoseconds. Our computational results provide molecular insights on dynamics surrounding protein glass transition in different chemical environments, which could assist in the development of bioprotective compounds.

20051A 計算モデリングを用いたアブラナ科植物の自家不和合性を制御するタンパク質 SRK/SP11 複合体の包括的理解
Comprehensive understanding of SRK/SP11 protein complexes of Brassicaceae using computational modeling

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S-locus receptor kinase (SRK) in pistil and a small ligand protein, *S*-locus protein 11 (SP11) in pollen are responsible for Brassicaceae self-incompatibility. If both proteins are derived from the same *S*-locus, the pollen will be rejected to prevent self-pollination. Although two haplotypes of their complex crystal structures have been determined, there remain more than 25 haplotypes with unknown structure. Here we report that most of the SRK and SP11 structures could be generated by using Rosetta combined with accelerated MD simulations. Our modeled complexes revealed that the binding mode between SRK and SP11 varies among the subgroups of haplotypes, and the residue-level difference in the same subgroups controls the self/nonself-discrimination.

20052A Effect of the divalent cation for the activity of alcohol dehydrogenase from *Sulfolobus tokodaii*

Shuichiro Goda[1,2], Sho Takashima[2], Kosei Kajiyama[2], Yuka Nagano[2], Takuro Uchida[2], Hideaki Unno[2], Tomomitsu Hatakeyama[2] ([1]*Fuc. Sci. Eng., Soka Univ.*, [2]*Grad. Sch. Eng., Nagasaki Univ.*)

Alcohol dehydrogenase from *Sulfolobus tokodaii* was produced as recombinant enzyme in *Escherichia coli*. The enzymatic activity of the produced enzyme was activated by heating. Tertiary structures were determined by X-ray crystallography. The results showed that the magnesium ion near the NAD was replaced by zinc by heating. Whereas, magnesium ion in this produced enzyme was not replaced by the dialysis for the EDTA solution. This result indicates that the replace of the divalent cation was occurred only by heating. The concentration of zinc in crude extract of E. coli was larger than that of magnesium. Therefore, this enzyme is preferred to bind magnesium in the E. coli cell. The temperature of production may affect the divalent cation selectivity.

20053A 細菌機械受容チャネル MscL の G46D 変異体を用いた張力感受活性化機構の考察に関するシミュレーション研究
Computational Study Focusing on the Mechano-Gating in the Bacterial Mechanosensitive Channel MscL Using G46D GOF mutant

Yasuyuki Sawada[1], Ken'ichi Hashimoto[2], Hisashi Kawasaki[2], Masahiro Sokabe[3] ([1]*Dept. Nutrition Nagoya Univ. Economics Fac. Human Life Sci.*, [2]*Biotechnology Res Ctr, Univ Tokyo*, [3]*Mechanobiology Lab. Nagoya Univ. Grad. Sch. Med.*)

The bacterial mechanosensitive channel MscL is constituted of homopentamer of a subunit with two transmembrane helices. One of the major issues 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 effect of changes in membrane environment, we modeled G46D experimentally GOF mutant as well as WT embedded in POPC membrane and performed MD simulations for opening of MscLs for 200 ns. As a result, G46D MscL showed faster opening than WT and it was found that D46 located in protein-lipid-water boundary interacted strongly with lipids than G46 in WT, thus it is suggested that an efficiency on sensing membrane tension is seemed to be increased in G46D MscL.

20054A* LI-cadherin 遺伝子上の SNP に伴う大腸がん転移リスク上昇の分子メカニズム
Molecular basis of increased risk of colorectal cancer metastasis caused by SNPs in LI-cadherin gene

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Liver Intestine-cadherin (LI-cadherin) is a member of cadherin superfamily, which is responsible for calcium ion-dependent cell adhesion. Expression of LI-cadherin is observed on cancer cells such as colorectal cancer (1). Previous research on genomic analysis of patients of colorectal cancer has shown that the single nucleotide polymorphisms (SNPs) at 343rd and 2216th bases of LI-cadherin gene increase the risk of lymph node metastasis of colorectal cancer (2). We discussed how the amino acid mutations caused by SNPs increased the metastatic potency using biochemical methods, cell-based assay and MD simulation. (1) T. Hinoi et al., (2002) Gastroenterol., 123, 1565-1577, (2) R.-Y. Chen et al., (2012) World J. Gastroenterol., 18, 7251-7261

20055A Aβ 産生抑制タンパク質 ILEI の活性中心の同定
Identification of the active center of the Aβ production suppressor protein ILEI

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Alzheimer's disease accounts for about 60% of all dementia and has become a major social problem. Alzheimer's disease is caused by the accumulation of Aβ peptides in the brain, but no effective treatment has yet been developed. We have identified the secreted protein ILEI (FAM3C) as a promising therapeutic lead. We have previously shown that ILEI reduces Aβ production by decreasing APP-CTF, a precursor protein of Aβ, and that this activity requires the binding of presenilin-1, a constituent protein of the γ-secretase complex involved in Aβ production. The purpose of this study was to elucidate the structure-function relationships that lead to the development of therapeutic agents based on ILEI. In this study, we elucidated the active center of ILEI by Alanine scanning.

20056A GTP-チューブリンはどのようにして微小管の核を生成するか? (1) 直線型オリゴマーの形成
How do GTP-tubulins nucleate microtubules? (1)Formation of straight oligomers

Rie Ayukawa[1], Seigo Iwata[1], Hiroshi Imai[2,5], Shinji Kamimura[2], Masahito Hayashi[1], Kien Ngo[1], Itsushi Minoura[1], Seiichi Uchimura[1], Tsukasa Makino[1], Hideki Shigematsu[6], Ken Sekimoto[3], Benoit Gigant[4], Etsuko Muto[1] ([1]*RIKEN CBS*, [2]*Chuo Univ.*, [3]*Paris Univ.*, [4]*Paris-Saclay Univ.*, [5]*Osaka Univ.*, [6]*RIKEN BDR*)

Nucleation of microtubules is essential for cellular activities, but its mechanism remains a mystery for decades. Combining rapid flush negative stain electron microscopy and kinetic analysis, we demonstrate that the formation of straight oligomers with critical size is essential for nucleation. Both GDP- and GTP-tubulin form single-stranded oligomers with a broad spectrum of curvatures but, upon nucleation, the curvature distribution of GTP-oligomers is shifted to produce a minor population of straight oligomers. With tubulin having the Y222F mutation in the β subunit, the proportion of straight oligomers increases and nucleation accelerates. The study suggests that cellular factors involved in nucleation promotes it via stabilization of straight oligomers.

20057A GTP-チューブリンはどのようにして微小管の核を生成するか? (2) オリゴマーのラテラルな相互作用
How do GTP-tubulins nucleate microtubules? (2)Lateral association of oligomers

Seigo Iwata[1], Rie Ayukawa[1], Hiroshi Imai[2,5], Shinji Kamimura[2], Ken Sekimoto[3], Benoit Gigant[4], Etsuko Muto[1] ([1]*CBS, RIKEN*, [2]*Chuo Univ.*, [3]*Paris Univ.*, [4]*Paris-Saclay Univ.*, [5]*Osaka Univ.*)

To understand how GTP-tubulin overcome the energy barrier for nucleation, we calculated the size of critical nucleus from the kinetics of tubulin polymerization and compared it with the actual size of structural intermediates towards the microtubules. The analyses showed that in the very initial stage of the nucleation, tubulin dimers assemble to single-stranded oligomers, majority of which are below the critical size. In contrast, the oligomers above the critical size are all multi-stranded. Our observation indicates that the passage of the energy barrier for nucleation is achieved by the formation of multi-stranded complex.

20058A クライオ電子顕微鏡を用いたシトクロム酸化酵素とシトクロム c の複合体構造解析
The structural analysis of cytochrome *c* oxidase complexed with cytochrome *c* using cryo-electron microscopy

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Cytochrome *c* oxidase (CcO) pumps protons coupled with O_2 reduction reaction. Each proton-pump reaction is driven by sequential electron transfer from cytochrome *c* (Cyt *c*) to O_2 bound to O_2 reduction site. The crystal structure of bovine CcO complexed with Cyt *c* provides a suggestion for the soft interaction enabling rapid exchange of substrate. In this study, we determined the complex structure of CcO and Cyt *c* at pH 6.8 and 8.0 using cryo-electron microscopy. Both structures were similar to the crystal structure. Their electron transfer pathway between Cyt *c* and CcO were shorter than that in the crystal, while the residues not in direct contact with CcO were further away from CcO. Our findings strongly support the soft and tight interaction between CcO and Cyt *c*.

20059A 重み付きアンサンブル法による Pin1 異性化のパスサンプリング
Obtaining path ensemble of Pin1-catalyzed cis-trans isomerization by weighted ensemble simulation

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Pin1 recognizes specifically phosphorylated serine/threonine (pSer/pThr) and catalyses the slow interconversion of the peptidyl-prolyl bond between cis and trans forms. In this study, we attempted to apply weighted ensemble simulations to obtain a comprehensive path ensemble of this isomerization process and to reveal the underlying molecular mechanism. Both the dual-histidine motif, H59/H157 and the basic residues, K63/R68/R69, were found to be used to anchor both side of the peptidyl-prolyl bond, the aromatic ring in Pro and the phosphate in pSer, respectively, facilitating the rotation of the torsion angle by relaying the hydrogen-bond partner of the main-chain oxygen in pSer from C113 in cis form to R68 in trans form, through S154 at the transition state.

20060A 水素結合経由の J 値の定量的解析
Quantitative analysis of J value via hydrogen bonds

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Understanding of weak interactions such as hydrogen bond is particularly important for studying structure and expression of function of biomacromolecules. J value via a hydrogen bond derived NMR is attractive to understand the nature of hydrogen bonds in protein. We focused on Ferredoxin that has been subjected to high-resolution X-ray crystal structure analysis to compare the NMR analyses using J value. Preparing the deuterated protein and utilizing TROSY based measurements, we obtained good quality data. We are analyzing the relationship between the geometries and the J values of the bifurcated hydrogen bonds.

20061A Design of cyclic and linear peptides interacting with transition metal ions

Rikako Morishita, Atsuo Tamura (*Grad. Sch. Sci., Kobe Univ.*)

In this study, we try to design peptides that selectively interact with transition metal ions. Histidine and amino acids with carboxyl groups on the side chains are commonly found in the metal binding sites of metal-binding proteins and are generally known to be involved in binding to metal ions. Therefore, cyclic peptides with four inward residues to interact with the metal ions were designed. In addition, we prepared a linear peptide with the same sequence to compare how cyclization affects the peptide structure and its interaction with the metal ions. In our experiments, we examined the structure and interaction of these peptides with metal ions by CD measurements. These results suggest these peptides selectively interact with specific metal ions, such as Au(III).

20062A 細胞壁を持たない細菌のチューブリンの解析
Analysis of bacterial tubulin in cell wall-less bacterium

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Spiroplasma eriocheiris is a cell wall-less bacterium, lacking most genes involved in cell wall synthesis except ftsZ and sepF genes. In *Bacillus subtilis*, the tubulin homolog FtsZ protein assembles into a ring structure at cell division site and SepF stabilizes the FtsZ polymers. To clarify the roles of FtsZ and its regulatory protein SepF in *S. eriocheiris*, these proteins were overproduced in *Escherichia coli* and purified. The purified SeFtsZ showed the GTP-dependent polymerization, which was promoted by SeSepF. Electron microscopy revealed that SeFtsZ polymer showed a thin filament structure and that SeFtsZ and SeSepF formed a ring structure, suggesting that SeSepF stabilized the polymerization of SeFtsZ and increased SeFtsZ filament curvature.

20063A* コレステロールが膜貫通ペプチドの二量体化に与える影響に関する分子動力学的解析
Effect of cholesterol on the dimerization of transmembrane peptides analyzed by the molecular dynamics simulations

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Membrane proteins play important roles in living organisms, and their functions are closely related to the nature of lipids. A previous study revealed that membranes containing cholesterol inhibit dimerization of transmembrane peptides with GxxxG motifs compared to pure POPC membranes. However, the mechanisms at the atomic level have not been clarified yet. We tackled this problem by using the molecular dynamics (MD) method. We conclude that cholesterol inhibits dimerization of transmembrane peptides through the conformational changes of the peptide dimer induced by an increase in the membrane thickness.The weak hydrogen bonding network(Cα-H-O) between main chains observed in the pure POPC membrane system was not observed in the cholesterol-containing membrane system.

20064A 残基間平均距離統計に基づく方法によるフラボヘモグロビンのフォールディング機構予測
Prediction of folding mechanism of flavohemoglobins using techniques based on inter -residue average residue distance statistics

Maho Osugi, Takeshi Kikuchi (*Dept. Bioinf. Col. Biosci. Ritsumeikan Univ.*)

In this study, we predict their folding mechanisms of flavohemoglobins, a chimeric protein of myoglobin and reductase, based on the inter - residue average distance statistics. Mainly using the ADM(Average Distance Map) method, the location where the structural domain is formed was predicted and compared with the three-dimensional structure of a sequence homologous protein whose structure is known. The origin of folding in the whole sequence is at both ends of the sequence, and it is predicted that Rosmann fold of flavodoxin fold is most likely to fold. As a result of domain-by-domain analysis, in Sinorhizobium meliloti 1021, which is one of the seven target flavohemoglobins, the predicted starting residues in the globin domain were 17-Leu, 106-Ile and 122-Trp.

20065A ドッキングシミュレーションによる Cyclin-dependent kinase-like 5 の基質タンパク質の同定
Identification of Cyclin-dependent kinase-like 5 substrate protein using docking simulation technique

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One of the causative proteins of the developmental disorder Rett syndrome is Cyclin-dependent kinase-like 5 (CDKL5). CDKL5 is a Ser / Thr protein kinase that regulates intracellular signal transduction and metabolism by phosphorylating substrate proteins. However, there are many unclear points regarding the physiological function of CDKL5 mediated by the substrate protein. The identification of the substrate protein of CDKL5 is thought to lead to the elucidation of the mechanism of Rett syndrome. In this study, docking simulations were performed to identify candidate substrate proteins for CDKL5. A complex of CDKL5 and a protein was obtained by ZDOCK and MEGADOCK followed by an MD simulation to examine stability of binding between a substrate protein and CDKL5.

20066A 構造研究のためのタンパク質連結法の開発
Development of protein ligation techniques for structural studies

Takumi Suzuki (*Grad. Sch. Sci., Univ. TMU*)

Investigation of the multidomain protein by NMR is hampered by overlap of the signals, although applications of NMR to multidomain systems is awaited. To overcome this problem, we developed protein ligation methods for domain selective labeling. First, application of highly active sortase for domain ligation. Sortase A catalyzes not only a proteolysis but also a ligation. To ligate proteins in a short time under conditions of 4 degrees, we designed the highly active sortase A. Second, click reaction for protein ligation using unnatural chemically modified amino acids. To utilize a click reaction using an azide and an alkyne, iodoacetamide as a linker and co-expression system for introduction of unnatural amino acid contains an alkyne group were adopted.

20067A* ネガティブ染色電子顕微鏡法により明らかにされた繊毛ダイニンの新規構造
Novel isolated ciliary dynein structure revealed by negative stain EM

Yici Lei[1], Hiroshi Imai[1], Akira Fukunaga[1], Shinji Kamimura[2] ([1]*Dep. Biol. Sci., Grad. Sch. Of Sci., Osaka Univ.*, [2]*Dept. Biol. Sci., Chuo Univ.*, [3]*Dept. Life Sci., Prefect. Univ. Hiroshima*)

Dynein is phylogenetically classified into three sub-families; ciliary, cytoplasmic and intra-flagellar transport (IFT) species. Structures of the cytoplasmic and the IFT dynein species have been extensively studied. However, for ciliary dynein species, only limited structural information is available. Here, we report a novel purification method for ciliary dynein. This method enabled us to obtain dynein particles with much higher purity than the previously published methods. By analyzing the particles with negative-stain EM, we have found novel ciliary dynein structures. Based on the structural analysis, we propose dynein's regulatory mechanism that is probably common to all dynein species.

20068A カメレオンモデルの二面角ポテンシャルの改良による NtrC の構造転移の解明
Conformational transition of NtrC elucidated by the improvement of dihedral angle potential in chameleon model

Taisei Nagata, Masaki Sasai, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*)

NtrC receiver domain is a single domain protein which exhibits allosteric transition with the register shift of an α-helix. To better understand this allosteric transition, we calculated the free energy landscape of the transition by using chameleon model (Terada et al., J. Phys. Chem. B 117, 12864 (2013)). By this model, two-state allosteric transition is reproduced as a result of locally cooperative structural changes. However, free energy barrier seemed too high for NtrC, seemingly because of the problem in modeling the secondary structure changes. We therefore modified the definition of the dihedral angle potential of the chameleon model. This modification preserved two-state allosteric transition but lowered free energy barrier as expected.

20069A Expression and Purification of Intact Small Peptides through a Novel Calmodulin-Fusion Protein System

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A kind of peptides with strong antibacteria activity called antimicrobial peptides (AMPs) become the focus of research. To provide amounts of AMPs to support related research, recombinant overexpression is the best choice. But traditional system by using *Escherichia coli* has problems with proteolysis and host toxicity. In this research, we used calmodulin as a fusion protein to overexpress cecropin P1, which is difficult to be got using thioredoxin as fusion protein. Another AMPs called fowlicidin-1 cannot be expressed by simple calmodulin fusion system. We invented a novel coexpression system with extra calmodulin to express fowlicidin-1 with strong activity in a large amount. All products were simply labeled with stable isotopes for structure analysis by NMR.

20070A RNA 結合タンパク質 FUS の液液相分離を制御するペプチドの探索
Search for peptides to control liquid-liquid phase separation of RNA binding protein FUS

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FUS forms solid amyloid fibers through the formation of liquid droplets, causing neurodegenerative diseases. Here, we took an experiment-based approach to search for the peptide targeting and controlling the liquid droplets. First, we investigated the effect of 19 amino acids on the liquid droplets of FUS using turbidity measurements and differential interference contrast microscopy. We found that the arginine and tyrosine suppressed the droplet formation. Second, we investigated the effect of polymerization of effective amino acids, and found that poly-arginine promoted the droplet formation. These results suggest that arginine additives break the cation-pi interactions between FUS molecules, but the poly-arginine can link multiple FUS molecules.

20071A 天然変性タンパク質 LAF-1RGG ドメインの一分子蛍光分光測定による構造特性評価
Conformational properties of the intrinsically-disordered RGG domain of LAF-1 detected by single-molecule fluorescence spectroscopy

Michiko Kimura[1,2], Saya Nakano[1,2], Hiroto Takahashi[1], Hiroyuki Oikawa[1], Satoshi Takahashi[1] ([1]*IMRAM, Tohoku Univ.*, [2]*Grad. Sch. Life Sci., Tohoku Univ.*)

LAF-1 RGG is an intrinsically disordered domain having the low complexity sequence that is necessary and sufficient for the phase separation of the RNA/protein assemblies called P granules. To investigate the mechanism of phase separation, we labeled fluorescence dyes to the N and C termini of LAF-1 RGG and examined its conformation by using single-molecule Forester resonance energy transfer. We observed that the LAF-1 RGG was collapsed even in the presence of denaturant. The collapse might be caused by the interaction between arginine and tyrosine residues of LAF-1 RGG, which is assumed to be important for the droplet formation. We are preparing a mutant whose tyrosines are all replaced with serine. We would like to report results for the mutant.

20072A Cryo-EM revealed unique and diverse binding schemes of the microtubule inner proteins at the inner junction region of cilia

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Cilia and flagella are important organelles of eukaryotic cells. Cilia and flagella share a same architecture called as 9+2 structure where nine doublet microtubules are bundled. The doublet microtubule is stable structure composed of complete A-tubule and incomplete B-tubule. B-tubule is tethered to the A-tubule by several microtubule inner proteins (MIPs) at the inner junction (IJ) region. Detailed architecture and protein identities of the IJ region have not been characterized. Here, we have obtained near-atomic resolution structures of the IJ region by cryo electron microscopy. Combined with mass spectrometry, we have identified new IJ proteins and built a model of the IJ region. Our model revealed complex and novel binding schemes of MIPs to the tubulin lattice.

20073A 生きた細胞における DXT 法を用いた nAChR のリガンド依存的な分子内部運動の計測
Ligand-dependent intramolecular motion of nAChR in living cells detected by DXT

Koichiro Oishi[1], Yuri Nishino[1], Hiroshi Sekiguchi[2], Yasuhiro Kashino[1], Yuji C. Sasaki[3], Atsuo Miyazawa[1] ([1]*Grad. Sch. Sci., Univ. Hyogo*, [2]*JASRI*, [3]*Grad. Sch. Sci., The Univ Tokyo*)

Diffracted X-ray tracking (DXT) is one of the methods for capturing intramolecular motions of a protein in function at a single-molecule level with synchrotron X-ray. So far, DXT has been used only for purified proteins. The muscle type nicotinic acetylcholine receptor (nAChR) is important for signal transduction between motor nurons and muscles. Ligand-dependent molecular dynamic study of nAChR would help to understand the signaling mechanisms of Cys-loop receptor family. However, mammalian nAChRs are difficult to purify and do not work without appropriate boundary lipids. In this study, we examined the fatal X-ray dose and the temperature condition for living cell, and captured the ligand-induced intramolecular motion of the nAChR expressed on living myoblast by DXT.

20074A Characterization of properties of microtubule inner protein FAP85

Yoshitoki Shibao[1], Corbin Black[2], Muneyoshi Ichikawa[1], Junya Kirima[4], Kazuhiro Oiwa[3], Khanh-Huy Bui[2], Tomoya Tsukazaki[1] ([1]*NAIST*, [2]*McGill University*, [3]*NICT*, [4]*University of Hyogo*)

Flagella drive the motility of eukaryotic cells like Chlamydomonas and human sperm. Doublet microtubule is a main component of flagella and stabilized by the microtubule inner proteins (MIPs). FAP85 is a MIP which stabilizes microtubule and facilitates microtubule growth (Kirima and Oiwa, 2018), but the details of FAP85's effects on tubulin lattice have not been characterized. Our preliminary EM results showed that there were more sheet structures when tubulin was co-polymerized with FAP85 compared with a condition without FAP85. FAP85 constructs and crystallization conditions are currently under screening to obtain crystals of FAP85 protein for X-ray crystallography. Based on the structural data obtained, FAP85's effects on microtubule will be discussed.

20075A Binding mode analysis of Hepatitis B virus X protein to DDB1 with Fluorescent based technology detecting Protein-Protein Interactions

Katsumi Omagari (*Department of Virology, Nagoya City University Graduate School of Medical Sciences*)

The hepatitis B virus X protein (HBx) interacts with a cellular protein, DNA-damage-binding protein 1 (DDB1) which implicates in DNA repair and cell cycle regulation, to stimulate viral activity. DDB1 binds several intracellular substrates and HBx of which binding sites have diverse amino acid sequences. To reveal whether HBx preferentially binds DDB1 rather than these substrates despite sequence diversity, we examined the binding specificity of DDB1 to the substrates in living cell through protein-protein visualization system, Fluorescent based technology detecting Protein-Protein Interactions (Fluoppi). Although the complex structure of HBx-DDB1 is similar to these of the substrates, the binding mode of HBx to DDB1 could be different from these of substrates.

20076A 大腸菌フェリチン変異体の荷電状態に関する研究
A study on the charge states of Escherichia coli ferritin mutants

Takumi Kuwata, Daisuke Sato, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. of Biosci., Soka Univ*)

Ferritin (Ftn) is a spherical protein composed of 24 identical subunits. It can accomodate metal or semiconducting materials inside the cavity of ~5nm diameter. Therefore, it is expected to utilize Ftn as a template to make inorganic nanoparticles. In this study, we made EQ and QE mutants of Escherichia coli ferritin (EcFtnA) by replacing Glu/Gln with Gln/Glu residues in order to control their net charges. Oppositly charged Ftns are useful to array nanoparticles. Electrophoretic mobility in the native-PAGE at pH8 was decreased with the number of EQ mutations. However, the mobility of QE mutants did not change from that of WT. These results indicated that there is a limit in the number of negative charges and that EcFtnA bears the negative charges maximally.

20077A* クライオ電子顕微鏡によるヒト PAC1 受容体の構造解析
Cryo-EM structure of the human PAC1 receptor coupled to an engineered heterotrimeric G protein

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Pituitary adenylate cyclase-activating polypeptide (PACAP) is a pleiotropic neuropeptide hormone. The PACAP receptor PAC1R, which belongs to the class B G-protein-coupled receptors (GPCRs), is a drug target for mental disorders and dry eye syndrome. Here we present a cryo-electron microscopy structure of human PAC1R bound to PACAP and an engineered Gs heterotrimer. The structure revealed that TM1 plays an essential role in PACAP recognition. A functional analysis demonstrated that the PAC1R-ECD functions as an affinity trap and is not required for receptor activation, whereas the GLP-1R-ECD plays an indispensable role in receptor activation. Our structural information will facilitate the design and improvement of better PAC1R agonists for clinical applications.

20078A Cryo-EM structure of *Thermus thermophilus* V/A-ATPase during the rotary catalysis

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V/A-ATPase is a rotary molecular motor which couples ATP hydrolysis/synthesis in V_1 with proton flow in V_o through rotation of central rotor apparatus. Previously, we reported electron cryo-microscopy (cryo-EM) structure of *Thermus thermophilus* V/A type ATPase entrapping inhibitory ADP in catalytic sites, suggesting ADP inhibited state. In this study, we report cryo-EM structures of the V/A-ATPase during the rotary catalysis. Resolving of rotary substates by 3D classification provides detailed pictures of the rotary motions that describe an entire ATP hydrolysis and conformational cycle. The local resolution of V_1 is sufficient to construct the atomic model, enabling us to discuss the mechanism for ATP hydrolysis by the V/A-ATPase that couple continuous rotary motion.

20079A タンパク質における連続する 3 つの残基で構成されるユニットの運動学的特性の解析
Analysis of the Kinematic Properties of Units Comprising Three Consecutive Residues in Proteins

Keisuke Arikawa (*Fcl. Eng., Kanagawa Inst. of Tech.*)

Units of three consecutive amino acid residues within proteins contain six movable backbone bond axes. Kinematically, a unit has the ability to modulate the relative spatial position and orientation between its both ends (RSE). By using the units, randomly sampled from the PDB, the specific distribution of their RSE was computed. This RSE distribution was compared to those obtained from units within single proteins and that obtained from artificial units whose six dihedral angles on their backbones were assigned using the Ramachandran probability. Moreover, for each unit, sterically feasible conformations while maintaining the original RSE were calculated based on the inverse kinematics formulation in robotics.

20080A Reconistitution of Cecytb-2 in Phospholipid Bilayer Nanodisc and Meaurments of its Ferric Reductase Activity

Hamed A. Abosharaf[1,2], Yuki Sakamoto[1], Mohammed El behery[1], Thoria Diab[2], Tarek M. Mohamed[2], Tetsunari Kimura[1], Motonari Tsubaki[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Fac. Sci., Tanta Univ.*)

Model organism C.elegans has seven homologs of cytochrome b561. Among them, Cecytb-2 was confirmed to be expressed in digestive organs. Cecytb-2 was expressed in Pichia pastoris cells, purified and then reconstituted into phospholipid bilayer nanodiscs. The reconstituted Cecytb-2 were more stable and more reducible by ascorbate than detergent-solubilized ones. We measured the oxidation of reduced heme of Cecytb-2 upon addition of ferric substrates under anaerobic conditions in both detergent micelle and nanodisc states. The putative ferric reductase activities in both states showed clear dependencies on the substrate concentrations. Further, we confirmed that the ferric substrates were converted to ferrous state by nitroso-PSAP assay.

20081A クライオ電子回折法による生体分子微小結晶の高分解能構造解析
High-resolution Structure Determination of Biomolecular Microcrystals by Cryo-Electron Diffraction

Kiyofumi Takaba, Koji Yonekura, Saori Maki-Yonekua (*SPring-8, RIKEN*)

Single-particle cryo-EM and cryo-electron diffraction are complementary techniques for structure analysis of various-sized molecules: The former is applied to larger-sized molecules that yield good image contrast in vitreous ice; The latter is available to undersized crystals of smaller molecules, which are hard to be solved by single particle analysis and to grow to a suitable size for X-ray diffraction even with the synchrotron radiation. We have performed electron diffraction experiments for small crystals of various samples such as complex organic compounds and peptides with a JEOL CRYO ARM 300 electron microscope, and succeeded in solving the structures beyond 1 Å resolution. We report these analyses, our development, and a perspective for further applications.

20082A* 液―液相分離によって形成される多相液滴の作成
Multiphase droplet formed by liquid-liquid phase separation

Kanji Tomohara, Yoshihiro Minagawa, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

In this work, we developed multiphase membrane-less droplets as reactors for synthetic cells. The mixture of intrinsically disordered protein (IDP) and two additional polymers, dextran (DEX) and polyethylene glycol (PEG), generated multiphase compartments, depending on the concentration of polymers. By probing these polymers with fluorescent dye, it was observed that IDP-rich droplets nested inside DEX-rich droplets, which were phase separated from PEG-rich phase. We will share the current progress on characterization of this multiphase system and discuss the future prospect of mimicking cellular functions by selectively recruiting enzymes and substrates in IDP-droplets.

20083A データベースアノテーションに基づく液滴の分析
Analysis of liquid droplets based on database annotations

Mitsuteru Iwatsuka[1], Motonori Ota[1], Satoshi Fukuchi[2], Hiroto Anbo[2] ([1]*Nagoya university*, [2]*Maebashi Institute of Technology university*)

We tried to identify features of liquid droplets based on SwissProt database. Firstly, we collected proteins in droplets. From the subcellular location annotation of SwissProt, a matrix of localizations was derived, in which each element represents co-occurrence of two names of localizations. We obtained functional information at keyword annotation, and derived a matrix showing co-occurrence of a keyword and a name of localization. From the matrices, dendrograms were constructed representing relationships among localizations, based on the co-occurrence of two localization, and that of a localization and a keyword. We found that two dendrograms were similar. They indicate three clusters. Keywords that characterize each of three clusters will be reported in the meeting.

20084A 免疫阻害機能の異なるリッサウイルス P 蛋白質 C 末端ドメインの構造比較
Structural comparison of the C-terminal domain of functionally divergent lyssavirus P proteins

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Lyssavirus P protein is a multifunctional protein that interacts with numerous host-cell proteins. The C-terminal domain (CTD) of P is important for inhibition of JAK-STAT signaling enabling the virus to evade host immunity. Among them, an extended, discrete hydrophobic patch on the surface is notable. Duvenhage virus P- CTD, which is functionally divergent from these species for immune evasion function. Here, we analyze the structures of the C-terminal domains of P of Duvenhage to gain further insight on the nature and potential function of the hydrophobic surface. Molecular contacts in crystals suggest that the hydrophobic patch is important to intermolecular interactions with other proteins, which differ between the lyssavirus species.

20085A High resolution X-ray analysis reveals a stable structure around the catalytic amino acid Asp52 in lysozyme-sugar complex

Ichiro Tanaka[1,2], Ryota Nishinomiya[1] ([1]*Grad. Sch. Sci. & Eng., Ibaraki Univ.*, [2]*Frontier Ctr, Ibaraki Univ.*)

The lysozyme mechanism of the hydrolysis reaction of lysozyme was first studied over 50 years ago; however, it has not yet been fully elucidated and various mechanisms are still being investigated. One reaction system that is commonly proposed is that the intermediate of lysozyme undergoes covalent ligand binding during hydrolysis. More recently, high resolution X-ray structural analysis was used to study lysozyme in complex with an N-acetylglucosamine tetramer. As a result, the carboxyl group of the Asp52 residue was found to form a relatively strong hydrogen bond network and had difficulty binding covalently to C1 of the sugar ring by rotating chi-angles around Asp52 side chains.

20086A シトクロム *c* が仲介する多段階電子伝達反応における呼吸鎖超複合体形成の機能的意義
Functional significance of formation of respiratory supercomplex for multiple electron transfer reaction mediated by cytochrome *c*

Wataru Sato, Peter Brzezinski (*Stockholm Univ. Fac. of Nat. Sci.*)

In respiratory chain, cytochrome *c* (Cyt *c*) mediates an electron between complex III (Cyt bc_1) and IV (C*c*O). Although the electron transfer (ET) of Cyt *c* with these redox partners have been examined, a detailed shuttle mechanism remains unclear because of the lack of information about Cyt *c* diffusion. Here, we focused on Cyt bc_1-C*c*O supercomplex formed by a supercomplex factor protein, Rcf1, and addressed the coupled ET via Cyt *c* in terms of kinetics. Change in Cyt *c* reduction level and molecular oxygen concentration upon the coupled ET showed that the reduced Cyt *c* directly donated an electron to C*c*O without release to bulk when the supercomplex was formed.

20087A* PaCS-MD/MSM を用いたタンパク質複合体の速度定数評価
Kinetic rate evaluation for protein complexes by PaCS-MD/MSM

Yoshiki Miyazawa, Phouc Duy Tran, Kazuhiro Takemura, Akio Kitao (*Grad. Sch. Life Sci Tech., Tokyo Tech*)

Association and dissociation of protein complexes are essential molecular processes in life. Kinetic rates are important quantities that measure the frequency of these events to characterize their time scales. Because of the limitation in computer power, conventional molecular dynamics cannot capture these rare events and thus cannot evaluate the kinetic rates. Previously, Parallel Cascade Selection Molecular Dynamics (PaCS-MD) combined with the Markov State Modeling (MSM), PaCS-MD/MSM, was shown to reproduce binding free energy and the kinetic rates of protein-peptide complexes. In this work, we successfully apply PaCS-MD/MSM to protein-protein complexes for the first time, and evaluate the binding free energy and kinetic rates.

20088A How internal cavities destabilize a protein

Ryo Kitahara[1], Mengjun Xue[2], Takuro Wakamoto[3], Frans A.A. Mulder[4] ([1]*Pharm. Sci., Ritsumeikan Univ.*, [2]*Dep. Chem. Univ. Washington*, [3]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [4]*iNANO, Univ. Aarhus*)

Proteins exist as ensembles of multiple conformations from the basic folded to the totally unfolded. Although transitions into lowly populated high-Gibbs energy states may lead to protein misfolding and aggregation, characterization of structure and stability of them are largely challenging. High-pressure NMR spectroscopy combined with H/D exchange and relaxation dispersion techniques were used to characterize the excited states of cavity enlarged variant L99A of T4-lysozyme in the pressure range of 0.1-250 MPa. We demonstrated that how internal cavities destabilized the protein. The energetic penalty of empty internal cavities of the protein was estimated to be 0.25 kJ/mL (36 cal/angstrom3) (Xue et al. PNAS 116, 21031-21036, 2019).

20089A クライオ電子線トモグラフィー法からの糸状仮足中のアクチン繊維とファシンのサブトモグラム平均化
Subtomogram Averaging of F-Actin with Fascin in Filopodia by Cryo-Electron Tomography

Atsuko Nakanishi[1], Naoko Kajimura[1], Shun Kurita[2], Takuo Yasunaga[3], **Kaoru Mitsuoka**[1] ([1]*Res. Ctr. UVHEM, Osaka Univ.*, [2]*Grad. Sch. Eng., Osaka Univ.*, [3]*Grad. Sch. Comp. Sci. Syst. Eng., KIT*)

A neuron is the main component of nervous tissue in all animals and migration of cells are important in the process of neural circuit formation. Filopodia are rod-like projections that extend beyond the leading edge of lamellipodia in migrating cells. In the filopodia, fascin stabilizes F-actin bundles and so understanding the interaction between F-actin and fascin is important. Cryo-electron tomography (cryo-ET) and subtomogram averaging allow high-resolution structural analysis of macromolecular complexes in the physiological conditions. In this study, we reconstructed the F-actin with fascin in situ using neuronal model cells (NG108-15 etc.). We used several different programs for the calculation and the resulted structures are compared.

20090A Could the biogenic zinc oxide nanoparticles inhibit the ATPase activity of ABC transporters?

Aliaa M. Radwan[1,2], Mai M. El-Keiy[2], Tarek M. Mohamed[2], Tetsunari Kimura[1] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Fac. Sci., Tanta Univ.*)

Zinc oxide nanoparticles (ZnO-NPs) have been used in different biological and biomedical applications. In addition, it is known that ZnO-NPs have cytotoxicity. This study aimed at clarifying whether the biologically synthesized ZnO-NPs have inhibitory effect on ABC transporters activity by conducting ATPase assay. Different concentrations of ZnO-NPs (0-0.01 mM) were added in the reaction mixture and the ATPase activity was estimated from the formation rates of inorganic phosphates in different concentrations of ATP. Michaelis-Menten analysis showed that ZnO-NPs did not affect the affinity between ATP and BhuUV, but decreased ATPase activity. The molecular mechanism of inhibitory effect of ZnO-NPs on ATPase activity in ABC transporter will be discussed.

20091A Cold adaptation and high thermal stability mechanism of glucokinase from psychrophilic bacteria are revealed by spin-labeling ESR

Akane Yato (*Grad. Sch. Adv Hea Sci., Univ. Saga*)

Generally, the cold-adapted enzyme has a high flexibility in structure, so that it is considered that it can maintain enzyme activity while a low temperature, and its thermal stability is decreased. However, our previous study revealed that glucokinase (GK) derived from psychrophilic bacteria, Pseudoalteromonas sp. AS-131 (PsGK) has a high thermal stability in spite of a cold-adapted enzyme, compared to GK derived from mesophilic bacteria, E.coli (EcGK). To clarify this unique mechanism, we measured the structural flexibility in the solution by using site-directed spin-labeling ESR. As a result, it was revealed that the structure of PsGK has duality, “rigid and flexible”, thus we conclude that it affects the function of PsGK.

20092A エネルギー準位統計とペプチドの分子進化
Energy level statistics and molecular evolution of peptide

Masanori Yamanaka (*CST, Nihon Univ.*)

We study the energy-level statistics of amino acids and peptides using random matrix theory. The energies of the molecular orbital and the Kohn-Sham orbital are calculated. We found that the statistics are between the Gaussian orthogonal ensemble and the semi-Poisson statistics, which means that the molecules are in a kind of the critical state in the sense of the random matrix theory. This result suggests that an amino acid in the critical state is a good starting point of protein synthesis. In the prolonging process of a peptide, the selection of the amino acid may be performed so that the whole molecule maintains the critical state among the huge number of combinations of amino acids.

20093A ドーパミン制御タンパク質 MAO-B のミトコンドリア膜中でのダイナミクス
The dynamics of dopamine-regulated protein MAO-B in the mitochondrial membrane

Masaki Ottawa[1], Lisa Matsukura[1], Naoyuki Miyashita[1], Ryuichi Harada[2], Yuichi Kimura[1], Shozo Furumoto[3] ([1]*BOST, KINDAI Univ.*, [2]*Med. Tohoku Univ.*, [3]*CYRIC, Tohoku Univ.*)

Monoamine Oxidase B (MAO-B), which is the integral mitochondrial outer membrane protein, works as the enzyme for the oxidation of dopamine, epinephrine, and so on. MAO-B controls the amount of dopamine and so on, and has been known to relate to Parkinson's disease. The structure of MAO-B is very similar to the structure of MAO-A. The previous experimental and simulation studies for MAO-A protein had suggested that the enzyme activity is affected by membrane environments. Here, we performed the long-time molecular dynamics simulation of MAO-B with the mitochondrial outer model membrane, to understand the dynamics of the entrance of the ligand-binding sites.

20094A* Engineering of genome editing protein Cas9 that slides along DNA faster and might enable efficient target search

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Genome editing protein Cas9 has been used in biological studies; however, has two defects: low efficiency and inaccuracy. Our earlier single-molecule experiments revealed that catalytically inactive Cas9 (dCas9), slides along DNA to much lesser extent than other DNA binding proteins. In this study, we tried to engineer Cas9 to slide along DNA faster by mutating Cas9 and adding a sliding-promoting peptide. We prepared several engineered Cas9 and analyzed them using single molecule fluorescence microscopy coupled with DNA garden. We found that the sliding-promoting peptide enhanced the sliding 3-fold and the mutation of the sites relevant to DNA binding did 90-fold. This strategy may help in reducing target-DNA search time and lead to efficient gene editing in the future.

20095A Influence of disulfide-closed loop structures on the stability of alpha-helix

Yuki Yanagida, Masamichi Ikeguchi, Kiyomi Yoshida, Kazuo Fujiwara (*Dept.of Biosci., Soka Univ.*)

CHIBLΔF is a fragment of β-lactoglobulin corresponding to the residue 97-142. It has a disulfide bond (Cys106-Cys119) and forms α-helices in the 98-107 and 114-135 regions. It has been shown that the helix content decreases when the disulfide bond is cleaved. From this result, we hypothesized that the loop formation reduces the conformations that can be taken in the loop and facilitates the nucleation of the helix. To prove this hypothesis, we constructed the three derivatives in which 1, 3, and 7 Gly residues were inserted between the residue 109 and 110. The CD spectrum showed that the helix decreased as the number of inserted Gly, suggesting that there is a relationship between the residue number in the loop and the helix stability.

20096A CNT aptamers selection and strucuture study

Ting-Chieh Chu, Huanwen Han, Ichiro Yamashita (*Graduate School of Engineering, Osaka University*)

We proposed a novel CNT/CNT junction for nanodevices. Outer-surface of cage shaped protein could be genetically modify to be a CNT linker. We attempted using the Ph.D.-12 phage display system (NEB) for the aptamer SELEX (Systematic evolution of ligands by exponential enrichment) and panning out high-affinity CNT aptamers. We got 107 sequences from 3 different CNT materials. We analyzed the hydrophobicity and 3D structure model (PEP-FOLD3) of all the sequences. The hydrophobic scores show pulsation and indicates that it is likely to form a helical structure. This is consistent with in-silico structural predictions. The helical structure plays an important role of CNT recognition.

20097A 逆並行 β-シート中の隣接ストランド間の Cα 距離の解析
Analysis of Cα distances between adjacent strands in anti-parallel β-sheets

Hiromi Suzuki (*Sch. Agri., Meiji Univ.*)

We selected 21,312 protein chains from PDB and analyzed amino acid pairs located on the adjacent strands in β-sheets. Average distances between Cα's of amino acid residues of adjacent anti-parallel strand pairs were 5.25Å and 4.50Å for hydrogen bond (HB) and non-hydrogen bond (nHB) pairs, respectively. The standard deviation of Cα distances for nHB pairs (0.33) was larger than that for HB pairs (0.25), reflecting the effect of HB. Cα distances for Cys-Cys of nHB pairs showed specific peak around 4.1Å. Cα distances between Asp and Arg or Lys tended to diverge more than those between Glu and Arg or Lys. These results indicated that side chain interactions had partial effect on Cα distances between adjacent strands in anti-parallel β-sheets.

20098A A method for producing recombinant cryptdin by enhancing inclusion body formation

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The cryptdin (crp) is an antimicrobial peptide found in mouse small intestine and there are six isoforms. For production of recombinant crp by *E. coli* with avoiding undesirable degradation, co-expression with an aggregation prone partner protein were used for accelerating the formation of stable inclusion body. By this method, crp4 could be expressed in large amount, but other crps could not. To identify the cause, we used cell free system and confirmed they were successfully synthesized at the ribosome level. For improving the expression efficiency, Origami2 strain was used to enhance the formation of inter-molecular disulfide bridges between the partner and target protein. It could be obviously observed that the expression level of crp family was increased.

20099A クライオ電顕データを用いた MD 力場の評価
Assessment of force-field accuracy using data of cryogenic electron microscopy

Tomotaka Oroguchi[1,2], Mao Oide[1,2], Taiki Wakabayashi[1,2], Masayoshi Nakasako[1,2] ([1]*Faclt. Sci. Tech., Keio Univ.*, [2]*RIKEN SPring-8 Center*)

Since results of MD simulations often display force field dependency. assessment of force field accuracy using experimental data of biomolecules in solution is essential for simulation studies. In this study, we propose the use of structural models obtained via cryo-electron microscopy (cryoEM). We assessed the accuracy of the six force fields (ff99SB-ILDN-nmr, ff14SB, ff15ipq, ff15FB, CHARMM22 and CHARMM36m) by comparing MD trajectories with the cryoEM structural model of hexameric glutamate dehydrogenase, which is reconstructed at a resolution of approximately 3 Å. The comparison enabled us to assess the validity of structures and conformational flexibility obtained by MD simulations using the force fields regarding both local and global structures.

20100A* TAT ロドプシン変異体に対する陽イオン結合の分光学的研究
Spectroscopic study of cation binding to a TAT rhodopsin mutant

Teppei Sugimoto, Kota Katayama, Hideki Kandori (*Nagoya institute of technology*)

TAT rhodopsin, found from marine bacterium SAR11 HIMB114, was named from the characteristic sequence motif in the helix 3, where the light-driven proton pump bacteriorhodopsin contains the DTD (D85, T89 and D96) motif. TAT rhodopsin possesses a neutral pKa of the Schiff base, and thus both protonated and deprotonated forms are present at the physiological pH. During the study of the molecular mechanism, we found cation binding, not only monovalent cations but also divalent cations, to the active center of a mutant of TAT rhodopsin. This is the first observation of the binding of divalent cations to the active center of rhodopsins. Molecular mechanism will be presented based on our spectroscopic investigations.

20101A Structural changes of a-synuclein along the lipid-binding and oligomerization revealed by fluorescence lifetime measurements

Ko Sasada, Ryosuke Matsubara, Koichi Fujii, Tetsunari Kimura (*Kobe Univ., Grad. Sch. of Sci.*)

Intrinsically disordered proteins (IDPs) form the specific three-dimensional structures when they bind with the target partner molecules. α-Synuclein (αSyn) is one of the IDPs whose structural changes along the binding with lipid membrane are well understood. But the roles of C-terminus part (96-140) in the membrane-binding and aggregation is still unclear at molecular level. Therefore, we use the fluorescence decay measurements with fluorescence resonance energy transfer and maximum entropy method analyses to characterize the distance between the fluorescent donor and acceptor and its distributions to clarify the structure of IDP and its fluctuation, respectively.

20102A* 単細胞緑藻由来の葉緑体 ATP 合成酵素完全複合体のワンステップ単離と制御機構の解析
One-step purification and functional analysis of the chloroplast ATP synthase complex

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Chloroplast ATP synthase (CF_oCF_1) has the redox regulation system, which is not observed in other kinds of F_oF_1. In order to elucidate the redox regulation in vitro, we aimed to purify the active CF_oCF_1 as complete complex by applying techniques for the purification of membrane-proteins. The obtained protein complex contained all known subunits of CF_oCF_1 with high purity and enough amount to conduct biochemical assays. Reduced CF_oCF_1 showed ATP synthesis activity but oxidized CF_oCF_1 did not. We therefore will apply these techniques for the mutant CF_oCF_1 complex expressed in chloroplasts and will elucidate redox regulation mechanisms by biochemical and structural biological methods.

20103A フォトンファクトリーにおける生体高分子の X 線溶液散乱
Current Status of BioSAXS at the Photon Factory

Nobutaka Shimizu, Kento Yonezawa, Masatsuyo Takahashi, Keiko Yatabe, Yasuko Nagatani (*KEK, IMSS, PF*)

Integrative structural biology (ISB) is the latest analytical approach that combines data from multiple experimental/theoretical methods in order to correctly understand the structural models for the biological system of interest. Small-angle X-ray scattering of biological macromolecules in solution (BioSAXS) has been employed well as one of the effective methods for ISB because it can obtain structural and physicochemical information in solution. We, Photon Factory support BioSAXS measurement and analysis under AMED's platform, BINDS, at the SAXS beamlines, BL-10C and BL-15A2. We will introduce the current status of our BioSAXS systems and the latest collaborative works as model studies in this presentation.
http://pfwww.kek.jp/saxs/index.html
https://www.binds.jp/

20104A 緩和モード解析を用いた NTL9 のシミュレーションデータの解析
Analysis of simulations of NTL9 using relaxation mode analysis

Ayori Mitsutake (*Dept. of Physics, Meiji Univ.*)

Because not only the most stable structure but also meta-stable structures and intermediate structures are included in trajectories in long simulations, it becomes to be necessary to develop dynamical analysis method to automatically extract reaction coordinates that identify these structures. We have developed relaxation mode analysis (RMA) to investigate dynamics and kinetics of protein simulations. RMA approximately extracts slow modes and rates from simulations. RMA was applied to folding simulations of NTL9 for which folding simulations were previously performed by Lindorff-Larsen et al. [1] Here, we present the results of RMA. [1] K. Lindorff-Larsen, S. Piana, R. O. Dror, and D. E. Shaw, Science, 334, 517 (2011).

20105A Theoretical Studies of Association-Dissociation of Plastocyanin by Coarse Grain Simulation

Dian Fitrasari, M.S. Arwansyah, Helmia Jayyinunnisya, Kazutomo Kawaguchi, Hidemi Nagao (*Kanazawa University*)

The complex plastocyanin has widely known as the electron transfer from cytochrome-f complex to PS I. However, theoretically barely describes the function of multi-subunit complex plastocyanin as carriers of a single PEG chain that has been developing for biological drugs (biologics) aims (Ravera, et. al., 2016). We are investigating the complex plastocyanin to know the association-dissociation process. MARTINI CG (coarse grain) simulation has been used for calculating the complex of plastocyanin. We obtain the equilibrium point of complex plastocyanin for the last 50ns is around 25Å and distance between complex plastocyanin that solved by Schmidt et al. (PDB:2GIM) is 27.847 Å. The free energy dissociation surface of complex plastocyanin obtains around 16 kcal/mol.

20106A 生体分子構造における形状と機能の関係
Shape similarity and functional similarity in biomolecular structures

Hirofumi Suzuki[1], Takeshi Kawabata[2], Kei Yura[1], Genji Kurisu[2] ([1]*Waseda Univ.*, [2]*IPR, Osaka-univ.*)

Shapes of biomolecular assemblies are important for their function. For example, some translation elongation factors share their overall shapes with tRNA to bind the same site on the ribosome, despite they are different types of molecules, such as protein and RNA. Such shape similarities with composition difference imply functional role in the molecular shapes. We have been developing Omokage search, a Web-based server to search three databanks, namely EMDB, PDB and SASBDB for molecules with shape similarity. We have recently made some improvements in the server, such as to narrow the search results by keywords and component similarity. In the poster session, we will discuss the improvement and some case studies using the new functions of Omokage search.

20107A Pressure-induced acceleration of the cyanobacterial circadian clock

Keita Mitsuhashi[1], Rina Sakurai[2], Soichiro Kitazawa[2], Kazuki Terauchi[1], Ryo Kitahara[2] ([1]*Grad. Sch. Life Sci., Univ. Ritsumeikan*, [2]*Depart. Pharm., Univ. Ritsumeikan*)

Cyanobacterial circadian clock consists of three proteins, KaiA, KaiB, and KaiC and ATP. While the circadian clock, namely the cycle of the KaiC phosphorylation, was inherently robust to temperature change, it was accelerated from 22 h at 1 bar to 14 h at 200 bar. This acceleration was caused by the pressure-induced enhancement of KaiC ATPase activity (Kitahara et al. Sci. Rep. 2019). Recently, pressure effects on the phosphorylation cycle were investigated up to 500 bar. Pressure-induced acceleration of the period-length was also shown in the short period mutant F470Y of KaiC. Based on the high-pressure studies, we will discuss the regulation mechanism of the cyanobacterial circadian clock.

20108A In-cell NMR analysis of an anticancer candidate compound against a chemokine-signaling protein FROUNT

Sosuke Yoshinaga[1], Takafumi Sato[1], Airi Higashi[1], Mitsuhiro Takeda[1], Yuya Terashima[2,3], Etsuko Toda[2,3,4], Kouji Matsushima[2,3], Hiroaki Terasawa[1] ([1]*Fac. Life Sci., Kumamoto Univ.*, [2]*Grad. Sch. Med., Univ. Tokyo*, [3]*RIBS, Tokyo Univ. Sci.*, [4]*Nippon Med. Sch.*)

The chemokines released from inflamed sites, are recognized by chemokine receptors on leukocytes, thus triggering leukocyte cell migration. In recent years, it has been found that cancer diseases occur when these chemokine signals are enhanced. Therefore, anticancer agents can be developed by controlling the chemokine signals. We found a cytoplasmic signaling protein of chemokine receptors (*Nature Immunol.*, 2005), as well as some compounds that control the signaling protein (*Nature Commun.*, 2020). The aim of this study is to develop an in-cell NMR system, which allows direct observation of intracellular proteins in cultured human cells, to evaluate the interactions between therapeutic candidate compounds and the target protein.

20109A Intrinsically Disordered Protein Studied by Multi-scale Divide-and-conquer Molecular Dynamics Simulation

Hiromitsu Shimoyama[1], Yasushige Yonezawa[2] ([1]*Kitasato Univ.*, [2]*Kindai Univ.*)

Calcineurin (CaN) is a eukaryotic Ca2+- and calmodulin (CaM)-activated serine/threonine protein phosphatase. CaN plays essential roles in cardiac, vasculature, and nervous system development. Calcineurin (CaN) includes an intrinsically disordered region (IDR), which folds into an alpha-helix upon binding with a calmodulin so that the CaN is activated. In this study, we proposed novel multi-scale divide-and-conquer molecular dynamics (MSDC-MD) and demonstrated that the MSDC-MD is able to sample the ordered conformation of the IDR even in solo situation. Furthermore, 100 ns of the MSDC-MD successfully sampled from wider conformational space than that of 400 ns of the conventional all-atom MD.

20110A* Saframycin A 生合成関連蛋白質のクライオ電子顕微鏡単粒子解析
Cryo-EM study on saframycin A biosynthesis related protein

Kiichi Honda[1], Takashi Matsui[2], Ryoko Komatsu[3], Ryo Tanifuji[4], Hiroki Oguri[4], Takeshi Yokoyama[1], Yoshikazu Tanaka[1] ([1]*Laboratory of Applied Biological Molecular Science, Graduate School of Life Sciences, Tohoku University*, [2]*Laboratory of Biophysics, Department of Physics, School of Science, Kitasato University*, [3]*Department of Applied Chemistry, Graduate School of Engineering, Tokyo University of Agriculture*, [4]*Department of Chemistry School of Science The University of Tokyo*)

Saframycin A, which is known to have antitumor activity, is biosynthesized by nonribosomal peptide synthetases (NRPSs); SfmA, SfmB, and SfmC. To develop a chemo-enzymatic assembly line that allows rapid and flexible access to saframycins and their variants, it is required to elucidate the molecular mechanism of NRPSs. In the present study, we investigated the structure of SfmC, a key enzyme of the biosynthesis of Saframycin A, using single particle cryo-electron microscopy (cryo-EM). SfmC was purified by Ni-affinity chromatography and subsequent size exclusion chromatography. The cryo-EM images of the purified SfmC were acquired with a Tecnai Arctica installed in RIKEN Yokohama campus. The cryo-EM single particle analysis showed polymorphism in the tertiary structure.

20111A A Singularity-Free Torsion Angle Potential for Coarse- Grained Molecular Dynamics Simulations

Cheng Tan[1], Jaewoon Jung[1,2], Chigusa Kobayashi[1], Yuji Sugita[1,2,3] ([1]*RIKEN Center for Computational Science*, [2]*RIKEN Cluster for Pioneering Research*, [3]*RIKEN Center for Biosystems Dynamics Research*)

Conventional torsion angle potentials used in molecular dynamics (MD) has a singularity problem when three particles are collinearly aligned. This problem is often encountered in coarse-grained (CG) simulations. Here we propose a new form of the torsion angle potential, introducing an angle-dependent modulating function. By carefully tuning parameters, our method can eliminate the problematic angle-dependent singularity while being combined with existing models. We optimized the modulating function for popular CG models of protein and nucleic acids based on the statistics over structures deposited on protein data bank. By comparing our design with previous methods, we found that our new potential has advantages in computational efficiency and numerical stability.

20112A* クライオ電子顕微鏡単粒子解析による百日咳壊死毒の構造解析
Cryo-electron microscopy single particle analysis of pertussis dermonecrotic toxin

Atsushi Tsugita[1], Takashi Matsui[2], Yasuhiko Horiguchi[3], Takeshi Yokoyama[1], Yoshikazu Tanaka[1] ([1]*Laboratory of Applied Biological Molecular Science, Graduate School of Life Sciences, Tohoku University*, [2]*Laboratory of Biophysics, Department of Physics, School of Science, Kitasato University*, [3]*Department of Molecular Bacteriology, Research Institute for Microbial Diseases, Osaka University.*)

Dermonecrotic toxin (DNT) is known as one of the major toxins produced by B. pertussis. However, the function of DNT in pertussis infection have not yet been clarified. Recently, it was revealed that DNT specifically binds to T-type voltage-gated Ca2+ channel Cav3.1 that is highly expressed in the central nervous system. This neurological disorder is present in up to 1% of pertussis patients and leads to severe sequelae (encephalopathy). To understand the molecular basis of DNT binding to Cav3.1 and causing pertussis encephalopathy, we performed single particle cryo-EM analysis of DNT. The obtained cryo-EM reconstruction depicted the entire structure of DNT. In this conference, we are going to discuss the function of DNT based on the revealed structure of DNT.

20113A Biflavonoids that inhibit ATPase and microtubule-gliding activities of mitotic kinesin Eg5

Tomisin H. Ogunwa[1], Sadakane Kei[1], Maruta Shinsaku[1], Miyanishi Takayuki[2] ([1]*Department of Bioinformatics, Graduate School of Engineering, Soka University, Hachioji, Japan*, [2]*Graduate School of Fisheries and Environmental Sciences, Nagasaki University, Nagasaki, Japan*)

Kinesin Eg5 is essential for the establishment and maintenance of bipolar spindles during mitosis. In our studies, we identified two biflavonoids (morelloflavone and kolaflavanone) from medicinal plants as potent Eg5 inhibitors. Morelloflavone (MRF) and kolaflavanone (KLF) suppressed Eg5 gliding along microtubules. The biflavonoids also inhibited both the basal and microtubule-activated ATPase activities of Eg5. Computational analysis predicted that the biflavonoids target and fit well into the allosteric pocket of Eg5. These data suggest that MRF and KLF are novel allosteric inhibitors of mitotic kinesin Eg5. It would be of considerable interest to evaluate the interaction mechanism and specificity of these inhibitors to Eg5.

20114A 分子動力学シミュレーションを用いた CDR-Grafting による合成 VHH における分子挙動の解析
Molecular dynamics analysis of structural effects of Grafting CDRs in synthetic VHHs

Seisho Kinoshita[1], Makoto Nakakido[1,2], Daisuke Kuroda[1,2], Jose M.M. Caaveiro[3], Kouhei Tsumoto[1,2,4] ([1]*Dept. of Bioeng., Sch. of Eng., Univ. of Tokyo*, [2]*Dept. of Chem. Biotech., Sch. of Eng., Univ. of Tokyo*, [3]*Grad. Sch. of Pharm. Sci., Kyushu Univ.*, [4]*Inst. of Med. Sci., Univ. of Tokyo*)

VHHs nanoantibodies are useful tools for biotechnological and medical applications. To improve their applicability, optimizations based on the understanding of molecular mechanisms and physicochemical properties are sought after. Herein we have exchanged the complementarity determining regions (CDR) between different scaffolds and performed physicochemical analyses, revealing that synthetic VHHs exhibited various affinities and thermal stabilities. To describe the molecular basis of these differences, we employed molecular dynamics simulations. From the comparison of the simulations with the experimental data, we noticed a correlation between the dynamics of the VHHs and their physicochemical parameters. In light of these data, we discuss possible molecular mechanisms.

20115A* 転写コアクチベータ CBP の KIX ドメインと転写因子の相互作用を標的としたペプチド阻害剤の合理的設計
Rational design of the peptide inhibitor targeting the interaction of the KIX domain of CBP with transcriptional activators

Nao Sato[1], Shunji Suetaka[1], Yuuki Hayashi[1], Munehito Arai[1,2] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Dept. Phys., Univ. Tokyo*)

Protein-protein interactions (PPIs) are involved in various diseases, and thus inhibition of PPIs is one of the promising ways of developing pharmaceutical drugs. The KIX domain of a general transcriptional coactivator CBP binds many kinds of transcriptional activators, including a mixed lineage leukemia protein MLL, but the interactions may cause leukemia and viral diseases. Here, we designed peptide inhibitors for the PPIs involving KIX. As a template of the peptide design, we used the transactivation domain (TAD) of MLL. Using the protein design software Rosetta and helicity prediction algorithm AGADIR, we designed mutants of the MLL TAD fragment that may bind KIX more tightly than the wild-type MLL. The details will be presented at the meeting.

20116A 分布推定アルゴリズムと勾配降下法最適化アルゴリズムによる単粒子解析初期モデル生成
Initial model generation in single particle analysis using Estimation of Distribution Algorithms and gradient descent optimization

Nobuya Mamizu[1,2], Takuo Yasunaga[1] ([1]*Grad. Sch. Comp. Sci., Kyushu Inst. Tech.*, [2]*SYSTEM IN FRONTIER INC.*)

In this research, we propose a method for determining the projection parameters for each particle and initial model generation for single particle analysis and 3D reconstruction. Using Estimation of Distribution Algorithms (EDAs), the proposed method evaluated the prior distribution for projection parameters in the model formula based on the reconstruction algorithm of RELION. Further, the optimization algorithm in the gradient descent method used in the field of machine learning for improving the convergence efficiency of the 3D density map is applied without directly calculating the gradients. We applied the method to simulation data and real EM data sets and then evaluated the possibility of initial model generation and the improvement of calculation speed.

20117A 粗視化ペプチドの安定構造探索に向けたアミノ酸間相互作用ポテンシャルの開発
Amino-Acid Pair Interaction Potentials for Coarse Grained Peptide Folding

Chieko Terashima, Yoshiaki Tanida, Hiroyuki Sato (*Fujitsu Laboratories Ltd.*)

Cyclic peptides are attractive research targets for drug discovery, but the conformational search of peptides is very time consuming. To accelerate the conformational search of peptides, we investigated coarse-grained model that treated amino-acid residue as an on-lattice particle interacting with amino-acid pair interaction potentials. However, interaction potentials from protein structures that have been used are not able to concern to artificial amino acids. To treat both natural and artificial types of amino acids and staples, new interaction potentials were developed by umbrella sampling. The new potentials were applied to explore the conformation of PLP-2 (cyclo-DLFVPPID) for their validation.

20118A 環状ペプチド中の隣接プロリンに特徴的な異性化
Characteristic isomerization of two adjacent prolines in a cyclic peptide

Yoshiaki Tanida, Chieko Terashima, Hiroyuki Sato (*Fujitsu Labs.*)

Finding characteristic features of cyclic peptides in structure are of great interest in middle molecule drug development using protein-protein interaction (PPI). The barrier height of cis-trans isomerization in proline residue is generally small than the others at room temperature. In this report, we investigated the structure of the two adjacent prolines in PLP-2 (cyclo-DLFVPPID). Using REST2, the major form was found to be cis type for the Val-Pro5 bond and trans type for the Pro5-Pro6 bond. This feature reproduces the solution NMR result.

20119A* マイコプラズマ・モービレのモーター構成タンパク質 MMOB1620 の SAXS による構造解析
Structural Analysis of MMOB1620, Component Protein of Mycoplasma mobile's Motor, by SAXS

Hiroki Sato[1], Hisashi Kudo[2,3], Yuuki Hayashi[3], Syunji Suetaka[3], Koji Ooka[4], Munehito Arai[3,4], Makoto Miyata[1,5]
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Mycoplasma mobile, a bacterium that parasitizes the gill of freshwater fish, glides by the force generated by a motor complex that evolved from F-type ATPase. In our lab, the motor whole structure has been revealed at a resolution of ~4.8 angstroms by electron cryomicroscopy (cryoEM). The structure and assignment of MMOB1620 (1620), a component protein, have not been clarified. Last year, we showed that it has a rod-shaped structure from small angle X-ray scattering. This year, size exclusion chromatography 90-degree light scattering measurement revealed that the molecule is a monomer, suggesting that some residues of 1620 were not visualized by cryoEM. 1620 protein deleted for the N-terminal flexible region was isolated for referring to the structure.

20120A Multiscale Modeling Approach for Conformational Search of Macrocyclic Peptides

Hiroyuki Sato, Chieko Terashima, Yoshiaki Tanida (*Fujitsu Laboratories Ltd.*)

We present an efficient multiscale modeling approach to search conformation of macrocyclic peptides. Firstly, lattice-based coarse-grained approach is carried out for conformational search. Then, atom-based conformation is determined by enhanced sampling method. The conformation of lattice model is identified using combinatorial optimization method with Fujitsu's Digital Annealer, and the conformational space of full-atom model is explored using REST2 method. We applied the approach to PawL-Derived Peptide PLP-2 as a test case, and the resulting conformation was in good agreement with the experimental conformation. We will discuss our approach in detail at the meeting.

20121A 非リボソーム分子機械によるペプチド合成の静電的ラチェット機構
Electrostatic ratcheting mechanism of peptide synthesis by non-ribosomal molecular machine

Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

While ribosome is the main molecular machine that synthesizes peptide, there exist non-ribosomal peptide-synthesizing machines. RimK is such a non-ribosomal molecular machine that synthesizes poly-α-glutamate, utilizing ATP hydrolysis energy, although not just its molecular mechanism but the glutamate binding sites have been unknown. We here conducted molecular dynamics simulation of RimK and found that glutamate binds to the positively charged surface of RimK on which the bound glutamate exhibits Brownian motion. We show that the structural change in RimK plays a ratcheting role in the Brownian motion, guiding glutamate to the site near ATP. We propose the mechanism of the poly-α-glutamate synthesis by RimK, the essential part of which is shared with ribosome.

20122A Local Structural Similarity of Mononucleotide Binding Sites Around Different Chemical Groups in Ligands

Shota Kawakami[1], Hafumi Nishi[2,3], Kengo Kinoshita[1,2] ([1]*Grad. Sch. Life Sci., Tohoku Univ.*, [2]*Grad. Sch. Info. Sci., Tohoku Univ.*, [3]*Fac. Core. Res., Ochanomizu Univ.*)

Examining the local structures of ligand-binding sites is important to elucidate the mechanisms of how proteins recognize ligands. Although mononucleotides interact with various proteins, few studies have performed an exhaustive comparison of ligand-binding site structures at the atomic level, focusing on the structures around different chemical groups in identical ligands. In this study, we performed an all-against-all comparison of mononucleotide binding sites at the atomic level for the structures around the phosphate group and the base group, respectively. Around the phosphate group, proteins from the same superfamily showed high similarity of local structure, but around the base group, the differences in their family or their ligands can reduce local similarity.

20123A* Secondary structure transformation of artificially designed peptide nanofibers

Minami Kurokawa[1], Mika Hirose[2], Akihiro Kawamoto[2], Atsuo Tamura[1] ([1]*Grad. Sch. Sci., Univ. Kobe.*, [2]*IPR,Univ. Osaka.*)

There are many natural fibrous proteins such as muscle fibers and spider silks. These fibers are composed of either α-helix or β-sheet, and it is quite unusual to transform between them. Thus we tried to design artificial peptides with the capability of changing the secondary structure in response to external environments. The designed peptides have 29 amino acid residues, named kp3 and kp4. CD and TEM observations showed that they transformed from α to β by pH change or heat, while maintaining the fibrous form. The β-structure of kp3 returned to α as time went by, whereas kp4 resulted in amyloid-like fibrillization that could never returned to α. To find out the reason for this difference, we have investigated characteristics of fiber structures with cryo-EM.

20124A 分子クラウディング環境における光活性化アデニル酸シクラーゼの光反応
Crowding effect on reaction dynamics of photoactivated adenylate cyclase

Hiroto Murakami, Masahide Terazima, Yusuke Nakasone (*Grad. Sch. Sci., Univ. Kyoto*)

In a living cell, it is highly crowded by macromolecules, which has a significant effect on protein reaction. To understand the crowding environment as a reaction field of proteins, we investigated the photoreaction of photoactivated adenylate cyclase (PAC), which is a blue light sensor to produce cAMP in a light dependent manner. Using the transient grating method, we found that the photoreaction rate and yield decreased upon addition of PEG200 as a crowding agent, which may be explained by an increase of the viscosity. When macromolecules such as BSA and Ficoll70 were used as crowders, however, the conformation of the active state of PAC was significantly changed, representing that the structure of the protein was strongly affected by the macromolecular crowding.

20125A 電子伝達系における複数のタンパク質複合体の複合体形成と構造安定性に関する理論的研究
Theoretical study on complex formation and conformational stability of multiple protein complexes in electron transport system

Rena Saito, Kazutomo Kawaguchi, Hidemi Nagao (*Grad. Comput. bio., Univ. Kanazawa*)

In the light reaction of photosynthesis, electrons are transferred from photosystem II (PSII) to photosystem I (PSI) via cytochrome b6f complex (Cyt f), plastocyanin (Pc) and so on. The structure of Cyt f and Pc in this process has been clarified experimentally. In our group, complex structure and reaction rate have been studied by Langevin dynamics simulation using a coarse-grained model. [S. Nakagawa, et al.,Mol.Phys. 2017] In this study, to investigate the dependence on the concentration ratio of Cyt f and Pc, we perform the Langevin dynamics simulation for multiple complex of Pc and Cyt f. The highest peak in the radial distribution function for the Cu-Fe distance shifts to a shorter distance with increasing the concentration of Pc.

20126A 高速原子間力顕微鏡を用いたアミロイドβ線維の伸長および抗アミロイドβ抗体による線維伸長阻害の観察
HS-AFM observation of Amyloid β elongation and inhibition by antibodies

Shogo Miyajima[1], Maho Yagi-Utsumi[2], Takayuki Uchihashi[1,2], Koichi Kato[2] ([1]*Dept of Phys, Nagoya univ*, [2]*EXCELLS*)

Amyloid fibrils are aggregates formed by proteins arranging regularly and are known to cause the neurodegenerative diseases such as Alzheimer's disease and Parkinson's disease. Amyloid β protein(Aβ) aggregates and elongates with ganglioside-bound Aβ as a seed, forming Aβ fibrils that are toxic to neurons. The IgG monoclonal antibodies 4396 C, 6E 10, and 4G8 are antibodies to Aβ, and in particular, 4396 C is known to inhibit Aβ fibril elongation, but how it actually functions has not been elucidated before. In this study, we used high-speed atomic force microscopy (HS-AFM) to directly visualize the binding of these antibodies to amyloid fibrils in real time. We also confirmed that inhibition of fibril elongation by 4396 C was concentration-dependent.

20127A Bayesian inference and Iterative Boltzmann approach to coarse-grained local potential of disordered proteins

Azuki Mizutani, Shoji Takada, Giovanni B Brandani (*Grad. Sch. Sci, Univ. Kyoto*)

Intrinsically disordered proteins (IDP) do not fold into specific structures and thus are difficult to be characterized by experiments at high resolution. Complementarily, MD simulations can be useful to study their structures and functions. We have been developing a Calpha-based coarse-grained (CG) MD method for IDPs. In this work, we improve on our previous version of the model by fitting the bond-angle potential to the statistics of the three residues involved, instead of the central one alone. We employ a Bayesian inference approach to overcome the issue of the small sample sizes used to fit the potential. Finally, we further adjust the potential using MD simulations and iterative Boltzmann inversion.

20128A NMR Studies on Cup s 7, an Novel Allergen from Cypress Pollen

Jingkang Zheng[1], Tomona Iizuka[1], Xiaoshaung Lu[1], Tomoyasu Aizawa[1,2] ([1]*Grad. Sci. Life Sci., Hokkaido univ.*, [2]*GI-CoRE Hokkaido univ.*)

Cup s 7 is a small cysteine-rich gibberellin regulatory protein (GRP) with 6 disulfide bonds, which was isolated from European cypress (Cupressus sempervirens) as the pollen allergen to make cross-reactivity with food allergens cause pollen-food allergy syndrome (PFAS). In our study, DNA sequence of Cup s 7 was newly identified by RNA-seq and the recombinant protein was overexpressed by *Pichia pastoris* . After the detailed examination of culture conditions, we successfully produced stable isotope-labeled samples for NMR experiment. The results clearly indicated that recombinant Cup s 7 formed a correct folding structure.

20129A* アミノ酸溶媒中における芳香族アミノ酸の溶解度
Solubility of aromatic amino acids in amino acid solutions

Akira Nomoto, Suguru Nishinami, Kentaro Shiraki (*Pure and Appl. Sci, Univ. Tsukuba*)

The characteristic of amino acids, e.g. solubility, hydropathy, and conformational parameter, is essential for understanding behavior of proteins for folding and aggregation. However, a new scale is necessary to understand the liquid-liquid phase separation (LLPS) of proteins which is triggered by the hydrophilic interactions between amino acid residues. Here we measured the solubility of aromatic amino acids (AAs) in the solution of natural amino acids (SAs). The solubility of AAs in the solutions of arginine, lysine and proline became 1.5-2.0 times higher than that in only water due to the attractive hydrophilic interaction between AAs and SAs. This simple parameter using solubility measurements would be a new scale to be reflected the interaction between amino acids.

20130A 経験ベイズ推定を用いた水の効果の最適化によるタンパク質デザイン
Protein design by optimization of role of water using empirical Bayes' estimation

Tomoei Takahashi[1], George Chikenji[2], Kei Tokita[1] ([1]*Grad. Sch. Inform. , Nagoya Univ.*, [2]*Grad. Sch. Eng. , Nagoya Univ.*)

In recent years, it has been found that the effect of water is closely related to protein stabilization. According to this, considering the effect of water on protein surface is a key point for protein design. Previously, based on statistical mechanics, we proposed a Bayesian design method in which the exhaustive conformational search is canceled by prior based on our original hypothesis for protein sequence evolution, and it successfully designed two dimensional lattice HP proteins. In this presentation, we update it by optimization of water effect on protein surface using empirical Bayes' estimation.

20131A* 脱水に応答して繊維構造を可逆的に形成するクマムシ固有の天然変性タンパク質の解析
Reversible fiber formation of tardigrade-unique intrinsically disordered proteins upon dehydration stress

Akihiro Tanaka, Tomomi Nakano, Takekazu Kunieda (*Dept. of Biol. Sci., Grad. Sch. of Sci., Univ. of Tokyo*)

Tardigrades can withstand almost complete dehydration, but the molecular mechanisms underlying the tolerance remain largely unclear. Recently, we identified several tardigrade-unique proteins which reversibly form fiber structures upon water-deficient stress when expressed in human cultured cells. We revealed that the fiber formation required the protein motifs, which were highly conserved among these proteins. Our mutational analysis suggested that the fiber formation relied on their helical coiled-coil structures although these proteins are predicted to be intrinsically disordered. These proteins may change their conformation to helical structure upon dehydration and form fiber structures, which may induce intracellular gelation beneficial for dehydration tolerance.

20132A* スピロプラズマのらせん反転機構
Helical reversal machinery of Spiroplasma

Yuya Sasajima[1], Takayuki Kato[2], Tomoko Miyata[3], Keiichi Namba[3,4,5], Makoto Miyata[1,6] ([1]*Grad. Sch. Sci., Osaka City Univ., Japan*, [2]*IPR., Osaka Univ., Japan*, [3]*Grad. Sch. Front. Biosci., Osaka Univ., Japan*, [4]*BDR & SPring-8 Center, Riken, Japan*, [5]*JEOL Yokogushi Res. Alliance. Lab. Osaka Univ., Japan*, [6]*OCARINA, Osaka City Univ., Japan*)

Spiroplasma are helical-shaped bacteria lacking peptidoglycan layer. They have a unique swimming system in which cells reverse the helicity from front to back. We analyzed the internal ribbon structure to elucidate the mechanism of the helical reversal. Electron microscopy revealed that the ribbon and Fibril, protofilament of the ribbon, have the same pitch of 350 nm with the helicity of swimming cells. Three-dimensional reconstructions of Fibril filaments from negative staining electron microscopy showed both the left-handed and right-handed helicity. Based on these results, we propose a swimming model in which the twist of the ribbon caused by Fibril accumulates in the longitudinal direction along the cell axis and pushes the medium backward to propel the cell body.

20133A* 多重平衡状態を持つ光スイッチング蛍光タンパク質「Kohinoor2.0」の開発と、細胞内小器官動態の超解像イメージングへの応用
Photoswitchable fluorescent protein with multiple equilibria states enables super-resolution imaging of intracellular dynamics

Ryohei Noma[1], Tethuichi Wazawa[1], Syusaku Uto[2], Kazunori Sugiura[1], Takeharu Nagai[1] ([1]*Nagai laboratory*, [2]*no affiliation*)

Reversible photoswitchable fluorescent proteins (RSFPs) are a kind of fluorescent proteins whose fluorescence can be turned on and off by light irradiation. Herein, we developed a RSFP, Kohinoor2.0, which was brighter than Kohinoor. Analysis of pKa revealed that the chromophore phenolate of Kohinoor2.0 was in multiple equilibria and increase of anionic mole fraction contributed to improvement of brightness, implying proton network involved in a histidine near the chromophore could give multiple equilibria states of Kohinoor2.0. In addition, we successfully performed super-resolution (SR) imaging with Kohinoor2.0 to visualize previously invisible dynamics of mitochondrial fine structure. Thus, Kohinoor2.0 opens a way of SR imaging of unrevealed intracellular dynamics.

20134A シアノバクテリア由来光受容タンパク質 GAF ドメインの立体構造解析
Structural study of a GAF domain of photosensor protein from Cyanobacteria

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A cyanobacterium synthesizes a photosynthetic pigment which absorbs red light under red-light condition. Conversely, under green-light condition, a photosynthetic pigment which absorbs green light is synthesized. This phenomenon is called “complementary chromatic acclimation”, regulated by RcaE protein, a photosensor protein, phosphorylating transcription regulatory proteins in a wavelength dependent manner. In order to elucidate the molecular mechanism of the structural change due to light absorption of RcaE, we are working on NMR structural analysis and X-ray crystallography of RcaE red light absorption form (15EPr) and green light absorption form (15ZPg).We are succeeded in obtaining the crystal structure of 15EPr. We are proceeding with the structural analysis.

20135B ウシミトコンドリア呼吸鎖酸素還元酵素の 1.3Å 分解能構造が示唆する二量体化機構
The 1.3 Å resolution structure of bovine mitochondrial respiratory oxygen reductase suggests a dimerization mechanism

Kyoko Shinzawa-Itoh[1], Miki Hatanaka[1], Kazuya Fujita[2], Naomine Yano[1], Yumi Ogasawara[1], Jun Iwata[2], Eiki Yamashita[3], Tomitake Tsukihara[2,3], Shinya Yoshikawa[2], **Kazumasa Muramoto**[1] ([1]*Grad. Sch. Life Sci., Univ. Hyogo*, [2]*Sch. Sci., Univ. Hyogo*, [3]*IPR, Osaka Univ.*)

Respiratory chain generates proton motive force coupled to electron transfer at high energy efficiency. Respiratory O2 reductases are broadly classified into A, B and C-types based on their molecular structures. The A-type O_2 reductase in bovine mitochondria forms both monomeric and dimeric structures, although all crystal and cryo-EM structures of other types O_2 reductases are monomeric forms. Previous study suggested that the dimerization of bovine enzyme was dependent on specifically arranged lipid molecules. To re-examine structural basis of dimerization, we improved the resolution of the crystal structure to 1.3 Å by optimizing the method for cryoprotectant soaking. The crystallographic and mass-spectrometric analyses revealed the factors involved in dimerization.

20136B ゲノム編集酵素の開発に向けたエングレイルドホメオドメインアレイの構造解析
Structural basis for an array of engrailed homeodomains toward the development of genome-editing enzymes

Tomoko Sunami, Yu Hirano, Taro Tamada, Hidetoshi Kono (*iQLS, QST*)

A small DNA binding protein to target desired sequences have the potential to become a scaffold of molecular tools such as genome-editing enzymes. We previously showed two engrailed homeodomains (EHDs) connected with a linker recognizes a target sequence twice as long as a single EHD in cells only when arginine 53 in each EHD in the tandem protein is mutated to alanine ((EHD[R53A])2). In this study, we determined the crystal structure of the (EHD[R53A])2-DNA complex. Most importantly, it shows the base-specific interactions necessary for the affinity and/or specificity of the wild-type EHD are preserved in (EHD[R53A])2. The mechanism of the specific recognition will be discussed based on the structure and cellular assays.

20137B　ナノディスクに再構成されたイネキシン 6 ギャップ結合ヘミチャネルの構造
Structures of the Innexin-6 gap junction hemichannels in nanodiscs

Batuujin Burendei[1], Ruriko Shinozaki[2], Masakatsu Watanabe[3], Tohru Terada[4], Kazutoshi Tani[5], Yoshinori Fujiyoshi[6,7], **Atsunori Oshima**[2,8] ([1]*Sch. Sci., Nagoya Univ.*, [2]*Grad. Sch. Pharm. Sci., Nagoya Univ.*, [3]*Grad. Sch. Frontier Biosci., Osaka Univ.*, [4]*III/GSII, Univ. Tokyo*, [5]*Grad. Sch. Med., Mie Univ.*, [6]*Adv. Res., TMDU*, [7]*CeSPIA, Inc.*, [8]*CeSPI, Nagoya Univ.*)

Gap junctions form intercellular conduits with a large pore size whose closed and open states regulate communication between adjacent cells. Here we show the cryo-electron microscopy structures of Caenorhabditis elegans innexin-6 (INX-6) gap junction proteins in an undocked hemichannel form. In the nanodisc-reconstituted structure of the wild-type INX-6 hemichannel, flat double-layer densities obstruct the channel pore. Comparison of the hemichannel structures of a wild-type INX-6 in detergent and nanodisc-reconstituted N-terminal deletion mutant reveal that N-terminal rearrangement and pore obstruction occur upon nanodisc reconstitution. Our results provide insight into the closure of the INX-6 hemichannel in a lipid bilayer before docking of two hemichannels.

20138B*　分子動力学シミュレーションを用いた、オレキシン 2 受容体の動的性質の研究
Dynamics of Orexin 2 Receptor Using Molecular Dynamics Simulations

Shun Yokoi, Ayori Mitsutake (*Meiji University*)

Orexinergic systems which comprise two peptide ligands, orexin-A and -B, and two G protein-coupled receptors (GPCR), OX1R and OX2R, are involved in regulation of sleep-wake rhythm. Such kind of neurological process are caused by GPCR activation. It's a process where ligand binding stabilizes a receptor conformation that allows for G-protein binding and downstream signaling. However the mechanism of activation remains unknown. So we performed and analyzed all-atom molecular dynamics (MD) simulations of OX2R. We execute not only original structure simulations but mutant ones. In this poster, we first show the results of the MD simulations and consider the dynamics of OX2R. Then, we discuss the implications of the mechanism binding between orexin peptides and the receptor.

20139B　酵母の DNA 複製開始機構の一分子観察に向けて
Toward single-molecule observation of yeast pre-replicative complex assembly and firing

Mayu Terakawa S., Tsuyoshi Terakawa (*Dep. Biophys, Grad. Sch. Sci., Kyoto Univ.*)

Eukaryotic DNA replication initiation is a highly complex process in which at least 18 proteins are involved. The molecular mechanism of DNA replication initiation remains elusive. The replication initiation can be divided into three steps: 1) Mcm2-7 is loaded onto the specific DNA sequence called ARS, 2) Cdc45 and GINS are loaded onto Mcm2-7 to assemble a pre-replicative complex, and 3) the firing factors make the pre-replicative complex capable of replicating DNA. In this study, we purified 18 proteins required to reconstitute in vitro DNA replication. Using magnetic beads pull-down assay, we confirmed that the purified proteins are properly loaded onto the ARS. This study paves the way for the single-molecule observation of replication initiation and firing.

20140B*　β 切断酵素と APP の生体膜中での相互作用と α 切断酵素の構造予測
Interaction Between beta-Secretase and APP in The Biological Membrane, and The Structure Prediction of The TM domain of alpha-Secretase

Kaori Yanagino, Naoyuki Miyashita (*Grad. Sch. BOST, KINDAI Univ.*)

Amyloid Precursor Protein (APP) is one of the key membrane proteins in the pathogenesis of Alzheimer's disease (AD). APP is usually cleaved by alpha-secretase in non-raft environments. However, APP is sometimes cleaved by beta-secretase in the lipid raft membrane, and amyloid-beta (Aβ) peptides are produced. The Aβ peptides are related to the AD. Currently, the transmembrane (TM) structures of beta- and alpha-secretase have not been solved experimentally. Here, we have performed the structure predictions of the TM domains of alpha- and beta-secretases using the replica-exchange molecular dynamics simulations (REMD). We also performed the Coarse-Grained model Molecular Dynamics simulations of the TM domain of beta-secretase and APP in the lipid raft environments.

20141B* マラリア原虫のトランスロコンである EXP2 ナノポアのチャネル電流計測
Channel current measurement of EXP2 nanopore as a translocon of the malaria parasite

Mitsuki Miyagi, Sotaro Takiguchi, Kazuaki Hakamada, Masafumi Yoda, Ryuji Kawano (*Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology*)

DNA sequencing by using nanopore has achieved and commercialized; the next step should be toward a peptide sequencing with the nanopore. Nanopore measurement requires high stability such as the mechanical stability including a bilayer lipid membrane (BLM), and the feasible pore size for the peptide sequencing. In this study, we focused on EXP2, which is a transmembrane site of the pore-forming translocon from the malaria parasite. As the first step for peptide sequencing, we here evaluated the stability of EXP2 nanopore in BLM and the capability of peptide translocation through the EXP2 nanopore.

20142B 四量体と二量体のヘモグロビン平衡混合物の構造の柔らかさの違いによる分離
Separation of tetramer-dimer mixtures mutant hemoglobin by structural flexibility

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Cavity mutant hemoglobin, rHb(βH92G) of human adult hemoglobin (Hb A) which has tetramer-dimer equilibrium, in which the proximal histidine of the β subunits are replaced by glycine in the presence of imidazole, shows larger dimer population than Hb A in tetramer-dimer equilibrium. Although charge distributions at the surface between tetramer and dimer in rHb(βH92G) seem to be almost the same, ion-exchange column chromatography of rHb(βH92G) yielded two main peaks, while isoelectric focusing of rHb(βH92G) did not separate to two positions. This suggests that difference of structural flexibility (or softness) between tetramer and dimer having an identical electric charge influences elution rate, and that enables us to separate the tetramer-dimer mixture.

20143B Assembly of a trimeric autotransporter transmembrane domain assisted by BamA embedded into the nanodisc

Eriko Aoki, Kazuo Fujiwara, Masamichi Ikeguchi (*Dept. of Biosci., Soka Univ.*)

Haemophilus Influenzae adhesin (Hia) is an outer membrane protein (OMP) and belongs to the trimeric autotransporter family. Although Gram-negative bacterial OMPs, including Hia, are thought to be inserted into the outer membrane by a β-barrel assembly machinery (BAM) complex, the insertion mechanism by BAM complex has not been fully elucidated. In this study, we investigated the assembly of Hia transmembrane domain (HiaTD) using empty and BamA-embedded nanodiscs. The results showed that BamA facilitates the assembly of HiaTD in vitro. Moreover, we investigated the effect of the truncation of BamA POTRA domains on the HiaTD assembly. The role of POTRA domains in the BAM-assisted HiaTD assembly will be discussed.

20144B ナノディスク再構成型ヘム ABC トランスポーターを用いた基質輸送機構の分光学的解析
Spectroscopic analysis of allocrite transport mechanism using nanodisc-reconstituted heme ABC transporter

Takuya Asada[1], Motonari Tsubaki[1], Yoshitsugu Shiro[2], Hiroshi Sugimoto[3], Tetsunari Kimura[1,4] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*Grad. Sch. Life Sci. Univ. of Hyogo*, [3]*RIKEN SPring-8*, [4]*K-CONNEX*)

ABC transporters are membrane proteins that use the energy of ATP to drive allocrite transport across biological membranes. Direct observation of transport process is necessary to essentially understand the transport mechanism. Therefore, I'm trying to spectroscopically visualize that process by using the heme import system; BhuUV-T. Moreover, I reconstituted heme transporter into the Nanodisc because the previous studies have shown that detergents interact with heme, complicating the observation of heme-transporter interaction. In this presentation, I will discuss the transport of heme and the ATP hydrolysis reaction using this ABC transporter nanodisc.

20145B 膜環境の違いがアルカン水酸化酵素の活性に与える影響について
An effect of membrane environment for the activity of alkane hydroxylase

Takaki Okamoto[1], Tomomi Kikuchi[2], Shingo Nagano[1], **Tomoya Hino**[1] ([1]*Grad. Sch. Eng., Tottori Univ.*, [2]*Grad. Sch. Sus. Sci., Tottori Univ.*)

Alkane hydroxylase (AlkB) catalyzes the regio-specific hydroxylation of the terminal carbon atom in the alkane molecule. AlkB is an integral membrane protein with the binuclear non-heme iron active center on the cytoplasmic side. Alkanes are extremely hydrophobic, therefore they are expected to be incorporated into AlkB after dissolving into the cell membrane, but the pathway of substrate incorporation into the substrate-binding pocket is largely unknown because the structure has not yet been resolved. In this study, we investigated the effect of the lipid environment on the substrate uptake of AlkB by comparing the activity after solubilizing with detergents or amphiphilic polymers. We found that the activity was significantly affected by the type of solubilizer used.

20146B* Investigating the dissociation process of DBD-p53/DNA complex by PaCS-MD and MSM

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The dissociation pathways for large biological molecules are still challenging. Therefore, in this study we applied the rare event sampling technique, parallel cascade selection molecular dynamics (PaCS-MD) in combination with the Markov state model (MSM) to generate dissociation pathways of DNA binding domain of p53 (DBD-p53), which binds to DNA forming DBD-p53/DNA complex. Using inter center of mass distance (inter-COM distance), inter center of mass coordinates and Cα coordinates as reaction coordinates, we built 1D, 3D and Cα MSM, respectively, to generate different dissociation pathways of DBD-p53/DNA complex and the sliding of p53. Our results indicate that the DBD-p53 prefers sliding along DNA than direct complete dissociation.

20147B Electrochemical studies of human neuroglobin and cytoglobin using nanostructured electrode

Yasuhiro Mie[1], Kyoka Takahashi[1], Itoga Yuka[2], Kenta Sueyoshi[2], Ryo Torii[2], Jingkai Shen[2], Takumi Tanaka[2], Hirofumi Tsujino[2], Taku Yamashita[3] ([1]*Bioproduction Res. Inst., AIST*, [2]*Grad. Sch. Pharm. Sci., Osaka Univ.*, [3]*Sch. Pharm., Mukogawa Women's Univ.*)

Human neuroglobin (Ngb) and cytoglobin (Cygb) are heme proteins expressed in the brain tissue and in many organs, respectively, and are believed to have important cellprotective roles. However, their molecular mechanisms are still under exploration. To gain further insights into this issue, we developed an electrochemical strategy using a facilely prepared nanostructured electrode. Immobilization of Ngb and Cygb onto the electrode surfaces enabled manipulation of the oxidation states of heme irons. Electrochemical responses in the presence and absence of potential substrates provided useful information for uncovering the molecular basis of Ngb and Cygb activities coupled with electron transfer reactions.

20148B スピンラベル ESR 分光法による HP1 の天然変性領域の動的構造解析： DNA 結合とリン酸化の影響
Structural dynamics of IDP region in heterochromatin protein HP1 by spin-labeling ESR: Effects of DNA binding and phosphorylation

Toshiaki Arata[1,5], Kazunobu Sato[4], Ena Hirai[4], Yuichi Mishima[5], Takeji Takui[4], Toru Kawakami[5], Hironobu Hojo[5], Risa Mutoh[6], Toshimichi Fujiwara[5], Makoto Miyata[1], Isao Suetake[2,3,5] ([1]*Dept. Biol., Grad. Sch. Sci., Osaka City Univ.*, [2]*Nakamura Gakuen Univ.*, [3]*Twin Research Center, Osaka Univ.*, [4]*Dept. Chem., Grad. Sch. Sci., Osaka City Univ.*, [5]*IPR, Osaka Univ.*, [6]*Dept. Phys., Fac. Sci.,Fukuoka Univ.*)

HP1 forms Ntail-CD-HR-CSD-CSD-HR-CD-Ctail. The rotational dynamics of nitroxide spin label[1] at the resudues of HR and Ntail IDR in HP1 was found to be extremely high on subnanosecond time scale, but immobilized with DNA on nanosecond time scale in glycerol where peptide backbone was immobilized. These results suggest that DNA binds to both HR and Ntail at the same time. Interestingly, phosphomimic mutation of Ntail reduced both HR and Ntail residual dynamics, suggesting that these two IDRs interact with each other. To see the geometry of HP1 including DNA binding region, we performed distance measurements at upto 8 nm sensitivity using pulsed ESR[1] by the spin labels located on 4 points of HP1 dimer or 2 points of monomeric mutant. 1. Arata, T. *IJMS* 21, E672 ('20).

20149B Reactive Coarse-Grained Molecular Dynamics Simulation for the Functional Dynamics of Lambda Exonuclease

Toru Niina, Shoji Takada (*Grad. Sch. Sci. Kyoto Univ.*)

Many of the cellular phenomena involve chemical reactions. To reveal the underlying physical mechanisms, it is important to observe the whole process of the phenomena including dynamics of molecules while chemical reactions are happening. While molecular dynamics (MD) simulation is a powerful tool to investigate microsecond-scale structural dynamic that does not involve chemical reactions, it is challenging to carry out a longer MD simulation that is coupled with chemical reactions. Here, we extended a well-established coarse-grained molecular model to simulate MD coupled with multiple chemical reactions of nucleic acid. Taking a hybrid Monte Carlo/MD approach, we investigated the functional dynamics of lambda exonuclease degrading a DNA strand.

20150B マイクロ秒時間領域で形成される一酸化窒素還元酵素反応中間体の分光解析
Characterization of reaction intermediate formed in the microsecond time domain of the catalytic reaction of nitric oxide reductase

Takehiko Tosha[1], Hanae Takeda[1,2], Tetsunari Kimura[3], Masaki Horitani[4], Yoshitsugu Shiro[2] ([1]*RIKEN SPring-8*, [2]*Univ. of Hyogo*, [3]*Kobe Univ.*, [4]*Saga Univ.*)

Bacterial nitric oxide reductase (NOR) catalyzes reduction of nitric oxide (NO) to nitrous oxide using two protons and electrons at a heme/non-heme iron catalytic center. The elucidation of the mechanism of the NOR-catalyzed reaction helps us understand how the enzyme effectively decomposes cytotoxic NO. Here, we utilized photosensitive caged NO as a trigger and NO source to observe NO reduction by NOR. The time-resolved IR measurements using caged NO showed that a NO-bound intermediate was formed within a few microseconds. The cryophotolysis of caged NO allowed us to trap the NO-bound intermediate, and its EPR measurements suggested the non-heme iron-NO species as the intermediate. The mechanism of the NOR-catalyzed reaction is discussed on the basis of the results.

20151B PyDISH: Database and analysis tools for heme porphyrin distortion in heme proteins

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Heme participates in a wide range of biological functions. While the mechanism of each function has been investigated for many heme proteins, the origin of the diversity of the heme functions is still unclear and a crucial scientific issue. We have constructed a database of heme proteins, named PyDISH (Python-based database and analyzer for DIStortion of Heme porphyrin), which also contains some analysis tools. The aim of PyDISH is to integrate the information on the structures of hemes and heme proteins and the functions of heme proteins. This database will provide the structure-function relationships focusing on heme porphyrin distortion and lead to the elucidation of the origin of the functional diversity of hemeproteins.

20152B Transient binding and non-rotational coupled motion of p53 revealed by sub-millisecond resolved single-molecule fluorescence tracking

Dwiky Rendra Graha Subekti[1,2], Satoshi Takahashi[1,2], Kiyoto Kamagata[1,2] ([1]*IMRAM, Tohoku Univ.*, [2]*Grad. Sch. Sci. Tohoku Univ.*)

Using a newly developed sub-millisecond single-molecule fluorescence microscopy, we revealed the unresolved dynamics of tumor suppressor p53 along DNA. The residence time distribution of p53 on DNA shows that, regardless of the salt concentration, >88% of p53 associated to DNA dissociated within a few milliseconds without demonstrating the 1D diffusion. The remaining binds DNA more stably and exhibit jumps and 1D diffusion whose frequencies (f) and coefficients (D) appear to be salt dependent. The plot of f against D at various salt concentrations showed a strong correlation of 0.85. These findings suggest multiple conformations of p53 causing such observed dynamics for the facilitation of the target search.

20153B リン脂質二重膜ナノディスクへの再構成に伴うヒト Steap3 の三価鉄還元酵素活性の増強
Enhancement of ferric reductase activity of human Steap3 upon reconstitution into phospholipid bilayer nanodisc

Ayane Nishi[1], Akito Nakata[1], Fusako Takeuchi[2], Tetsunari Kimura[1], **Motonari Tsubaki**[1] ([1]*Dept. of Chem., Grad. Sch. Sci., Kobe Univ.*, [2]*IPHE, Kobe Univ.*)

Steap3 is a major ferric reductase in developing erythrocytes and participates in cellular iron uptake. As a p53-targeted gene, it may act as a tumor suppressor by an unknown mechanism. Steap3 is considered to receive electrons from cytoplasmic NADPH via FAD. After the transmembrane electron transfer to heme b on the endosomal internal surface, they are used to reduce Fe3+ to Fe2+. To clarify the details of ferric reductase activity, we conducted and succeeded in the reconstitution of purified human Steap3 (expressed by Pichia pastoris system) into phospholipid bilayer nanodisc using various size of MSPs. Analyses showed significant enhancement of NADPH-dependent ferric reductase activities upon the reconstitution compared to those in the detergent micelle state.

20154B 分子動力学シミュレーションによって明らかになった SLC26A9 の塩素イオン輸送における細胞質ドメインの役割
Role of the cytoplasmic domains of SLC26A9 in chloride ion transport revealed by the molecular dynamics simulations

Satoshi Omori[1], Yuya Hanazono[2], Hafumi Nishi[1,3], Kengo Kinoshita[1,4,5] ([1]*GSIS, Tohoku Univ.*, [2]*Inst. for Quantum Life Sci., QST*, [3]*Faculty of Core Res., Ochanomizu Univ.*, [4]*ToMMo, Tohoku Univ.*, [5]*Inst. of Dev. Aging and Cancer, Tohoku Univ.*)

Solute Carrier 26 family member A9 (SLC26A9) is a membrane-transport protein that exhibits chloride transporter activity and plays essential roles for many physiological processes. The recent cryo-EM studies of homo-dimeric SLC26A9 claimed the unique chloride transport mechanism: the cytoplasmic domains mediate the interactions between the subunits. In this study, we performed the MD simulations of dimeric SLC26A9 with the full-length model and the cytoplasmic domain removal model. The chloride ions could access their binding sites in the full-length model, but be locked out in the removal model during the simulations. The results indicate that the cytoplasmic domains maintain the cooperative motions of the transmembrane domains to allow the access of the chloride ions.

20155B Time-resolved spectroscopic measurements on the transport dynamics of ABC transporter

Tetsunari Kimura[1,2], Sae Hayashi[1], Yuka Ikemoto[3], Yoshitsugu Shiro[4], Hiroshi Sugimoto[2] ([1]*Grad. Sch. Sci., Kobe Univ.*, [2]*RIKEN, SPring-8*, [3]*JASRI*, [4]*Grad. Sch. Sci., Univ. Hyogo*)

Comprehensive observations in structural and functional dynamics of biomolecular systems, which can express higher hierarchic functions by the assembly of proteins or their domains, are crucial to reveal their molecular mechanism. ABC transporters are one of the typical biomolecular systems, which can transport the allocrites through their channel in the transmembrane domain along the reactions of ATP in the cytosolic nucleotide-binding domain. Here, we focused to observe the allocrite transport, ATP hydrosis, and conformational changes in TMD by developing the time-resolved spectroscopy with microfluidic mixers, in which the reaction was triggered by the diffusional mixing of ATP to ABC transporter. The detailed mechanism of biomolecular systems will be discussed.

20156B 大腸菌 UvrD C 末端 40 アミノ酸欠損変異体の DNA 巻き戻しダイナミクス
DNA-unwinding dynamics of *Escherichia coli* UvrD lacking the C-terminal 40 amino acids

Hiroaki Yokota (*Grad. Sch. Creation New 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. To understand the role of the C-terminus amino acids of UvrD that are crucial to dimerization and unwinding activity, single-molecule direct visualization was performed for a UvrD mutant lacking the C-terminal 40 amino acids (UvrDΔ40C). I have already reported in the 2018 annual meeting that UvrDΔ40C unwound DNA in the form of an oligomer (dimer or trimer) as wildtype UvrD (*Biophys. J.* 2013). I will report that the involvement of multiple UvrDΔ40C molecules was also observed under a physiological salt concentration and for a duplex DNA substrate with a shorter 12-nt 3' ssDNA tail (*Biophys. J.* 2020).

20157B 高速原子間力顕微鏡によるタンパク質膜輸送装置 Sec の動態観察
Observation of Substrate Binding Sec Translocon and Structural Change of SecA with HS-AFM

Wataru Nagaike[1], Takamitsu Haruyama[2], Tomoya Tsukazaki[2], Takayuki Uchihashi[1,3] ([1]*Dept of phys, Nagoya univ*, [2]*NAIST*, [3]*EXCELLS*)

The SecYEG forms a complex with the cytosolic motor SecA ATPase to drive the proteins translocation. However, the dynamics of how the conformational change in SecA ATPase was coupled to the protein translocation remain elusive. In this study we applied high speed atomic force microscopy (HS-AFM) to directly capture conformational dynamics of the SecYAEG complex during the substrate translocation. By reconstituting the SecYAEG complex into a nanodisc and then incubating with an unfolded model substrate protein, we observed the SecYAEG incorporated with the substrate protein. In addition, a nucleotide-dependent conformational change in the structure of the PPX (pre-protein cross-linking) domain of SecA ATPase was successively visualized.

20158B Structure of the voltage-dependent potassium channel (hERG) using cryo-electron microscopy

Tatsuki Asai[1], Kano Suzuki[1], Naruhiko Adachi[2], Masato Kawasaki[2], Toshio Moriya[2], Toshiya Senda[2], Satoshi Ogasawara[1], Takeshi Murata[1] ([1]*Grad. Sch. Sci., Univ. Chiba*, [2]*KEK, Tsukuba*)

The toxicity of drugs remains an important issue for the pharmaceutical industry. And, about 30% of these problems result from arrhythmias of which inhibition of hERG has become the most frequent single cause. Recently, Mackinnon's group determined the structure of the hERG at 3.8 Å resolution using cryo-EM, which is showing the basic features of hERG functions. However, the resolution of the structure is not so high that the binding sites for drugs and potassium ions are indicated. In this study, we have solved the cryo-EM structure of the hERG at 3.9 Å resolution. In this structure, densities for potassium ions are observed at the selectivity filter of the hERG. Now, we are trying to solve the structure of the hERG with the drug at a higher resolution.

20159C 状態遷移機械を実装する多段階 DNA コンピューティング反応の最適化
Optimization of the multi-step DNA computing reaction that implements a state machine

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Displacement Whiplash PCR (DWPCR) is a unique DNA computing reaction that implements a state machine. In DWPCR, each single-molecule DNA, in principle, executes multi-step computation by repeating formation of a hairpin structure and polymerase extension reaction under an isothermal condition. DWPCR is expected to be applied for medical diagnosis using only an aqueous solution. However, state transition only up to two-step has been reported so far. In this study, we investigated the efficiency of DWPCR for achieving state transition of three-step and more. As a result, we found the problem in our design for the state transition of the second step and after. We discuss the solution and report optimization of the reaction conditions.

20160C 演題取り消し

20161C* DNA のメチル化パターン依存的な構造動態の解析
Structural Dynamics of DNA Depending on Methylation-Patterns

Takeru Kameda[1,2], Miho M. Suzuki[3], Akinori Awazu[4], Yuichi Togashi[2,4] ([1]*Graduate School of Science, Hiroshima University*, [2]*RIKEN Center for Biosystems Dynamics Research*, [3]*Graduate School of Medicine, Nagoya University*, [4]*Graduate School of Integrated Sciences for Life, Hiroshima University.*)

DNA methylation plays a crucial role of epigenetic regulation in eukaryotic gene expression. However, how it changes DNA mechanics is still unclear, although experimentally suggested by some reports. In this research, we performed fully atomic molecular dynamics simulation of double-stranded DNA including several biased patterns of DNA methylation. Through the analysis of base-step variables (i.e. relative positioning of nucleotides) of DNA, we observed characteristic changes of flexibility in three modes of base-step dynamics. We also confirmed that the changes in these specific modes affect the overall DNA geometry. Our finding may serve as basic knowledge to discuss the methylation-dependent DNA dynamics.

20162C クロマチンドメインのエントロピー駆動相分離による染色体コンパートメント形成
Entropic phase separation of chromatin domains to form chromosome compartments

Shin Fujishiro, Masaki Sasai (*Grad. Sch. Appl. Phys., Nagoya Univ.*)

Mammalian chromosomes are compartmentalized into active (A) and repressed (B) regions in interphase nuclei. Despite its functional importance, it is still unclear how the gigabase-scale compartments emerge from the sub-megabase chromatin domains. We hypothesize that this compartmentalization is realized through physical self-organization of chromatin segments having different densities. A genome-wide molecular dynamics simulation shows entropic phase separation of two types of chromatin segments into the A/B compartments. Our study proposes a new picture of chromosome organization; without assuming any specific chromatin-chromatin interactions, chromosomes are organized just as an entropic consequence of molecular crowding.

20163C* 分子動力学計算による p53-C 末端部位の DNA 結合機構の解明
DNA binding mechanisms of the p53 C-terminal domain elucidated by MD simulation

Yuta Taira, Duy Tran, Akio Kitao (*Titech*)

The tumor-suppresser protein p53 has two DNA binding domains; core domain and intrinsically disordered C-terminal domain. The latter non-specifically binds to DNA, which is considered to be essential for 1D sliding movement of p53 along DNA. However, due to the intrinsically-disordered nature of the domain, molecular mechanisms of the binding are still unclear . In this study, p53-DNA binding were simulated starting from distinct C-terminal structures distributed around a DNA duplex by multiple independent all-atom MD simulations. By observing p53 binding with the DNA in atomic level, we identified amino residues having high binding affinity with DNA. We also built Markov state model to investigate sliding movement of C-terminal domain along DNA of a micro second order.

20164C DNA curtain assay of nucleosome repositioning and collisions induced by translocases

Fritz Nagae, Shoji Takada, Tsuyoshi Terakawa (*Department of Biophysics, Graduate School of Science, Kyoto University*)

In eukaryotic DNA transactions such as transcription, DNA replication, or DNA repair, various translocases (e.g., polymerases, helicases, and endonucleases) inevitably encounter a nucleosome, the basic unit of chromatin. Previous studies suggest that a single nucleosome start repositioning upon encounter with the translocases. However, the effect of an array of nucleosomes on the repositioning remains elusive. We conducted single-molecule fluorescence microscopy using a DNA curtain set up to observe collision between nucleosomes induced by translocases. As a result, we observed the collision-induced nucleosome deposition, which might be a molecular mechanism underlying nucleosome depletion in various DNA transactions.

20165C 核膜近傍におけるクロマチン構造形成と RNA 輸送モデルの構築
Model construction of chromatin structure formation and RNA transport near the nuclear membrane

Nozomu Imai, Shin Fujishiro, Masaki Sasai (*Dept. Appl. Phys., Nagoya Univ.*)

mRNA and other RNA involved in translation are transposed from the interior of nucleus through nuclear pore to cytoplasm, but it is still unclear how the pathway of RNA transport is formed in the nucleus. In this study, we simulated a chromatin system to analyze how the pathway is formed. The system is composed of heterochromatin and euchromatin regions near the nuclear membrane, RNA, and nuclear pores, and their movement was simulated with the Langevin equation. We investigated the regions where RNA passes through to reach the nuclear pore. The simulation result suggested that RNAs are mainly distributed in the phase boundary of euchromatin and heterochromatin regions.

20166C ArsInsC 配列及び DNA 反復配列の物理的特性・機能性解析
Analysis of physical properties and functionalities of ArsInsC and DNA repeat sequences

Tappei Oda, Masashi Fujii, Naoaki Sakamoto, Akinori Awazu (*Dept. of math. and life sci. Hiroshima Univ.*)

Genome DNA contains coding regions with genetic information for protein synthesize and non-coding regions. There are various types of non-coding regions playing a variety of roles such as maintenance of chromosomal structures and gene regulations. Insulator is one of typical gene regulatory non-coding regions. Recent study suggested some of insulator regions exhibit their activities through the formations of chromatin loops. However, some non-looping regions such as ArsInsC and CCGNN repeat were found to show insulator activities without chromatin looping but the mechanism of them were still unknown. In this study, we simulated ArsInsC and DNA repeat sequences to clarify the mechanism of insulator activity without chromatin looping from their physical properties.

20167C* 並列的な自己集合を基盤とした DNA 演算のナノポアデコーディング
Nanopore decoding for DNA computing based on parallel self-assembly

Sotaro Takiguchi, Ryuji Kawano (*Department of Biotechnology of Life Science, Tokyo University of Agriculture and Technology*)

DNA computing has been attracted attention as a tool for solving mathematical problems because of its huge parallelism and low energy consumption. However, it is usually time-consuming to decode the output information from the molecule to the human recognizable signal in the conventional system. Here, we report a method of a nanopore decoding, which can perform rapid and label-free recognition of oligonucleotides, for mathematical DNA computation. Moreover, we attempted to apply the methodology of DNA-based parallel computing and nanopore decoding to the identification of the expression pattern of microRNA from tumor cells. Our data showed the feasibility of nanopore decoding, and its methodology would be applied to the rapid cancer diagnosis.

20168C Local chromatin motion, chromatin quantity and nuclear volume

Shiori Iida[1], Yuji Itoh[2], Kayo Hibino[1,2], Kazuhiro Maeshima[1,2] ([1]*Dept. of Genetics, Sch. of Life Sci., SOKENDAI*, [2]*Genome Dynamics Lab., Natl. Inst. of Genetics*)

During cell-cycle progression from G1, S to G2, the genome chromatin doubles with replication accompanied by increasing nuclear volume. Here we examined whether these nuclear environmental changes affect local chromatin motion in living human cells using single-nucleosome imaging with oblique illumination microscopy. We revealed that local chromatin motion was not significantly changed with nuclear growth from G1 to G2 phase. Furthermore, we showed that local chromatin motion did not alter in the cells with large G2-like nuclei by replication inhibition. These results indicated that neither the amount of genome chromatin nor nuclear volume does not affect local chromatin dynamics. Physical factors that impact on chromatin motion in living cells will be discussed.

20169C* 分子動力学シミュレーションによる転写開始複合体の全原子構造モデリング
Modeling Atomistic Structure of Transcription Initiation Complex with DNA Bubble by Molecular Dynamics Simulation

Genki Shino, Shoji Takada (*Dept. of Biophys., Div. of Bio. Sci., Grad. Sch. of Sci., Kyoto Univ.*)

The molecular mechanism of transcription initiation process has been actively studied by using cryo-electron microscopy and biochemical experiments. The transcription of eukaryotic protein-coding genes results from forming transcription initiation complex on the promoter DNA, consisting of RNA polymerase II and the six general transcription factors, and DNA opening. However, the details of DNA opening remain unclear. To address this problem, we performed coarse-grained molecular dynamics simulations to model DNA bubble in transcription initiation complex, followed by the back-mapping to fully-atomistic structures.

20170C Toward the construction of artificial organelles with controllability based on liquid-liquid phase separation of DNA nanostructures

Yusuke Sato (*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

Recent studies revealed that membraneless organelles are formed by liquid-liquid phase separation (LLPS), where specific molecules are accumulated for efficient chemical reactions or controlling biological functions. We aim to construct artificial organelles with controllability based on DNA nanotechnology that allows for controlling LLPS of DNA molecules. We established a system in which the addition of a trigger nucleic acid into a solution can induce LLPS of DNA nanostructures and designed an accumulation mechanism of functional enzymes into the DNA-microdroplets. We plan to expand this technique for the photo-controllable artificial organelles. This study would provide a tool to construct organelle-like functional modules for artificial molecular systems.

20171C* DNA によるミクロ相分離 droplet の安定化と新しい人工細胞系の検討
Stabilization of micro phase-separated droplet and examination of new artificial cell system

Moe Yabuta, Yoshihiro Minagawa, Hiroyuki Noji (*Department of Applied Chemistry, Graduate School of Engineering, University of Tokyo*)

Sustainable growth and division are necessary for the construction of autonomous artificial cells, and for that purpose, it is ideal that internal replication and cell growth are linked. Recently, it is reported that DNA is concentrated inside the phase separation droplets formed with Dextran (Dex) and Polyethylene Glycol (PEG). However, it hasn't been reported that phase separation is stabilized by concentrated molecules. Therefore, we examined how the critical concentration of phase separation is affected by DNA. As a result, we found that phase separation is stabilized depending on the length of concentrated DNA. We conclude Dex/PEG droplets can be used as a potential container for artificial cells.

20172C* Large scale simulation of DNA hydrogel

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DNA hydrogels are self-assembled molecular aggregates based on the formation of networks of DNA polymeric chains. Their properties are based on the DNA sequence, and they have been studied for their prospective use in DNA computing, delivery of medicines and biosensing. To understand the formation dynamics and test theoretical sequence designs, optimization based on simulations are required. However, DNA hydrogel particles size varies between 1~20 micron, and simulations in this scale for long time intervals are still not viable in most coarse-grained molecular dynamics. In order to simulate the formation of DNA hydrogels, we propose a stochastic, in-lattice coarse grained model. Using this model, we simulated the formation of DNA hydrogel in unprecedented scales.

20173D 銅アミン酸化酵素のプロトン化状態についての QM/MM 解析
QM/MM study for the protonation states of copper amine oxidase

Mitsuo Shoji[1,2], Takeshi Murakawa[3], Yasuteru Shigeta[1], Hideyuki Hayashi[3], Toshihide Okajima[3,4] ([1]*Univ. Tsukuba*, [2]*JST-PRESTO*, [3]*Osaka Medical College*, [4]*Osaka Univ.*)

Copper amine oxidases (CAOs) catalyze the oxidative deamination of biogenic amines critical in a variety of metabolisms. In this presentation, we have theoretically explored the unique protonation states of the key catalytic residue of aspartate (Asp298) and the prosthetic group of topaquinone (TPQ) in the CAO from Arthrobacter globiformis (AGAO) in order to gain deeper insight into the crystal structure determined by the recent neutron diffraction (ND) method. The quantum mechanics/molecular mechanics (QM/MM) calculations suggest that the ND structure is closest to the state with the protonated Asp298 and the TPQ enolate form. The TPQ keto form can coexist in the fully protonated state.

20174E Application of a Deep-Learning Technique to Predict the Hydration Structure around Proteins

Kosuke Kawama[1], Takashi Yoshidome[1], Mitsunori Ikeguchi[2,3], Masateru Ohta[2] ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*RIKEN*, [3]*Grad. Sch. of Med. Life Sci., Yokohama City Univ.*)

Hydration is an imperative factor to understand a variety of biological processes such as protein folding, ligand binding, and so on. With all-atom molecular dynamics simulation, three-dimensional distribution function of water molecule around a protein is obtained as hydration structure. However, its high computational cost hinders the application to a large number of proteins. In the present study, we propose that a hybrid of the 3D-RISM theory, a solution theory, and a deep-learning technique can resolve the issue. The hybrid enables us to successfully reproduce the three-dimensional distribution function of water molecule, and to compute the distribution function of water molecule for a protein within 10 seconds.

20175E リガンド結合サイトにおける水和の包括的解析：3D-RISM 理論アプローチ
Comprehensive Analysis of the Hydration of Small Molecule Binding Sites in Ligand-Free Protein Structures: 3D-RISM Approach

Takashi Yoshidome[1], Mitsunori Ikeguchi[2,3], Masateru Ohta[2] ([1]*Dep. of Appl. Phys., Tohoku Univ.*, [2]*RIKEN*, [3]*Grad. Sch. of Med. Life Sci., Yokohama City Univ.*)

To examine the hydration states of ligand binding sites, the three-dimensional distribution function for the water oxygen site, g(r), was computed for 3,706 ligand-free protein structures based on the corresponding small molecule-protein complexes using the 3D-RISM theory. Based on the g(r) for the crystallographic binding pose of the ligand, hydrogen bond interactions are dominant in the highly hydrated regions while weak interactions such as CH-O are dominant in the moderately hydrated regions. The polar heteroatoms of the ligand occupy the highly hydrated and less hydrated regions in the crystallographic (correct) and wrongly docked (incorrect) poses, respectively. Thus, the g(r) of polar heteroatoms may be used to distinguish the correct binding poses.

20176E Analysis of urea effect for binding free energy of lysozyme-$(GlcNac)_3$

Simon Hikiri, Nobuyuki Matubayasi (*Grad. Sch. Eng. Sci., Osaka Univ.*)

In order to elucidate physical origin of the urea effect on the lysozyme-$(GlcNac)_3$ binding at atomic level, we employ all-atom molecular dynamics and calculate the change in the binding free energy ($\Delta\Delta F$) with the solution environment through the energy-representation method. In a thermodynamic cycle, $\Delta\Delta F$ can be calculated from the free energy change of transfer of the solute consisting of the lysozyme and ligand from pure-water environment to a water-urea mixture and the explicit estimation of the conformational entropy of solute is unnecessary due to the variational principle. Therefore, we focus on solvation free energy (SFE) of the solute. SEF is decomposed into the electrostatic, van der Waals, and excluded-volume components to identify the key component.

20177E Simulation-based machine-learning approach for the water dynamics

Taku Muzukami[1], Viet Cuong Nguyen[3], Hieu Chi Dam[2] ([1]*Materials Science, JAIST*, [2]*Knowledge Science, JAIST*, [3]*HPC systems Inc*)

Water plays an important role in biological systems. The functions of biomolecule express in a hydrated environment that have mechanisms tightly influenced by water interaction. A simulation-based machine-learning approach is presented that quantitatively analyzes the structure and dynamics of hydration water. We focus on the motive behavior of all water molecules observed in the classical molecular dynamic simulations. Our approach consists of 1) The clustering technique that categorizes the atomistic motion to create descriptors, and 2) The machine-learning technique that predict a physicochemical feature of molecule on the feature space. By means of the methodology, we will report the prediction for the local potential energy of water and the dynamics.

20178E* MED26 による TAF7 と EAF1 認識における多様な結合様式に関する分子動力学研究
Molecular dynamics study on the multiple binding modes of MED26 torecognize EAF1 and TAF7

Satoshi Goto[1], Kota Kasahara[2], Hidehisa Takahashi[3], Hidehisa Takahashi[2] ([1]*Grad. Sch., Life Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*, [3]*Grad. Sch. Med., Yokohama City Univ.*)

The N-terminal domain of MED26(MED26NTD), a subunit of the mediator complex, functions as a molecular switch by interacting with transcription factors such as TAF7 and EAF1 in the eukaryotic transcriptional process. However, the molecular mechanism of how MED26NTD recognizes these proteins remains to be clarified. In this study, we investigated this molecular mechanism by using a multi-canonical MD simulation for models of MED26NTD-TAF7 and MED26-EAF1 complexes. The resultant conformational ensembles were analyzed using clustering. As a result, TAF7 and EAF1 peptides were recognized by MED26NTD in different binding sites with high flexibility. This implies that these complexes are fuzzy complexes.

20179E ヌクレオチド三リン酸の結合による細胞混雑中の蛋白質間相互作用の減少
Reduced protein-protein interactions in the cellular crowding with binding of nucleoside triphosphates

Isseki Yu[1], Michael Feig[2], Yuji Sugita[3] ([1]*Maebashi Institute of Technology*, [2]*Michigan State University*, [3]*RIKEN Theoretical Molecular Science Lab.*)

Recently, ATP, one of the most abundant metabolites in cell, was found to inhibit the aggregation of intrinsic disordered proteins (IDPs). To understand the effect of ATP and other metabolites on the protein-protein interaction from the microscopic viewpoint, we performed all-atom molecular dynamics (MD) simulations of cytoplasm by changing the metabolite or ion concentration. We found that the nucleoside triphosphates, including ATP, show long time binding with sidechains of ARG and LYS in proteins, while other metabolites or ions diffuse rapidly to the bulk phase. Such stable bindings of nucleoside triphosphates on the protein surface result in the enhancement of the electrostatic repulsive interaction between macromolecules.

20180E 異なる配列と構造のペプチド周囲の水和ダイナミクスを MD シミュレーションで明らかにする
MD simulations reveal hydration dynamics around peptides with different sequences and structures

Takuya Takahashi[1], Shingo Nobunaga[1], Takuya Azami[2], Ryoi Ashida[2], Takuya Fujisawa[2], Kota Kasahara[1] ([1]*Coll. Life Sci., Ritsumeikan Univ.*, [2]*Grad. Sch., Life Sci., Ritsumeikan Univ.*)

MD simulations were performed on various peptides as protein model molecules, and the effects of their physicochemical properties and structure on the hydration dynamics were analyzed. In order to advance the theoretical elucidation of hydration water dynamics, we developed several analysis software and approximation functions to the time correlation function of rotational movement as well as the analysis of the translational movement and the number of hydrogen bonds. Specifically, we used polyglutamic acids with different charge state and structure, and some other hydrophobic polypeptides as the protein models. We also evaluated the effect of water models, solvent ions and force fields on hydration dynamics.

20181E 分子動力学法を用いたポリグルタミン酸周囲の水和ダイナミクス解析
Analysis of hydration dynamics around polyglutamic acid using molecular dynamics method

Takuya Fujisawa[1], Takuya Takahashi[2], Kota Kasahara[2] ([1]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*)

Hydration water dynamics carry important roles for elucidating the behavior of protein. In this study, I used an 8-residue glutamic acid polypeptide (PGA) and observed hydration water dynamics by analyzing the results of molecular dynamics simulation by selecting three indices: self-diffusion coefficient in translational motion, relaxation time in rotational motion, and number of hydrogen bonds. As results, the mobility of water molecules was low when PGA deprotonate and negatively charged, and has an α-helix structure. Further, the water model also affects the hydration dynamics; the order of water mobilities is as follows: TIP4P-D > TIP3P = SPC/E > TIP5P. Influences of the shielding effects of solvents on the hydration dynamics would be studied in the future work.

20182F Loop extrusion of chromatin at surfaces modulates the growth dynamics of transcriptional condensates

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Experiments by super-resolution microscopes have shown that superenhancers colocalize with transcriptional condensates, which form due to the phase separation of transcription factors and cofactors. We here treat a transcription condensate as a microemulsion stabilized by chromosome, which is grafted at the surface of the condensate via superenhancers. Our theory predicts that the surface tension of the condensate decreases with decreasing the loading time of cohesin because the loop extrusion increases the local concentration of chromosome segments at the surface, enhancing the excluded volume interactions between the segments. This implies that the loop extrusion process modulates the coarsening dynamics of transcription condensates.

20183F* 細胞性粘菌の脱分化過程における細胞質 pH の測定
Measurement of cytosolic pH changes during dedifferentiation of *Dictyostelium* cells

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Dictyostelium discoideum cells aggregate to form a multicellular body when the cells are starved. We introduced pH-sensitive fluorescent proteins into *Dictyostelium* cells and visualized cytoplasmic pH at the multicellular stage using confocal fluorescence microscopy. The result showed that the cytoplasmic pH of prestalkcells was lower than that of presporecells. We also found that the cytoplasmic pH of the prestalkcells was increased by disaggregating the multicellular body to induce dedifferentiation. These findings indicate that cytoplasmic pH imaging can visualize both differentiation and dedifferentiation processes in *Dictyostelium* cells.

20184F 合成遺伝子回路における細胞間相互作用依存的な発現と分化多能性
Cell-cell interaction-dependent expression of a synthetic genetic circuit and its relevance to pluripotency

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There are several dynamical-systems studies, in which cellular differentiation is represented as the state transitions driven by cell-cell interaction-dependent gene regulatory networks. Inspired by this concept, we synthesized a genetic circuit of three genes in *E.coli*, which mimics a network predicted to show a stem-cell-like behavior. A theoretical study on this network has suggested that oscillatory expression is essential to pluripotency. Our computational analysis predicted that the oscillatory dynamics also emerge with the constructed circuit, and the time-lapse microscopy indicated such dynamics *in vivo*. The expression dynamics coupled with cell growth and depended on culture conditions, especially cell density.

20185G 小胞輸送を担う分子モーターの分子数とダイニン阻害剤の影響
Effect of the dynein inhibitor dynarrestin on the number of motor proteins transporting synaptic cargos

Kumiko Hayashi[1,3], Miyamoto Miki[1], Shinsuke Niwa[2] ([1]*Grad. Sch. Eng., Tohoku Univ.*, [2]*FIRS, Tohoku Univ.*, [3]*JST, PRESTO*)

Synaptic cargo transport by the motor proteins kinesin and dynein in the axons of hippocampal neurons was investigated using non-invasive measurement of transport force based on non-equilibrium statistical mechanics. Although direct physical measurements such as force measurement using optical tweezers are difficult in an intracellular environment, the proposed non-invasive estimations enabled enumerating force producing units (FPUs) carrying a cargo comprising the motor proteins generating force. The number of FPUs served as a barometer for the stable and long-distance transport by multiple motors, which was then used to quantify the extent of damage to axonal transport resulting from dynarrestin, a dynein inhibitor.

20186G X 線繊維回折解析による真核生物鞭毛軸糸の Ca^{2+}濃度依存的らせん対称性変化
[Ca^{2+}]-dependent changes in the helical symmetry of *Chlamydomonas* and *Ciona* flagellar axonemes revealed by X-ray fiber diffraction

Kazuhiro Oiwa[1], Kenta Ishibashi[1,2], Kogiku Shiba[3], Kazuo Inaba[3], Hiroyuki Iwamoto[4], Hitoshi Sakakibara[1] ([1]*Nat. Inst.Info.Commun.Technol*, [2]*Osaka Univ. CiNet*, [3]*Shimoda Marine Res. Cent. Univ. Tsukuba*, [4]*JASRI, SPring-8*)

Eukaryotic flagella change their waveforms coupled with intracellular [Ca^{2+}]. To obtain insight into the mechanism, we have investigated the spatial arrangement of axonemal components in their flagellar axonemes under different [Ca^{2+}]. The axonemes aligned in a physiological solution by continuous shear-flow were exposed to X-ray generated in the synchrotron radiation facility SPring-8 BL40XU. Changes in X-ray fiber diffraction patterns at different [Ca^{2+}] suggests the change in the helical symmetry of nine doublet microtubules in the axoneme. The response of *Ciona* sperm flagella to the change in [Ca^{2+}] was the mirror image of that of *Chlamydomonas*. These results suggest the helical symmetry of doublets plays a role in the generation of the flagellar waveform.

20187G KIF1A/UNC-104 によるシナプス小胞前駆体輸送の数理モデル 2
Mathematical modeling of synaptic vesicle precursor transport by KIF1A/UNC- 104 2

Ryo Sasaki[1], Ryota Shinagawa[1], Kimiko Nagino[1], Kazuo Sasaki[1], Shinsuke Niwa[2], Kumiko Hayashi[1,3] ([1]*Dep. Appl. Phys., Grad. Sch. of Eng., Tohoku Univ.*, [2]*FRIS, Tohoku Univ.*, [3]*JST, PRESTO*)

UNC-104/KIF1A transports synaptic vesicles(SVPs)along microtubule tracks in neurons. When not hauling cargo vesicles, UNC-104/KIF1A assumes to be an autoinhibited form to reduce the wasteful consumption of ATP. This regulatory system controls the efficiency of neuronal transport; the absence of such a system leads to reduced numbers of UNC-104/KIF1A that actively transports SVPs and defects in the generation of vesicles pools and synapses. In order to quantitatively understand howthe number of active UNC-104 is related to vesicle pool formation and synapse creation,we observed the distribution and motility of fluorescent-labelled SVPs in C. elegans neurons and perfomed numerical simulations of transport SVPs by UNC-104 based on those observations.

20188G Computer simulation of molecular shuttles driven by biomolecular motors in external force field

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Biomolecular motors, such as kinesin, together with functionalized microtubules, can be used for the transport of cargos on Lab-on-a-Chip devices. These nanoscale transport systems, termed as molecular shuttle, move in wiggling motions characterized with the path persistence length, which is a key parameter determining the transport efficiency. However, the relationship between the path and filament persistence length remains unclear. Here, to provide better insights, we have developed a computer simulation with implicit-explicit scheme to simulate 3D movement of microtubules propelled by kinesins. This study revealed that the path persistence length differed from the filament persistence length, contradicting a previous theoretical prediction.

20189G The Impact of Defective Motors on Biosensor Integrated with Actin Filaments and Myosin

Samuel Macharia Kang'iri[1], Takahiro Nitta[1,2] ([1]*ELECTRONICS AND INFORMATION SYSTEMS ENGINEERING DIVISION, FACULTY OF ENGINEERING, GIFU UNIVERSITY*, [2]*APPLIED PHYSICS COURSE, FACULTY OF ENGINEERING, GIFU UNIVERSITY*)

Myosins are biomolecular motors that work together with actin filaments to generate forces in vivo. This actin-myosin system can be used in vitro for applications such as making stand-alone biosensors. However, upon myosins binding to the sensor surface, some become defective. The defective myosins impede the propulsion of the actin filaments, preventing analyte transportation and hence the biosensor functionality. Here, we developed a 3D Brownian dynamics simulation to reproduce movements of actin filaments gliding over active and defective myosins. We found that 80% of active myosins were required to sustain actin filament propulsion. This ratio can be used as an allowable minimum in biosensor design.

20190G* キネシン分子の空間配置が輸送複合体の運動に与える影響の評価
Molecular layout of kinesin affects the collective movement of DNA origami-based transport complex

Kodai Fukumoto[1], Yuya Miyazono[2], Hisashi Tadakuma[3], Yoshie Harada[1] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sch. Front. Sci., Univ. Tokyo*, [3]*SLST, ShanghaiTech Univ.*)

Intracellular transport is central to the cellular phenomena, where multiple motors orchestrate their function. However, it remains elusive how the molecular layout affects the cargo transport. To elucidate the effect of molecular layout, DNA origami is useful as a scaffold to assemble motors in a spatially well-defined manner. Here, we have made DNA origami-based transport complexes, where we integrated teams of kinesins containing SNAPf-tag and positively charged lysine-tag, and measured the movement on axonemes. The velocities of the complexes remained constant, while the run lengths differed with different kinesin layout. Our findings reveal the layout effect on cargo transport and suggest a platform to study the coordination behavior of motor proteins.

20191G キネシン・ダイニンによる軸索輸送速度の極値統計解析
Extreme value analysis of axonal transport velocity of kinesins and dyneins

Takuma Naoi[1], Kimiko Nagino[1], Kazuo Sasaki[1], Shinsuke Niwa[2], Kumiko Hayashi[1,3] ([1]*Dep. Appl. Phys., Grad. Sch. Eng., Tohoku Univ.*, [2]*FRIS, Tohoku Univ.*, [3]*JST, PRESTO*)

Extreme value analysis (EVA) is a branch of statistics that is incorporated in several applications (such as disaster prevention) for predicting extreme values from the observed data. We conducted EVA to examine axonal transport velocity, and focused on the transport of synaptic vesicle precursors (SVPs) in DA9 motor neurons of C. elegans. Generally, SVPs are anterogradely transported by UNC-104 kinesins and retrogradely transported by cytoplasmic dyneins. The motion of SVPs was observed by employing fluorescence microscopy and the velocity was measured through kymograph analysis. It was observed that the maximum velocity of retrograde transport was greater than that of anterograde transport. Furthermore, we have discussed the results based on mathematical modeling.

20192G 外眼筋の X 線回折像に対する BDM の効果
Effect of BDM on the structure of extraocular muscle revealed by x-ray diffraction

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We have performed X-ray diffraction experiments of the extraocular muscles (EOM) and found that EOM showed no sampling peaks at 0.05 /nm on the first myosin layer line (MLL) which is evidently observed in the fast skeletal muscle. In this study, we obtained X-ray diffraction patterns of EOM with BDM, which is known to increase stable population of myosin intermediate. EOM showed no sampling peaks at 0.05 /nm on the MLL even in the presence of BDM suggesting that the lack of the peak was not due to BDM sensitive mobile myosin heads but structural characteristics of EOM. Electron micrograph revealed that M-line of the EOM was sparse compared with that of the fast skeletal muscle, confirming that EOM have structural characteristics different from fast skeletal muscle.

20193G 1 分子・多分子実験から迫る、心機能に特化した心筋ミオシンの性質
Molecular properties of single cardiac myosin adapted for heart functions revealed by single- and multi-molecule approaches

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Despite many reports about the properties of single cardiac myosin, it still remains unclear what the properties of cardiac myosin ensemble are and how the properties of single myosin affect its ensemble behaviors. Thus, we measured forces of cardiac myofilaments and revealed unique properties of cardiac myosin ensemble, which are distinctively different from those of skeletal myosin ensemble. We also evaluated dynamic responses of single cardiac and skeletal myosins under loads, suggesting that the reverse stroke is a unique feature of cardiac myosin. Combining these results with simulations of cardiac myofilaments and sarcomeres showed that the reverse stroke is a key to enhancing force outputs of cardiac myofilament and facilitating efficient heart contractions.

20194G ウシミトコンドリア由来 ATP 合成酵素の内在性阻害因子 IF_1 の 阻害機構解明
Elucidation of inhibition mechanism by IF_1, a natural inhibitor protein for bovine mitochondrial ATP synthase

Ryohei Kobayashi, Sougo Mori, Hiroshi Ueno, Hiroyuki Noji (*Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

F_1-ATPase (F_1) is a catalytic domain of ATP synthase (F_oF_1). Although the physiological role of F_oF_1 is ATP synthesis, F_1 hydrolyzes ATP when proton motive force collapses in a cell or F_1 is isolated from F_o. To prevent wasteful consumption of synthesized ATP, mitochondrial F_1 has an inhibitory subunit, IF_1, which inhibits ATP hydrolysis, but doesn't inhibit ATP synthesis. Despite extensive structural analysis of F_1-IF_1 complex, the regulation mechanism by IF_1 still remains controversial. Here, to elucidate how IF_1 inhibits catalysis of F_1, we have analyzed IF_1-inhibited form in biochemical assay and single-molecule rotation assay. Our results suggested that IF_1 inhibition is composed of two rate-limiting reactions; loose binding process and tight locking process.

20195G The N-terminal β-strand of single-headed kinesin-1 is involved in the off-axis force-generation and resultant rotation pitch

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In *in vitro* gliding assays, most kinesins rotate the gliding microtubules in a corkscrew motion. To elucidate the molecular mechanisms of kinesins corkscrew, we performed a 3D tracking of a Qdot bound to microtubules translocated by monomeric kinesin-1s under various conditions. Alternations in ionic strength, kinesin and ATP concentrations changed both gliding and rotational velocities, but the rotation pitch remained left-handed and constant at about 0.3 μm. It was found that point mutations in the N-terminal cover-strand shortened the rotation pitch. Our findings confirm that the rotation of gliding microtubules is an intrinsic property of kinesin and demonstrate that changes in the active or retarding force originating from cover-strand modulate the rotation pitch.

20196G 心筋サルコメアにおける Fhod3 と cMyBP-C の同定
Identification of Fhod3 and cMyBP-C in cardiac sarcomere

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Fhod3, formin homology protein, interacts with cMyBP-C, myosin filament related protein, in C-zone of cardiac sarcomeres. Although their interaction has been suggested to regulate cardiac sarcomere assembly and maintenance of homeostasis, the details of sarcomere disruption induced by the loss of the interaction are unknown. Thus, we obtained 3D-structures of cardiac sarcomere from three phenotypes, wild type and two types of the cMyBP-C deletion mutant with/without Fhod3 over-expression by electron tomography. In the cross-section in the C-zone of the cardiac sarcomeres of these mutant mice, the myosin filaments arrays were disturbed. Also, we found some cross-links between thick and thin filaments in the WT C-zone, which presumably correspond to cMyBP-C.

20197G キネシンと微小管による印刷可能な人工筋肉のコンピュータシミュレーション
Computer simulation of printable artificial muscles composed of engineered kinesins and microtubules

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Muscle tissues and motor proteins can be seen as flexible and highly efficient actuators and have been studied for driving robots. We developed an artificial muscle composed of engineered kinesins and microtubules whicn can be printed in various shapes. However, the contraction mechanism of the artificial muscle hasn't yet been clarified, making difficult predictions of the contraction movement of printed artificial muscles. A computer simulation enables to analyze contraction properties of various shapes without experiments. In this study, we developed a simulation that reproduced the contraction movement of the printed artificial muscle. Our study provides insights on the contraction mechanism leading to practical use of the artificial muscle.

20198G ウニ胚形態形成の細胞骨格観察に基づくモデル化
Modeling of sea urchin gastrulation based on cytoskeleton imaging

Kaichi Watanabe[1], Yuta Kurose[2], Yuhei Yasui[1], Naoaki Sakamoto[1], Akinori Awazu[1] ([1]*Grad. Sch. of Integrated Sciences for Life, Univ. Hiroshima*, [2]*Grad. Sch. Sci, Univ. Hiroshima*)

Gastrulation is one of the most important and universal processes for morphogenesis. Sea urchin embryo is the typical model organism of morphogenesis showing clear gastrulation. We found H+/K+-ATPase ion pump activity play important roles to proceed the gastrulation; gastrulation was inhibited and embryo exhibited anomalous shape when the activity of H+/K+-ATPase was suppressed. In this study, we first obtained fluorescence imaging data of cytoskeleton, extracellular matrix, and pH of sea urchin embryo. Based on imaging, we developed a mathematical model to reproduce the normal and H+/K+-ATPase inhibition induced anomalous gastrulation processes. By these studies, we reveal the contributions of inter- and intrarcellular chemo-mechanical couplings to gastrulation.

20199G ATP 合成酵素の c リングの回転は c サブユニットでのプロトンの受け取りと放出および a サブユニットとの静電相互作用が協調して引き起こされる
Cooperation of proton release/uptake and electrostatic interaction between a subunit and c subunit drive c-ring rotation in ATP synthase

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In FoF1 ATP synthase, proton translocation through Fo drives rotation of c subunit oligomer ring (c-ring) relative to a subunit. In order to clarify the cooperativity of the roles between adjacent c subunit, we compare the activity of ATP synthase having hetero mutation at conserved glutamic acid residue in c subunit by genetically fused ten of c subunits. Among double mutation, the activity was decreased as the distance between two of mutations was increased. This result indicates that there is a mechanism in which two or more c subunits cooperate. Molecular dynamics simulation suggested that cooperation of each role of the three c subunits adjacent to the a subunit: proton release/uptake, electrostatic interaction with a subunit drive the rotation of c-ring.

20200G Performance of step-finding algorithm based on the Schwarz Information Criterion depends on noise and data points per dwell-time

Monique Honsa[1,2], Kimitoshi Takeda[2], Akihiro Otomo[2,3], Hanjin Liu[4], Tomohiro Shima[4], **Ryota Iino**[2,3] ([1]*LMU Munich*, [2]*IMS*, [3]*SOKENDAI*, [4]*U Tokyo*)

Molecular motors, such as kinesins and rotary ATPases, move with small steps. This step-motion is disturbed by thermal fluctuations and measurement noises that diminish the performance of step-finding algorithms evaluating the step-size of these motors. To examine the performance of the step-finding algorithm based on the Schwarz (or Bayesian) Information Criterion (SIC) [1, 2], we simulated trajectories of motors including forward and backward steps and added Gaussian noise. We examined a dependency between the correctness of the SIC algorithm and the amplitude of the Gaussian noise as well as the number of data points per dwell-time.

20201G 自由エネルギーランドスケープのスイッチングとパワーストロークを考慮した筋収縮の三状態モデル
Three-state model of muscle contraction with switched free energy landscapes and power stroke

Kaima Matsuda, Masaki Sasai, Tomoki P. Terada (*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya. Univ.*)

Muscle contraction is generated by the relative sliding of actin and myosin filaments. With coarse-grained molecular dynamics calculation of actomyosin system, we have previously proposed that free energy landscape experienced by myosin head switches from symmetric one to asymmetric one, corresponding to the weakly bound state and strongly bound state, respectively (Nie et al., PLoS Comput. Biol. 2014). In this study, we have constructed three-state model of myosin heads diffusing on free energy landscape with 36 nm period and extended this model by considering 5 nm power stroke. Comparison of these models with quick tension recovery experiments showed that T1 fits the experimental data better whereas T2 does not by considering the power stroke.

20202G 体温に温めた心筋細胞に備わる収縮リズム恒常性
Contraction Rhythm Homeostasis in cardiomyocytes warmed to body temperature

Seine A. Shintani (*Dep. of Biomedical Sci., College of Life and Health Sci., Chubu Univ.*)

It has been suggested that the rapid drop in blood pressure that occurs with a slow decrease in [Ca^{2+}] preceding early diastolic filling is related to the mechanism of rapid sarcomere lengthening associated with spontaneous tension oscillation. We analyzed a new type of sarcomeric oscillation. Sarcomeres in cardiomyocytes warmed at 38-42 °C oscillated with both slow, Ca^{2+}-dependent frequencies and fast, Ca^{2+}-independent frequencies. Our experimental observations revealed that the amplitude of the fast sarcomeric oscillation was high and low at low and high [Ca^{2+}], respectively; nevertheless, the oscillation period was kept constant. Our simulations suggest that this regular rhythm is maintained by the unchanged cooperative binding behavior of myosin molecules.

20203G 電子顕微鏡構造解析により明らかにされた細胞質ダイニンの休止状態の解除メカニズム
Release mechanism of the shutdown state of cytoplasmic dynein revealed by electron microscopy

Kazuki Iwasaki[1], Yui Kurume[1], Hiroshi Imai[1], Shinji Kamimura[2], Rieko Shimo-kon[1], Ryosuke Yamamoto[1], Takahide Kon[1] ([1]*Grad. Sch. Sci., Osaka Univ*, [2]*Dept.Biol.Sci.,huo Univ.*)

Cytoplasmic dynein is a motor protein, which transports intracellular cargoes along microtubules in eukaryotic cells. Not all the dynein binds to microtubules. Most of the dynein are in the shutdown state in cytoplasm without binding to microtubules. Cryo-EM structure of the dynein in the shutdown state has been published. However, it is not known how the dynein releases the shutdown state. Here, we examined the structure variation of the dynein in the shutdown state by employing negative stain EM. We found several novel structures in addition to the previously published shutdown structure. Based on our observation, we propose a new release mechanism of the shutdown state of cytoplasmic dynein.

20204G 動く幽霊~高度好塩菌ハロフェラックス・ボルカニ~
Motile ghosts of the halophilic archaeon, Haloferax volcanii

Yoshiaki Kinosita[1,2], Richard Berry[2] ([1]*Molecular Physiology Lab., RIKEN*, [2]*Department of Physics, University of Oxford*)

Archaea swim using the rotary motor, archaellum (archaeal flagellum. Unlike the bacterial flagellar motor (BFM), ATP hydrolysis probably drives both motor rotation and filamentous assembly in the archaellum. However, direct evidence is still lacking due to the lack of a versatile model system. Here we present a membrane-permeabilized ghost system that enables the manipulation of intracellular contents. We observed high nucleotide selectivity for ATP driving motor rotation and negative cooperativity in ATP hydrolysis. Second, the response regulator CheY increased motor switching from CCW to CW rotation. Finally, we constructed the torque-speed curve at various [ATP]s and discuss rotary models in which the archaellum has characteristics of both the BFM and F1-ATPase.

20205G 汎用 3 次元モデリングソフトウェア Blender を利用したタンパク質超分子構造の動的性質の理解
Understanding Supermolecular Structure and Dynamic Property of Proteins using a general purpose 3D Graphics Modeling Software Blender

Yutaka Ueno[1], Kaoru Katou[1], Akira Kakugo[3], Kento Matsuda[3], Akihiko Konagaya[2] ([1]*AIST Tokyo*, [2]*Tokyo Tech., Dept. of Computer Scinence*, [3]*Hokkaido Univ., Graduate School of Chemical Science and Engineering*)

Since understanding functions of proteins and their dynamics property requires building 3D models of these molecular complexes,a general purpose 3D computer graphics modeling software, Blender is used with polygon models for proteins at mezoscale. In addition to the filament model of skeletal muscle illustrated in textbooks, a structural model of smooth muscle filaments based on recent high resolution microscopic studies was proposed. The modeling method was also applied to understand an artificial muscle material built with microtubule and kinesin. These 3D models allow us to evaluate molecular interaction on force generation and functions of accompanied regulatory proteins. .

20206G NMR による海洋性ビブリオ菌べん毛モーターの回転方向を制御する回転子タンパク質 FliG の構造変化の解析
NMR analysis of the conformational change in FliG that switches the rotational direction of the flagellar motor in marine bacterium *Vibrio*

Tatsuro Nishikino[1], Seiji Kojima[2], Michio Homma[2], Yohei Miyanoiri[1] ([1]*Inst. for Protein res., Osaka Univ.*, [2]*Div. Biol. Sci. Grad. Sch. Sci., Nagoya Univ.*)

FliG, one of the rotor components of flagellar motor, consists of 3 domains called FliG-N, -M and -C. From the cell motility assay for various *Vibrio fliG* mutants, we have revealed that FliG involves rotational switching between counterclockwise (CCW) and clockwise (CW) directions. To understand the molecular mechanism of CW-CCW switching, we study the structure and dynamics of *Vibrio* FliG by NMR. From 2D HSQC measurements for FliG mutant defective in switching, we found that the relative orientation between FliG-M and FliG-C domains are related to the CW and CCW states in FliG. In this presentation, we will also discuss about structural dynamics of FliG.

20207G* Multiple step photo regulation of mitotic kinesin Eg5 using a novel photochromic Inhibitor composed of Spiropyran and azobenzene

Islam Md Alrazi, Kei Sadakane, Happy Ogunwa Tomisin, Shinsaku Maruta (*Soka University, Graduate School of Engineering, Department of Bioinformatics*)

Mitotic kinesin Eg5 is ATP driven motor protein and one of the targets for cancer therapy. In this study, we demonstrated that novel photochromic compound SPSAB which is composed of Spiropyran and Azobenzene shows multi-step inhibitory activities for Eg5. SPSAB exhibited three isomer formation states, SP-Trans (VIS), MC- Cis (UV), and MC- Trans (in the dark). The three states of SPSAB showed different inhibitory activities for basal, microtubules activated Eg5 ATPase, and microtubules gliding. SP- Trans isomer showed the most potent inhibitory activity among the three states. The microtubule concentration-dependent inhibition of Eg5 ATPase activities indicated that SPSAB bind to subsite apart from the well-known inhibitor binding site, L5 pocket.

20208G Modeling of condensin hinge/DNA structure by molecular dynamics simulations guided by atomic force microscopy

Hiroki Koide[1], Noriyuki Kodera[2], Shveta Bisht[3], Christian Haering[3], Shoji Takada[1], Tsuyoshi Terakawa[1] ([1]*Department of Biophysics, Graduate School of Science, Kyoto University*, [2]*Nano Life Science Institute (WPI-NanoLSI), Kanazawa University*, [3]*Cell Biology and Biophysics Unit, Structural and Computational Biology Unit, European Molecular Biology Laboratory (EMBL)*)

Condensin is a protein that condenses chromatin by its loop extrusion activity. Previous studies proposed the molecular mechanisms for the loop extrusion, which assumes the binding of double-strand (ds) DNA to the hinge at the interface of the condensin subunits, Smc2 and Smc4. Using coarse-grained molecular dynamics (CGMD) simulations guided by an atomic force microscopy image, we modeled the hinge structure with transient open conformation. We then predicted the structure of the hinge/dsDNA complex in which the hinge is either in open or closed conformation using CGMD simulations. The simulation results suggest that there are dsDNA binding surfaces both inside and outside of the hinge, and the binding is regulated by opening and closing of the hinge.

20209G キネシン 1 二量体の前頭部における微小管からの解離抑制の直接観察
Direct observation of the suppression of the leading head of kinesin-1 dimer from detachment from microtubule

Kohei Matsuzaki[1,2], Michio Tomishige[1] ([1]*Dept. Phys., Col. Sci. Eng., Aoyama Gakuin Univ.*, [2]*Dept. Appl. Phys., Grad. Sch. Eng., Univ.Tokyo*)

Kinsin-1 is a motor protein that moves processively along microtubules. To move in a hand-over-hand manner, the trailing head should detach from the microtubule before the leading head detaches, however there is no quantitative evidence whether the detachment of the leading head is suppressed or the detachment of the trailing head is accelerated. In this study, we observed binding/unbinding of the leading head by using a heterodimer composed of wild-type and E236A mutant heads. High-speed dark-field microscopic observations showed that the detachment rate of the leading head was 16 times slower than that of the trailing head of wild-type homodimer, supporting the idea that the leading head is suppressed from ATP hydrolysis by a backward orientation of the neck linker.

20210G ミオシン VI の歩行運動に対するランドスケープ描像
A landscape-based view on the stepping movement of myosin VI

Tomoki P. Terada[1], Qing-Miao Nie[2], Masaki Sasai[1] ([1]*Dept. Appl. Phys., Grad. Sch. Eng., Nagoya Univ.*, [2]*Dept. Appl. Phys., Zhejiang Univ. Tech.*)

Myosin VI walks towards the minus end of the actin filament with a large and variable step size of about 25-36 nm. Using a same computational method as we have used for myosin II, we have theoretically characterized the free energy landscape experienced by the leading head to compare the two proposed models of myosin VI. Our results showed that the leading head is pulled toward the minus end of the actin filament according to the energy bias in the actin-myosin interactions, leading to the variable step size of movement in both two models. However, the large stepping size is realized only in the Spudich model, because in the Houdusse-Sweeney model, unfolding of the three-helix bundle gives rise to the entropic force to shorten the distance between two heads.

20211G 微小管とキネシンの結合におけるチューブリン C 末端の役割
Role of C-terminal tail of tubulin in microtubule-kinesin binding

Yuta Taguchi, Yukinobu Mizuhara, Jun Ohnuki, Mitsunori Takano (*Dept. of Pure & Appl. Phys., Waseda Univ.*)

In our previous MD study, we observed biased Brownian motion of single-headed kinesin along the microtubule (MT). Although kinesin appears to be able to bind not only to the intra-tubulin-dimer junction region but also to the inter-tubulin-dimer junction region, it preferentially binds to the intra-dimer junction. Here we study the binding preference mechanism by all-atom MD simulations. For high-speed calculation, we use the Generalized-Born/Surface-Area (GB/SA) model, with calibration of the SA term to remedy the overstabilization of the protein-protein interaction. We then analyze binding free-energy profiles at both junctions and investigate how much the Coulomb interactions between kinesin and C-terminal tails of tubulins contribute to the binding preference.

20212G* べん毛モーター固定子の協働的な集合によるトルクの自律的制御
Cooperative stator assembly of bacterial flagellar motor for autonomous torque regulation

Kenta Ito, Shuichi Nakamura, Shoichi Toyabe (*Grad. Eng., Tohoku Univ.*)

Torque-generating stator units of the bacterial flagellar motor has a mechanosensitive dynamic structure. With a larger load on the motor, the number of the stator units N increases. We used the electrorotation method to reduce the load for releasing all the stator units, and observed the reassembling process. With a large number of motor-torque traces, we quantified the kinetics of the stator assembly and the free energy for each N. We found that cooperativity among the stator units drives the stator-binding; the binding of the first stator unit is unstable, while that of the followings is stable. I modeled the energetics and kinetics of the torque regulation based on the results, showing that the cooperativity leads to a sensitive and robust torque regulation.

20213G 光てこによる *Volvox*1 個体が生じる推進力の直接測定
Direct force measurement of a swimming *Volvox* spheroid by a high-speed optical lever system

Katsuya Shimabukuro[1], Kosaku Horinaga[1], Kazumo Wakabayashi[1], Hikaru Emoto[1], Noriko Ueki[2], Ken-ichi Wakabayashi[3], Noriyo Mitome[1,4] ([1]*Chem. Bio. Eng., NIT Ube College*, [2]*Sci. Res. Cent., Hosei Univ*, [3]*CLS, Tokyo Tech*, [4]*Tokoha Univ.*)

We report a new experimental system using modified atomic force microscopy to directly measure forces of swimming microorganisms. A cantilever deflection by collision of swimming microorganisms was monitored at high speed. The force generated by a single microorganism can be calculated from the vertical displacement and the stiffness of a cantilever. To evaluate the capability of this system, we measured forces generated by swimming in two *Volvox* species, *V. rousseletii* (~5000 cells) and *V. carteri* (~2000 cells) and found that their forces were 16.2 ± 9.0 nN and 6.6 ± 3.6 nN, respectively, which are relatively higher that those of estimated by Stokes' law. This is the first demonstration of direct force measurement generated by swimming microorganisms.

20214G 高速イメージングで明らかになった遊泳するボルボックスの速度周期性
Periodic fluctuations detected in the swimming velocity of a *Volvox carteri* spheroid by high speed imaging

Naoki Uemura, Tatsuya Suehiro, Midori Nosaka, Katsuya Shimabukuro (*Chem. Bio. Eng., NIT Ube College*)

Our direct force measurement of a swimming *Volvox carteri* spheroid has demonstrated that the spheroid can produce a force around several nN. The magnitude of the force, however, was not constant, oscillated at 30Hz frequency, indicating that a swimming spheroid can change its velocity in the same manner as the force. To examine this, we observed the *Volvox* motility at 0.2 ms time resolution under a bright microscope and found that the velocity fluctuates periodically as expected. Previous studies of the solution flow along a *Volvox* spheroid showed 30Hz-periodicity, presumably due to the metachronal wave generated by *Volvox* flagella. We are currently investigating the relation between a spheroid motility and flagella beating and will report our recent results.

20215G* 好熱菌由来 F_1-ATPase の完全な化学力学共役は至適生育温度において破れる
The perfect mechanochemical coupling of thermophilic F_1-ATPase breaks at the optimum growth temperature

Tomoaki Okaniwa[1], Yohei Nakayama[1,2], Eiro Muneyuki[1] ([1]*Grad. Sch. Sci. Eng.*, [2]*Grad. Sch. Eng.*)

We found that the thermodynamic efficiency of a rotary molecular motor, F_1-ATPase (TF_1) derived from thermophilic Bacillus PS3, is lower than 100% at the optimum growth temperature (65°C) in contrast to the previous research at 25°C (Toyabe et al., 2011). In this study, we developed the experimental methods to measure mechanical work performed by TF_1 in the single-molecule experiment at such a high temperature. In addition to the decrease of the efficiency, we found that TF_1 showed irregular behavior such as backward steps without external torque at 65°C. Our results suggest the possibility that the thermodynamic efficiency of TF_1 may not be 100% in vivo and provided a clue to the requirements for TF_1 to exhibit high efficiency.

20216G ATP 加水分解を選択的に抑制する F_1-ATPase の速度論的制御機構
Kinetic ratchet mechanism of F_1-ATPase selectively suppresses hydrolysis of ATP

Yohei Nakayama, Shoichi Toyabe (*Grad. Sch. Eng., Tohoku Univ.*)

We investigated how the inhibited state of F_1-ATPase selectively supresses the hydrolysis of ATP without affecting the synthesis of ATP. Its rotational motion was observed in single molecule experiments with the electrorotation method. We found that the application of the external torque reduced the fraction of the inhibited state irrespective of its direction, and the torque dependence of the fraction was mainly regulated by the duration of the inhibited state. Considering the detailed analysis of the dynamics of activation from the inhibited state, we construct a kinetic ratchet model where the selective suppression of ATP hydrolysis results from the asymmetry of the magnitude of the transition rates, not of the potential energy.

20217G Mixed motility assay を用いたフォトクロミック Eg5 阻害剤の Eg5 阻害機構の解析
Analyze inhibitory mechanism of kinesin Eg5 with photochromic Eg5 inhibitor using mixed-motility assay

Kei Sadakane[1], MD Alrazi Islam[2], Happy Ogunwa Tomisin[2], Shinsaku Maruta[1,2] ([1]*Sci. & Eng., Soka Univ.*, [2]*Grad. Sch. Eng., Soka Univ.*)

Mitotic kinesin Eg5 is one of the targets for the cancer therapy. It is known that there are several small molecules which exhibit specific potent inhibition for kinesin Eg5. We have previously succeeded to regulate Eg5 activity using photochromic Eg5 inhibitor analogues; ACTAB, DSPPA and BDPSB. Especially, trans isomer of BDPSB exhibited potent inhibition on the Eg5 activity, whereas cis isomer showed almost no inhibition. However, inhibitory mechanism of the photochromic Eg5 inhibitors is still obscure. In this study, we studied which step in Eg5 ATPase cycle is inhibited by the photochromic Eg5 inhibitors utilizing mixed motility assay and stopped flow. Preliminary results suggested that BDPSB inhibits Eg5 ATPase at the same step with STLC.

20218G DNA ナノチューブ上に構築されたダイニン線形アレイの集団運動性
Collective motility of dynein linear arrays built on DNA nanotubes

Ryota Ibusuki[1], Misaki Shiraga[2], Akane Furuta[1], Maki Yoshio[1], Hiroaki Kojima[1], Kazuhiro Oiwa[1,2], Ken'ya Furuta[1] ([1]*Adv. ICR. Res. Ins., NICT. Kobe*, [2]*Grad. Sch. Sci., Univ. Hyogo*)

Dynein motors usually work as a group inside cells. Despite the importance of the intracellular functions of dynein, the effect of inter-dynein interactions on collective motility remains poorly understood due to the difficulty in building large dynein ensembles with defined geometry. Here, we describe a method to construct linear arrays of tens to hundreds of cytoplasmic dynein monomers on a DNA nanotube. The collective motility of dynein ensembles was affected by the stiffness of a DNA nanotube or motor-motor distance built on DNA. Furthermore, we observed cyclical buckling of DNA nanotubes on microtubules, reminiscent of ciliary/flagellar beating. These results highlight the importance of the geometric arrangement of dynein motors on their collective motility.

20219G Increasing speed of single-molecule kinesin movement in vitro

Keitaro Shibata[1], Misaki Sagawa[2], Hiroaki Kojima[1], Ken'ya Furuta[1] ([1]*Adv. ICT. Res. Ins., NICT*, [2]*Grad. Sch. Sci., Univ. Hyogo*)

Kinesin is a motor protein that moves along microtubules upon ATP hydrolysis and is involved in intracellular anterograde transport. The intracellular transport is usually operated at a speed of 1-5 μm/s, while in vitro reconstituted kinesin movement has not achieved such a high speed, making the fundamental mechanisms of intracellular transport difficult to understand. Here, we reconstituted the movement of single molecules of kinesin-1 under conditions that are close to the intracellular environment and identified the conditions that enable kinesin-1 to move at a faster speed. We are working on the stepping behavior and ATPase turnover of kinesin-1 under the optimum condition to elucidate the mechanisms underlying the high-speed intracellular transport.

20220G Single-molecule analysis of artificial kinesin-1 dimers and trimers with different linker lengths

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Here we investigated motions of artificial kinesin-1 dimers and trimers with different linker lengths connecting heads. We found all dimers and trimers tried moved processively but much slower than the wild-type (690 nm/s) at 1 mM ATP. On the other hand, the trimer with long linker showed longer run-length (3.8 μm) than the wild-type (2.7 μm), whereas dimer with long linker showed shorter run-length (1.2 μm). Furthermore, dimer with short linker moved faster (130 nm/s) than that with long linker (82 nm/s) with similar run-length (1.0 μm), whereas trimer with short linker moved slower (60 nm/s) than that with longer linker (105 nm/s) with shorter run-length (1.3 μm). We will discuss effect of the number of heads and linker length on the coordinated motion of kinesin-1.

20221G* バーチャル電極上の電場によるキネシンと微小管の駆動システムの制御
Controlling fundamental functions of the kinesin-microtubule by the electrical field on the virtual cathode

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The kinesin-microtubule (MT) system attracts much attention as a key component for nanotechnological applications such as analyte detection and biosensing due to the fundamental function of driving through inter molecular electrostatic interactions. On-demand controlling of the gliding MT is requested for developments to such biomechanical applications. Controlling the fundamental functions of the kinesin-MT system is also important for reducing molecular design costs. So, we propose the on-demand control of the fundamental kinesin-MT system by using the virtual cathode that can locality-selective change in the electrical field. In this report, we show virtual cathode induced pausing and changing direction of a target gliding MT.

20222G* ダイナクチンサイドアームのコンフォメーション多様性
Conformational diversity of dynactin sidearm

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Dynactin is a principal regulator of the minus-end directed microtubule motor dynein. The sidearm of dynactin is essential for binding to microtubules and regulation of dynein activity. Here, we report the flexible nature and diverse conformations of dynactin sidearm observed by electron microscopy. Using nanogold labeling and deletion mutant analysis, we determined the domain organization of the sidearm. Furthermore, single particle analysis revealed that dynactin sidearm adopted several characteristic conformations and that they were in equilibrium under physiological conditions. These conformational diversities of the dynactin complex provide clues to understanding how it binds to microtubules and regulates dynein.

20223G Constructing a simplified axoneme-like system using *Chlamydomonas* outer arm dynein and DNA nanotubes

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Flagellar beating is generated by thousands of dynein motors distributed along the axonemal microtubule. To understand how the individual dynein motors contribute to the organized beating waveforms, we set out to build a simplified axoneme-like system using DNA nanotubes as a template. As a first step, we introduced a specific tag to an intermediate chain 2 of *Chlamydomonas* outer arm dynein (OAD) for a linkage between dynein and DNA nanotube. Purified tagged OAD retained microtubule gliding activity and load-dependent microtubule-binding behavior when applied force by an optical trap. Using electron microscopy, we observed that OAD were aligned in a single row on a DNA nanotube. The cooperative movement of the dynein-DNA nanotube complex will be discussed.

20224G V/A-ATPase の膜内在性ドメイン V_o のプロトン漏洩防止機構
Mechanical inhibition of isolated Vo from V/A-ATPase for proton conductance

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V-ATPase is an energy converting enzyme, coupling ATP hydrolysis/synthesis in the hydrophilic V_1 domain, with proton flow through the V_o membrane domain, via rotation of the central rotor complex relative to the surrounding stator apparatus. The isolated V_o domain of the eukaryotic V-ATPase can adopt a physiologically relevant auto-inhibited form in which proton conductance through the V_o domain is prevented, however the molecular mechanism of this inhibition is not fully understood. Using cryo-EM, we determined the structure of both the holo V/A-ATPase and isolated Vo at near-atomic resolution, respectively. These structures clarify how the isolated V_o domain adopts the auto-inhibited form and how the holo complex prevents formation of the inhibited V_o form.

20225G* FliL は低負荷条件下で大腸菌べん毛モーターの回転を支援する
FliL assists flagellar motor rotation in *Escherichia coli* under low load condition

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Since bacteria explore various environments, the performance of their flagellar motors needs to be optimized in response to external conditions. FliL, one of regulatory factors of the flagellar rotation, was reported to assist motor torque generation at high load in *Vibrio*, *Salmonella*, etc., but its function in *E. coli* remains unclear. In this study, we observed the effect of *E. coli* FliL on the motor speed over a wide range at single motor levels. We found that cells expressing FliL (called FliL+) can rotate their motors faster than Δ*fliL* cells at not high but low load. The maximum motor speed of FliL+ and Δ*fliL* cells near zero load were up to 300 Hz and 200 Hz, respectively. These results suggest that FliL in *E. coli* functions to assist motor rotation at low load.

20226G *Enterococcus hirae* 由来 V-ATPase のナトリウムイオン濃度に依存した回転運動の 1 分子解析
Single-molecule analysis of rotation of *Enterococcus hirae* V-ATPase depending on sodium ion concentration

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Enterococcus hirae V-ATPase (EhV_oV_1), composed of two rotary motors, functions as a sodium ion (Na^+) pump driven by ATP hydrolysis. EhV_oV_1 converts chemical energy into electrochemical potential across the cell membrane via mechanical rotation. Here we observed ATP-driven rotation of detergent-solubilized EhV_oV_1 in a wide range of Na^+ concentrations ($[Na^+]$s) to elucidate coupling mechanism between V_o and V_1. Even at high ATP concentration, rotation rate decreased to ~10 rps by decreasing $[Na^+]$, indicating Na^+ binding to V_o becomes rate-limiting. Furthermore, at low $[Na^+]$, EhV_oV_1 showed small steps close to 36°, presumably reflecting structural symmetry of V_o rotor ring. We will present detailed analysis of $[Na^+]$ dependence of rotation rate, step size, and dwell time.

20227G Autonomous molecular swarm robots realized by sequential transfer of DNA signal

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Autonomous molecular swarm robots that can communicate to each other and start swarming according to their DNA based molecular memory have been successfully designed and constructed, by integrating sequential transfer of DNA signal and microtubule (MT) kinesin molecular motors. Three kinds of DNA tethered MTs prepared using Cu free click chemistry, DNA signal on the first MT propelled on kinesin coated substrate in the presence of chemical energy, ATP, is transferred to the second MT through physical contact, which consequently activates swarming of the second and the third MTs. A multi-step chemical reaction between isolated DNA strands on MTs through individually traceable and sequential collisions realizing transfer of information has been achieved.

20228G* 演題取り消し

20229G 鞭毛波形切り替えメカニズムの数理モデル
A mathematical model for mechanism of flagellar waveform change

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We studied Ca^{2+}-dependent waveform changes of Chlamydomonas flagella using the numerical simulation, in which antagonistic pairs of cross-bridges worked against the elastic load. Since the X-ray diffraction of Chlamydomonas flagella at different [Ca^{2+}] suggests the change in the axial helical symmetry of the doublets, we incorporated this helical symmetry into the simulation as the nm-shift between positions of dynein and their binding sites on the adjacent doublet. In the simulation, a pair of the cross-brides working antagonistically against the elastic load showed stable oscillations. Their amplitude and frequency varied with the amount of the shift, suggesting the waveform changes might be coupled with changes in the helical arrangement of the axonemal components.

20230G The Helical Arrangement of Axonemal Structures Depends on the Region of the Flagellum

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From X-ray fiber diffraction studies, we found that the Chlamydomonas flagellar axoneme has a helical arrangement of structures (BSJ2019). However, it is still unknown where the origin of the arrangement is. Here, we observed axonemes by negative staining electron microscopy to get hints of it. Analyses of those electron micrographs using the ImageJ FFT plugin showed that there was a helical arrangement of the axonemal structures away from the base of the flagellum. However, it did not show a signal indicating a helical arrangement near the base. Considering that the mutant lacking radial spokes also shows a helical arrangement, it is suggested that the origin of the helical arrangement of axonemal structure is the interactions between peripheral microtubules.

20231G ビーズ-DNA 複合体および DNA ナノチューブを利用した人工分子モーターの実現を目指して
Towards the realization of artificial molecular motor using beads-DNA complex and DNA nanotube

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The molecular motor is composed of functional domains such as the ATPase moiety, hinge, and stator-binding site. The functions of each domain has been elucidated. However, it remains to be understood how the domains work together coordinately to achieve the robust and efficient function of the motor. Realization of artificial molecular motor would be a promising approach to understand such cooperativity. As the first step along this challenge, we aim to realize an artificial molecular motor using DNA and beads. We have constructed DNA nanotube as the rail for the motor movement. Complex of beads and DNA will roll on the rails with digesting "fuel" DNA molecules. Here, we report the ongoing experiments towards the realization of artificial molecular motor.

20232G 単極毛性細菌 *Vibrio cholerae* におけるべん毛モーター回転切り替えの協同性
Low cooperativity of flagellar motor switching in *Vibrio cholerae* the bacterium of a single polar flagellum

Hirotaka Tajima[1,2], Masatoshi Nishikawa[1], Yuki Miura[3], Yoshiyuki Sowa[1,2,3], Ikuro Kawagishi[1,2,3] ([1]*Dept. Front. Biosci., Hosei Univ.*, [2]*Res. Cent. Micro-Nano Tech., Hosei Univ.*, [3]*Grad. Sch. Eng., Hosei Univ.*)

Vibrio cholerae shows chemotaxis by modulating the rotation of the polar flagellum. Binding of phosphorylated CheY to the flagellar motor component FliM induces clockwise rotation of the motor which otherwise rotates counterclockwise. By enhancing CheY phosphorylation, repellents cause tumbling of the peripherally flagellated bacterium *Escherichia coli*. *V. cholerae*, however, shows frequent switching of forward and backward swimming upon similar stimulation. Here we found that the binding cooperativity between CheY and FliM of *V. cholerae* is lower than that of *E. coli*, which is consistent with its repellent responses. We are currently examining the relation of cellular concentration of phospho-CheY and motor switching at the single-cell level.

20233G　CbM4 の持つ時計回りの運動活性の解析
Analysis of the clockwise motility of CbM4

Kohei Yoshimura, Takuma Imi, Takeshi Haraguchi, Masanori Tamanaha, Kohji Ito (*Grad. Sch. Sci., Chiba Univ.*)

In our study, we found that Chara braunii has four myosin XI's and also One of them, CbM4 (Chara braunii Myosin 4), was found to have clockwise motility. Furthermore, CbM4 forms a actin ring pattern that, under certain conditions, rotates steadily in a clockwise direction. We used CbM3 to determine the mechanism for establishing the asymmetry of CbM4. CbM3 has 90% of the same amino acid sequence as CbM4 but has no clockwise motility. We hypothesized that the 10% difference is important for establishing asymmetry, and we performed subdomain recombination experiments between CbM3 and CbM4. The results suggest that the clockwise motility may be dependent on the actin-binding site rather than the converter region, which is responsible for the conformational change.

20234G*　腸管病原性大腸菌が有するⅢ型分泌装置の ATPase の活性特性評価と HS-AFM を用いた構造ダイナミクスに対する考察
Characterization of the enzymatic property and structural dynamics of the T3SS ATPase from Enteropathogenic Escherichia coli

Aya Suzuki[1], Hiroshi Ueno[1], Ryo Kurosaki[2], Takayuki Uchihashi[2], Hiroyuki Noji[1] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*Grad. Sch. Sci., Univ. Nagoya*)

Type III secretion system (T3SS) ATPase complex from enteropathogenic E. coli (EPEC) is composed of the hexameric ATPase EscN, the central stalk EscO, and the peripheral stalk EscL, and it is essential for the injection of virulence effector proteins into host cells. Here, the enzymatic property of EPEC T3SS ATPase subcomplex (EscN/O) was characterized. Similar to the rotary ATPases, the ATPase activity of EscN/O gradually decreased with time and became stable. Besides, its activity was activated by the addition of detergent LDAO that relieves the ADP-inhibition of rotary ATPases, suggesting ADP-inhibition is a common inhibitory mechanism between EscN/O and rotary ATPases. Furthermore, the structural dynamics of EscN hexamer observed by high-speed AFM is discussed.

20235H　演題取り消し

20236H　演題取り消し

20237H Visualizing of neo-self phenomena in chimeric antigen receptor (CAR)-T cells

Hiroaki Machiyama, Ei Wakamatsu, Tadashi Yokosuka (*Dept. Immunol, Tokyo Med. Univ.*)

CAR-T is a recent remarkable advantages in cancer immunotherapy. Human CD19 CAR already applied to clinical use for B cell lymphomas. However little is known about the molecular mechanism how CAR introduces the activation signaling in T cells to kill the targets. To confirm if CAR-T cells are also spatio-temporally activated by various molecules in T cell signaling, we established an up-to-date CD19 CAR imaging system by the combination of TIRFM and lipid-bilayers. We found that CAR clustering serves as a signalosome in CAR-T cells and further discovered that endogenous T cell receptors (TCRs) closely localizing beside CARs participate in CAR-T cell activation without their cognate antigens. This would be the first evidence to visualize “neo-self” recognition by TCRs.

20238H ストレスファイバーの張力ホメオスタシスに関する研究
Theoretical consideration of homeostasis in stress fibers

Yuika Ueda, Daiki Matsunaga, Tsubasa Matsui, Shinji Deguchi (*Grad. Eng. Sci., Univ. Osaka*)

Stress fibers (SFs) have a unit structure called non-muscle sarcomeres. SFs are able to adapt to changes in the mechanical environment through their interactions and molecular exchange or turnover with their surrounding diffusive components. On the other hand, it is known that the tension in SFs has a specific set-point. This mechanism that keeps the level of the intracellular tension constant is called tensional homeostasis. Our group observed that SFs can collapse when they are subjected to fast compressive strains. In this study, using a probabilistic model of SFs that are subjected to cyclic stretch, I analyzed how collapse and maintenance of SFs can be affected by the applied mechanical stress.

20239H 支持脂質二重膜に固定したカドヘリンのモノマー・ダイマー間構造変換の高速 AFM による追跡
Chasing the transformation between monomer and dimer structure of cadherin anchored to supported lipid bilayer by high-speed AFM

Shigetaka Nishiguchi[1], Hiroki Oda[3,4], Takayuki Uchihashi[1,2] ([1]*ExCELLS*, [2]*Nagoya Univ.*, [3]*BRH*, [4]*Osaka Univ.*)

Homophilic binding of E-cadherins through their ectodomains is essential to epithelial cell-cell adhesion. The ectodomains of Drosophila E-cadherin (DE-cadherin) is composed of seven EC domains and others. We previously reported that the membrane-distal EC domains of DE-cadherin form knot-like structure and is essential for trans-homophilic binding; however, the binding structure has not been visualized by observing diffusive proteins. In this study, we anchored the DE-cadherin ectodomains to supported lipid bilayer and then observed them in solution by high-speed AFM. We observed the transformation between monomer and dimer structure of DE-cadherin, and found that the knot-like portion of DE-cadherin is the binding interface.

20240H 非接着状態がん細胞の転移能上昇に伴う細胞間接着強度の増加
Increase of intercellular adhesion strength of non-adherent cancer cells associated with the upregulation of their metastatic ability

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Adhesion of non-adherent cancer cells, as represented by circulating tumor cells (CTCs), plays critical role for the success of distant metastasis. In this study, intercellular adhesion strengths of such cancer cells were quantitatively measured by atomic force microscopy (AFM). Two cancer cells having different malignancies were captured to the AFM cantilevers, respectively, and were approached on the same kinds of cancer cells. In results, highly metastatic cancer cell adhered strongly each other, which were also confirmed by hanging drop tests. This result suggests high ability of cell cluster formation in highly metastatic non-adherent cancer cells, which is also consistent with a clinical result that abundance of CTC clusters strongly correlated with bad prognosis.

20241H* 損傷した細胞における細胞内粘性と生存確率の関係
Cytoplasmic Viscosity and Cellular Viability of the Damaged Cells

Hideaki Ota, Hideo Higuchi (*Department of Physics, School of Science, The University of Tokyo*)

Cellular viability decreases at cell damage. We found movements of cytoplasm decreased by the damages of reactive oxygen species and local heats. This finding will be related to glass-like high viscosity of cytoplasm reported recently. Here, to understand the relation between cytoplasmic viscosity and cellular viability, cells were damaged by photoactivation of IR700 during red laser illumination to cells, and then we counted the living or dead cells to calculate survival probabilities. Cytoplasmic viscosity was also measured by the recovery of Kusabira-fluorescence after the photobleaching. We found the strong photoactivation decreased the survival probabilities. We will discuss the relation between cytoplasmic viscosity and survival probabilities of the damaged cells.

20242H 繊毛への機械刺激依存的な、マウスノードクラウン細胞における mRNA 分解
Mechanical stimuli to a cilium activate mRNA decay in a mouse nodal crown cell

Takanobu A Katoh[1], Katsutoshi Mizuno[1,2], Hiroshi Hamada[1] ([1]*BDR, Riken*, [2]*School of Medical Sciences, University of Fukui*)

Nodal immotile cilia, hair-like protrusions on the surface of cells, sense a flow-dependent signal to determine the Left-Right patterning of the embryo. The cation channel Pkd2 is required for the sensing and triggers Cerl2 mRNA decay, however, it is still controversial how cilia sense the flow. To examine the mechanosensor hypothesis, we applied mechanical stimuli to nodal immotile cilia by the optical tweezers, and the decay of Cerl2 mRNA was monitored by the Tg mouse. The mRNA decay was recognized after the 1.5h stimulation, and significant mRNA decay was detected at 2h (58±29%; n=18). The mRNA decay was never detected under the treatment of GdCl3 (inhibitor of channel; n=6). These results suggest that mechanical stimuli activate mRNA decay via the Pkd2 channel.

20243H* 運動性細胞における Ras の興奮性制御に関わる GEF の同定
Identification of GEFs regulating the excitability of Ras in motile cells

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Cell polarity and migration are based on symmetry breaking in Ras activity on the plasma membrane in eukaryotic cells. Activated Ras forms an enriched domain that exhibits traveling waves even in the absence of external cues. However, how the dynamics is regulated via GEF has not been elucidated. We investigated the effect of over-expression of each GEF gene out of 25 genes by quantifying a fraction of the cells showing waves, a domain size and a wave period in Dictyostelium discoideum. As a result, 11 GEFs were found to be responsible for the regulation. In fact, the over-expression of these GEFs affected cell motility as well. These results suggest that multiple GEFs regulate a threshold of the excitability and spatiotemporal characteristics of the system.

20244H クラミドモナス軸糸運動の再活性化イメージング
High hydrostatic pressure induces vigorous flagellar beating in *Chlamydomonas* non-motile mutants lacking the central apparatus

Toshiki Yagi[1], **Masayoshi Nishiyama**[2] ([1]*Pref. Univ. Hiroshima*, [2]*Kindai Univ.*)

Chlamydomonas paralyzed-flagella (*pf*) mutants lacking the central pair of microtubules (CP) or radial spokes (RS) are non-motile under physiological conditions. Here, we show that high hydrostatic pressure induces vigorous flagellar beating in *pf* mutants. The beating pattern at 40 MPa was similar to that of wild type at 0.1 MPa. In addition, at 80 MPa, flagella underwent an asymmetric-to-symmetric waveform conversion, similar to the one triggered by an increase in intra-flagella Ca^{2+} concentration during cell's response to strong light. Thus, our study establishes that neither beating nor waveform conversion of cilia/flagella requires the presence of CP/RS in the axoneme.

20245H 細菌バイオフィルムと骨代謝の ASEM 免疫電顕と cryo-TEM による観察
Observation of biofilm and bone metabolism in aqueous liquid using immuno-labeled ASEM and cryo-TEM

Chikara Sato[1], Shinya Sugimoto[2], Eiko Sakai[3], Mari Sato[1], Naoki Kasahata[1], Masami Naya[1] ([1]*Health & Medical Res.Inst, AIST.*, [2]*Dept. Bacteriol., The Jikei Univ. Sch. Med.*, [3]*Dental Pharmacology,Nagasaki Univ.*)

ASEM observed microbes in situ in natural aqueous buffer, decreasing the risk of changes of the surrounding water-rich biofilm and mucin. Filamentous structures of bacteria culture and on tissue revealed by PTA staining suggest the formation of biofilms, confirmed by immuno-EM in solution targeting dsDNA. Bone absorption [1], and axonal segmentation controlling neuron trafficking was also visualized in combination with immuno-labeling [2]. MRSA biofilm formation was monitored by ASEM [3] and cryo-TEM. [1] Sato et al. Scientific Reports 9, 7352, 1-13 (2019). [2] Kinoshita et al. Sci. Rep. 7, 41455, 1-14 (2017). [3] Sugimoto et al. Sci. Rep. 6, 25889, 1-13 (2016)

20246H Tension at adherens junction inhibits proliferation and promotes differentiation of keratinocyte carcinoma cells

Oleg Dobrokhotov, Masahiro Sokabe, Hiroaki Hirata (*Grad. Sch. Med., Nagoya Univ.*)

Cell density-dependent inhibition of proliferation (termed contact inhibition of proliferation, CIP) is a well-appreciated phenomenon that distinguishes normal cells from cancer cells. Previously we have shown that actomyosin-generated forces at the adherens junctions (AJ) are required for CIP in normal keratinocytes. In keratinocyte carcinoma cells impairment of actomyosin contractility is associated with overproliferation both in vivo and in vitro, while exogenous application of tensile load to the AJs, by pharmacological treatment or mechanical stretch, inhibits proliferation and promotes differentiation in keratinocyte carcinoma cells under the condition that cells form AJs. Thus targeting AJs tensile status might be used as a novel approach for skin cancer therapy.

20247H 細胞質中における p52SHC は GRB2 の細胞膜移行を負に制御する
p52SHC in the cytoplasm negatively regulates GRB2 translocation to the plasma membrane

Ryo Yoshizawa[1,2], Nobuhisa Umeki[2], Masayuki Murata[1], Yasushi Sako[2] ([1]*Grad.sch.arts and ahi., the univ. Tokyo*, [2]*Wako Inst., Riken*)

p52SHC (SHC) and GRB2 are adapter proteins to propagate RTK signals to the RAS/MAPK pathway. The recruitment of these proteins to active RTKs have been thought synchronous. However, we recently found that translocation dynamics of SHC was sustained though that of GRB2 was transient, and these protein's functions are not redundant for MAPK activation. Here, we examined the effects of SHC on the GRB2 translocation. Co-expression of SHC3F that cannot bind with GRB2 induced sustained translocation of GRB2. FCCS analysis revealed that cytoplasmic interaction of GRB2 with SHC was increased but not with SHC3F after cell stimulation. These results suggest that phosphorylated SHC in the cytoplasm acts as negative regulator for membrane translocation of GRB2.

20248H 細胞内脂肪滴の普遍的相挙動
Liquid-liquid crystal phase transitions in intracellular lipid droplets

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Lipid droplets are cytoplasmic organelles involved in energy homeostasis and handling of cellular lipids and proteins. The core structure is composed of two kinds of neutral lipids, triglycerides and cholesteryl esters, which are coated by a phospholipid monolayer and proteins. Despite the liquid crystalline nature of cholesteryl esters, the connection between the lipid composition and physical states is poorly understood. Here, we present a intracellular phase diagram of lipid droplets, semi-quantitatively consistent with the in vitro phase diagram, and reveal that cholesterol esters cause the liquid-liquid crystal phase transition under near-physiological conditions. Our findings contribute to a better understanding of their biological functions and diseases.

20249H 陰圧条件下における金魚ケラトサイト細胞の移動速度の上昇
Enhanced movement of fish keratocyte cells under negative pressure conditions

Akihiro Yamazaki, Hitoshi Tatsumi (*Kanazawa Inst. of Technology*)

Vacuum assisted closure is being increasingly used for wound management, a system that promotes healing by exposing damaged areas to local negative pressure. However, the mechanism of the action of vacuum assisted closure remains unknown especially when applying negative pressure directly to cells. In this experiment, we examined the changes seen in cultured goldfish keratocytes directly exposed to a negative pressure, and analyzed the behavior of keratocytes. Under the negative pressure conditions, the rate of cell movement gradually increased, the shape of the cells became thinner (increased cell aspect ratio), and the space between the cells was enlarged.

20250H 1 細胞自律的な細胞内温度制御の分子機構
A cell-autonomous control of intracellular temperature by mitochondrial thermogenesis

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Intracellular temperature affects a wide range of cellular functions. However, it remains unclear whether temperature in individual cells is controlled as response to the fluctuation of environmental temperature. Using two mechanistically distinct intracellular thermometers, we found that Δ9-fatty acid desaturase DESAT1, which is essential for regulating the membrane lipid composition via biosynthesis of unsaturated fatty acids, increases the intracellular temperature of steady-state Drosophila S2 cells via mitochondrial respiration. The mitochondrial respiration was enhanced by cold exposure in a DESAT1-dependent manner. From these findings, we propose a novel cell-autonomous mechanism for intracellular temperature control during environmental temperature changes.

20251H 蛍光顕微鏡法による単一デスミンフィラメントの可視化
Visualization of single desmin filaments by fluorescence microscopy in vitro

Masashi Sato, Keigo Murakami, **Kuniyuki Hatori** (*Grad. Sch. Sci. Eng., Yamagata Univ.*)

Desmin, type 3 of intermediate filament (IF) protein, assembles into IFs depending on ionic strength and divalent cation. Morphology of IFs is mainly studied by electron microscopy. To gain a better understanding of the assembly mechanism, we approached the visualization of desmin IFs conjugated with tetramethylrhodamine (TMR) under a fluorescence microscope. An incubation of urea-denatured desmin with TMR-maleimide at molar ratio of 1:6 induced the label ratio of 0.45. After an initiation of desmin assembly by adding KCl, the diluted sample to 1 μg/ml was observed. Desmin developed into IFs (average 3 μm in length) for 24 h after the initiation. As KCl concentration was increased to 150 mM, IFs associated each other via side-to-side interactions.

20252H* 収縮するアクトミオシン構造の綱引きで決まる細胞サイズ液滴内の位置対称性
A tug-of-war between contractile actomyosin structures determines the positioning symmetry in cell-sized droplets

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Symmetric or asymmetric positioning of intracellular structures such as nucleus and spindles steers various cellular processes. Previous studies have shown that the actin cytoskeleton is involved in the positioning, however, its mechanism is still unclear. Here, we construct an in vitro artificial cell as a physical model of positioning, where actin-intact cytoplasmic extracts and nucleus-like clusters are confined within emulsion droplets. We find that periodic centripetal actomyosin waves push clusters to the center, while percolation of actomyosin network pulls clusters to the edge. Combining the molecular perturbations and an active gel theory, we show that a tug-of-war between two distinct actomyosin structures determines the positioning symmetry.

20253H* NF-κB mediated transcriptional regulation in B-cell

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NF-κB signaling pathway shows a threshold response upon B-cell receptor (BCR) activation and is thought to be associated with cell fate determination. This research aims to explore the relationship between NF-κB activity and transcriptional regulation on super enhancers (SEs), which are enhancers bound by transcription factors such as NF-κB. The induction of SE formation is investigated through fluorescence imaging of RelA-GFP in DT40 cells combined with omics analysis (single-cell RNA-seq and ATAC-seq). Results of multi-omics analysis were validated using RNA fluorescence in situ hybridization (RNA-FISH). Our analysis indicates that BCR-mediated gene expression is regulated in an all-or-none manner, beneficial for the cells to remove noise for cell determination.

20254H 神経シナプスでの AMPA 受容体数密度の動的制御：1 分子イメジングによる解明
Dynamic regulation of the AMPA receptor number density in the neuronal synapse as revealed by single-molecule imaging

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The AMPA subtype of ionotropic glutamate receptor (AMPAR) is at the heart of synaptic plasticity: Upon nerve excitation, its number is increased, and subunit compositions are modulated in the synapse. However, how such regulations occur is not totally known. Here, our single-molecule tracking revealed that AMPAR and its regulatory protein TARP 2 frequently entered and exited from the spine, with three dwell-lifetime components on the order of 1, 10, and 100 s. When AMPAR entered a spine, 30% (70%) were entrapped there for a period of the order of 100 s (1 and 10 s). This result suggests that the AMPAR number and the subunit compositions in the spine are dynamically maintained in the resting state, and that, upon stimulation, they could be modulated quite readily.

20255H γ-tubulin は中心子トリプレット微小管形成に寄与する
γ-tubulin functions in assembling centriolar triplet microtubules

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While the γ-tubulin ring complex is a key player in nucleating cytoplasmic microtubules, little is known about whether it also nucleates triplet microtubules in centrioles/basal bodies. We recently isolated novel *Chlamydomonas* mutants (*bld13-1* and *bld13-2*) that show defects in flagellar assembly and cell division, phenotypes common to known centriole-deficient mutants. Genetic analyses showed that these defects are caused by a single dominant-negative mutation in the γ-tubulin gene at conserved residues (T292I or E89D). Interestingly, electron microscopy of the mutant centrioles revealed that 1-6 protofilaments in a particular position of the triplet are frequently missing. These results provide evidence that γ-tubulin functions in assembling triplet microtubules.

20256H 2 本の内べん毛の同調した回転は細菌の遊泳を制御する
Coordinated rotation of dual endo-flagella controls bacterial swimming

Toshiki Kuribayashi, Shuichi Nakamura (*Grad. Sch. Eng., Tohoku Univ.*)

Leptospira is a spirochete bacterium possessing periplasmic flagella (PFs) at both ends, and can move in liquid using two PFs. Although rapidly harmonized operation of dual motors allows the bacteria to explore environments, it remains unknown how they are coordinated during swimming. To elucidate the coordination system, we focused on the motility of the spirochete lacking PFs at one of the cell-ends accidentally, and compared the behavior of such “single-bent” cells with the intact ones. Our results showed a change of switching rate and the possibility of such coordination.

20257H 細胞の間隙で働く接着性 GPCR の蛍光 1 分子観察
Single molecule observation of adhesion GPCR accumulated at the cell-cell interface

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Adhesion GPCRs (G-protein coupled receptors) are quite important for cell adhesion as well as communication for establishing proper organization of cells. CELSR, one of the adhesion GPCRs, is involved in cell adhesion through homophilic trans-interaction at the cell-cell interface. However, a precise mechanism of adhesion remains unclear. By applying newly developed single fluorescent molecule observation technique at the cell-cell interface, we found that CELSR is highly accumulated at the interface. Whereas most of CELSR proteins are immobilized and some of them form cis-dimers, diffusing trans-dimers are also observed. This suggests that the trans-dimer bound to actin filaments through unidentified proteins serves as a minimal unit for adhesion.

20258H* マイクロ構造化ハイドロゲル上を移動する細胞の核形態変化の定量解析
Quantitative analysis of dynamic changes in nuclear morphology in cells migrating on microstructured gelatin hydrogel

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The physical properties of cell culture substrate affect various cellular processes, such as migration, proliferation and differentiation. The signaling involves the physical network structure from cell adhesion structure via actin fibers to cell nucleus. To understand the signaling mechanism of mechanotransduction, we focused on the dynamic changes in the morphology of the nucleus, based on the hypothesis that the magnitude and direction of the forces transmitted to the nucleus will change dynamically with actin reorganization in migrating cells. We analyzed the morphological changes of the nucleus in fibroblasts migrating on gelatin hydrogel substrates with micro-pillar and hole arrays and estimated the mechanical effect on the cell nucleus.

20259H ADP により調節されるマウス気管繊毛の運動活性
Motility of murine tracheal cilia modulated by ADP

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Exclusion of harmful materials from trachea is supported by the increase in amplitude and velocity of ciliary beating. To investigate modulation of ATP-dependent ciliary motility by ADP, we observed beating of individual demembranated cilium from trachea of mice under the 3D tracking microscope with a fluorescent bead attached to the tip as a probe. Although beating frequency was unchanged, increased amplitude and velocity were observed in the presence of 50-150 μM ADP with the maxima at 50 μM. The ciliary beating is assumed to share a common mechanism of activation by ADP with previously reported flagellar beating. Thus ADP is not solely the product of ATP hydrolysis, but in fact plays a key role in mucociliary clearance.

20260H 熱量および蛍光滴定により推定されたタウ-DNA 結合熱
Tau-DNA binding heat estimated by calorimetric and fluorescence titrations

Kan Matsuda, Junta Kashima, Hideyuki Komatsu (*Dept. Biosci. Bioinf., Kyushu Inst. Tech.*)

The microtubule-binding protein tau also binds to polyanions such as nucleic acids, heparin and polyglutamic acid. DNA has been reported to bind to tau in the nucleus of brain neurons (Marie V. et al. *Front. Neurosci.* **8** (2014) 1-11). We here focus on the thermodynamic properties of tau-DNA interaction. First, the DNA-binding of tau was confirmed by a displacement assay using an intercalational fluorescent dye GelRed. The tau-DNA interaction was then analyzed using isothermal titration calorimetry. Unexpectedly, little heat was observed when DNA was titrated into tau solution, suggesting the tau-DNA interaction unaccompanied by enthalpy change. Thus, the binding may be driven by entropy. Possible mechanisms will be discussed in this presentation.

20261H* クラミドモナス繊毛交互打ち変異株の単離と解析
Isolation and analysis of Chlamydomonas mutants showing alternate ciliary beatings

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Chlamydomonas reinhardtii is a unicellular green alga that swims by beating two cilia simultaneously like human's breaststroke. The simultaneous beatings of two cilia are essential for C. reinhardtii cells to show phototaxis because they change their swimming direction by beating one of the two cilia stronger than the other. However, how the two cilia beat simultaneously is a long-standing question. By screening for phototaxis mutants, we isolated mutants that beat cilia alternately (termed alt mutants). Among newly isolated six mutants, we identified a causative gene for a mutant tentatively named alt6.

20262H Response of plural phagocytosis is regulated by the attached order of antigens as far as macrophages can recognize the time differences

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To investigate whether the first local phagocytosis regulates the initiation of the other phagocytosis, we attached plural antigens to stimulate single macrophage. After the attachment of first antigen on the surface of the cell, we attached the second on the opposite side, and then attached the third between them, using optical tweezers. Two types of phagocytosis manner were observed depending on the timing of attachment of the third antigen;(1)three antigens were phagocytosed sequentially as the attached order, and (2)the second and third antigens were phagocytosed simultaneously regardless the attached order. The result suggests that the response of plural phagocytosis is followed by the attached order as far as macrophages can recognize the time difference.

20263H Dominant factor for cease phagocytosis after excess intake of antigens is explained by the volume regulation with 0.62-μm encapsulation

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Two candidates of dominant factor for cease phagocytosis after excess intake of antigens are thought to be surface area-saturated and volume-saturated regulation. The serial phagocytosis experiment predicted volume-saturated regulation can explain as far as the volume increase of macrophage is larger than antigen volume increase. We developed a precise volume increase measurement assay with capillary tube for aspiration of a macrophage, and measured its length increase to estimate cell volume increase. The increase of cell volume was larger than the volume antigen and was estimated to have 0.62 μm envelope surrounding the antigen. The results indicated the 0.62-μm encapsulated volume regulation is ruling index for defining the maximum number of serial phagocytosis.

20264H Measurement of the temporal rotation change of individual cells' trajectory in collective cell migration in agarose microchannels

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To understand the hidden rule in collective cell migration as fluid-like mechanics, we measured the rotation of individual cells in 2-dimentional cell sheet. We microfabricated agarose gel microchannels in its thin layer with a spot heating of focused 1480 nm infrared laser. We observed the cell trajectory of migration in the micro channel in time lapse and calculated rotation by plotting the position coordinates of a cell in each time. The rotation of cell was observed, however it was not continuous but changing over time. The results indicate the existence of rotation means the collective cell migration is not similar to the incompressible fluid. Fluctuation of cell density is also indicated by the fluctuation of the rotation of cell trajectory.

20265H Maximum limit of phagocytosis is explained by the shortage of consumable cell membrane with 0.9 μm envelope in phagosome

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The maximum number of antigens after excess intake were examined with serial phagocytosis exploiting optical tweezers with 2 to 40 μm non-digestible IgG-polystyrene spheres. Experimental results showed the size dependency of maximum number of antigens was observed, whereas it was not explained by simple maximum volume nor maximum surface area model. Membrane model with hypothesis of flexible 5-hold expansion of cell membrane explained the experimental results of antigens larger than 4.5 μm. Moreover, considering 0.9 μm envelope adding to the antigen radius, the membrane model satisfied whole sizes of antigens. If we allow the existence of 0.9 μm envelope in phagosomes, the maximum limits of phagocytosis are determined by the shortage of the consumable cell membrane.

20266H Velocity split after passing through the wide-narrow-wide capillary tube caused by short-term memory in collective cell migration

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Collective cell behavior was observed with the flexible diameter-controlled (32 μm-120 μm) 3D capillary inside the gelatin gel. In a straight capillary, the cells exhibited an overall constant velocity. In the simple changing widths (narrow-wide/wide-narrow), the velocity decreased/increased proportionally to their diameter changes as predicted by fluid-like manner, respectively. In a series of changing widths (wide-narrow-wide), the migration of the cells was slow at the first wide region and fast at the narrow region, however, varied into three velocity modes after passing through this three-width-channel. This indicates the existence of short-term memory stored in cells and that the variety of modes are caused by the change of width while the memory remains.

20267H PM2.5 antigens maintains efficiency of engulfment ability in serial phagocytosis of single macrophages with on-chip free-flow method

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For understanding the influence of indigestible particles like PM2.5 to phagocytosis ability in macrophages, we examined the time course of one-by-one series phagocytosis of indigestible 2-μm polystyrene spheres (PS) by combining free-flow method and optical tweezer method. IgG-BSA decorated PS showed shortest-interval of series phagocytosis, which was ten times faster than Zymosan in engulfment frequency, and was engulfed up to 50 particles within 2 h maintaining constant intervals until reaching to the maximum number. The results suggest (1) no change of reaction rate constant against the history of phagocytosis numbers, and (2) IgG-BSA decorated indigestible micro particles in blood can give serious shortage of macrophages within a short time.

20268H 好気及び嫌気性条件で酸化及び還元型αディフェンシン cryptdin-4 の抗菌メカニズムの検討
Antibacterial mechanism of an α-defensin, cryptdin-4 in redox status under aerobic and anerobic conditions

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Crptdin-4(crp4), a kind of antimicrobial peptides from mouse small intestine, has been studied. But the molecular mechanisms of membrane disruption have yet to be determined. The oxidized form (crp4oxi) with 3 disulfide bonds and reduced form (crp4red) in disordered structure have been found with different bactericidal performances under aerobic and anerobic conditions. In this study, crp4oxi was found to exert stronger bactericidal activity against *E. coli* in aerobic condition while membrane permeabilization was remarkably weaker compared to crp4red. Membrane fragmentation of bacteria had been proved only in crp4oxi. Those results clearly showed the differences of bactericidal mechanisms towards redox peptide and under different cultured conditions.

20269H 多電極電位システムを用いたハイスループット心毒性検査法の実用化を目指した少数心筋細胞集団薬剤応答の解析
Analysis of small size of cardiomyocyte population's drug response for high-throughput cardiotoxicity test using multi-electrode system

Kentaro Kito, Naoki Tadokoro, Masahito Hayashi, Tomoyuki Kaneko (*Laboratory for Reconstructive Cell biology, Department of Frontier Bioscience, Hosei University*)

Drugs have side effects, some of which cause arrhythmias. In particular, cardiotoxicity test is indispensable in drug discovery. However, the cardiotoxicity test is needed high cost and a lot of time. In our previous study, we constructed high-throughput cardiotoxicity test prepared 64 populations of individually pulsating chick embryo-derived cardiomyocytes using agarose microfabrication technology on a multi electrode system. In this study, we added E-4031, hERG channel blocker, in the system for cardiotoxicity test. As a result, pulsation arrest due to QT interval prolongation was measured, and recovery of pulsation due to washout was also measured. It was suggested that this high-throughput cardiotoxicity test was valuable for side effect detection of drugs.

20270H 大腸菌走化性応答適応過程の高い再現性を実現する簡易培養方法の構築
Construction of simple culture method that realizes high reproducibility of Escherichia coli chemotaxis response adaptation process

Hiroto Tanaka, Yasuaki Kazuta, Amina Yano, Hiroaki Kojima (*Adv ICT Res Inst, NICT*)

In order to develop solution evaluator, we have used the Adaptation process of Chemotactic response of Escherichia coli (ACE) as a method to quantify (visualize) characteristics of chemical solution. A problem of using ACE in quantifying solution characteristics was that fluctuation of ACE, which would due to E. coli growth, was observed for each culture. In order to overcome the problem, we tested various culture procedures with the aim of improving reproducibility of AEC. As a result, we succeeded in constructing a culture procedure that realizes high reproducibility of AEC, though culture total volume is small compared to the conventional method. At annual meeting, we would like to discuss the possibilities of the culture method together with the report.

20271H Hysteresis is not remained in macrophages after engulfment in fluctuation of movement angles with a single-point series phagocytosis assay

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To investigate the ability of memorization in previous phagocytosis, the time-course change of macrophage motility during a series of engulfment of indigestible antigens was measured. We contacted IgG-BSA coated polystyrene beads as model antigens on a single identical point of the macrophage using optical tweezers, recorded every 5 s for 30 min and analyzed its movement especially angle dependence from the gravity center position of macrophage, during a series of 14 engulfment. Angles of macrophage fluctuated randomly between -0.4 and 0.4[rad/s] regardless of engulfment process. The result suggests that hysteresis is not remained after each engulfment process at least from the view point of fluctuation of movement angles.

20272H* アガロース微細加工技術を用いた環状心筋細胞ネットワークによる伝導異常モデルの構築
Construction of conduction abnormality model by circular cardiomyocyte network using agarose microfabrication technology

Koji Emura, Masahito Hayashi, Tomoyuki Kaneko (*LaRC, FB, Grad.Sci&Eng, Hosei Univ.*)

Arrhythmia is a fatal disease caused by conduction abnormality. Therefore, a system for measuring conduction abnormality is required. In this study, Closed-loop shaped cardiomyocyte network was fabricated by Agarose-Microchamber. The field potential of the network was measured by using Multi-Electrode Array system. Two kinds of phenomena observed. One was that conduction was transmitted in one direction. The other was that conduction propagated in two directions from the origin, and conduction collided on the opposite side. Moreover, the beating origin was the part with a high proportion of fibroblasts. It is considered that fibroblasts were the starting point of the beating because they reduce the resting potential of cardiomyocytes.

20273H Width-dependent concave velocity distribution in collective migration is explained by two fluid-like behavior rules

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We investigated the rule of fluid-like behavior in two-dimensional collective cell migration in agarose microchannel patterns. Straight microchannels from 15 μm to 200 μm were fabricated with a spot heating of a focused infrared laser, we measured the structure dependency of the velocities of the front of epithelial cell sheets. The velocity maintained constant regardless of their extension length, whereas the convex width dependency in velocity was observed: 8.8 μm/h as peak velocity at 30 μm-width and decreased both in narrower and wider channels. These width dependencies should be explained by two rules as fluid-like behavior; (1) velocity is decreased by cell width compression, and (2) velocity is decreased by increase of random walk-like behavior as width increase.

20274H 高静水圧によるウニ精子細胞内カルシウム濃度への影響
Effects of high hydrostatic pressure on intracellular Ca2+ concentration of sea urchin swimming live sperm

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Intracellular Ca2+ concentration plays a critical role in living cells. The Ca2+ concentration is well regulated by membrane proteins and intracellular organelles. Here, we have developed a novel assay to estimate the intercellular Ca2+ concentration by combining the sea urchin sperm flagellar motility analysis and the high-pressure technique. We examined effects of high hydrostatic pressure up to 60 MPa on swimming live sperm of sea urchin, Anthocidaris crassispina. To our surprise, the applied pressure induced changes in the swimming path curvature of live sperm depending on the Ca2+ concentration of extracellular solution. This result suggests that high pressure would shift the intracellular Ca2+ concentration of swimming live sperm.

20275H 生細胞における１分子イメージングと超解像顕微鏡法を用いた動態と相互作用の定量解析
Quantification of dynamics and kinetics using single-molecule and super-resolution imaging in living cells

Yuma Ito, **Makio Tokunaga** (*Sch. Life Sci. Tech., Tokyo Tech.*)

We introduced a method to quantify dynamics and kinetics of spatiotemporal interactions in living cells using single-molecule tracking and super-resolution analysis. Moving subtrajectory analysis defines the dynamics and kinetics of molecules, and is superior to standard analysis methods by revealing details on the temporal and spatial variation of the movement. Combining with multi-color simultaneous single-molecule imaging, we quantified the dynamics and localization of histone and RNA Polymerase II molecules. Analysis on localization-localization and localization-dynamics relations brings us multimodal information about dynamics differences and interactions between molecules. These are valuable in clarifying various types of molecular features.

20276H １分子イメージングで明らかになった糖鎖によるエクソソーム機能制御
Regulation of exosome function by glycans as revealed by single-molecule imaging

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Exosomes are extracellular vesicles which have been drawing an extensive attention as a carrier for cell-cell communication, and the issue of metastatic organotropism may be resolved by studies of exosomes. Recent studies suggested tumor-derived exosomes bind to specific target cells which may be determined by integrin subtypes in the exosomes. However, the detailed mechanisms are unknown. Here, we tried to unravel the mechanisms by super-resolution microscopy and simultaneous single-molecule imaging. We found that glycans of exosome surface control the binding affinity of exosomes to extracellular matrix and the target cells, and determine the internalization pathways. We discuss the role of N-linked glycans of integrin on the binding and uptake of exosomes.

20277H アクチンの重合と脱重合の熱測定
Calorimetry of actin polymerization and depolymerization

Shouron Kure, Hideyuki Komatsu (*Dept. Biosci. Bioinf., Kyushu Inst. Tech*)

Polymerization and depolymerization of actin are responsible for various cell functions. The assembly and disassembly of actin molecules accompany with large changes of thermodynamic parameters (changes of Gibbs energy, enthalpy and entropy), of which qualitative analysis is essential for biophysical understanding of cell functions. The effect of temperature on equilibrium between monomer and polymerized actin has showed that actin polymerization is an endothermic process driven by entropy. Therefore, we try to directly observe heat generation accompanying actin polymerization/depolymerization using isothermal titration calorimetry. For this purpose, this study seeks to optimize the experimental conditions for calorimetry of actin polymerization and depolymerization.

20278H 線虫 MEC-2 および相互作用チャネル蛋白質の構造・生化学的解析
The structural and biochemical analyses of MEC-2 and its partner channel proteins in *C. elegans*

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Stomatin-like protein (slipin) is a protein family that has a conserved SPFH motif. The slipin is conserved in eukaryotes and prokaryotes and controls the activity of various channels/transporters. MEC-2 is a putative slipin that regulates MEC-4, a neuronal sodium channel in *C. elegans*. To understand the mechanism of channel regulation by MEC-2, we solved the structure of the middle domain of MEC-2 and performed biochemical analysis. The structure revealed that the middle domain adopts a typical SPFH fold and forms a thin triangular plate made of three subunits. Glu270, whose substitution with lysine causes thermotaxis in *C. elegans*, locates on one side of the plate. The trimer may be a functional form of MEC-2, because MEC-4 also forms a trimer.

20279H ヒト iPS 細胞を用いた原腸形成時の自己組織化運動
Self-organizing movement during gastrulation using human iPS cells

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Human gastrulation occurs from monolayers of epiblasts to form three layers (mesoderm, endoderm, and ectoderm). However, the dynamics of the layer formation are largely unknown. We hypothesized that the layer formation can be reproduced by mixing cells in a confined space, strongly adherent cells attach on culture dish to form the basal layer, on which the weakly adherent cells for an upper layer. We cultured mesodermal and epiblast like cells derived from human iPS cells in a confined circular cell culture area with a diameter of 1 mm. We also investigated the concentration of laminin required for cell adhesion on the basal layer. The cell motility in this confined area will be investigated using time-lapse analysis.

20280H マウス気管の繊毛運動による喘息原因物質キチンの輸送
Observation of ciliary motility of murine trachea and epithelial transport of chitin involved in the development of asthma

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In the trachea, numerous hair-like structures called cilia are found on the apical surface of epithelia. They make cooperative asymmetric beating motions to generate mucus flow, which transport harmful particles back toward the larynx. These particles are involved in allergic inflammation, but their behaviors in relation to ciliary motility remain still unclear. Here chitin, a potent adjuvant of asthma, was introduced into half cylinders of dissected murine tracheae and observed along with motions of cilia under a fluorescence microscope. We showed that velocity of chitin translocation clearly depends on the flow rate determined by ciliary motility, and chitin tends to be trapped in between cilia under low-viscous conditions.

20281H リアルタイムフィードバック制御による機械的刺激に影響を受けた心筋細胞の拍動
Beat sequence of cardiomyocytes affected by to mechanical stimulus with real-time feedback control

Shota Nozaki, Kazuki Mammoto, Takashi Miyazawa, Ryuta Watanabe, Yuta Moriyama, Ryu Kidokoro, Toshiyuki Mitsui (*Aoyama Gakuin University*)

It is important to control physiological properties, interbeat intervals and contract length, of cardiac cells motivated by clinical applications using iPS cell-derived cardiomyocytes. The key to control them may lay in the adjustability, synchronization, of cardiomyocytes to the others. We have fabricated an instrumentation to apply mechanical stimulus to cells imitating the beat motions of cardiomyocytes. Cardiomyocytes were extremely sensitive to the mechanical stimulus particularly in the phase differences between autonomous beats and external stimuli. In this presentation, we demonstrate artificial beat-like stimulus to cells with adjusted phase differences by a real-time feedback control. We also present the preliminary results of the phase-controlled stimulus.

20282H 心筋梗塞の治療のための in vitro 移植モデルにおけるペースメーカーの入れ替わり
Pacemaker switching of in vitro transplantation model for heart infarction

Toru Nakamura, Chiho Nihei, Masahito Hayashi, Tomoyuki Kaneko (*Laboratory for Reconstructive Cell biology, Department of Frontier Bioscience, Hosei University, Grad. School of Science and Engineering*)

Transplantation of cultured cardiomyocyte sheet is a hopeful treatment for heart infarction. However, the mechanism of beating synchronization between the heart and cell sheet is still unclear. We constructed an in vitro transplantation model in which a tissue piece of atrium from chick embryo contacts with a primary cultured cell sheet on a Multi Electrode Array (MEA). We measured and analyzed the extracellular potential. Although the beating interval of the tissue piece and cell sheet mismatched just after the contact, the beating synchronization was observed 2 to 3 days after. Pacemaker was not fast beating region but stable beating one. In all cases where tissue piece was pacemaker region, the region switched to cell sheet a few hours later.

20283H 圧力がミトコンドリアの機能に及ぼす影響
Effects of pressure on mitochondrial activity

Yoshiki Oie[1], Yoshihiro Ohta[2] ([1]*Grad. Sch. Sci., Tokyo University of Agriculture and Technology*, [2]*Tokyo University of Agriculture and Technology*)

In a physiological circumstance, cells function in response to various mechanical stimuli. Pressure is one of the mechanical stimuli which mainly acts on the membrane. Since organelles are membranous system, organelles might function in response to pressure. In the present study, we measured the mitochondrial response to pressure in terms of the membrane potential. When isolated mitochondria were placed under +200 mmHg, mitochondria gradually lost their membrane potential within 10 min. On the other hand, mitochondria under atmospheric pressure kept their membrane potential. These results suggest that mitochondria are would be a pressure sensor. The mechanism by which mitochondria lose their membrane potential will be discussed.

20284H タウ–微小管とタウ–ヘパリン相互作用の等温滴定熱測定の比較
Comparative analysis between isothermal titration calorimetries of tau–microtubule and tau–herparin interactions

Junta Kashima, Rio Okamoto, Hideyuki Komatsu (*Dept. Biosci. Bioinf., Kyushu Inst. Tec*)

Tau binds and stabilizes microtubules (MTs). In order to investigate the thermodynamics of binding-induced changes of tau conformation and MT stabilization, we have analyzed tau–MT interaction by an isothermal titration calorimetry (ITC). The thermgram of each titration contained the fast steep and the slow gradual exothermic changes. Only latter heats depend on the molar ratio of tau/tubulin, suggesting that the gradual exotherm is related to tau conformation and/or MT stabilization. In addition, tau–polyanion (heparin) interaction was analyzed as a model of acidic amino acid cluster of MT surface. Unexpectedly, heat of binding was not observed. The heat can be separated into that from tau–MT electrostatic interaction and that from tau-induced MT stabilization.

20285H ミトコンドリア電子伝達系のプロトンポンプ活性の単一細胞検出
Detection of proton pump activities in mitochondrial electron transfer chain in a single cell level

Yoshiki Suganuma, Masato Miura, Hiroko Kashiwagi, Yoshihiro Ohta (*Tokyo University of Agriculture and Technology, Department of Biotechnology and Life Sciences.*)

Mitochondria play an important role in ATP synthesis. For this function, three types of proton pumps in the electron transfer chain generate proton motive force (pmf) to facilitate ion transport across the membrane. Since the decrease in the activities of these proton pumps are involved in many disease, the method for sensitive detection of the activity of each proton pump in a single cell level is anticipated. To analyze these proton pump activities, we have measured the membrane potential changes upon addition of substrates and inhibitors in a single cell level. Here we report the membrane potential changes of mitochondria in the cells with the mutation of each proton pump and FoF1-ATPase. The decreases in the activity of each proton pump were successfully detected.

20286H 単細胞 FRET とべん毛モーター回転による CheYp 濃度の同時観察による適応系のメカニズム解明
Elucidation of mechanism for adaptation system through the simultaneous observation CheYp by single cell FRET and flagellar motor rotation

Takuma Nakagawa, Tatsuya Yamakoshi, Che Yong-Suk, Hajime Fukuoka, Akihiko Ishijima (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

E. coli reset the sensitivity of chemotaxis system to stimuli by adaptation. During adaptation, CheY-P concentration ([CheYp]) and flagellar motor-rotation are thought to be closely related, however it is not understood well. Therefore, we simultaneously measured the motor-rotation and [CheYp] via FRET between CheY-YFP and CheZ-CFP at single cell. After adding serine, [CheYp] rapidly decreased to zero and then gradually increased. The recovery time of [CheYp] and the steepness for recovery of [CheYp] were dependent on the serine concentration. The fitting for recovery time of [CheYp] by incomplete gamma function suggest that several hundreds of reaction-steps present in the process of adaptation. Using these quantitative parameters, we discuss a model of adaptation.

20287H Simultaneous observation of chemotactic response and intracellular behavior of chemotaxis proteins at single *E. coli* cell

Taro Yuri, Takuma Nakagawa, Keisuke Nishitani, Yong-Suk Che, Yumiko Uchida, Akihiko Ishijima,
Hajime Fukuoka (*Grad. Sch. Frontier Biosci., Osaka Univ.*)

E. coli swims toward favorable environment by chemotaxis signaling system. However, relation between the intracellular behavior of chemotaxis proteins (Che-proteins), such as activity and localization, and the magnitude of chemotactic response is not unclear at single cell level. To quantitatively understand this relation, we constructed functional fusions of fluorescence protein and Che-proteins, and we are trying to simultaneously measure the chemotactic response through the motor-rotation and behavior of Che-proteins, such as the binding of CheY to flagellar motor, the change in localization of Che-proteins, and the receptor's activity thorough FRET. We will discuss signaling process based on the experimental results quantitatively measured at single *E. coli* cell.

20288H CheB の細胞内動態とべん毛モーター回転の同時計測
Simultaneous measurement of flagellar motor rotation and Dynamics of CheB localization during chemotactic response

Keisuke Nishitani[1], Tatsuki Hamamoto[2], Yong-Suk Che[1], Akihiko Ishijima[1], Hajime Fukuoka[1] ([1]*Grad. Sch. Frontier Biosci. Osaka Univ.*, [2]*OIST. Grad. Univ.*)

Chemotaxis system adapt to stimuli by the activity of CheR and CheB. However, the relation between intracellular dynamics of CheB and CheR and cellular behavior is not understood well. Therefore, we simultaneously observed localization of CheB and flagellar rotation after adding repellent at single cell. Immediately after adding repellent, the motor switched to CW rotation and the polar localization of CheB-GFP increased (0.54 ± 0.32 s^{-1}). Several tens of seconds, the motor gradually resumed rotational switching and the localization of CheB was reduced (1.01 ± 0.75 s^{-1}). Therefore, we succeeded in measuring the response and adaptation to repellent as the localization and the cellular response; localization of CheB represents the active state of receptor cluster.

20289H 回転方向に依存したべん毛モーターの回転揺らぎの高時間分解能測定。
High temporal resolution measurement of rotational fluctuation of flagellar motor depending on rotational direction

Koki Murai, Akihiko Ishijima, Hajime Fukuoka (*Grad. Sch. Frontier Biosci. Osaka Univ.*)

Flagellar motor of E. coli rotates in clockwise (CW) and counterclockwise (CCW) directions. In this study, we investigated the rotational fluctuation depending on the rotational direction by measuring the rotation of bead attached flagellum with high temporal (1250 fps) resolution. The apparent rotational centers and the rotational radius of CCW rotation was widely distributed than those of CW rotation. The tracking of the bead position every sampling frame revealed the rotational center and the rotational radius transiently change during CCW rotation . To clarify the cause of fluctuation during CCW rotation, we are trying to measure and analyze a moment this transient changes using an ultra-high speed camera (20K fps) and we will discuss these results at the meeting.

20290H 心筋細胞における拍動間隔の温度依存性
Temperature dependence of beating rate in cardiomyocytes

Kohei Oyama, Masahito Hayashi, Tomoyuki Kaneko (*Laboratory for Reconstructive Cell Biology, Department of Frontier Bioscience, Hosei University, Grad School of Science and Engineering*)

Cardiomyocyte beats slower at low temperatures. Heart is temporarily cooled during the transplant and hypothermia therapy. However, the transition process of beating pattern during rapid temperature change (4 to 37℃ within 18 min) remains unclear; we investigated Inter-Spike Interval (ISI) and Field Potential Duration (FPD) of cardiomyocyte sheet from chick embryo by multi-electrode array. Stopped beating at lower temperatures resumed at 20℃, and ISI decreased to at 37℃. FPD increased from 20 to 31℃, and then decreased to at 37℃. Moreover, ISI fluctuation increased from 28 to 33℃, at which temperature FPD prolonged. This study suggests that FPD doesn't monotonously decrease as temperature raise and ISI and FPD interacted through different thermosensitive factors.

20291H 走化性タンパク質 CheRCheB の存在と大腸菌スイッチング同調
Requirement for Chemotaxis Protein CheR and CheB for the switching coordination between two flagellar motors on E. coli cell

Tatsuki Hamamoto[2], **Yumiko Uchida**[1], Yong-Suk Che[1], Akihiko Ishijima[1], Hajime Fukuoka[1] ([1]*Grad. Sch. Frontier Biosci. Osaka Univ*, [2]*OIST Grad. Univ*)

Chemotaxis system of E. coli controls cellular swimming by turning the rotational direction of flagellar motor. We have shown the switching of two flagellar motors is coordinated without stimuli. Here we investigated whether the change in methylation level of receptor by CheB/CheR is required for this switching coordination. E. coli cells expressing Tsr mutants with fixed methylation levels showed no switching coordination in the absence of CheB/CheR. Trg, which natively lacks the CheR tether-site (NWETF), conferred no switching coordination, but Trg-NWETF chimera conferred. Therefore, we suggest the activity of receptor cluster fluctuates by the change in methylation level to cause the change in CheYp concentration, and this change induces the switching coordination.

20292H* レプトスピラ経皮侵入に関わる運動の重要性
Significance of motility for percutaneous invasion of the spirochete *Leptospira*

Keigo Abe[1], Toshiki Kuribayashi[1], Kyosuke Takabe[2], Shuichi Nakamura[1] ([1]*Department of Applied Physics, Graduate School of Engineering, Tohoku University*, [2]*Faculty of Life and Environmental Sciences, University of Tsukuba*)

Leptospira is a zoonotic bacterium, infecting the mammals through wounded dermis. The pathogens' motility is known to be an essential virulence factor, but its practical role for percutaneous infection remains unknown. We hypothesized the relevance of the force produced by *Leptospira* to their pathogenicity. We measure the swimming force using optical tweeze and showed that they produce ca. 20 pN and the propulsive power is ca. 4×10^{-16} W. These results suggest that *Leptospira* can produce a large force while maintaining high efficiency when penetrating gel-like viscous materials. We will also report our recent results of the stiffness measurement of the *Leptospira* cell body, which could correlate with pathogenicity.

20293H* 蛍光および反射干渉顕微鏡による細胞ー基板界面でのがん細胞膜の分子パッキングの評価
Evaluation of molecular packing of cancer cell membrane at cell-substrate interface by fluorescence and interference reflection microscopy

Hayata Noro[1], Mai Fujii[1], Shodai Togo[1], Mami Watanabe[1], Masami Suganuma[2], Naritaka Kobayashi[2], Ryozo Kawamura[1,2], Seiichiro Nakabayashi[1,2], Takahisa Matsuzaki[2], Hiroshi Yoshikawa[1,2] ([1]*Dept. of Chem., Saitama Univ.*, [2]*Div. of Strateg. Res. and Dev., Grad. Sch. of Sci. and Eng., Saitama Univ.*)

A number of studies suggested that membrane of various cancer cells seems to be more dynamic compared to that of normal cells. However, how such dynamic membrane affects cancer biology related to metastasis (e.g., adhesion and migration) still remains unclear. In this study, we evaluated molecular packing of cancer cell membrane at the cell-substrate interface by using a new optical microscopic system that combined fluorescence microscopy and interference reflection microscopy. We found that molecular packing of membrane of mouse melanoma cells at adhesion area tend to be looser compared to that at non-adhesion area. In the presentation, we will explain the detail results of mouse melanoma cells with different malignancy.

20294H* 細胞接着界面の膜分子配列性の評価：がん細胞と正常細胞の比較
Characterization of molecular packing of cell membranes at cell-substrate interface:Comparison between cancer cells and normal cells

Mai Fujii[1], Hayata Noro[1], Syodai Togo[1], Mami Watanabe[1], Masami Suganuma[2], Naritaka Kobayashi[2], Ryuzo Kobayashi[1,2], Seiichiro Nakabayashi[1,2], Takahisa Matsuzaki[2], Hiroshi Y. Yoshikawa[1,2] ([1]*Grad. Chem., Univ. Saitama*, [2]*Division of Strategic Research and Development, Grad. Sci. Eng., Univ. Saitama*)

In this study, we have investigated molecular packing of membrane of cancer cells (MCF-7) and normal cells (MCF-10A) at cell-substrate interface. Here, we obtained two dimensional maps of molecular packing and morphology of cell membrane by using fluorescence microscopy with polarity-sensitive dye (Laurdan) and reflection interference microscopy, which can determine cell-substrate distance with the resolution of a few nanometers. As the results, we found that both types of cells showed looser molecular packing at adhesion area compared to non-adhesion area. In addition, we also found that molecular packing of cancer cell membrane at adhesion area were more inhomogeneous, indicating characteristic physical features of cancer cell membrane.

20295H 人工多細胞型分子ロボットの自動生産に関する研究
Toward Automated Production of Multicellular Molecular Robots

Ryo Shimizu[1], Satoshi Murata[1], Shin-ichiro Nomura[1], Yuki Suzuki[4], Ibuki Kawamata[1], Gen Hayase[3], Taro Toyota[2] ([1]*Murata/Nomura Lab, Univ. Tohoku*, [2]*Toyota Lab, Univ. Tokyo*, [3]*MANA*, [4]*FRIS, Univ. Tohoku*)

Artificial cells that mimic real cell functions where the basic unit of living organisms, are being actively studied. In particular, artificial multicellular structures that are composed of multiple compartments can be expected to have a variety of functions in the same complex such as the sensing, production of materials, and the motion, etc. We have recently developed a new method for preparing the multi-compartments by hydrating porous polymers using osmotic pressure difference. In this research, we tackle to develop a method of mechanically mass-producing artificial multicellular molecular robots by automating this process. Here we will introduce the machine connecting between the wetware and the hardware.

20296H 繊毛の初期屈曲形成に重要な根元局在型マイナーダイニン
Requirement of minor-type axonemal dyneins localized to the proximal region for the initial bend formation of cilia

Tomohiro Komatsu, Ayuna Sahara, Yusuke Kondo, **Toshiki Yagi** (*Dept. Life Sci. Prefectural Univ. Hiroshima*)

Cilia have more than ten types of dyneins. *Chlamydomonas* has thirteen different type of ciliary dyneins, three of which are minor-type dyneins localized to the proximal region. We had isolated the mutants missing the respective minor-type dyneins, and found that the mutants displayed WT-like motility. To explore the functional properties of these dyneins, here we compared cilia movements in wild type and mutant cells with very short flagella (~3 um, 1/4 of full length) regenerating after cilia amputation. Wild-type cilia displayed vigorous bending movements, but in contrast, most of mutant cilia displayed no movement. This suggests that minor-type dyneins generate a significant force to produce the bend formation at the proximal region.

20297H Formation of actin cortex structure by myosin motor activity

Mitsusuke Tarama, Tatsuo Shibata (*RIKEN BDR*)

Actin filaments, together with myosin motors, construct various cellular-scale structures. Among them, the actin cortex is a ubiquitous structure among eukaryotic cells. It is a network structure on the inner face of the cell membrane that maintains the cell morphology. The actin filaments that form this cortex are long rigid filaments with a persistence length around 20 micrometers, which is comparable to the typical size of a cell. Due to their length, it should be entropically unfavourable for these filaments to accumulate around the membrane as this restricts their rotational degrees of freedom. Our in silico study shows that the cortical structure is formed nevertheless, as a result of the myosin motor activity which compensates the depletion force.

20298I* 抗菌ペプチド・マガイニン 2 と脂質膜の相互作用に対する膜電位の効果
Effect of Membrane Potential on Interaction of Antimicrobial Peptide (AMP) Magainin 2 (Mag) with Single GUVs

Or Rashid Md. Mamun[1], Moghal Md. Mizanur[1], Billah Md. Masum[1], Hasan Moynul[1], Yamazaki Masahito[1,2,3] ([1]*Grad. Sch. Sci. Tech., Shizuoka Univ.*, [2]*Res. Inst. Ele., Shizuoka Univ.*, [3]*Grad. Sch. Sci., Shizuoka Univ.*)

Membrane potential, Δφ, plays a vital role in the damage of plasma membrane and lipid bilayers by AMPs (1) and entry of cell-penetrating peptides (2). In the BP conference last year, we demonstrated that the rate constant of Mag-induced pore formation increases with increasing negative Δφ. Here we examined the effect of Δφ on the interaction of Mag with single GUVs. We found that the binding constant of carboxyfluorescein-labeled Mag (CF-Mag) to the GUV membrane increased with negative Δφ. In the interaction of Mag and CF-Mag mixture, CF-Mag locates in the outer leaflet of single GUVs until just before pore formation. Based on these results, we discuss the effect of Δφ on Mag-induced pore formation. (1) J. Biol. Chem. 294, 10449, 2019, (2) Biophys. J. 118, 57, 2020.

20299I* 蛍光プローブでラベルされていない細胞透過ペプチド・トランスポータン 10 の巨大リポソーム内腔への侵入の検出
Detection of the Entry of Nonlabeled Cell-Penetrating Peptide (CPP) Transportan 10 (TP10) into Single Giant Unilamellar Vesicles (GUVs)

Madhabl Lata Shuma[1], Md. Mizanur Moghal[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.*)

We have developed a new method to detect the entry of nonlabeled CPPs into single GUV lumens without pore formation in the GUV membrane (1). In this method, we investigate the interaction of CPPs with single GUVs containing large unilamellar vesicles (LUVs) whose lumens contain a high concentration of calcein. If the CPPs enter the GUV lumen and interact with these LUVs to induce calcein leakage, the fluorescence intensity due to calcein in the lumen increases. Using this method, we found that nonlabeled TP10 entered single DOPG/DOPC-GUVs and DOPC-GUVs without pore formation in the GUV membranes. The rate of entry of TP10 into the GUV lumen increased with TP10 concentration. We discuss the entry of nonlabeled TP10 into single GUVs. (1) Biochemistry, 59, 1780, 2020.

20300I* 脂質分子の二分子層膜横断（フリップ・フロップ）に対する浸透圧の効果
The effect of osmotic pressure on the transbilayer movement (flip-flop) of lipid molecules

Samiron Kumar Saha[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.*)

In the last year BP conference, we demonstrated the estimation of osmotic pressure (Π)-induced membrane tension (σ_{osm}) in DOPG/DOPC-GUVs in a buffer containing a physiological concentration of salts. The experimental values of σ_{osm} agreed with their theoretical values. Here we examined the effect of Π on the rate constant (k_{FF}) for the transbilayer movement (flip-flop) of lipid molecules in single DOPG/DOPC-GUVs using our method (1). We found that the values of k_{FF} increased with increasing Π, indicating that k_{FF} increased with σ_{osm}. The relation between k_{FF} and membrane tension is almost the same as that obtained by the micropipette method (1). These results support the existence of pre-pores in stretched lipid bilayers. (1) J. Chem. Phys., 148, 245101, 2018

20301I 脂質・コレステロールによって制御される上皮成長因子受容体の膜貫通・膜近傍ドメインの多量体形成機構
Lipid-cholesterol regulation of the oligomerization in transmembrane and juxtamembrane domains of epidermal growth factor receptor

Ryo Maeda[1], Takeshi Sato[2], Yasushi Sako[1] ([1]*Cellular Informatics Lab., RIKEN*, [2]*Kyoto Pharmaceutical Univ.*)

Transmembrane (TM) helix and juxtamembrane (JM) domains bridge the extracellular and intracellular domains of epidermal growth factor receptor, EGFR. Although dimerization of TM and JM domains is thought to play a crucial role in regulation of EGFR kinase activity, the underlying kinetic mechanisms remain unclear. Here, combining single-pair FRET imaging and nanodisc techniques, we showed that cholesterols in the membrane stabilized close dimer conformations among TM-TM and JM-JM domains in the TM-JM peptides. Furthermore, we found that cholesterols induced assembly of TM-JM peptides in cooperation with lipid PS and Thr654 phosphorylation. The current results indicated that cholesterols can help the EGFR clustering, resulting in the intracellular signal regulation.

20302I* 抗菌ペプチド・ラクトフェリシン B(4-9)の大腸菌、スフェロプラスト、および巨大リポソームの内腔への侵入に対する膜電位の効果
Effect of Membrane potential on Entry of Antimicrobial Peptide (AMP) LfcinB (4-9) into Single *E. coli* Cells, Spheroplasts, and GUVs

Farzana Hossain[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.*)

Recently we demonstrated that membrane potential (Δφ) plays a vital role in AMP lactoferricin B (LfcinB)-induced membrane damage in plasma membrane and lipid bilayers (1). Here we examined the effect of Δφ on the activity of AMP LfcinB (4-9), a shorter version of LfcinB, which can enter *E. coli* cells and GUVs without membrane damage (2). A protonophore CCCP suppressed the entry of fluorescent probe-labeled LfcinB (4-9) (Rh-LfcinB (4-9)) into *E. coli* cells and spheroplasts. Rh-LfcinB (4-9) entered single GUVs of *E. coli* lipid without pore formation, and the rate of its entry increased with negative membrane potential. Based on these results, we discuss the effect of Δφ on the activity of LfcinB (4-9). (1) *J. Biol. Chem.* 294, 10449, 2019, (2) Biochemistry, 56, 4419, 2017.

20303I* アミロイド線維形成とリン脂質二分子膜破壊との関係性の解明
Investigation of relationships between amyloid fibril formation and phospholipid bilayer destruction

Hiroki Takayama[1], Kaori Mageshi[1], Kenichi Morigaki[2], Eri Chatani[1] ([1]*Graduate School of Science, Kobe University*, [2]*Biosignal research center, Kobe University*, [3]*Graduate School of Agricultural Science, Kobe University*)

Neurodegenerative diseases and amyloidosis occur by accumulating aggregated proteins in living tissues. One of the important issues to be investigated for understanding the mechanisms of disease development is cell death that accompanies amyloid deposition, although details of which are unclarified. Here, with amyloid β and insulin, we observed the process of the formation of amyloid fibrils and destruction of phospholipid liposomes simultaneously by using thioflavin T and sulforhodamine B, respectively, as fluorescent probes. As a result, the destruction of liposomes with a negatively charged head group was observed in both proteins, while uncharged liposomes were hardly destructed. Furthermore, in insulin, the involvement of liposomal fluidity was also suggested.

20304I Regulation of actin dynamics by phosphoinositides

Yosuke Senju (*RIIS, Univ. Okayama*)

Actin cytoskeleton provides forces for vital cellular processes involving membrane dynamics. Membrane phosphoinositides regulate many actin-binding proteins including cofilin, profilin, mDia2, N-WASP, ezrin, and moesin. However, the underlying mechanisms have remained elusive. By applying a combination of biochemical assays, photobleaching/activation approaches, and atomistic molecular dynamics simulations, we revealed that these proteins interact with membranes through multivalent electrostatic interactions, without specific binding pockets or penetrations into the lipid bilayers. Thus, membrane-interaction mechanisms of actin-binding proteins evolved to precisely fulfill their specific functions in cytoskeletal dynamics.

20305I 高速 AFM によるハブ毒液由来脂質分解酵素 PLA2 の膜認識機構の解明
Membrane recognition mechanism of phospholipase A_2 from habu snake venom revealed by high-speed AFM (HS-AFM)

Magoto Kamiya[1], Mikihiro Shibata[2,3], Naoko Oda-Ueda[4], Ayumi Sumino[2,3] ([1]*Grad. Sch. Math. & Phys., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*, [3]*InFiniti, Kanazawa Univ.*, [4]*Dept. Pharm. Sci., Sojo Univ.*)

PLA2 is one of phospholipase A_2 contained in habu snake venom. Previously, we have found that the PLA2 hydrolyze phospholipid bilayer selectively at membrane edge. Here, we analyzed adsorption behavior of the PLA2 on planar area and edge of the membrane by HS-AFM. PLA2 showed remarkably higher affinity at the membrane edge than planar surface of the membrane, indicating that selective degradation at the membrane edge is due to the selective adsorption of the PLA2 at the membrane edge. When melittin, an amphipathic peptide that forms pores in flat area of the membrane, was added prior to subsequent PLA2 addition, PLA2 rapidly expanded pore size. We propose that PLA2 functions as pore-expander of the cell membrane by cooperative interaction with some pore-forming events.

20306I 2 種類のリン脂質種からなるモデル生体膜の構造に対するコレステロールとラノステロールの影響の比較
Comparative study of the effects of cholesterol and lanosterol on the structure of model biomombrane formed by two phospholipid species

Akira Matsumoto, Hiroshi Takahashi (*Grad. Sch. Sci and Tech., Gunma University*)

Cholesterol is a molecule that controls the physical properties of biological membranes. Lanosterol is a cholesterol precursor in the cholesterol biosynthetic pathway, and has been proposed to be an ancestor molecule of cholesterol from the viewpoint of molecular evolution [1]. In this study, small-angle X-ray scattering was used to investigate the effect of these two sterols on the membrane structure of a phospholipid binary mixture system. As a result, it was found that the two sterols have different effects on the membrane thickness in the gel phase and the liquid crystal phase. We will discuss the obtained result from the viewpoints of sterol induced condensing effect on lipid packing. [1] Mouritsen & Bagatolli, "Life-As Matter of Fat" Ch.14,(2016)

20307I* 細胞サイズ閉じ込め中の拡散に対する界面の効果
Effects of membrane interface properties on diffusion in cell-sized confinement

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To investigate the effects of intracellular environment such as macromolecular crowding and membrane confinement on molecular diffusion in cells, we analyzed molecular diffusion inside cell-sized droplets of highly concentrated solution of polysaccharide dextran and its monomer unit glucose. We found that the diffusion slowed down in small highly concentrated dextran droplets covered with a lipid layer than in bulk unlike glucose, which is consistent with our previous study using Bovine Serum Albumin (BSA) and Polyethylene glycol (PEG). When we incorporated PEGylated lipid for the membrane, the slowing effect weakened. We will discuss the membrane effect from the hydrophilic-hydrophobic interaction between crowder polymers and membrane lipids.

20308I 相分離リポソームを用いた膜タンパク質の高濃度再構成
High-density reconstitution of membrane protein into phase-separated liposome

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Towards functional analysis of membrane proteins in conditions like cells, membrane proteins have been reconstituted within liposomal membranes. However, the density of reconstituted membrane proteins is much lower than that in biomembranes. In this work, we use phase-separated liposomes like heterogeneous biomembranes to increase the density of reconstituted membrane protein alpha-hemolysin (α-HL). We found that the reconstituted α-HL density within membranes increases with an increase in cholesterol ratio. In addition, under the same density of α-HL, membrane stability of the phase separated liposomes is higher than that of homogeneous liposomes. We will explain the mechanism how the highly condensed membrane proteins are stabilized within phase-separated liposomes.

20309I 鞭毛で泳ぐ単細胞緑藻クラミドモナスを用いて巨大リポソームを内側から動かす
Driving a giant liposome from inside by a flagellating unicellular green algae *Chlamydomonas*

Shunsuke Shiomi[1], Masahito Hayashi[1], Tomohiro Uemura[2], Tomoyuki Kaneko[1] ([1]*LaRC, FB, Hosei Univ.*, [2]*FB, Hosei Univ.*)

Liposomes are used in drug delivery systems. However, it has no driving force and cannot be actively transmitted to the target site in the living body. To control the driving direction of liposomes, the phototaxis in *Chlamydomonas* were utilized with its driving force. As the first step, *Chlamydomonas* was encapsulated into the liposome using by emulsion transfer method. The encapsulated *Chlamydomonas* swam as if it hit the membrane from the inside of the liposome with flagella. The driving force of *Chlamydomonas* caused the liposomes to move together. We were able to drive the liposomes using a simple method of encapsulating *Chlamydomonas* inside the liposomes. In the future, I would like to research the detailed mechanism of the driving of liposomes by *Chlamydomonas*.

20310I ラベルされていない抗菌ペプチド・PGLa と単一 GUV との相互作用
Interaction of Nonlabeled Antimicrobial Peptide PGLa with Single Giant Unilamellar Vesicles (GUVs)

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In the interaction of a mixture of PGLa and fluorescence dye-labeled PGLa (CF-PGLa) with single GUVs, the time course of the fluorescence intensity (FI) of the GUV membrane due to CF-PGLa showed a two-step increase from a steady value to another before pore formation, and concomitantly the FI of the GUV lumen increases (1). This result indicates that CF-PGLa enters the lumen before pore formation. Labeling of fluorescent dye to peptides may affect its behavior. Here, we investigated the interaction of nonlabeled PGLa with single GUVs held at the tip of a micropipette by applying the new method to detect the entry of nonlabeled peptides into a GUV (2). We show the results and discuss them in the conference. (1) BBA, 1860, 2262, 2018, (2) Biochemistry, 59, 1780, 2020.

20311I Epigallocatechin gallate induces the burst of giant unilamellar vesicles in the tension-dependent manner

Naoya Sugita[1], Mika Terada[1], Yukihiro Tamba[1], Masahito Yamazaki[2] ([1]*Natl. Inst. Tech., Suzuka Coll.*, [2]*Shizuoka Univ.*)

We investigated the process of burst of a giant unilamellar vesicles (GUVs) induced by epigallocatechin gallate (EGCg) and succeeded in observing the evolution of a pore in the GUV membrane. In this report, we examined the effect of membrane tension on the EGCg-induced bursting of DOPC-GUVs using micropipete aspiration method. 100μM EGCg induced burst of aspirated GUVs as a result of pore formation. The fraction of burst of GUVs decreased with increasing the applied tension in the range of low tension which did not induced rupture of aspirated GUVs. We also analyzed the EGCg-induced fractional change in area of the GUV membranes under above low applied tension. Based on these results, we discuss the mechanism of the EGCg-induced pore formation in the membrane.

20312I 筋小胞体 Ca ポンプの M2 ヘリックス:膜貫通部分のエネルギー共役における役割
Role of transmembrane portion of M2 helix in energy coupling of sarcoplasmic reticulum Ca pump

Takashi Daiho, Kazuo Yamasaki, Satoshi Yasuda, Jun-ichi Kawabe (*Asahikawa Med. Univ. Biochem.*)

The Ca pump catalyzes Ca-transport coupled with ATP-hydrolysis. In the transport cycle, the three cytoplasmic domains N, P, and A change their organization state, and the motion of A domain functions in regulating Ca gating. The long M2 helix connects with A domain by a linker loop, and changes its structure together with A domain movement. We have previously shown that the transmembrane part (M2m) and cytoplasmic part (M2c) of M2 play distinct roles in the energy coupling. Moreover, Ala substitution of Gly105 at the border of M2m/M2c results in slow EP isomerization and uncoupling. So, Gly105 functions as a flexible hinge for a critical knee-like joint of M2. In this study, we have found that the defects of G105A could be restored by an additional mutation at M2m.

20313I* 脂質分子混み合い効果によるバクテリオロドプシン間実行相互作用の解析
Crowding effects induced by lipid molecules on effective interactions between bacteriorhodopsins

Keiju Suda[1], Ayumi Suematsu[2], Rho Akiyama[1] ([1]*Kyushu University, science faculty, department of chemistry*, [2]*Kyushu sangyo University*)

We studied the depletion effects induced by lipid molecules on the effective interactions between transmembrabe proteins in a lipid bilayer. We focused on crystallization of bacteriorhodopsin (bR), a kind of transmembrane protein. Critical concentration ratio for crystallization (CCR) between bR trimer and monomer was calculated to compare the experimental results reported by M.P.Krebs(1999). Asakura-Oosawa theory and Modified Asakura-Oosawa theory were adopted to analyze the CCR. Our results showed lipid molecule's crowding effect should be dominant to effective interactions between membrane proteins.

20314I* ナノサイズリポソームの脂質膜への融合条件の調査
Examination of fusion condition of nano-sized liposome to lipid membrane

Chika Arisaka, Kouki Kamiya (*Grad. Sch. Sci and Tec., Univ. Gunma*)

Various membrane proteins existing in cells perform signal transduction, ion transport, and energy production. It is technically difficult to prepare liposomes in which a plurality of types of membrane proteins are reconstituted, because the types of surfactants required to solubilize membrane proteins from cells are different for each membrane protein. In this study, we prepared liposomes with reconstituted membrane proteins using the pulse jet method, and examined the fusion conditions for planar membranes of nano-sized liposomes. This experimental method succeeded in reconstitution of membrane proteins in cell liposomes.

20315I ハイドロゲル固体試料中で見られた紫膜の特異な積層構造の形成機構
Formation Mechanisms of Anomalous Purple Membrane Stacking in Hydrogels

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Bacteriorhodopsin (bR), a photo-receptor membrane protein, is a possible candidate for industrial application. We have reported that purple membranes (PM) became stacked in poly(vinyl alcohol) (PVA) hydrogel, whereas an isotropic periodic structure of PMs was formed in PVA solution before gelation. In this work, we studied the PM stacking mechanisms focusing on the PM periodic structure in PVA solution, since the PM stacking is likely advantageous for the application. It was shown that the PM periodic structure in PVA solution was formed on the balance of an electrostatic repulsive force and an attractive depletion force between PMs. The PM stacking required both a porous network of the hydrogels and the PM periodic structure in polymer solutions.

20316I ベシクル凝集構造の力学モデル
Mechanical Model of Vesicle Aggregates

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In the morphogenesis of multi-cellular organisms, proteins govern cell arrangements and cell shapes by regulating the mechanical balance. In this study we have investigated the relationship between mechanical parameters and the morphology of model multi-cellular organisms composed of phospholipid GUVs. The adhesion strength and volume-to-area ratio of vesicle aggregates (doublets, triplets and quartets) were controlled by tuning the inter-membrane interactions and thermal expansion, respectively. We reproduced observed morphologies by minimizing the total energy consisting of adhesion, bending, and surface energy terms, which reveals the mechanism governing the morphogenesis.

20317I In vitro selection using cDNA display for liposome binding peptides to generate antibacterial peptides

Takeru Yoshinobu, Naoto Nemoto (*Graduate School of Science & Engineering, Saitama University*)

In the past years, bacterial infections have been generally treated with antibiotics. However, drug resistant bacteria have emerged. Recently, antibacterial peptides (ABPs) that selectively kill bacteria attract attention. ABPs kill bacteria by forming pores in the cell membrane that causes cytoplasm to flow out. Therefore, resistant bacteria have less incidence of emergence. In this study, we tried to obtain peptides that bind to bacterial membrane as the first step for obtaining ABPs. As a cell model, a liposome with the same composition of bacterial membrane was the target for in vitro selection using cDNA display with a completely random peptide library in 36-residue amino acids. After 6 rounds of selection, the results by NGS analysis will be reported.

20318I* Pattern Formation by Mechanochemical Feedback between Membrane Deformation and the Brusselator Model

Naoki Tamemoto, Hiroshi Noguchi (*ISSP, Univ. Tokyo*)

The shape of biological membrane plays an important role in living cells. The mechanism of membrane deformation by proteins in thermal equilibrium has been studied so far, but in nonequilibrium has not been well studied. Here, we investigated non-equilibrium pattern formation by mechanochemical feedback between membrane deformation and chemical reactions by coupling dynamically triangulated membrane simulations and the Brusselator model. The formation of a stable pattern with membrane deformation was observed, and the transition from the oscillation pattern to the stable pattern was also confirmed. Our results demonstrate the importance of the mechanochemical feedback on the pattern formation on the deforming membranes.

20319I ナノサイズリポソーム融合による細胞サイズ GM1 非対称膜リポソームの構築
Construction of cell-sized GM1 asymmetric vesicles using nano-sized vesicle fusion method

Masato Suzuki[1], Kouki Kamiya[1,2] ([1]*Sci. & Tech., Univ. Gunma*, [2]*Grad. Sci. & Tech., Univ. Gunma*)

Ganglioside (GM1) exists in an outer leaflet of living cells. Large amount of GM1 is localized on the nervous system, and GM1 is important for the regulation and control of cell differentiation and reproduction. In this study, cell-sized asymmetric GM1 vesicles were prepared by applying jet flow to a planar lipid bilayer which was fused with nano-sized lipid vesicles containing the GM1. The formation of asymmetric GM1 vesicles was confirmed by observing fluorescent-labeled choler toxin on the asymmetric GM1 vesicles because the choler toxin specifically binds to GM1. When the choler toxin was added to the outer solution of the vesicles, the fluorescence of choler toxin was only observed on the vesicles containing GM1 on the outer leaflet.

20320I 電位依存性プロトンチャネルの細胞内側からの制御
Intracellular regulation of the voltage-gated proton channel

Akira Kawanabe, Yuichiro Fujiwara (*Kagawa Univ.*)

The voltage-gated proton channel (Hv1) consists of four transmembrane helices (S1-S4) which act as a voltage sensor and a proton permeation pathway (Sasaki et al. 2006). Its activity is known to be regulated by various extracellular molecules, ions, inhibitors, and unsaturated fatty acids (Kawanabe&Okamura 2016). However, the effects of intracellular molecules on Hv1 remains unclear. In this study, we analyzed the proton currents of mouse Hv1 using patch-clamp technique. Application of nucleotides, lipids or ions to the inside-out patch membranes influenced the amplitude of the proton currents. We will discuss the molecular mechanisms and physiological significance of these regulations. COI:No

20321I Artificial bilayers on hydrogel for channel current recordings

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The purpose of our study is to develop high-throughput measuring technologies for ion channel current. We previously reported channel proteins immobilized on a hydrogel bead are directly incorporated into planar artificial lipid bilayers. Improving this technology, we reconstituted channel proteins on solid substrates such as silicon and gold needles into artificial bilayers and measured single channel currents. Here, we show a technology to form much more stable bilayers on hydrogel or solid substrates for channel current recordings, which enables us to measure channel currents efficiently. We measured single channel currents of several types of channel such as gramicidin, alpha-hemolysin, Kcsa, and BK.

20322I イノシトールリン脂質による KcsA の制御
Functional coupling between phosphoinositides and KcsA studied by lipid-bilayer recording

Takunari Kiya, Akira Kawanabe, Yuichiro Fujiwara (*Kagawa Univ.*)

The biological membrane is composed of various lipids and plays important roles in cell signaling. Phosphoinositides (PIPs) are known to modulate the functional properties of various ion channels (Kv,Kir,Cav etc). It is reported that the activity of KcsA, which is considered as a model of potassium channel, is regulated by membrane phospholipids. However, no study has reported whether PIPs modulate the function of the KcsA channel. In this study, we analyzed the activity of KcsA in the presence of PIPs using a contact bubble bilayer method. We observed that the open probability of KcsA became higher, when some PIPs were mixed in the phosphatidylcholine membrane in the side of inner leaflet. We will discuss the molecular mechanisms of the functional coupling. COI:No

20323I* 自動顕微鏡計測により見出された，定常流れ場における細胞サイズのリポソームへの分子濃縮
Automated direct observation unveiled hydrodynamic accumulation of molecules into cell-sized liposomes against a concentration gradient

Hironori Sugiyama[1], Toshihisa Osaki[2,3], Shoji Takeuchi[2,4], Taro Toyota[1,5] ([1]*Grad. Sch. Arts and Sci., The University of Tokyo*, [2]*IIS, The University of Tokyo*, [3]*KISTEC*, [4]*Grad. Sch. Info. Sci. Tech., The University of Tokyo*, [5]*UBI, The University of Tokyo*)

Constructing chemical cell models based on cell-sized liposomes can clarify an unexplored chemical logic behind the complexity of living cells. To efficiently develop liposome-based artificial cells, an automated experimental platform to directly observe cell-sized liposomes was recently constructed based on the microfluidics (termed as MANSIONs). By MANSIONs, we found that without proteins, cell-sized liposomes under hydrodynamic environment repeatedly accumulate small molecules against a concentration gradient. Notably, an analogue of adenosine triphosphate was also accumulated. The current findings can solve the low permeability of phospholipid membrane, one of fundamental bottleneck in liposome-based artificial cells.

20324I 平面脂質膜の組成の違いによる OmpG の膜への挿入の違いについて
Differences of OmpG into the planar lipid membranes with various compositions

Toshiyuki Tosaka[1], Koki Kamiya[2] ([1]*Sci. & Tech., Univ. Gunma*, [2]*Grad. Sci. & Tech., Univ. Gunma*)

An outer membrane protein G (OmpG) from gram-negative bacteria is pore forming protein. The monomeric OmpG pore is formed from 14 anti-parallel β-strand. The role of OmpG pore integrated into a cell membrane uptakes ions and small molecules. Recently, nanopore proteins such as OmpG integrated into an artificial cell membrane have been used as nanopore sensors. In this study, we investigate differences of reconstitution of OmpG into the planar lipid membrane with different composition. Electric currents of OmpG reconstituted into the planar lipid bilayer were observed by a path clamp method of the artificial cell membrane. We obtained the specific current amplitude of OmpG. The signals of OmpG into the planar lipid membranes with various compositions were measured.

20325I 油中水滴エマルションにおけるヒドロキシプロピルセルロースのパターン形成とダイナミクス
Pattern formation and dynamics of hydroxypropyl cellulose in water-in-oil emulsion

Kazunari Yoshida[1], Keitaro Horii[2], Azusa Saito[2], Akito Takashima[2], Izumi Nishio[2] ([1]*Grad. Sch. Sci. Eng., Yamagata Univ.*, [2]*Col. Sci. Eng., Aoyama Gakuin Univ.*)

The living cells enclose highly condensed molecules; hence, the living cells are too complicated. The simple model systems of living cells, such as liposomes, water-in-oil (W/O) emulsion, and oil-in-water (O/W) emulsion, are quite beneficial for clarifying the Physico-chemical behaviors of phase-separation in living cells. We revealed that the dynamic behaviors of aqueous HPC droplets coated by different phospholipid single layers and mineral oil (W/O emulsions) with an increase in the temperature. We revealed that the pattern formation depends on the head group of phospholipids (without lipid, choline, and ethanolamine).

20326I Effect of lipid quality on the association of membrane bound proteins with phosphoinositide-containing membranes

Eiji Yamamoto[1], Junko Sasaki[2], Takehiko Sasaki[2], Mark S. P. Sansom[3] ([1]*Department of System Design Engineering, Keio University*, [2]*Medical Research Institute and Graduate School of Medical and Dental Sciences, Tokyo Medical and Dental University*, [3]*Department of Biochemistry, University of Oxford*)

Association of peripheral membrane proteins with cell membranes is important for cell signaling and trafficking. Pleckstrin homology (PH) domains are lipid recognition module of peripheral membrane proteins. Here, using molecular dynamics simulations, we investigate the PIP concentration dependency of the interaction of a PH domain with biological membranes. The binding energy of the PH domain with more than two PIPs is comparable to experimental values [Science Adv. 6, eaay5736 (2020)]. Local nanoscale clustering of PIPs bound to the PH domain changes the strength and orientation of the PH domain on the membrane in a concentration dependent manner. Moreover, we will present the effect of acyl chain difference in PIPs on the association of a PH domain with membranes.

20327I 気液界面における人工肺サーファクタント膜へのコレステロールの影響
Effect of cholesterol on a model lung surfactant monolayer at the air-water interface

Masahiro Hibino[1], Saki Izumi[2] ([1]*Div. Sustain. Environ. Eng., Muroran Inst. Tech.*, [2]*Dept. Appl. Sci., Muroran Inst. Tech.*)

Lung surfactant is a complex mixture of lipids and proteins at the air-water interface of the alveolus. Early studies using isotherms suggested any amount of cholesterol is detrimental to the proper functioning of the lung, since the ability of the lung surfactant to reach a low surface tension was inhibited in most of the studies. Meanwhile, it is important to note that cholesterol forms the major neutral lipid component of lung surfactants. The function of cholesterol in the lung surfactant remains mostly unknown. Here we investigate effects of cholesterol on the ternary monolayer using isotherms, surface elastic modulus and fluorescence microscopy. The results indicate any negative effects of low cholesterol concentration can be countered with the ternary system.

20328I 自動生成される人工多細胞体とその電気的活性について
On multicellular lipid compartments and their electrical activity

Shin-ichiro Nomura (*Dep. Robotics, TOHOKU Univ.*)

We study artificial multicellular structures, self-growing ensembles of vesicles whose membranes are combinations of phospholipid and viscous amphipathic molecules. The vesicles grow from a porous gel, and an osmotic pressure difference between the interior of the gelt and its surrounding drives the growth. The growing ensembles exhibit spike-like dynamics in electrical potential recorded on the electrodes inserted in the ensembles. The evidence of neuromorphic electrical activity in multicellular systems of lipid vesicles is a promising indication of feasibility of future designs of self-growing artificial proto-brains.

20329I 分子シミュレーションによるリポソームにおける膜タンパク質拡散解析
Molecular dynamics simulation of the diffusion of membrane proteins on vesicles

Diego Ugarte, Shoji Takada (*Dept. Biol., Sch. Sci., Kyoto Univ., Japan*)

Membrane proteins play an essential role in lipid membranes, participating in different biological processes such as signaling and transport. Furthermore, many of these proteins are not freely diffusing on the membrane but rather forming macromolecular clusters. Thus, protein mobility is still actively studied. In this work, we use our newly developed lipid force-field iSoLF, together with a well-tuned protein model, to perform coarse-grained molecular dynamics simulations of membrane proteins on small unilamellar vesicles (SUV) of POPC. We study the effect of vesicle size, i.e., curvature, and protein-multimerization on the lateral and rotational diffusion coefficient.

20330I* Observation Protein-Protein Interactions in α-hemolysin

Misa Yamaji, Ryuji Kawano (*Tokyo University of Agriculture and Technology*)

We describe single-molecule behavior of a small protein at confined nanospace of α-hemolysin (αHL) and their protein-protein interactions (PPIs) between the nanopore and the small protein. Ion current recording of αHL nanopore with a hairpin DNA (hpDNA) reflects the change as the position of the hpDNA interacted with the αHL inner wall. We have previously reported that analyzing the blocking current changes enables us to show the behavior of hpDNA. In this study, we tried to probe PPIs in nanospace using a small protein having a β-hairpin structure (SV28) instead of hpDNA. As a result, the blocking levels varied depending on salt concentration and pH. It suggests that we can observe the PPIs between αHL and SV20 depending on the outer environment of the nanospace.

20331I* Outer membrane phospholipaseA (OmpLA)を用いた細胞モデルの構築
Creation of complex-functional cell model using outer membrane phospholipase A

Seren Ohnishi, Koki Kamiya (*Grad. Sci., Univ.Gunma*)

Outer membrane protein (Omp) family that is expressed in E.coli outer membranes is responsible for transporting ions or small molecules. Outer membrane phospholipase A (OmpLA) catalyzes phospholipids to lyso-phospholipids and concomitant fatty acid, in the presence of calcium ion. We show that OmpLA into the lipid bilayer also have transportation function of ions or small molecules. In this study, by a reconstitution of OmpLA into giant lipid vesicles, we develop a complex-functional cell model for transporting molecules through the OmpLA nanopore and for budding small vesicles by changing the membrane curvature by the OmpLA enzyme activity. The giant lipid vesicles containing OmpLA will be contributed to regulate cell functions, and recognize and kill cancer cells.

20332I* α-ヘモリシンナノ空間における β ヘアピンペプチドのイオン電流記録
Ion current recording of a β-hairpin peptide in confined α-hemolysin nanospace

Miyu Fukuda, Misa Yamaji, Ryuji Kawano (*Department of biotechnology and life science, Tokyo University of Agriculture and Technology*)

We report the channel current recordings of the β-hairpin peptide (1U0P) which is stayed inside in α-hemolysin (αHL) nanopore. Unzipping behavior of hairpin DNA has been studied using the current recordings with αHL nanopore. We next try to record the unzipping behavior of hairpin peptide instead of the DNA. In the nanopore measurements, intramolecular interactions can be investigated by changing the blocking current signals and these signals will provide insight into the folding pathway and kinetics of the protein. In this study, we synthesize 1U0P by the PURE system, and also we measure the ion currents of 1U0P stayed inside in the nanopore.

20333I 大腸菌が引き起こすリポソームの形態変化パターン解析
Analysis of morphological change patterns of liposomes driven by encapsulated *E. coli*

Mai Hayakawa, Masahito Hayashi, Tomoyuki Kaneko (*LaRC, FB, Grad. Sch. Sci. & Eng., Hosei Univ.*)

Investigating morphological changes of cell-size liposomes can be applied to control the deformations of lipid membranes. In this study, we aimed to investigate the factors of the morphological changes of liposomes driven by encapsulated *E. coli*. As a result, some liposomes deformed by *E. coli*-membrane contact forces, forming warp, ellipsoid, and tube shapes. We observed the liposomes containing four different densities of *E. coli*, and found that 93% of the liposomes changed their shapes at the highest density. Although only 11% of liposomes larger than 15 μm deformed, 93% of liposomes smaller than 15 μm deformed. These findings suggest that we can control the shape of liposomes by their size and the density of encapsulated *E. coli*.

20334I* Construct analysis system between peptide local structure in lipid membrane and membrane deformation

Kayano Izumi, Ryuji Kawano (*Department of Biotechnology and Life science, Tokyo University of Agriculture and Technology*)

In this presentation, we studied correlation between liposome deformation and peptide local structure in lipid membrane by using microscopic observation and capacitance measurement. A few studies have reported that some peptides have liposome deformability. Using microscope, we observed liposome deformation by peptides. From the results, we assumed that liposome deforming pattern and peptide local structure could be associated. To exam this, we measured membrane capacitance of peptides. As the capacitance includes membrane deforming parameters, it is possible to detect the deformation. To analyze the capacitance, we attempt to classify liposome deformation by the type of peptide local structure. We believe that our method will be analyzing tool of liposome deformation.

20335I サイズ選択性を有する DNA オリガミ人工チャネル
Size-selective molecular transportation by DNA origami channel

Shoji Iwabuchi[1], Ibuki Kawamata[1,2], Satoshi Murata[1], M. Shin-ichiro Nomura[1] ([1]*Rob. Eng., Univ. Tohoku*, [2]*Nat. Sci., Fuc. Core Res., Univ. Ochanomizu*)

Development of an artificial cell or molecular robot which can work in a microenvironment has attracted attention. As their “body”, closed-lipid bilayer membrane called liposome has been adopted, but the membrane inhibits the input of a hydrophilic molecular signal from the environment. In this work, we design an artificial channel composed of DNA origami. The channel structure has a pore with 10 nm in diameter, which is larger than conventional artificial channels. By using additional DNA strands, we have also designed molecular mesh to control transportation. The structure was confirmed by TEM. The passage of molecules through the liposomal membrane and the blockade of the transport by the input of single-stranded DNA has been observed by confocal microscopy.

20336I* Protein crowder as a modulator of Min wave generation for cell division

Saki Nishikawa, Shunshi Kohyama, Nobuhide Doi, Kei Fujiwara (*Faculty of science and technology, Keio University*)

The Min system, which determines the cell division plane of bacteria, is known to exhibit dynamic intracellular localization of Min proteins (Min waves). It has been reported that the addition of a protein crowder like BSA or cell extract is essential for the generation of Min waves in the cell sized confinement. However, general properties required for the Min wave generation in the cell size confinement have not yet been clarified. Here we investigated this property by using column fractions of cell extract or purified proteins and found that multiple proteins can emerge Min waves in the cell size confinement by molecular weight dependent manner. These results indicated that multi-molecular environment is critical for shaping spatiotemporal regulation in cells.

20337I 脂質二分子膜に働く光捕捉力の検証
Lateral diffusion in lipid bilayers biased by optical forces

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For artificial control of synaptic transmission in neuronal networks, we have applied optical trapping to manipulate molecular dynamics of neurotransmitter receptors on neurons. Here we study how optical forces influence diffusion properties in artificial lipid bilayers as a model of cell membranes to clarify optical trapping dynamics of cell surface molecules. When a 1064-nm laser beam was focused on lipid bilayer labeled with fluorescent dyes within patterned polymeric bilayers, two-photon excitation fluorescence intensity increased at the laser focus. The lateral diffusion in lipid bilayers derived from fluorescence correlation spectroscopy slightly increased with irradiation time and laser power, suggesting that the diffusion is biased by optical trapping forces.

20338I* 細胞膜の物理的状態の制御に向けた生物活性ナノ材料の設計並びに評価
Design and Evaluation of Bioactive Nanomaterials toward Control of Physical Properties of Plasma Membrane

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The formation/deformation of lipids rafts associated with information exchange through the plasma membrane. Here, we report the formation/deformation of model lipid raft, Lo-phase domains on giant unilamellar vesicles, can be controlled with surface-modified gold nanorod(AuNR) covered with high-density lipoprotein (HDL), The AuNR induce the collapse of Lo domain spontaneously and cholesterol-loaded the AuNR generate Lo domain triggered by laser irradiation. We also developed new surface HDLs for pathogenic-like conditions. They attached on model and plasma membrane under low pH conditions selectively. Our strategy to develop bioactive and smart raft-manipulator will be a way to control lipid rafts on cells and, in the future, become a new therapeutic method.

20339J* 線虫の低温耐性を制御する新規の GPCR 型温度センサー分子
Novel GPCR-type temperature receptor in cold tolerance of *C. elegans*

Kohei Ohnishi, Toru Miura, Tomoyo Ujisawa, Akane Ohta, Atsushi Kuhara (*Inst. for Integrative Neurobiology, Konan Univ., Japan*)

ASJ and ADL thermo-sensory neurons regulating cold tolerance of *C. elegans* is a useful model for studying temperature sensation (Ohta et al., *Nat. commun*, 2014; Ujisawa et al., *PNAS*, 2018). To identify novel thermo-sensor, we performed RNAi for about 1000 GPCRs, as a result, 86 knocked-down animals showed abnormal cold tolerance respectively. Expression analysis showed that 16 GPCRs were expressed in ASJ or ADL. We constructed KO mutants of respective 16 GPCRs by using CRISPR/Cas9, and one of these GPCR mutants showed abnormal cold tolerance. Ectopic expression of this GPCR gene conferred the temperature responsiveness on non-warm sensitive ASE gustatory neuron, suggesting that we identify the novel GPCR-type temperature receptor.

20340J* ヒトムスカリン性アセチルコリン受容体 (M_2) のリガンド認識機構の理解に向けた赤外分光研究
Infrared spectroscopic study for elucidating ligand recognition mechanism of human M_2 muscarinic acetylcholine receptor

Kohei Suzuki[1], Kota Katayama[1], Ryoji Suno[2], Yuji Sumii[1], Norio Shibata[1], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech*, [2]*Kansai Medical University. Medical.*)

M_2 muscarinic acetylcholine receptor (M_2R) is a prototypical GPCR that responds to acetylcholine (ACh) and mediates various cellular responses in the nervous system. Recently, by use of attenuated total reflection (ATR)-FTIR spectroscopy, we reported the spectral changes upon ligand-binding to M_2 for the first time. The observed vibrational signals originate from ligand, protein, lipid, and protein-bound waters. Here, for in-depth understanding of the ligand recognition mechanism by M_2, we attempted to distinguish these vibrational modes. Vibrational bands of ligand were successfully identified by ^{13} C-labeled ACh, and the analysis of X-H stretches provides information of hydrogen-bonding network. We will propose the model structure based on the present results.

20341J Clostridium 属細菌の走化性アッセイ法の確立
Establishment of Methods for Chemotaxis Assays of *Clostridium* spp.

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Clostridium species are spore-forming, obligate anaerobic bacteria. At least some of them, including a notorious food pathogen *C. botulinum*, possess peritrichous flagella and are motile. However, their chemotaxes have been barely studied thus far. In this study, by using *C. sporogenes*, a non-toxigenic surrogate of *C. botulinum*, we tried to establish methods for quantitative analysis of their chemotaxis abilities. As a first step, we started to optimize conditions for their swarming in soft agar medium. Via stepwise dilution of a standard medium, we succeeded in observing clear swarm rings, suggesting that they are actually chemotactic. Further optimizations of swarm conditions are currently underway to screen attractants and repellents for *Clostridium* spp.

20342J* 非平衡流動場における脂質膜へのアミロイドβ凝集の単分子観察
Single Molecule Observation of Amyloid β Aggregation to Lipid Membrane under Non-equilibrium Fluidic Condition

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Alzheimer's disease is characterized by the aggregation of amyloid β (Aβ) peptides under interstitial fluid (ISF) flow to form amyloid plaque on the surface of brain cells, although its molecular mechanism is still under debate. ISF flow has roles to regulate (i) continuous supply and removal of Aβ, and (ii) intra- and inter-molecular structural changes of Aβ. Since previous studies investigated under closed conditions such as Petri dishes, unlike in vivo, we focused on the behavior of Aβ molecules on the cell membrane under non-equilibrium fluid flow. Single molecule observation provided insights into a time-course change in degree of polymerization. A new model involving ISF flow for the initial process of Aβ plaque formation and nerve cell collapse was proposed.

20343K 線虫 *C. elegans* を用いた異なる感覚情報の統合に関わる神経回路モデル
The model of neural circuit integrating different sensory information in *C. elegans*

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We are studying cold acclimation in nematode *C. elegans* as experimental model for analyzing neuronal systems. *kqt-2* mutant defective in potassium channel showed abnormal cold acclimation. Because the strength of this abnormality depended on the size of diameter in agar medium plate, we expected that other environmental stimuli except for temperature affect cold acclimation. We found that *KQT-2* regulate cold acclimation in ADL thermo-sensory neuron which connects to oxygen sensory neuron. The abnormal cold acclimation of *kqt-2* mutant was suppressed by *gcy-35* mutation defective in an oxygen receptor. Our genetic results indicated that a neuronal circuit integrating two different sensory modalities, temperature and oxygen, that modifies cold acclimation.

20344K 海馬で合成される男性・女性ホルモンやストレスホルモンによる記憶シナプスの早い non-genomic な制御
Rapid non-genomic modulation of synapses by hippocampus-synthesized androgen, estrogen and stress steroid

Suguru Kawato[1,2], Mika Soma[1,2], Mari Ikeda-Ogiue[1,2], Minoru Saito[2] ([1]*Dep. Urology, Grad Sch Medicine, Juntendo Univ.*, [2]*Dep. Life sciences, College Humanities and Sciences, Nihon Univ.*)

Neurosteroids (sex steroids and stress steroids) are synthesized in the hippocampus, center for learning and memory. Rapid action of neurosteroids has been extensively studied in the hippocampus over more than decades, and a significant progress has been achieved in clarification of essential molecular mechanisms. Dihydrotestosterone (DHT), testosterone (T), estradiol (E2) and corticosterone (CORT) trigger synaptic (membrane) sex steroid receptors (AR and ER) and glucocorticoid receptor (GR), leading to rapid modulation of dendritic spines in hippocampal slices. In downstream, kinase-dependent signaling regulates non-genomic modulation of dendritic spines for not only sex steroids but also stress steroids. Kinases are, for example, MAPK, LIMK, PKA and PKC.

20345K 線虫において脂肪酸代謝経路のβ酸化で働く HADH が低温馴化を制御する
HACD-1 that is beta-oxidation of fatty acid metabolism regulates cold acclimation in intestine and sensory neurons in C. elegans

Akihisa Fukumoto[1], Atushi Kuhara[1], Akane Ohta[1], Misaki Okahata[1], Youhei Minakuti[2], Atushi Toyoda[2] ([1]*Inst. for Integrative Neurobio., Konan Univ.*, [2]*NIG, Japan*)

We are studying temperature acclimation of nematode C. elegans to reveal how animals appropriately respond to temperature change. We found that expression level of hacd-1 was changed depending on temperature change by using RNA sequencing analysis with next generation sequencer. HACD-1 codes HADH 3-hydroxyacyl-CoenzymeA dehydrogenase which catalyzes a beta oxidation reaction. hacd-1 mutant showed abnormal temperature acclimation when animals transferred to higher cultivation temperature. HACD-1 were observed in several head neurons and intestine. The abnormal cold acclimation of hacd-1 mutant was rescued by expressing hacd-1 cDNA in either intestine or sensory neurons. These results suggest that HACD-1 regulate cold acclimation in intestine and sensory neurons.

20346K 細胞間の活動同期性に基づく神経クラスタの統計的推測
Statistical inference of neuronal ensembles based on synchronous activity among neurons

Shun Kimura, Koujin Takeda, Yuishi Iwasaki (*Grad. Sch. Sci. Eng., Univ. Ibaraki*)

We propose a stochastic neuronal ensemble inference method generalized to continuous neuronal activity data in order to clarify relationship between neuronal activity and behavior of target animal. In this method, we aim to infer neuronal ensembles and ensemble activities from time series data of neuronal activity by Markov chain Monte Carlo method. The proposed method is based on Bayesian inference method with generative model, which is derived from prior knowledge of neuronal activity. To validate our proposed method, we apply it to real activity data from C. elegans. As a result, we can classify neurons into ensembles with similar activation timings, and also infer ensemble activities.

20347K Integrated signaling from thermosensoryneurons at a tail interneuron regulates cold acclimation

Haruka Motomura, Satoko Fujii, Makoto Ioroi, Atsushi Kuhara, Akane Ohta (*Institute for integrative Neurobiology, Konan Univ.*)

C. elegans can alter its temperature tolerance depending on past environmental exposure (Ohta et al., Nat. commu, 2014; Okahata et al., Science Adv., 2019). Here we found that a neural circuit containing ASJ thermosensory neuron located in the head, PVQ interneuron in tail and RMG interneuron in head functioned as regulator of cold acclimation. Optical calcium imaging revealed that neural activity in ASJ, PVQ and RMG of wild-type fluctuated with changes in temperature, and PVQ neural activity decreased in *deg-1* mutant, defective in ASG thermo-sensation. Our results suggest that temperature signaling from ASJ and ASG are integrated into PVQ. Thus, we identified body-wide neural circuit as the modulatory mechanism of temperature acclimation.

20348K 内因性カンナビノイドによる小脳 GABA シナプス伝達のシナプスタイプ別制御
Endocannabinoids regulate cerebellar GABAergic transmission in a synapse type-dependent manner

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Endocannabinoids (eCBs) act as ubiquitous modulators of synaptic transmission via the activation of cannabinoid receptors (CBRs). Cerebellar Purkinje cells (PCs) make inhibitory synaptic contacts not only with neurons in the deep cerebellar nuclei (DCN), but also with globular cells. However, the modulatory actions of eCBs on GABA release from PC axon terminals remain unknown. We showed that the type 1 and 2 CBR agonist WIN55212 did not affect inhibitory postsynaptic currents in globular cells or large DCN neurons. These neurons did not elicit depolarization-induced suppression of inhibition. These results indicate the lack of a functional role of CBRs at PCs' axon terminals, suggesting that the actions of eCBs are selective to distinct synapses in the cerebellum.

20349K A method to differentiate neurite non-invasively with needle agarose microfabrication technology

Yuhei Tanaka, Haruki Watanabe, Kenji Shimoda, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

We have developed the agarose microfabrication technology for stepwise control of neurite elongation during cultivation to mimic in vivo differentiation. However, it has limitations such as damage to neurons during additional microstructure formation close to cells due to the resolution limit of focused infrared laser. To overcome the limitation, we converted permeable 1064-nm laser into heat by 2 μm absorption target on the tip of the microneedle, and manipulated this target to agarose microstructure for additional fabrication. We have succeeded in guiding and differentiating neurites with no damage to neurons during cultivation by additional stepwise fabrication with 2 μm resolusion, indicating this improvement can overcome the potential limitation of cell damage.

20350K 微小多電極解析のための神経細胞の 1 細胞レベル長期培養環境の最適化
Optimization of the long-term cultural environment of isolated single neurons for micro-multielectrode analysis

Kenji Shimoda, Yuhei Tanaka, Haruki Watanabe, Kenji Yasuda (*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

We examined the optimal cultivation conditions of isolated neurons in micro structures for multielectrode analysis. We compared the 14-day viability of isolated rat hippocampal cells on electrodes in 50-μm round shaped microchambers with four types of adhesion factors; poly-L-lysine (PLL), poly-D-lysine (PDL), laminin, and polyethyleneimine. The isolated neurons grew for 14 days on PLL-coated electrodes in microchambers, whereas the neurons did not grow on other adhesion coatings. In contrast, all the four adhesion coatings worked well without any apparent difference for neurons' growth when microchambers and microelectrodes did not place. The results indicate that PLL coating has an ability to coat the 3D-structured porous metal surface.

20351K 1 神経突起の伸長を長期間観察さるための改良された μm 分解能のアガロース微細加工技術の評価
Evaluation of an improved μm resolution agarose microfabrication technology for long-term individual neurite elongation observation

Haruki Watanabe[1], Yuhei Tanaka[1], Kenji Shimoda[1], Kenji Yasuda[1] ([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]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [4]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*)

We have developed an improved μm resolution agarose microfabrication technology and applied this technology for long-term observation of isolated single neurite elongations. Using micropatterns with 2 μm resolution in agarose layer, a hippocampal cell placed in the chamber with a diameter of 20 μm, and individual neurites isolated in the microchannels with 2 to 5 μm were successfully observed. Elongation rates were varied 0.26 μm /min to 0.40 μm /min in elongation area and were not continuous but stepwise such as elongated 100 μm for 384 min, and then stopped for 635 min in the 2-μm channel. The results indicate this assay can isolate a single neurite and measure elongation rate for the long-term, and the precise manner of neurite's straight elongation.

20352K マウス海馬の長期増強を膜電位感受色素によるイメージングで観察する
Imaging analysis of the long-term potentiation of the mouse hippocampal activity

Yoko Tominaga, Makiko Taketoshi, **Takashi Tominaga** (*Inst Neurosci Tokushima Bunri Univ.*)

Optical imaging techniques with voltage-sensitive dye (VSD) is an essential method to probe the neural circuit activity. Here we present that our fast single-photon wide-field VSD imaging technique can)be applied to show the neural circuit activity change caused by the long-term potentiation (LTP) in the mouse hippocampus. LTP at the hippocampal circuit is the cellular model of the brain's learning and memory functions. We achieved LTP measurements over 12 hrs (every 30 sec) with 0.1 ms/frame recordings. We will show that averaged data across many slices can give a quantitative evaluation of the circuit activity. The robust LTP assessment should be useful in many applications.

20353K　プリオンタンパク質ノックアウトマウスにおける小脳長期抑圧障害
Impairment of cerebellar long-term depression in prion protein-deficient mice ectopically expressing PrPLP/Dpl

Yasushi Kishimoto[1], Moritoshi Hirono[2], Ryuichiro Atarashi[3], Suehiro Sakaguchi[4], Tohru Yoshioka[5], Shigeru Katamine[6], Yutaka Kirino[1] ([1]*Kagawa Sch. Pharm. Sci., Tokushima Bunri Univ.*, [2]*Dep. Physiol., Wakayama Med. Univ. Sch. Med.*, [3]*Fac. Med., Univ. of Miyazaki*, [4]*KOSOKEN, Tokushima Univ.*, [5]*Kaohsiung Medical Univ.*, [6]*CICORN, Nagasaki Univ.*)

Prion protein (PrP^C) knockout mice, named as the Ngsk *Prnp*$^{0/0}$mice, show late-onset cerebellar Purkinje cell (PC) degeneration because of ectopic overexpression of PrPLP/Dpl. Our previous study indicated that the mutant mice also exhibited alterations in cerebellum-dependent eyeblink conditioning, even at a young age. Thus, this electrophysiological study was designed to examine the synaptic function of the cerebellar cortex in Ngsk *Prnp*$^{0/0}$mice. We showed that Ngsk *Prnp*$^{0/0}$mice exhibited impaired cerebellar long-term depression. $GABA_A$-mediated inhibitory postsynaptic currents recorded from PCs were also weakened in Ngsk *Prnp*$^{0/0}$mice Thus, the Ngsk *Prnp*$^{0/0}$mouse model can contribute to study underlying mechanisms for impairments of synaptic transmission and motor learning.

20354K　ミミズ短期記憶におけるセロトニンの関与
Involvement of serotonin in short-term memory of earthworms

Yoshiichiro Kitamura, Toshiaki Nakahara, Hikaru Takahashi (*Dept Math Sci Phys, Col Sci Eng, KGU*)

Involvement of serotonin in short-term memory of the earthworm Eisenia fetida was investigated. We previously reported that habituation by repeated tactile stimulus to the body wall in the earthworm is induced assumedly due to via serotonin-nitric oxide (NO)-cGMP signaling. In this study, we investigated effect of several serotonin-related reagents on establishment of habituation. Administration of serotonin $5\text{-}HT_2$ and $5\text{-}HT_3$ receptor antagonist similarly impaired memory formation. From these results, it is revealed that serotonin signaling through both $5\text{-}HT_2$ and $5\text{-}HT_3$ receptors related to short-term memory formation in the earthworm.

20355L　蟻はピンクノイズで探索する
Ants run on a treadmill with the pink noise

Tomoko Sakiyama[1], Naohisa Nagaya[2], Ryusuke Fujisawa[3] ([1]*Soka University*, [2]*Kyoto Sangyo University*, [3]*Kyushu Institute of Technology*)

The investigation of the locomotion mechanism of animals helps us to understand both the inherent movements of animals. Little is known about the detailed movement patterns for exploratory behaviours of ants. This is perhaps because the difficulty for dealing with small insects on a restricted flat field. Here, we tackle this problem using the spherical treadmill, called ANTAM, and investigate the diffusiveness of Japanese wood ants' walks. Overall, we found that individual ant walkers presented super-diffusive movements to some extent. However, the diffusiveness of individual movements depended on the time and varied. Interestingly, advanced analysis proved that the travel paths of individual walkers exhibited pink noise as a universal property.

20356L*　隠れマルコフモデルと逆強化学習法による生物複数戦略の同定
Identification of multiple strategies by inverse reinforcement learning with hidden-Markov model

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Animals adapt environments by developing behavioral strategies and flexibly switch multiple strategies in a context-dependent manner. Understanding how animals control the multi-strategy is important for elucidation of whole process in decision making. However, there is difficulty to examine the multi-strategy due to complexity of animal behaviors. By modeling multi-strategy switching by hidden-Markov model, we developed inverse reinforcement learning method to decode multiple strategies and detect their switching from behavioral data. By applying this method to C.elegans thermotaxis, we found that worms actively switch two independent strategies for directed migration toward specific temperature and isothermal migration.

20357L 睡眠の剥奪はショウジョウバエによる食物臭の嗜好性を変化させる
Sleep deprivation alters food odor preference in Drosophila

Fuminori Tanizawa[1,2], Hiroyuki Takemoto[3] ([1]*Kaisei Senior High School*, [2]*Future Scientists' School, Shizuoka University*, [3]*Research Institute of Green Science and Technology, Shizuoka University*)

We investigated the effect of sleep deprivation on preference of food-related odors in Drosophila melanogaster adults. In the experiment, 50 flies could choose in a 500ml container between two bottles filled with 10 ml of apple cider vinegar (ACV) and broth respectively for 16 hours. Flies whose sleep had been disturbed with intermittent rotation stimuli during night-time preferred ACV to broth, while flies without sleep deprivation and those rotated during daytime showed lower preference for ACV over broth. Moreover, increase of responses to ACV and decrease of responses to broth were observed in the experiments using single odor. These results suggested that sleep has a role in food odor preference and foraging behavior of fruit flies.

20358L 壁近くのゾンビ化した単鞭毛クラミドモナスの遊泳
Swimming of zombifield monoflagellated Chlamydomonas near wall

Ken Nagai (*JAIST*)

In this study, we used the uni1-1 strain of Chlamydomonas reinhardtii(CR), most of which are mono-flagellated. To clarify swimming behaviours caused by intrinsic noise, motility of the living ones with one flagellum and demembranated cell models with one flagellum were investigated. A cell model is prepared by killing CR with non-ion surfactant. The prepared cell models swim only in ATP solution. Near surface, both living CR and cell models rotated with axes perpendicular to the surface. Seen from the outside, counterclockwise rotation was observed more frequently and the ratio between counterclockwise and clockwise were almost the same in the both cases. This indicates that the rectification of rotation is induced by hydrodynamical interaction between CR and a wall.

20359L* 報酬と好奇心によって駆動される行動を表現する意思決定モデル
A decision-making model for reward and curiosity-driven behavior

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Animals learn new uncertain environments for survival and reproduction. Such adaptive behaviors have been modeled by reinforcement learning, which is the theory for describing only rewards-seeking behaviors. However, animals do not only rationally exploit rewards, but also explore environment even without rewards so as to minimize uncertainty of the environment owe to their curiosity. Here, we developed a new decision-making model of two-choices task, in which rewards are given at different probabilities at each choice, based on free energy principle. This model is appropriate to describe animal behaviors motivated by both rewards and curiosity.

20360M マウス桿体視細胞においてロドプシンを介するが光オフで生じるプロテインキナーゼ A の活性化
Rhodopsin-mediated Light-off-induced Protein Kinase A Activation in Mouse Rod Photoreceptor Cells

Shinya Sato[1], Takahiro Yamashita[2], Michyuki Matsuda[1,3] ([1]*Grad. Sch. Biostud., Univ. Kyoto*, [2]*Grad. Sch. Sci., Univ. Kyoto*, [3]*Grad. Sch. Med., Univ. Kyoto*)

Light-induced dopamine release in the retina reduces cAMP in rod photoreceptor cells, which is thought to mediate visual desensitization. However, fine time course of the cAMP dynamics in rods remains elusive due to technical difficulty. Here, we visualized cAMP dynamics in mouse rods by two-photon live imaging of retinal explants of PKAchu mice, which express a biosensor for cAMP-dependent protein kinase (PKA). Unexpectedly, we detected prominent light-off-induced PKA activation in the illuminated rods upon photopic light stimulation. Our data suggest that, upon photopic light stimulation, rhodopsin and dopamine signals are integrated to shape the light-off-induced cAMP production and following PKA activation. This may support the dark-adaptation of rods.

20361M 光合成酸素発生系における *g*=5 S_2 状態の分子構造
Molecular Structure of the S_2 State with a *g*=5 Signal in the Oxygen Evolving Complex of Photosystem II

Hiroyuki Mino, Shota Taguchi, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Uni.*)

The Mn_4CaO_5 cluster, located in the photosystem II (PS II) protein complex, is the core machinery for photosynthetic oxygen evolution. In the intermediate S_2 state, two kinds of EPR signals, the g = 2 multiline and g=4.1 signals, have been observed. Upon depletion of the extrinsic proteins, another S_2-state EPR signal was detected at g = 5. The signal has a hyperfine spacing with about 3 mT. This signal was related to the distortion of the manganese cluster, which is derived from the modification of the chemical bond. Based on these observations, another molecular structure of the S_2 state, a 'distant Mn' structure, was discussed as an intermediate state between the S_2 (g = 4) and S_3 states.

20362M QM/MM-MD による光回復酵素-紫外線損傷 DNA 複合体の逐次修復反応中における反応中間体の観測に成功
QM/MM-MD approach for photolyase-UV-damaged DNA complex achieved that observe an intermediate in the successive DNA repair reactions

Ryuma Sato[1], Hiroshi Watanabe[2,3], Junpei Yamamoto[4], Makoto Taiji[1] ([1]*RIKEN*, [2]*Keio univ, KQCC*, [3]*PRESTO JST*, [4]*Osaka univ*)

There are two major types of UV-induced DNA lesions, cyclobutane pyrimidine dimer (CPD) and pyrimidine-pyrimidone (6-4) photoproduct ((6-4)PP). It has been known that photolyases (PLs) exert the DNA repair function. The details of DNA repair mechanism of CPD and (6-4)PP have been explored by theoretical and experimental studies, but the repair mechanism has not been perfectly clarified. To observe the successive repair reaction, we performed the QM/MM-MD simulations for PL and UV-damaged DNA complexes and emphasized that we established comprehensive picture of the repair mechanism by integrating the previous models.

20363M 光化学系Ⅱにおける D1-Asp170 の His 変異体の新規なアミノ酸変換
Novel amino acid conversion of a His mutant of D1-Asp170 in photosystem II

Yuichiro Shimada[1], Tomomi Kitajima-Ihara[1], Ryo Nagao[1,2], Takumi Noguchi[1] ([1]*Grad. Sch. Sci., Nagoya Univ.*, [2]*Res. Inst. Interdiscip. Sci., Okayama Univ.*)

Our recent FTIR and LC-MS study showed that the His mutant of D1-D170, which provides a carboxylate ligand to the Mn cluster in PSII, had mainly Asp at D1-170 (Kitajima et al., 2020), but its mechanism has not been resolved yet. To clarify the mechanism of this D1 conversion, we labeled His residues in the D1-D170H mutant with ^{13}C-His and analyzed isolated PSII complexes using FTIR. Flash-induced S_2/S_1 FTIR difference spectrum of ^{13}C-His-labeled D1-D170H PSII showed clear changes in the symmetric COO^- stretching region indicative of incorporation of a ^{13}C-COO^- group. This observation suggests that His170 in D1-D170H was post-translationally modified to Asp most likely by oxidation of His catalyzed by Mn^{3+}, which was photo-produced in the Mn-cluster binding site.

20364M Clarification of proton transfer pathways in water photolysis in photosystem II

Ayane Sugiyama, Yuichiro Shimada, Takumi Noguchi (*Division of Material Science, Graduate School of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8602, Japan*)

A number of theoretical studies have suggested that D1-D61 is involved in proton extraction from water. However, it is not clear which channel is responsible for the proton emission and water uptake in each S-state transition. To identify the channels through which the proton release of the water photolysis takes place, oxygen evolving activity and delayed light fluorescence (DL) measurements of D1-D61A, D2-K317A, D1-E65A, D2-E312A, D1-R334A mutants on Cl-channels were performed. As a result, the oxygen evolving activity and transition efficiency were reduced in each mutant. These results suggest that the Cl- channel functions as a proton release pathway during the water photolysis.

20365M 光化学系Ⅱの第二キノン電子授与体 Q_B の反応における D1-His252 の役割
Role of D1-His252 in the reaction of the secondary quinone electron accepter Q_B in photosystem II

Tomoyuki Kobayashi[1], Yuichiro Shimada[1], Ryo Nagao[2], Takumi Noguchi[1] ([1]*Grad. Sch. Sci, Nagoya Univ.*, [2]*Res. Inst. Interdiscip. Sci., Okayama Univ.*)

The secondary quinone electron accepter Q_B in PSII is converted to plastoquinole upon double reduction. The nearby His residue, D1-H252, has been proposed to be involved in the reactions of Q_B, but its mechanism remains unresolved. In this study, we investigated the role of D1-H252 by characterizing a D1-H252A mutant using delayed luminescence (DL) and quantum mechanical (QM) calculations. DL measurements showed that H252A mutation lowered the $E_m(Q_B^-/Q_B)$ and decreased the efficiency of the Q_B photoreaction. QM calculations reproduced the E_m downshift by mutation, although the H-bond interaction of Q_B was little affected because of the replacement of His with water molecules. It was suggested that D1-H252 plays roles in controlling E_m and facilitating the Q_B exchange.

20366M 光化学系Ⅱにおけるキノン電子受容体 Q_A・Q_B 間の電子移動の時間分解赤外分光検出
Time-resolved infrared detection of electron transfer between quinone electron acceptors Q_A and Q_B in photosystem II

Honami Ito, Yuki Kato, Takumi Noguchi (*Grad. Sch. Sci, Nagoya Univ.*)

Electron transfer from the primary quinone Q_A to the secondary quinone Q_B in PSII is controlled by the protein environment, but its mechanism remains unresolved. So far the Q_A-to-Q_B electron transfer has been investigated only by fluorescence detection, which indirectly monitors the redox state of Q_A. In this study, we applied time-resolved infrared (TRIR) spectroscopy to directly monitor the Q_A-to-Q_B electron transfer. The time course of the flash-induced absorption change at 1745 cm^{-1}, where the specific signal of Q_B^- exists, showed a rise with a time constant of 500-600 μs. This rise disappeared in the presence of DCMU, which inhibits electron transfer by binding at the Q_B site, confirming that the detected TRIR signal originates from the Q_A-to-Q_B electron transfer.

20367M Mutational analysis of the mechanism of an absorption red shift in a marine bacterial Cl^--pumping rhodopsin

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A marine bacterium, *Rubrivirga marina*, possesses two Cl^--pumping rhodopsins in which only four amino acid residues are different near the retinal chromophore. Interestingly, the absorption maximum of one of them is 29-nm red shifted compared with the other, suggesting that one or a few residues possibly induce a large spectral shift. To obtain clues to the spectral tuning mechanism, we performed a comprehensive mutational analysis by generating 30 types of single or multiple mutants, and found amino acid substitutions that can explain a part of the spectral shift. In the presentation, we will discuss the effects of the mutations with an additional mutation at a site distant from the chromophore.

20368M FTIR spectroelectrochemical study on the mechanism of the pH dependence of the redox potential of the non-heme iron in photosystem II

Yuki Kato, Hiroki Watanabe, Takumi Noguchi (*Grad. Sch. Sci., Nagoya Univ.*)

The redox potential E_m of the non-heme iron, locating between Q_A and Q_B in PSII, is known to be ~+400 mV with a pH dependence of ~-60 mV/pH. However, the cause of this pH dependence remains unresolved. In this study, to clarify the mechanism of the pH dependence, we examined $E_m(Fe^{2+}/Fe^{3+})$ and the protonation structures of proteins around the non-heme iron in a pH range of 5.0~7.5 using FTIR spectroelectrochemistry. A linear pH dependence of $E_m(Fe^{2+}/Fe^{3+})$ with -58 mV/pH was observed over this pH range. Fe^{2+}/Fe^{3+} difference spectra showed changes in His CN bands at pH 5.5~7.5 and in Glu COO^- bands at pH 5.0~6.5. We thus concluded that nearby His and Glu residues are responsible for the pH dependence of $E_m(Fe^{2+}/Fe^{3+})$ in the higher and lower pH regions, respectively.

Poster

20369M Spectroscopic properties and energy transfer dynamics of two different forms of acpPC from dinoflagellate *Symbiodinium*

Hayata Yamamoto[1], Keisuke Kawakami[2], Hiroko Uchida[3], Akio Murakami[3], Nobuo Kamiya[4], Daisuke Kosumi[5] ([1]*Dept. of Sci. and Tech., Kumamoto Univ.*, [2]*RIKEN*, [3]*Research Center of Island Seas, Kobe Univ.*, [4]*ReCAP, Osaka City Univ.*, [5]*IINA, Kumamoto Univ.*)

Photosynthetic antenna apparatus efficiently capture sunlight and transfer the energy to reaction centers. Chlorophyll *a*/*c*-peridinin protein complex (acpPC) is an integral membrane complex from dinoflagellate, and contains major carotenoid peridinin (per) and minor carotenoid diadinoxanthin (ddx). Per exhibits an intramolecular charge transfer (ICT) state located nearby the S_1 state, leading to the generation of a strongly coupled S_1/ICT state. Consequently, per efficiently transfers the absorbed energy to nearby Chl *a* via S_1/ICT state. On the other hand, ddx plays a photoprotective function by dissipating excitation energy as heat. In this study, we isolated the two different fractions of functional acpPC from dinoflagellate *Symbiodinium* sp.strain SGCH-03.

20370M Energy transfers in PSI of cyanobacterium, red alga, and dinoflagellate

Hiroki Serikawa[1], Hayata Yamamoto[1], Keisuke Kawakami[2], Hiroko Uchida[3], Akio Murakami[3], Kimiko Nagayoshi[4], Toshinari Kuroki[4], Susumu Takio[5], Nobuo Kamiya[6], **Daisuke Kosumi**[7] ([1]*Dept. of Sci. and Tech., Kumamoto Univ.*, [2]*RIKEN*, [3]*Research Center of Island Seas, Kobe Univ.*, [4]*Daiichi Seimou Co., Ldt.*, [5]*CWMD, Kumamoto Univ.*, [6]*ReCAP, Osaka City Univ.*, [7]*IINa, Kumamoto Univ.*)

Natural photosynthetic organisms capture sunlight energy and transfer it to reaction centers (RC) where charge separation takes place to gain electro-chemical potentials. Photosystem I (PS I) is the photosynthetic pigment-protein complex consisting of core antenna and RC. One of the spectroscopic interests of PSI is a presence of red-chlorophylls (Chl) with strong excitonic interactions between Chl molecules.It has been reported that the presence of red-Chl in PSI realizes the efficient energy transfer from b-carotene to Chl a. In the present study, we performed fs pump-probe spectroscopies on the isolated PSI-trimer from a thermophilic cyanobacterium, dinoflagellate, and red alga to clarify the detailed energy transfer dynamics of carotenoid to Chl.

20371M 新しいタイプの光サイクル型動物オプシンの創製
Construction of a novel type of photocycle animal opsin

Kazumi Sakai[1], Yoshinori Shichida[2], Yasushi Imamoto[1], Takahiro Yamashita[1] ([1]*Grad. Sch. Sci., Univ. Kyoto*, [2]*Res. Org. for Sci. and Tech., Univ. Ritsumeikan*)

Opsins are universal photoreceptive proteins in animals and have diversified photoreaction mechanisms. Most opsins are called as bistable opsins which photo-convert between stable dark and active states. By contrast, vertebrate rhodopsin is a mono-stable opsin which photo-converts to a metastable active state that cannot revert to the dark state. Recently, we identified a unique opsin, Opn5L1. Opn5L1 forms the active state in the dark and deactivates by light. And the dark state thermally reverts to the dark state after photoreception. Thus, Opn5L1 can be classified as a photocyclic opsin. Here we constructed a novel type of photocyclic opsin from vertebrate rhodopsin as a template. We will discuss the mechanism of this opsin different from (that of) Opn5L1.

20372M AUREO1-LOV ドメインの光誘起構造変化
Light-induced conformational switching of the LOV domain in aureochrome-1

Itsuki Kobayashi, Hiroto Nakajima, **Osamu Hisatomi** (*Grad. Sch. Sci., Osaka Univ.*)

Photozipper (PZ) protein is an N-terminally truncated aureochrome-1 comprising a LOV domain and a basic leucine zipper domain. Blue light induces PZ dimerization and subsequently increases its affinity for the target DNA. We found that substitutions of Phe298 and Gln317 in PZ affected the monomer-dimer ratio and affinity for the target DNA both in the dark and light states. A clear correlation was detected between the dimer fraction and DNA affinity of each PZ mutant. Our results suggest the existence of a conformational equilibrium and that its shift by a synergistic interaction between the chromophore and protein moiety probably enable BL-regulated switching of aureochrome-1.

20373M* 演題取り消し

20374M* 低温赤外分光測定による(6-4)光回復酵素の修復メカニズム解明
Elucidation of the repair mechanism of (6-4) photolyase by low-temperature FTIR spectroscopy

Katsuya Maeda[1], Mai Kumagai[1], Daichi Yamada[2], Yuma Terai[3], Junpei Yamamoto[3], Hideki Kandori[1] ([1]*Nagoya Inst. Tech*, [2]*Univ. Hyogo.*, [3]*Osaka Univ.*)

(6-4) photolyases is a DNA repair enzyme that reverts UV-induced (6-4) photoproducts into normal bases. (6-4) photolyase is able to repair both T(6-4)T and T(6-4)C, where the OH and NH2 groups are bound at C5 position of 5' side, respectively. Until now, researches have been conducted mainly on T(6-4)T, and the repair mechanism of T(6-4)C is believed to be the same as T(6-4)T without detailed analysis. Here, we studied the repair mechanism by low-temperature light-induced difference FTIR spectroscopy. We attempted to identify vibrations of the repair intermediates by isotope labeling, and extract the difference from the comparison of the spectra of T(6-4)T and T(6-4)C. We will discuss the DNA repair mechanism based on the obtained results.

20375M* カチオンチャネルロドプシン *Ts*_Rh3 における C 末端領域の重要性
Importance of the C-terminal region in cation channel rhodopsin *Ts*_Rh3

Rintaro Tashiro[1], Kumari Sushmita[2], Suneel Kateriya[2], Hideki Kandori[1], Satoshi Tsunoda[1,3] ([1]*Nagoya Inst. Tech.*, [2]*Jawaharlal Nehru Univ.*, [3]*JST PRESTO*)

We here report a novel microbial rhodopsin *Ts*_Rh3. It is a member of channelrhodopsins, and functions as a light-gated cation channel. *Ts*_Rh3 consists from a 7 transmembrane rhodopsin domain followed by a long cytoplasmic domain about 560 amino acids which encodes a peptidoglycan binding domain. By electrophysiological measurement, we found that the open lifetime of the channel differs depending on the C-terminus length. It is assumed that the charged amino acids in the C-terminal region affect the kinetics of *Ts*_Rh3, we performed mutation studies in detail. As a result, R287A and R291A mutants showed altered open lifetime compared to WT. Thus, interaction between the rhodopsin domain and the C-term region via arginine residues mediates the channel properties.

20376M 高速 AFM によるロドプシンクラスター上トランスデューシン動的過程の観察
Dynamic process of G protein transducin on rhodopsin cluster observed by high-speed AFM

Kazuhiko Hoshikaya[1], Hayato Yamashita[1], Fumio Hayashi[2], Kenichi Morigaki[3,4], Masashi Fujii[5,6], Akinori Awazu[5,6], Masayuki Abe[1] ([1]*Graduate School of Engineering Science, Osaka University*, [2]*Graduate School of Science, Kobe University*, [3]*Biosignal research center, Kobe University*, [4]*Graduate School of Agricultural Science, Kobe University*, [5]*Graduate School of Science, Hiroshima University*, [6]*Graduate School of Integrated Sciences for Life, Hiroshima University*)

Rhodopsin (Rh) likely forms supramolecular structures such as dimers and dimer rows in retinal disc membrane. Single molecule-imaging [1] and simulation study [2] revealed Rh dynamics in native discs and the formation mechanism of Rh supramolecular structures. In this study, we observed single molecule dynamics of transducin (Gt) on Rh clusters by using high-speed AFM. Movies showed that Gt diffuses over Rh clusters consisting of dimer rows in the dark. Upon light illumination some of Gt molecules transiently stayed on Rh clusters. These single molecular observations will elucidate the functional role for Rh supramolecular structures. [1] F. Hayashi et al, *Comm. Biol.* (2019) [2] Y. Kaneshige et al, *PLOS ONE* (2020)

20377M Biophysical characterization of different members of TAT rhodopsins: a new group of microbial rhodopsins

Kentaro Mannen[1], Takashi Nagata[1,2], Oded Béjà[3], Keiichi Inoue[1] ([1]*Inst. Solid State Phys., Univ. Tokyo*, [2]*PRESTO, JST*, [3]*Biol., Israel Inst. Tech.*)

TAT rhodopsin, a microbial rhodopsin found in an α-proteobacterium, SAR11 HIMB114, was recently reported to exhibit unique properties in photochemical dynamics. This rhodopsin shows photoisomerization of retinal chromophore like other microbial rhodopsins, but it reverts to the original state in less than 10 microseconds without further latter intermediates. In this study, we found several new TAT rhodopsins and similar homologues. To reveal whether the unique properties are shared in common with the newly discovered TAT rhodopsins and similar homologues, their absorption spectra and pH dependence were investigated using spectroscopic methods. Based on the results, we will discuss the diversity of the molecular properties of TAT rhodopsins.

20378M Actinotalea fermentans におけるヘリオロドプシンの発現
Expression of Heliorhodopsin in Actinotalea fermentans

Rei Abe-Yoshizumi, Ai Muto, Hideki Kandori (*Nagoya Inst. Tech.*)

Heliorhodopsin (HeR; 48C12) is a new family of rhodopsin, discovered in 2018. Slow photocycle suggests sensor function, whereas the interaction partner remains unknown. Functional analysis of HeR is not easy because of the difficulty to culture HeR-containing native cells. In this study, we identified the HeR gene from an actinomycete named *Actinotalea fermentans*, which can be cultured in the laboratory. To clarify the physiological function of HeR, we first tried RT-PCR and immunoblotting to determine whether HeR was expressed in native cells. RT-PCR revealed that AfHeR was expressed regardless of the light conditions during culture. In addition, we are preparing antibodies against AfHeR and are trying to detect them in native cells.

20379M 絶対嫌気性緑色硫黄光合成細菌における Rieske/cyt*b* 複合体と *c* 型シトクロム間の相互作用解析
Studies on interaction between Rieske/cyt*b* complex and *c*-type cytochromes in strictly anaerobic photosynthetic green sulfur bacteria

Hiraku Kishimoto[1], Takahiro Nagaoka[1], Chihiro Azai[2], Risa Mutoh[3], Hideaki Tanaka[4], Yohei Miyanoiri[4], Genji Kurisu[4], Hirozo Oh-oka[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Col. Life Sci., Ritsumeikan Univ.*, [3]*Fac. Sci., Fukuoka Univ.*, [4]*Inst. Protein Res., Osaka Univ.*)

Cytochrome (cyt) *bc* complexes in photosynthetic electron transport chain contain three transmembrane proteins, cyt *b*, cyt c_1 or cyt *f*, and Rieske ISP. They conduct electron transport reactions coupled with proton translocation across membranes, resulting in the production of proton motive force to synthesize ATP. Photosynthetic green sulfur bacteria were strictly anaerobic and contain the most primitive Rieske/cyt*b* complex. We tried to purify it under anaerobic conditions to explore the structure-function relationship. We observed the interaction between the ^{15}N-labeled Rieske ISP and cyt *c*-556 by NMR measurements and identified the interaction sites on the Rieske ISP. We are now preparing ^{15}N-labeled cyt *c*-556 to identify the sites interacted with the Rieske ISP.

20380M 脊椎動物の非視覚オプシン Opn5 の多様化の起源の探索
Origin of diversification of vertebrate non-visual opsin Opn5

Takahiro Yamashita[1], Kengo Fujii[1], Kazumi Sakai[1], Yasushi Imamoto[1], Hideyo Ohuchi[2], Yoshinori Shichida[3] ([1]*Grad. Sch. of Sci., Kyoto Univ.*, [2]*Grad. Sch. of Med., Dent. and Pharm. Sci., Okayama Univ.*, [3]*Ritsumeikan Univ.*)

Opsins are the photoreceptive proteins for visual and non-visual photoreception in animals and are classified into several groups based on their amino acid sequences. Opn5 forms an independent opsin group whose members are found in not only vertebrates but also a wide range of invertebrates. Our analysis of the molecular properties showed that vertebrate Opn5 is diversified into four subgroups based on their spectral sensitivities and their binding preference for retinal isomers. In this study, to get insight into the evolutionary origin of diversified vertebrate Opn5, we analyzed Opn5 genes found from invertebrates including deuterostomes and protostomes. We would like to discuss the diversity of the molecular property of Opn5 widely found in bilateral animals.

20381M* アニオンチャネルロドプシン吸収波長制御機構の解明
Mechanism of absorption wavelength shifts in anion channelrhodopsin mutants

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Anion channelrhodopsins (ACRs) are light-gated anion channels that are used as neural silencing tools in optogenetics. To be used for a fiberless optogenetics approach via the lanthanide micro-particles that can reduce damage to the tissue, the absorption wavelength is yet short. Using a quantum mechanical/molecular mechanical approach, we analyzed the mechanisms of how the protein environment shifts the absorption wavelength in ACR from Guillardia theta (GtACR1). Investigation of ~200 mutant structures shows that mutations at T101, C133, P208, and C237 can increase the absorption wavelength. In particular, T101A GtACR1 was expressed in E. coli and the measured absorption wavelength was 10 nm higher than that of wild type, consistent with the calculated wavelength.

20382M AUREO1-LOV の光誘起構造変化に関与する水素結合
Hydrogen bonds involved in the light-induced conformational switching of AUREO1-LOV

Yumiko Adachi, Hiroto Nakajima, Osamu Hisatomi (*Graduate School of Science, Osaka University*)

Hydrogen bonds are involved in the conformational stabilization of biomolecules, including DNA and proteins. To elucidate the roles of hydrogen bonds on the conformational change of light-oxygen-voltage (LOV) domain, we prepared site directed mutants of an N-terminally truncated aureochrome-1 (Photozipper, PZ) consisting of a LOV domain and a basic leucine zipper domain. Blue light induces dimerization of PZ and subsequently increases its affinity for the target DNA. We found that substitutions of Gln332 to Ala in Jα helix caused aggregation of PZ even at 37 ℃, suggesting that the hydrogen bond between Cys283 and Gln332 increases the thermal stability of PZ. Hydrogen bonds may play important roles for stabilization of LOV domains.

20383M* 新たに同定した水素結合ネットワークによる植物由来(6-4)光回復酵素の補因子 FAD の光依存的還元反応の制御
A newly identified hydrogen-bonding network modulates photoreduction of the flavin cofactor in plant (6-4) photolyase

Yuhei Hosokawa[1], Ryuma Sato[2], Martin Saft[3], Pavel Muller[4], Klaus Brettel[4], Lars-Oliver Essen[3], Shigenori Iwai[1], Junpei Yamamoto[1] ([1]*Grad. Sch. Eng. Sci., Osaka Univ.*, [2]*Riken*, [3]*Dept. Chem., Philipps Univ.*, [4]*I2BC, CEA, CNRS*)

(6-4) photolyases ((6-4)PLs) are flavoproteins able to repair a UV-induced DNA lesion called (6-4) photoproduct using blue light. To achieve the repair, their flavin adenine dinucleotide (FAD) cofactor needs to be reduced through a tryptophan (Trp) chain in a light-dependent manner, called photoreduction. How do (6-4)PLs stabilize a charge-separated state between FAD and Trp during the photoreduction process? In this study, we proposed that an H-bonding network around the terminal Trp plays a key role in stabilizing the charge-separated state in plant (6-4)PL. This hypothesis was supported by UV/vis spectroscopy and structural analyses with hydrogen-deuterium exchange mass spectrometry (HDX-MS) and molecular dynamics (MD) simulation.

20384M* 分光学的手法による霊長類青感受性視物質の光反応構造解析
Photochemical dynamics of a primate blue-sensitive pigment by spectroscopic study

Shunpei Hanai[1], Kota Katayama[1], Takuma Sasaki[1], Hiroo Imai[2], Hideki Kandori[1] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech*, [2]*Prim. Res. Inst. Kyoto Univ.*)

Color pigments have 11-cis-retinal as the chromophore. Light absorption causes cis-trans isomerization, followed by conformational changes of the protein moiety. Our recent UV-visible spectroscopy study for primate blue pigment (MB) showed that all intermediates except for Meta-II state accumulated at specific temperature are converted into the initial state by light. Light-induced difference FTIR spectroscopy for BL intermediate formed from the initial intermediate Batho state provided the distinct vibrational signals of retinal, peptide backbone, and protein-bound waters in comparison with that of Batho state. Here, to understand the spectroscopic basis underlying MB specific photoreaction, we will extend the spectroscopic studies using site-directed mutagenesis.

20385M* Rhodococcus 属細菌が有するヘリオロドプシンの物性および生理機能の探索
Study on physiological functions and physical properties of heliorhodopsin possessed by Rhodococcus bacteria

Ai Muto, Rei Abe-Yoshizumi, Hideki Kandori (*Nagoya Inst. Tech.*)

Although rhodopsins have been believed to be composed of two families, type-1 and type-2, a new rhodopsin family, Heliorhodopsin (HeR), was recently discovered through functional metagenomics analysis. More than 600 organisms contain HeR genes, but few can be cultured. Consequently, function of HeR is still unknown, despite sensor function is postulated. In this study, we successfully cultured a Rhodococcus bacterium that possesses two HeRs. We now try functional analysis by use of native cells. In parallel, molecular properties of the HeRs are studied by expressing them in *E. coli*. Function of HeR will be discussed based on the present results using native cells.

20386M 光応答転写因子 Photozipper における二量体形成過程の高速 AFM 観察
High-speed AFM observation on dimer formation of a light-sensing transcription factor, Photozipper

Akihiro Tsuji[1], Kento Nomura[1], Hayato Yamashita[1], Osamu Hisatomi[2], Masayuki Abe[1] ([1]*Grad. Sch. of Eng. Sci., Osaka Univ.*, [2]*Grad. Sch. of Sci., Osaka Univ.*)

Transcription factors (TF) regulate various gene expression by binding to the target DNA sequences. Although the dimerization of TF is crucial for its DNA binding, the single molecular dynamics of dimer formation remains to be visualized. Photozipper (PZ) is a TF consisting of a basic leucine zipper DNA binding (bZIP) domain and a light-oxygen-voltage-sensing (LOV) domain. Biochemical and spectroscopic studies suggested that blue light induces the reversible dimerization of monomeric PZ and increases its affinity for the target DNA sequence. Here, we report the observation of PZ molecules using high-speed AFM in the dark and light states. Also, high-speed AFM movies visualized the monomer-dimer transition of PZ molecules.

20387M 光による植物細胞の膜電位制御系の開発
Development of an light regulatory system of membrane potential in plant cell

Masae Konno[1,2], Hiromu Yawo[1], Hideki Kandori[3,4], Keiichi Inoue[1] ([1]*ISSP, Univ. Tokyo*, [2]*JST, PRESTO*, [3]*Life Sci. Appl. Chem., Grad. Sch. Eng., NIT*, [4]*OBTRC, NIT*)

Membrane potential regulates various physiological responses in plant. However, it is difficult to control the membrane potential spatially and temporally using conventional methods. To regulate the membrane potential in plant cells by light, we applied optogenetic approach to plant cells. Six microbial rhodopsins were transiently or constitutively expressed in *Arabidopsis* T87 cells. The localization to the plasma membrane was observed in light-driven sodium pump (KR2), light-gated cation (*Gt*CCR4) and anion channels (*Gt*ACR1). Light-dependent membrane potential changes were detected in the cells expressed *Gt*CCR4 and KR2 with light illumination at 530 nm. Based on these results, we will discuss about the details of optogenetic control of membrane potential in plant cells.

20388M* ビブリオ属のブループロテオロドプシンが示す異常な pH 依存的吸収変化のメカニズム
Mechanism of unusual pH-dependent color change in blue-proteorhodopsin from *Vibrio califitulae*

Mizuki Sumikawa (*Nagoya Inst. Tech*)

Proteorhodopsins(PRs) are light driven proton pumps found in marine bacteria, which are classified into blue-absorbing (BPR) and green-absorbing (GPR) forms. Previously, we converted BPR from LC1-200 strain into GPR by simple pH change through pH 2, but the mechanism was fully unknown. In this study, we found the same pH effect for BPR from *Vibrio califitulae* (*Vc*BPR), but not for standard BPR. We investigated the molecular mechanism by use of mutation, and successfully identified key amino acid residues. Structural model to explain the unusual pH-dependent color change in specific BPR will be presented.

20389M* 新規ロドプシンフォスホジエステラーゼ（Rh-PDE）8 種の分子特性
Molecular properties of eight novel rhodopsin phosphodiesterases (Rh-PDEs)

Masahiro Sugiura[1], Satoshi Tsunoda[1], Masahiko Hibi[2], Hideki Kandori[1] ([1]*Nagoya Institute of Technology*, [2]*Graduate School of Science, Nagoya University*)

Enzyme rhodopsin is a new family of microbial rhodopsins. They exhibit light-dependent catalytic functions such as guanylyl cyclase (Rh-GC) and phosphodiesterase (Rh-PDE). Here, we report molecular properties of 8 novel Rh-PDEs which have been identified from several choanoflagellates recently. PDE activity and its substrate specificity toward cAMP or cGMP varied among them, where activities of MrRh-PDE and SrRh-PDE are cAMP and cGMP specific, respectively. We investigated absorption wavelength of seven Rh-PDEs using UV-vis spectroscopy, revealing that absorption maxima ranged from 490 to 525 nm. Based on the experimental data and amino acid sequences, we propose a novel absorption wavelength control mechanism.

20390M* 内外の配向でのセンサリーロドプシン II の表面増強赤外分光法
Surface-enhanced infrared spectroscopy on sensory rhodopsin 2 tethered with the inside or outside facing orientation

Jingyi Tang[1], Insyeerah Binti Muhammad Jauhari[1], Yuji Furutani[1,2] ([1]*Grad. Sch. Eng., Nagoya Inst. Tech.*, [2]*OptoBioTech. Research Center, Nagoya Inst. Tech.*)

Sensory rhodopsin 2 (SRII) is a seven-transmembrane photo-receptor, which is activated by blue-green light. The N-terminus faces the outside and the C-terminus faces the inside of the cell. To discuss the differences in the structural changes between the outside and inside region of SRII, we applied surface-enhanced infrared absorption spectroscopy (SEIRA), which increase the infrared absorption intensity of the region near the surface of the gold thin film. We modified the gold surface with linker molecules possessing Ni-NTA and tethered the SRII proteins with His-tag at C-terminal or N-terminal to control the orientation. Then, the light-induced FTIR difference spectra were measured in the SEIRA configuration, and compared the results of them.

20391M 電子励起状態における、フィコシアノビリンの構造変化に関する理論的研究
Exploring the structural changes of phycocyanobilin in the excited states

Kenji Mishima[1], Mitsuo Shoji[1,2], Yasufumi Umena[3], Yasuteru Shigeta[1] ([1]*CCS. Univ. Tsukuba*, [2]*JST-PRESTO*, [3]*Jichi Medical University*)

In this talk, we present our recent theoretical work on the peculiar properties of the chromophore in the C-phycocyanin (C-PC), phycocyanobilin (CYC), based on the time-dependent density functional theory and natural bond orbital (NBO) methods. The scope is to unravel their key features upon light absorption and transmission occurring in natural photosynthesis. To this aim, we compute the photoabsorption spectra, which reflects the presence of three different orientations of the CYC in C-PC. The NBO geometrical analyses of the bond lengths, interatomic angles, and dihedral angles evidenced that the intermolecular interactions of the propionic acid side chains play a crucial role in the determination of the excited state molecular conformations.

20392M 対称 I 型ヘリバクテリア反応中心光捕集過程の理論解析と光化学系 I との比較
Theoretical analysis of light harvesting mechanism of homodimeric type-I Heliobacterial reaction center: comparison to PSI

Akihiro Kimura[1], Hirotaka Kitoh[2,3], Yasuteru Shigeta[3], Shigeru Itoh[1] ([1]*Department of Physics, Graduate School of Science, Nagoya University*, [2]*JST, PRESTO*, [3]*Center for Computational Sciences, University of Tsukuba*)

The structure of type-I Heliobacterial reaction center (hRC), one of 4 types of RCs, was reported in 2017. In this study, we theoretically analyzed light harvesting mechanisms of hRC based on an exciton model to reproduce the experimental spectroscopies on hRC. Excitonic couplings and site energies on hRC were accurately calculated by quantum chemical calculations. Poisson-TrESP method and FED method were used to calculate the excitonic couplings between any two pigments. The site energy of each pigment in hRC was calculated by the CDC method. Reproducing the experimental transient spectroscopies, we compared the light harvesting mechanisms of hRC with those of photosystem I (PSI) focusing on the differences of pigment arrangements/species between hRC and PSI.

20393M 錐体・桿体視細胞の外節における脂質環境の解析
Analysis of the lipid environment in outer segment membranes of rod and cone photoreceptor cells

Shuji Tachibanaki[1], Keiji Seno[2], Tateki Matsui[1], Masahiro Ueda[1] ([1]*Grad. Sch. of Frontier Biosci., Osaka Univ.*, [2]*Facultiy of Med., Hamamatsu Univ. Sch. of Med.*)

In vertebrate retina, there are two types of visual photoreceptor cells: rods and cones. The sensitivity of rods is ~100 times higher than that of cones. We found that the signal amplification is 5 times larger in rods than in cones, and this partially explains the higher sensitivity of rods. In this study, to know the molecular mechanism of larger signal amplification in rods, we focused on the lipid compositions of cellular membranes in outer segment (OS), where the enzymatic reactions to generate the responses occur. As a result, we found that rods and cones have different lipid compositions: Rods have less raftophilic phospholipids and cholesterols than cones. Based on our results, we will discuss the effect of lipid environments in OS on signal amplification.

20394M 固体 NMR による内向きプロトンポンプロドプシン Schizorhodopsin のレチノール発色団の構造解析
Structure of retinal chromophore in Schizorhodopsin as studied by solid-state NMR

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Schizorhodopsin (SzR) found in Asgard archaea is a light-driven inward proton transporter [K. Inoue et al. (2020) Sci. Adv. 6, eaaz2441]. It is assumed that the structure of the retinal-binding pocket having a unique Phe-Ser-Glu (FSE) motif is deeply related with unidirectional proton transport. Here, we show solid-state NMR results of SzR embedded into DOPC/DOPE membrane. From the 13C-13C DARR and CP-MAS NMR spectra, 14- and 20-13C signals of the retinal in SzR appeared at 124.3 and 15.4 ppm, indicating 13-trans, 15-anti configuration. 15N NMR signal of the protonated Schiff base appeared at higher field resonance than those of other microbial rhodopsins. We will discuss about the structure of retinal-binding pocket in SzR.

20395M 共役二重結合系を延長したレチナールアナログによる赤色感受性チャネルロドプシンの更なる長波長シフト
Red-Shift of Red-Activatable Channelrhodopsin Using One-Double-Bond-Inserted Retinal Analogs

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Optogenetics application for animal tissues demands the red-tuned channelrhodopsin driven by deep red light which passes through the biological optical window. Red-activatable channelrhodopsin (ReaChR) is a red-shifted variant of cation channelrhodopsin, which is a promising template to develop further red-shifted channelrhodopsin. Here we incorporated one-double-bond inserted A1- and A2-retinal analogs into ReaChR apoprotein. The binding experiment demonstrated that they were accommodated in the chromophore binding pocket of ReaChR to form the red-shifted pigments. However, some of these analogs showed significantly low photosensitivity, suggesting that the specific chromophore/protein interaction is required to improve the photoactivity of ReaChR analogs.

20396M 紅色光合成細菌の LH2 タンパク質の色素改変：色素のサイトエネルギーとタンパク質内励起エネルギー移動への影響
Pigment modification in LH2 proteins from purple photosynthetic bacteria: effects on pigment site-energy and intracomplex energy transfer

Yoshitaka Saga[1], Yuji Otsuka[1], Madoka Yamashita[1], Shiori Nakagawa[1], Yuto Masaoka[2], Tsubasa Hidaka[2], Yutaka Nagasawa[2] ([1]*Fac. Sci. Eng., Kindai Univ.*, [2]*Grad. Sch. Life Sci., Ritsumeikan Univ.*)

The pigment manipulation in photosynthetic proteins is promising for understanding of the functional mechanisms. We focus on LH2 proteins in purple photosynthetic bacteria and demonstrate that energy-donating B800 bacteriochlorophyll (BChl) a can be modified with various types of (B)Chl pigments. The red-shifts of the Qy bands of Chls induced by insertion into the B800 pockets were smaller than those of BChls. The intracomplex energy transfer from Chls in the B800 site to energy-accepting B850 BChl a in LH2 was slower than that in native LH2. In contrast, BChl b in the B800 site transferred excitation energy to B850 BChl a at a similar rate to the case of native LH2 despite the increase of the spectral overlap between the energy donor and the accepter.

20397M* Aureochrome-1 における LOV コアから活性ドメインへの情報伝達機構
Signal transduction from LOV core to effector domain in Aureochrome-1

Hiroto Nakajima, Itsuki Kobayashi, Osamu Hisatomi (*Grad. Sci. Sci., Univ. Osaka*)

Aureochrome-1 (AUREO1) contains a basic leucine zipper (bZIP) domain and a light-oxygen-voltage-sensing (LOV) domain. Blue light induces dimerization and increases the affinity of AUREO1 for the target DNA. To elucidate the signal transduction from photoexcited LOV core, we prepared nine site-directed mutants of N-terminally truncated AUREO1 (PZ), with amino acid substitutions in the hydrophobic β-sheet region and in the hinge region between A'α and LOV core. Mutations in the hydrophobic region altered the hydrodynamic radii and affinities to DNA, although mutations in the hinge region have minor effect on these properties. Our data suggested that light signal is transduced via the hydrophobic β-sheet region of LOV core and activates the bZIP domain of AUREO1.

20398M 天然アニオンシャネルロドプシン GtACR1 の分子機構に関する理論的研究
Theoretical study on molecular mechanics of natural anion channel rhodopsin GtACR1

Takafumi Shikakura, Cheng Cheng, Shigehiko Hayashi (*Kyoto Univ. Graduate School of Science*)

Channelrhodopsins are photo-sensitive channel proteins with a retinal chromophore and are utilized in optogenetics. Recently a structure of an anion-conducting channelrhodopsin, GtACR1, was determined by X-ray crystallography. We theoretically examined protonation states of counter ion groups (Glu68 and Asp 234) and distributions of water molecules and a Cl- anion in a putative channel which are key properties for photo-sensitive ion channel conduction. Ab initio QM/MM free energy geometry optimizations revealed tight coupling of the protonation states and distributions of water molecules and a Cl- anion, providing a molecular insight into electrostatic environment in the anion conducting channel.

20399M Theoretical study of electron transport between cytochrome f and plastocyanin by using a coarse-grained simulation

Kazutomo Kawaguchi, Hidemi Nagao (*Inst. Sci. Eng., Kanazawa Univ.*)

An electron is transported from cytochrome f (Cyt f) in cytochrome b6f complex to photosystem I via plastocyanin (Pc) during photosynthetic electron transport. Electron transport rate is different among some species. We have shown that the electron transport rate can be predicted by using the Langevin dynamics simulations with a coarse-grained model developed in our previous study [S. Nakagawa, et al., Mol. Phys. 2017; K. Kawaguchi, et al. Mol. Phys. 2016]. In this study, we investigate a dependence of the electron transport rate due to species differences. We perform the Langevin dynamics simulation for Cyt f-Pc complex in cyanobacteria, algae, and higher plants and show that complex formation of Cyt f and Pc is reflected in species differences.

20400M 緑色硫黄細菌のルブレドキシン-酸素酸化還元酵素への電子供与系
Electron transfer path to the rubredoxin-oxygen oxidoreductase in green sulfur bacteria

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Green sulfur bacterium *Chlorobaculum tepidum* is an obligate anaerobe performing anoxygenic photosynthesis. In its genome, rubredoxin (Rd) and Rd-oxygen oxidoreductase (ROO) genes are present, but putative NADH-rubredoxin oxidoreuctase gene is missing. In this work, Rd and ROO were prepared as recombinant forms, and the dioxygen reduction activity was confirmed with ferredoxin-NAD(P)+ oxidoreductase (FNR). FNRs from *C. tepidum* and *Bacillus subtilis* catalyzed the rubredoxin reduction at high rates. In the presence of NADPH, FNR and Rd, ROR supported the dioxygen reduction at comparable rate to those of the other bacterial ROOs. Our results suggest that Rd and ROO participate the removal of dioxygen in *C. tepidum* cells, and FNR can support the rubredoxin reduction.

20401M *Heliobacterium modesticaldum* 由来反応中心における励起エネルギー移動および初期電荷分離に関する研究
Studies on excitation energy transfer and primary charge separation in the reaction center complex from *Heliobacterium modesticaldum*

Risa Kojima[1], Hayata Yamamoto[2], Chihiro Azai[3], Chiasa Uragami[4], Hideki Hashimoto[4], Daisuke Kosumi[5], Hirozo Oh-oka[1] ([1]*Grad. Sch. Sci., Osaka Univ.*, [2]*Grad. Sch. Sci & Tech., Kumamoto Univ.*, [3]*Coll. Life Sci., Ritsumeikan Univ.*, [4]*Fac. Sci & Tech., Kwansei Gakuin Univ.*, [5]*IINA, Kumamoto Univ.*)

The kinetics of excitation energy transfer and charge separation process in the photosynthetic reaction center of *Heliobacterium modesticaldum* were investigated with femtosecond transient absorption spectroscopy at room temperature. After laser-flash excitation, the equilibration of spectral changes among antenna bacteriochlorophyll (BChl) *g*s completed in less than 0.2 ps, indicating a very rapid excitation energy transfer among them. The decay-associated difference spectra (DADS) revealed a trapping process with a time constant of 20 ps to form the initial charge separation state of $P800^{+}A_0^{-}$. The 20 ps component showed the bleaching at 816 nm and would derive from the excited red-BChl *g*s or might be due to the exciton coupling between P800 and accessory BChl *g*.

20402M 光吸収計算によって現れた C-フィコシアニンの 6 量体構造の機能的な意味
Functional meaning of hexamer structure of C-phycocyanin revealed by calculation of absorption wavelength

Hiroto Kikuchi (*Dept. of Phys. Nippon Med. Sch.*)

C-phycocyanin (C-PC) is the main constituent of the rod of phycobilisome (PBS) which is a giant peripheral light-harvesting protein complex. The C-PC monomer structure is composed of two chains which are called α and β subunits, and aggregate to form disc-shaped trimers $(\alpha\beta)_3$ having rotational symmetry. This trimer is a structural-block unit and assembles the rod of PBS. The two structural-blocks does not stack in the same direction to form an $(\alpha\beta)_6$-hexamer, and are associated face-to-face to form it. The two $(\alpha\beta)_6$-hexamer are associated back-to-back to form through a linker protein. In this study, functional role of hexamer structure of C-PC revealed by calculation of absorption wavelength is discussed.

20403M Connecting the spectral properties to the structure of photosystem I containing Chlorophyll-*f*

Rin Taniguchi[1], **Yutaka Shibata**[1], Toshiyuki Shinoda[2], Tatsuya Tomo[2], Shen Ye[1] ([1]*Tohoku Univ., Grad. Sch. Sci.*, [2]*Tokyo Univ. Sci., Fac. Sci.*)

Recently, several cyanobacteria producing specifically red-shifted pigment chlorophyll (Chl)-*f* were discovered. PSI of such species, *Halomichronema hongdechloris*, shows two red-shifted fluorescence bands at around 750 nm and 810 nm due to Chl-*f*. In this study, we try to connect the spectral properties of the *H. hongdechloris* PSI to the seven Chl-*f* identified by the recent cryo-EM study. To this end, we conducted the fluorescence polarization anisotropy analysis of single PSI complexes at low temperature. We observed clear polarization anisotropies of fluorescence bands at 750 nm. This band can be assigned to Chl-*f*s with the transition dipole moments either parallel or perpendicular to the membrane normal. We are accumulating data to achieve more convincing assignments

20404M 海洋性藻類 *Guillardia theta* における微生物ロドプシンの遺伝子発現解析
Gene expression analysis of microbial rhodopsins from marine algae *Guillardia theta*

Yumeka Yamauchi[1], Masae Konno[1,2], Keiichi Inoue[1,2], Hideki Kandori[1,3] ([1]*Life Sci. & Appl. Chem., Nagoya Inst. Tech.*, [2]*ISSP, Univ. Tokyo*, [3]*OBTRC, Nagoya Inst. Tech.*)

Microbial rhodopsins are photoreceptive proteins working as light-driven ion transporters, light sensors or light-activated enzymes. Cryptophyta *Guillardia theta* has 46 microbial rhodopsin-like genes on its nuclear genome, whose physiological roles remain unknown. Here we investigated the cell growth of *G. theta* and the expression of the rhodopsin-like genes in native cells. Light was essential for cell growth and the cell color changed from brown to green under nitrogen depletion. We found 29 genes being expressed, and the expression patterns of 25 genes were analyzed. Under nitrogen depletion conditions, expression of several genes was enhanced or reduced. We will discuss the mechanism and physiological roles of the rhodopsin-like proteins in *G. theta*.

20405M Theoretical study on molecular mechanism of a light-driven ion transport of Halorhodopsin

Ryo Oyama, Taisuke Hasegawa, Shigehiko Hayashi (*Grad. Sch. Sci., Kyoto Univ.*)

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.

20406M Disruption of water-mediated H-bond network in rhodopsin mutations cause night blindness

Kota Katayama[1], Yuri Takeyama[1], Akiko Enomoto[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 bound with 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. The mutations, G90D and T94I are night blindness-causing mutation that exhibit different physicochemical characteristics associated with the dark activation. To elucidate the molecular mechanism by which two mutations affect rhodopsin dark activation, we performed light-induced difference FTIR spectroscopy of both mutants. Our results show an altered H-bond network around the central transmembrane region of mutant rhodopsin, which is reminiscent of the active Meta-II state.

20407M クロロフィル *f* をもつ光化学系 I 複合体の構造
Structural of photosystem I complex with chlorophyll *f*

Toshiyuki Shinoda[1], Koji Kato[2], Ryo Nagao[2], Seiji Akimoto[3], Jian-Ren Shen[2], Fusamichi Akita[2,4], Naoyuki Miyazaki[5,6], Tatsuya Tomo[1] ([1]*Fac. Sci., Tokyo Univ. Sci.*, [2]*RIIS., Okayama Univ.*, [3]*Grad. Sch. Sci., Kobe Univ.*, [4]*PRESTO, JST*, [5]*IPR., Osaka Univ.*, [6]*TARA., Tsukuba Univ.*)

Chlorophylls (Chls) play pivotal roles in energy capture, transfer and charge separation in photosynthesis. In 2010, Chl *f* containing cyanobacterium was discovered in Australia. We isolated photosystem I (PSI) complexes from this cyanobacterium, and analyzed their high-resolution structures by cryo-electron microscopy [1]. The structure showed that PSI binds 83 Chl *a* and 7 Chl *f*, and Chl *f* are associated at the periphery of PSI. Among the seven Chl *f*, six form a cluster with rather short inter-molecular distances. It is suggested that this cluster was involved in energetically unfavorable uphill energy transfer. We will discuss the roles of Chl *f* based on the structural and spectroscopic analyses.
1] Kato et al., Nat. Commun. 11 238 (2020)

20408M* In situ visualization of reversible state transition in live *Chlamydomonas* cells by noninvasive excitation spectral microscopy

Xianjun Zhang[1], Yuki Fujita[1], Ryutaro Tokutsu[2], Jun Minagawa[2], Shen Ye[1], Yutaka Shibata[1] ([1]*Tohoku Univ., Grad. Sch. Sci.*, [2]*NIBB, Div. Environ. Photobiol.*)

Efficient photosynthesis is maintained by the movement of the antenna complex (LHCII) between PSII and PSI to balance the excitation rates of the two PSs (State transition). However, in situ visualization of the rearrangement of LHCII in live cells is limited. In this work, the home-built noninvasive excitation spectral microscopy was used. The system provided powerful spectral information covering the Qy bands of chlorophyll (Chl)-*a* and also Chl-*b* exclusively bound to LHCII. We could construct intracellular mapping of the relative intensity of the Chl-*b* component which directly reflected the reversible migration of LHCII. The rearrangement of LHCII upon state transition was clearly visualized in live *Chlamydomonas* cells for the first time.

20409M Anion binding to mutants of the Schiff base counterion in heliorhodopsin
Anion binding to mutants of the Schiff base counterion in heliorhodopsin

Manish Singh[1], Kota Katayama[1], Oded Beja[2], Hideki Kandori[1] ([1]*Nagoya Inst. Tech*, [2]*Israel Inst. Tech*)

Heliorhodopsins (HeRs), a new family of microbial rhodopsins hold a unique topology, the N-termini face the intracellular side and C-termini face the extracellular side. HeRs (n=195), contains only one negative, most conserved residue Glu (E), corresponding to Asp (D85) in bacteriorhodopsin (BR). Here, we examined the possible anion binding into wild type and Glu mutants of HeRs. For bacterial HeR-48C12 and archaeal TaHeR, we prepared the E/A, E/Q, E/D and explored the Cl- binding effect by UV-visible spectroscopy. Experimental results clearly showed no Cl- binding for wild type and E/D mutant but significant Cl- ion interaction for E/A and E/Q mutants. Moreover, wild type, E/D, E/A and E/Q mutants also followed a similar pattern with other ions (Br-, I- and NO3-).

20410M* 光化学系 I 反応中心の電子移動におけるクロロフィルエピマー化の影響
Effect of chlorophyll epimerization on the electron transfer in photosystem I reaction center

Koji Mitsuhashi[1], Keisuke Saito[1,2], Hiroshi Ishikita[1,2] ([1]*Grad. Sch. Eng., Univ. Tokyo*, [2]*RCAST, Univ. Tokyo*)

In oxygenic photosynthesis, photosystem I (PSI) catalyzes the sunlight-driven electron transfer, which occurs through pseudo-symmetric A and B blanches. In the reaction center of PSI, there is the primary electron donor, P700, composed of two chlorophylls PA and PB, which belong to the A blanch and the B blanch, respectively. PB is chlorophyll a (Chla) and PA is Chla', the C13 epimer of Chla. It was observed that the electron transfer is asymmetric. Using quantum mechanics / molecular mechanics module, we investigated the effect of PA epimerization on the electron transfer in PSI. Our calculation shows that epimerization of PA causes the localization of LUMO of P700 on PA, which may be related to the asymmetric electron transfer in PSI.

20411M* 光化学系 II 水分解触媒部位の交換カップリングの起源
Origin of exchange couplings of the Mn_4CaO_5 cluster in photosystem II

Shunya Nishio[1], Keisuke Saito[1,2], Hiroshi Ishikita[1,2] ([1]*Fac. Eng., Univ. Tokyo*, [2]*RCAST., Univ. Tokyo*)

Photosynthesis is a process, which converts light energy into chemical energy. The Mn_4CaO_5 cluster in photosystem II (PSII) has four water ligands. The S2 state has two conformations, the open cubane and the closed cubane. From electron paramagnetic resonance (EPR) studies, it has been suggested that the exchange coupling between Mn3 and Mn4 (J_{34}) must be $|J_{34}| > \sim 30$ cm^{-1} in the closed cubane conformation. Based on the crystal structure, we calculated the exchange couplings, using a quantum mechanical/molecular mechanical approach. The results show that $|J_{34}| > \sim 30$ cm^{-1} when W1 is OH^-. Further details of the relationship between the Mn3-Mn4 distance and the exchange coupling will be discussed.

20412M Simultaneous Mapping of Fluorescence Spectra and Lifetimes of Chlorophylls Revealed Accumulation of Quenched LHCII

Yuki Fujita, Xianjun Zhang, Touru Kondou, Yutaka Shibata (*Organic Physical Chemistry Lab., Tohoku Univ.*)

A mechanism called state transition is known as a function to regulate relative antenna sizes of two photosystems (PSs) by shuttling of light harvesting complex (LHCII). Here we conducted direct observations of their movement within a cell by using the home-built high-resolution cryogenic microscope. The system provides simultaneous observations of fluorescence (FL) spectra and lifetimes. We could resolve inhomogeneous distributions of PSs within Chlamydomonas cells at 80 K and estimate the quantum yield of LHCII in the subdivided PSII-rich and PSI-rich regions. From this measurement, short lifetime and high intensity signal of LHCII were observed in the PSI-rich regions, suggesting the accumulation of isolated and FL-quenched LHCII in the PSI-rich region.

20413M アゾベンゼン挿入 DNA と T7RNA ポリメラーゼの光転写制御ダイナミクス
Dynamics of photo-regulated transcription reaction of T7 RNA polymerase and azobenzene-tethered DNA

Gennosuke Takekawa (*Grad. Sch. Sci., Kyoto Univ.*)

T7 RNA polymerase (T7RNAP) catalyzes the synthesis of RNA from DNA. Recently, it was revealed that an insertion of azobenzene into the T7 promoter DNA can control the enzymatic activity of T7RNAP in a light dependent manner. In this system, the Azo_{trans}-DNA terminates transcription by inhibiting a binding of T7RNAP to DNA, whereas the Azo_{cis}-DNA facilitates the binding of T7RNAP and melting the unwinding region, which promotes the transcriptional reaction. In this study, we investigated the time-resolved interaction dynamics between T7RNAP and Azo-DNA initiated by an isomerization of azobenzene using the transient grating (TG) method. We will also discuss differences in kinetics depending on the azobenzene insertion position.

20414M 青色光センサータンパク質 VVD の光反応ダイナミクス
Photoreaction dynamics of blue light sensor protein VVD

Takafumi Nakayama, Andrea Mussini, Yusuke Nakasone, Masahide Terajima (*Grad. Sch. Sci., Univ. Kyoto*)

VVD is a blue light sensor protein, which is involved in a regulation of circadian cycle in fungi. Since it forms dimer upon blue light irradiation, it has been widely used as an optogenetic tool. Although the crystal structures of both dark- and light-states of VVD have been reported, however, its reaction dynamics has not been clarified yet. In this study, we investigate the photo-induced reaction dynamics of VVD by the transient grating (TG) method to understand the molecular mechanism of signal transduction. We found that the diffusion coefficient (D) decreased upon photoexcitation and its reaction rate depended on the concentration of VVD. Hence the decrease of D has been attributed to the dimerization reaction. The details of the photoreaction will be discussed.

20415M* The gate-keeper role of a highly conserved helix-3 tryptophan for ion transport of the channelrhodopsin chimera, C1C2/ChRWR

Yujiro Nagasaka[1], Shoko Hososhima[2], Keiichi Inoue[1], Hideki Kandori[2,3], Hiromu Yawo[1] ([1]*ISSP., Univ. Tokyo*, [2]*Grad. Sch. Eng., Nagoya Inst. of Tech*, [3]*Optobio., Nagoya Inst. of Tech*)

C1C2/ChRWR, a chimera between channelrhodopsin (ChR)-1 and -2 from Chlamydomonas reinhardtii, is a light-gated cation channel. Its helix-3 tryptophan (W163) is one of the aromatic amino acids forming the retinal binding pocket around the all-trans retinal (ATR) and is highly conserved among microbial rhodopsins. Here, we replaced W163 of C1C2/ChRWR with a smaller aromatic residue phenylalanine to investigate its contribution on the ion transport. The W163F mutation strongly attenuated the passive transport of cations with the manifestation of outward H+ pump activity. It is suggested that W163 has a role of the “gate keeper” which places the structure involved in channel gating at the optimum position (Nagasaka et al., Biophys. Physicobiol. in press).

20416O 演題取り消し

20417O 天然の原核生物由来カルシウムチャネルにおけるイオン透過選択性の進化とその決定残基の同定
The selectivity determinant and evolution of a native prokaryotic voltage-dependent calcium channel

Katsumasa Irie[1], Takushi Shimomura[1,3], Yoshiki Yonekawa[2], Hitoshi Nagura[1], Michihiro Tateyama[3], Yoshinori Fujiyoshi[4] ([1]*CeSPI, Nagoya univ.*, [2]*Grad. Pharm. Med. Sci., Nagoya univ.*, [3]*Div. Biophys. Neurobio., NIPS*, [4]*CeSPL,TMDU*)

Voltage-dependent Ca^{2+} channels (Cavs) are indispensable for coupling action potentials with Ca^{2+} signaling in living organisms. Prokaryotic Navs can obtain Ca^{2+} selectivity by negative charge mutations of the selectivity filter, but native prokaryotic Cavs had not yet been identified. Here, we report the first identification of a native prokaryotic Cav, CavMr. Although the CavMr selectivity filter is less negatively charged than that of artificial prokaryotic Cavs, CavMr exhibits high Ca^{2+} selectivity. The glycine residue of the CavMr selectivity filter is a determinant for Ca^{2+} selectivity. This residue is conserved in subdomains I and III of eukaryotic Cavs, which provide new insight into the Ca^{2+} selectivity mechanism conserved from prokaryotes to eukaryotes.

20418O* Effects of Oligopeptides on Growth of Primitive Vesicles

Akiko Baba[1], Kazuki Yokoyama[1], Ulf Olsson[2], Masayuki Imai[1] ([1]*Department of Physics, Faculty of Science, Tohoku University*, [2]*Department of Chemistry, Faculty of Science, Lund University*)

A milestone from molecular assemblies to the cellular life is interplay between biopolymers that carry essence of life and vesicles that is container of life. In the prebiotic era, it is likely that oligonucleotides or oligopeptides encourage growth and division of primitive fatty acid vesicles. The effect of primitive biopolymers on the growth of vesicle probably depend on the sequence of nucleotides or amino acids, which determine the fitness landscape toward the cellular life. To demonstrate this pathway, we have measured the growth rate of fatty acid vesicles in the presence of oligonucleotides or oligopeptides. The fatty acid vesicle shows that the growth rate depends on the type of amino acids and the sequence of amino acids in the oligopeptides.

20419O* ベシクル表面上での情報分子成長
Growth of Information Molecules on Vesicle Surface

Yuto Hachiya[1], Hikaru Hatori[1], Syoichi Toyabe[2], Steen Rasmussen[3], Masayuki Imai[1] ([1]*Phys, Tohoku Univ.*, [2]*Appl. Phys., Grad. Sch. Eng., Tohoku Univ.*, [3]*Phys, Chem Pharm, Univ. Southern Denmark*)

To synthesize information molecules in the prebiotic environment, primitive ingredient molecules should be accumulated in reaction fields where reactants and products form mutual-catalytic reaction networks. Vesicle surface is a promising candidate for the reaction field. Prebiotic molecules having hydrophobic segments are anchored to the membrane, which enhances the reaction efficiency due to the dimensionality and the amphiphilic environments. In this study we demonstrate that vesicle surface promotes synthesis of information molecules by measuring ligation rate of oligonucleotides anchored on the vesicle surface. The obtained ligation rate is compared with that in bulk solution, which shows the advantage of vesicle interface as a reaction field.

20420O 膜のないドロップレット内での RNA ゲノムの自己複製
Translation-coupled RNA replication in membrane-free droplets

Ryo Mizuuchi[1,2], Norikazu Ichihashi[1] ([1]*Komaba Institute for Science, Univ. Tokyo*, [2]*JST PRESTO*)

The construction of artificial cells helps understand cellular functions and provide novel cell-like reactors. Gene-expression, a key phenomenon of living cells, has been integrated with various biological processes typically in lipid-based compartments. However, the demonstration of such complex reactions in artificial cells based on liquid-liquid phase separation (LLPS) was challenging. Here, we combined a cell-free gene-expression system with a genomic RNA within LLPS-based droplets and demonstrate RNA self-replication by its encoded protein. The droplets concentrated both the genomic RNA and translation proteins, and also facilitated the replication of the genomic RNA by segregating it from parasitic replicators despite the lack of membranes.

20421O Study on evolutionary fluctuation-response relationship in multicellular development

Chikara Furusawa[1,2] ([1]*BDR, RIKEN*, [2]*UBI, Graduate School of Science, The University of Tokyo*)

The fluctuation-response relationship in evolution, e.g., a positive correlation between the amplitude of noise in gene expression and response to mutations, has been proposed based on theoretical models of replicating cells and experimentally confirmed by analysis of unicellular organisms. However, the fluctuation-response relationship in the evolution of multicellular development remains unclear. In this study, by using a simple computational model, we found that the fluctuation-response relationship generally emerges multicellular development when the high-dimensional expression dynamics representing the development is constrained on low-dimensional dynamics. Based on the result, general features in the evolution of multicellular development will be discussed.

20422O* 膜面上の高分子合成と連携した持続的なベシクルの自己生産
Sustainable Reproduction of Vesicles coupled with a Surface-Confined Template Polymerization

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Construction of autonomously reproducing molecular assembly system is one of the key approaches to understand what bridges non-living and living forms of matter. Here we show the sustainable reproduction of cell-sized vesicles coupled with a membrane-confined polymerization of aniline. Polyaniline emeraldine salt form(PANI-ES) is synthesized on the surface of vesicles composed of AOT. When AOT micelles are supplied to the AOT/PANI-ES vesicle, the AOT molecules are incorporated into the membrane, which leads to vesicle growth. Moreover, the vesicles also show spontaneous division if the membrane contains the second component such as cholesterol. By introducing cholesterol transporting mechanism, we succeeded in developing sustainable reproduction of AOT/PANI-ES vesicles.

20423O How combination of DNA recombination and translation error allows efficient evolution?

Kenta Mitsutomi, **Daisuke Kiga** (*Waseda Univ, Dept Electrical Eng and Biosci*)

Although the present translation system has high fidelity, early life had a genetic code with low fidelity. What would have been the outcome of protein evolution at early life? For directed evolution with such codes, we have created codes with adjustable low fidelity by engineering of cell-free translation. Adjustable misincorporation by our low fidelity codes, intriguingly, can accelerate directed evolution by smoothing protein fitness landscape on DNA sequence space. In order to evaluate combined effect between DNA recombination and translation errors in terms of efficient evolution, we performed in silico evolution where we varied recombination and translation error rate. Interestingly, complexity of interactions among residues defined which parameter was dominant.

20424O* 進化実験による最も単純な等温条件下 DNA 複製機構の探索
Minimization of Elements for Isothermal DNA Replication by an Evolutionary Approach

Hiroki Okauchi[1], Yoshihiro Sakatani[2], Kensuke Otuka[2], Norikazu Ichihashi[1,2] ([1]*Dept. Life Sci., Univ. Tokyo*, [2]*Dept. Bioinfo. Eng., Univ. Osaka*)

DNA replication is one of the central functions of the cell. The complexity of modern DNA replication systems raises a question: is it possible to achieve a simpler continuous isothermal DNA replication using fewer proteins? We searched such replication using an evolutionary approach. Through a long-term serial dilution experiment with phi29 DNA polymerase, we found that large repetitive DNAs spontaneously appear and continuously replicate. The repetitive sequence is critical for this replication scheme. This study revealed that continuous isothermal DNA replication can be achieved in a scheme simpler than that employed by modern organisms, providing an alternative strategy for simpler artificial cell synthesis and a clue to possible primitive forms of DNA replication.

20425O ホストパラサイト相互作用による表現型可塑性の進化
Evolution of Phenotypic Plasticity in Host-Parasite Interactions

Naoto Nishiura, Kunihiko Kaneko (*The University of Tokyo Graduate School of Arts and Sciences*)

To study the evolution of the genotype-phenotype mapping, we employed a simple model for gene expression dynamics.The network consists of genes that mutually activate or inhibit each expression.The population of each parasite increase in proportion to the host with the corresponding phenotype.Then the growth rate of each hosts is decreased by the parasite attacks.In the absence of parasite interaction, the host's phenotype with expressing all fitness genes emerged.Under the presence of sufficient interaction with parasites, the host population evolves into multiple groups with different phenotypes.To examine how the interaction will enhance the phenotypic diversity, we computed the phenotypic variance from two perspectives: genetic mutation and phenotypic plasticity.

20426O* 高分子混雑環境下でのミクロ相分離が創成する細胞様構造体
Emergence of cell-like structure through micro phase separation in a crowding macromolecular solution

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Living cells maintain their lives through an orderly manner under a crowding environment with various kinds of biopolymers. Using aqueous/aqueous phase separation, we reported the formation of cell-sized droplets entrapping biomacromolecules in a spontaneous manner. Here, we further apply this experimental strategy for a solution system containing phospholipid. It will be shown that artificial primitive cells covered by the lipid membrane, incorporating DNA molecules inside them, also spontaneously generated. Interestingly, such cell-like structure emerges in a spontaneous manner, through the simple mixing procedure for the solution containing DNA and lipids. Physico-chemical mechanism on the self-organization of cell-like structure will be discussed in the conference.

20427O* 人工膜小胞内リン脂質合成による自律的細胞分裂機構の構築
Development of a self-reproducing vesicular system driven by internal phospholipid synthesis

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Autonomous self-reproduction is essential to the propagation and evolutionary adaptation of life. Thus, designing and engineering artificial cells capable of growth and division can contribute to our understanding of primitive self-reproduction and evolution of life. Here, we developed a simple self-reproducing system in which liposomes undergo a coupled process of growth and division driven by internal phospholipid synthesis mediated by a soluble enzyme FadD10. Continuous supply of precursors needed for the lipid synthesis leads to the dynamic shape transformation followed by the division of some liposomes, seemingly caused by the internal reaction of FadD10. This system will be a versatile platform for realizing an autonomous self-reproduction in artificial cells.

20428O* 細菌アクチン MreB からスピロプラズマ遊泳モーターへの進化
Development of *Spiroplasma* swimming motor from bacterial actin, MreB

Daichi Takahashi[1], Ikuko Fujiwara[1,2], Makoto Miyata[1,2] ([1]*Grad. Sch. Sci., Osaka City Univ.*, [2]*OCARINA, Osaka City Univ.*)

Spiroplasma are helical bacteria of the phylum *Tenericutes* that evolved from *Firmicutes* including *Bacillus subtilis*. *Spiroplasma* swim by helicity switching with kinks traveling along the cell, in which five classes of bacterial actin homolog MreBs are involved in the force generation. We analyzed sequences of *Spiroplasma* MreBs (SMreBs). The maximum likelihood phylogeny showed that all SMreBs formed a clade adjacent to the radiation of MreBH, an MreB isoform of *Firmicutes*. Sequence comparisons of SMreBs and *Bacillus* MreBs revealed significant differences in functions such as protofilament interactions, ATP hydrolysis, and membrane binding. These features may support the SMreBs have adopted functions responsible for the unique mechanism of *Spiroplasma* swimming.

20429O 遺伝暗号における適応度地形の解析
Analysis of the fitness landscape of the genetic code

Yuji Omachi[1], Nen Saito[1], Chikara Furusawa[1,2] ([1]*Grad. Sch. Sci. UTokyo*, [2]*RikenBDR*)

The genetic code is the rule to translate one codon into one amino acid. Almost all the organisms share the same genetic code, which is termed as the standard genetic code (SGC). It was suggested that the SGC is evolutionarily optimized to minimize translation errors or mutations. To understand how robust and how unique the SGC is, comparisons between SGC and randomly generated genetic codes in computer simulation is a comprehensive approach. In this study, we apply multicanonical Monte Carlo to efficiently sample random genetic codes with high robustness. Using this method, we discuss the fitness landscape of genetic codes and the optimality of SGC.

20430O ~Parasite による Host 多様化の促進~ 原始的な多様性は如何にして生まれたか？
Host diversification promoted by parasites: prebiotic diversity in evolution

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Existent lives have been diversified such as ecosystems. Here, they are involved in complicated interactions, and these often essential for sustainable coexistence of diversified lives. In prebiotic world as well, diversification is a general phenomenon, for it is needed to complicate functions so that self-replicatable RNA (host) suggested in RNA world evolved to present complex lives. In this study, we discuss how prebiotic diversity expands with examining host evolution. In this evolution, parasitic RNAs endangering hosts appear. As a result of simulation work, asymmetric resistance against parasites is essential for initial diversification of host. This was observed in a long-term evolution of host. Hereafter, we will evaluate how larger diversity emerges.

20431P Selection originating from protein stability/foldability: Relationships between protein folding free energy, sequence ensemble and fitness

Sanzo Miyazawa

Assuming that mutation and fixation processes are reversible Markov processes, we prove that the equilibrium ensemble of sequences obeys a Boltzmann distribution with $\exp(4N_e\, m(1 - 1/(2N))$, where m is a Malthusian fitness and N_e and N are the effective/actual population sizes. On the other hand, the maximum entropy model indicates a Boltzmann distribution with $\exp(-\psi_N)$ for homologous sequences, and a protein folding theory does a canonical ensemble with $\exp(-\Delta G_{ND}/(k_B\, T_s))$ or $\exp(-G_N/(k_B\, T_s))$ for a constant amino acid composition; ψ_N is the sum of one body and pairwise interactions, and ΔG_{ND} is a folding free energy. Based on the equilvalency among these quantities, T_s and protein evolution are analyzed for some proteins. (DOI:10.1016/j.jtbi.2017.08.018)

20432P 自己集合ペプチドのオリゴマー形成に関する分子動力学的解析
Capturing oligomerization process of self-assembly peptides by using molecular dynamics simulations

Kota Kasahara[1,3], Junya Okigawa[1], Hiroki Terazawa[2], Qilin Xie[3], Satoshi Goto[2], Hayato Itaya[2], Katsufumi Nakayama[3], Takuya Takahashi[1] ([1]*Coll. Life. Sci., Ristumeikan Univ.*, [2]*Grad. Sch. Life Sci, Ritsumeikan Univ.*, [3]*Coll. Pharm. Sci., Ritsumeikan Univ.*)

Although self-assembly peptides are of interest in biophysics, the molecular details of assembly formation are still unclear, especially for its oligomerization process. Here, we studied oligomerization process of self-assembly peptides including 8-residue segment in amyloid-βby using our original molecular dynamics (MD) method, named VcMD. As a result, higher stability of β-sheet structures was observed in models with higher number of peptides. In addition, the model consisting of four peptides energetically favored the states with two-stranded β-sheet surrounded by two unstructured peptides rather than three- and four-stranded β-sheet. This implies non-specific interaction of unstructured peptides enhances formation of β-sheet.

20433P* Protein Data Bank に基づくタンパク質-ペプチド結合予測のための相互作用パターンの網羅的な分類と分析
Comprehensive classification and analysis of interaction patterns for protein-peptide binding prediction based on the Protein Data Bank

Keiichiro Sato[1], Kota Kasahara[1,2], Takuya Takahashi[1,2] ([1]*Grad. Sch. Life Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*)

The molecular principles for protein-peptide specific recognition is poorly understood. Although many studies have tackled this problem based on structural information stored in the Protein Data Bank (PDB), it is difficult to extract knowledge about rules of specific interactions from the PDB. Here, we have applied a pattern recognition technique to classify molecular interactions comprehensively by focusing on the spatial distribution of ligand atoms around a receptor residue. As a result, we found 2,771 interaction patterns. Statistics on the non-redundant dataset showed that approximately 50% of the peptide atoms interacted with at least one interaction pattern. In addition, they interacted with one of 1,838 interaction patterns.

20434P 演題取り消し

20435P* 荷電性残基の分布がタンパク質の液-液相分離に与える影響の解明に向けた分子動力学シミュレーション
Molecular dynamics simulations to dissect effects of charge distributions in protein sequence on the liquid-liquid phase separation

Hiroki Terazawa[1], Junya Okigawa[2], Kota Kasahara[2], Hiroshi Imamura[2], Minoru Kato[2], Takuya Takahashi[2] ([1]*Grad. Sch. Life Sci, Ritsumeikan Univ.*, [2]*Coll. Life Sci, Ritsumeikan Univ.*)

Liquid droplets of proteins formed by liquid-liquid phase separation (LLPS) are known to have important roles in living cells. However, little is known for the mechanisms of how charged amino acid residues work in the droplet formation. Here, we conducted coarse-grained molecular dynamics simulations to analyze the effects of charged amino acid residues on the phase behaviors of proteins by mutating the sequence to have diverse charged distributions. As a result, sequences which have localized charges formed droplets with sea-urchin like morphology while those with spread charge distributions did not. In addition, we found that electrostatic interactions between oppositely charged residues enhance LLPS. Our results imply charge distribution is a key factor of LLPS.

20436P 分子動力学シミュレーションによるアクチン構造ゆらぎの解析
Structural flexibility of actin studied by molecular dynamics simulation

Ryotaro Koike, Motonori Ota (*Grad. Sch. Info., Nagoya Univ.*)

Actin is one of the abundant proteins within a cell, and polymerizes to a filament. In the polymerization, actin changes its structure from the globular (G) form to the filamentous (F) one. Actin also adopts two distinct forms; open (O) and cofilin-bound (C) forms. The structural changes among these forms are fundamental to the functional cycle of actin. We performed molecular dynamics simulations of actin in several different states and examined the structural flexibilities using principal component analysis. We found that each of three major components in the F form correlates with the structural transition of G-F, G-O and F-C forms, respectively. This result indicates that three distinct fluctuations are essential in the functional transitions.

20437P* PC4 天然変性領域の VP16 結合の制御メカニズムの解明
Simulation study of the mechanism of PC4 unstructured region which regulates binding with VP16

Qilin Xie[1], Kota Kasahara[2], Masafumi Nakayama[1], Takuya Takahashi[2] ([1]*Coll. Pha Sci., Ritsumeikan Univ.*, [2]*Coll. Life Sci., Ritsumeikan Univ.*)

The transcriptional cofactor PC4 has an unstructured region in the N-terminal domain (PC4ntd). Previous studies reported that the C-terminal domain of PC4 (PC4ctd) binds to VP16, and PC4ntd regulates this binding. However, the mechanisms at the atomic level are not clear. This study investigates the mechanisms of VP16 binding regulation using the virtual-system coupled canonical molecular dynamics (VcMD) method. We constructed the simulation model including the PC4-VP16 complex and a peptide derived from PC4ntd. Conformational sampling was enhanced along with the intermolecular distance between PC4-VP16 complex and PC4ntd peptide to study how PC4ntd interacts to the complex. As a result, we found direct interactions of the Lys residues in the Lys-rich region of PC4ntd.

20438P ウニ初期胚の核及び核内動態の蛍光イメージング観察・解析
Imaging analysis of inter- and intra-nuclear dynamics of sea urchin embryo

Miko Imada[1], Ayaka Sugiyama[2], Sayaka Hayashi[2], Kaichi Watanabe[1], Yuhei Yasui[1], Naoaki Sakamoto[1], **Akinori Awazu**[1] ([1]*Dept. Math and Life Sciences*, [2]*Dept. Math and Life Sciences*)

During early developmental processes of animals from fertilization to cell differentiations and morphogenesis, cell nuclei and intra-nuclear structures change in their structural features through various dynamical processes. In this study, the detailed imaging analysis of nuclei and cell-dependent chromosome structures and dynamics in sea urchin embryo were performed to consider the regulatory relationships between the progress of developmental stages as multicellular system and cell nuclear states-dependent gene regulations of each cell.

20439P 不凍タンパク質の予測及び解析
Prediction and analysis of antifreeze protein

Ryosuke Miyata, Kentaro Shimizu, Tohru Terada, Yoshitaka Moriwaki (*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

Antifreeze protein (AFP) is a protein that contributes to the maintenance of life by preventing recrystallization of ice in the living body. In addition, AFP is widely used in industries such as food processing, cryopreservation of foods, tissues and organs, medical treatment, and development of antifreezing materials. In this study, we collected a wide range of AFP sequences from UniProtKB and developed a predictor of AFPs from amino acid sequences. The features used for the prediction are amino acids, amino acid dipeptides, several AAindeces, and Composition, Transition, Distribution (CTD) patters. We also investigate the important characteristics of AFPs by analyzing the features that contributed to the prediction.

20440P 酵母の胞子形成の時系列マイクロアレイデータに対する効果的な非階層的クラスタリング手法開発の検討
Consideration of efficient non-hierarchical clustering method for time series microarray data of sporulation of S. cerevisiae

Aoi Tani[1], Masahiro Sugimoto[2], Takanori Sasaki[1] ([1]*Fac. Adv. Math. Sci., Meiji Univ.*, [2]*RDCMIT, Tokyo Med. Univ.*)

On the development of organism, the expression levels for specific genes change with time. In this study, we aimed at efficient clustering for time series microarray data of sporulation of S. cerevisiae, and applied clustering method which combined two kinds of non-hierarchical methods. Specifically, k-means++ which determines initial values by weighted probability distribution and c-means method which calculates membership values for each cluster were partially applied. By clustering for all 6,118 genes of S. cerevisiae by k=28, DESs contained related genes for sporulation were grouped together in 3 clusters. In this presentation, we will discuss whether DEGs in each cluster corresponds to the functional genes in each step during sporulation (early, middle, and late).

20441P DTX: 新規ヒト創薬ターゲット探索のための統合化ウェブツールの開発
DTX: An integrative web tool for exploring new potential drug targets in humans

Atsushi Hijikata, Masafumi Shionyu, Tsuyoshi Shirai (*Facult. Biosci, Nagahama Inst. Bio-Sci. Tech.*)

One of the major bottlenecks of the new drug development is identifying the potential targets for intervention. To tackle this problem, we have developed a new web tool, named Drug Target eXcavator, shortly DTX (http://harrier.nagahama-i-bio.ac.jp/dtx/), for identifying potentially new drug targets by integrating information of relations among diseases, therapeutic drugs, disease-related genes/proteins as well as drug target proteins. The DTX interface enables to search for paths from a disease to a drug by using the relation among them. We found that 9,036 disease-drug pairs were connected by one of 13 patterns of the shortest paths. Systematic analyses with DTX would reveal hidden relations among the proteins would be important for an efficient drug target discovery.

20442P DR-SIP: Predicting the Quaternary Structures of Homo-oligomeric Transmembrane Proteins

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Proteins commonly form quaternary complexes to perform their biological functions. The main computational method used to predict these complexes is molecular docking which is mostly limited to predicting dimers. Here we introduce a new docking protocol, Distance Restraints- and Cyclic Symmetry-Imposed Packing (DR-SIP), which can predict the quaternary structures of homo-oligomeric transmembrane proteins (HoTPs) of any size (dimers or larger) without prior-knowledge of its native size. DR-SIP is able to recover 52.6% and 76.3% of HoTPs within the top-20 poses when given/not-given the complexes' native size, respectively. Predictions can be further improved by making use of distance-based experimental data such as those from single-molecule FRET (smFRET).

20443P 機械学習を利用した scRNAseq からの空間的遺伝子発現パターンの再構成
Prediction of spatial gene expressions from scRNAseq data by machine learning

Yasushi Okochi[1,2], Shunta Sakaguchi[3], Ken Nakae[4], Takefumi Kondo[3,5], Naoki Honda[1,6,7] ([1]*Laboratory for Theoretical Biology, Graduate School of Biostudies, Kyoto University*, [2]*Faculty of Medicine, Kyoto University*, [3]*Laboratory for Cell Recognition and Pattern Formation, Graduate School of Biostudies, Kyoto University*, [4]*Graduate School of Informatics, Kyoto University*, [5]*K-CONNEX*, [6]*Research Center for Dynamic Living Systems, Kyoto University*, [7]*Theoretical Biology Research Group, ExCELLS*)

Decoding spatial transcriptomes has become a fundamental technique for understanding multicellular systems; however, existing computational methods lack both accuracy and biological interpretability due to their model-free frameworks. Here, we introduced a model-based method to integrate scRNA-seq data with reference in situ hybridization data. To calibrate differences between these datasets, we developed a biologically interpretable model that uses generative linear mapping. Perler accurately predicted the spatial gene expression from scRNA-seq data. Furthermore, the reconstructed transcriptomes did not over-fit the ISH data. These results demonstrated that Perler is a biologically interpretable framework for accurate reconstruction of spatial transcriptomes.

20444P 蛍光増強 RNA アプタマーと cDNA ディスプレイを用いた高感度抗原検出法の開発
Development of a highly sensitive antigen detection method using fluorescence-enhanced RNA aptamer and cDNA display

So Higashide, Naoto Nemoto (*Graduate School of Science & Engineering, Saitama-University*)

Immuno-PCR is a high-sensitive antigen detection method by combining the specific antibody-antigen reaction with PCR amplification. However, the linking of DNA with antibody on a one-to-one basis is complicated and PCR is not easy to use outside the medical sites and laboratories. Thus, a convenient highly sensitive antigen detection method has been required. The cDNA display is a linking method which a protein conjugate with its coding cDNA on a one-to-one basis via a puromycin molecule. A fluorescence enhanced RNA aptamer can enhance the fluorescence of a specific dye neary 1000-fold by binding the dye. In this presentation, we will report a new method for easy and high-sensitive detection of a target antigen without PCR by combining the RNA aptamer with cDNA display.

20445P 機械学習を用いた PLP 結合タンパク質の予測
Prediction of PLP-binding proteins by using machine learning-based methods

Masafumi Shionyu, Tomohiro Hatta, Atsushi Hijikata (*Fac. Biosci., Nagahama Inst. Bio-Sci. Tech.*)

Pyridoxal 5'-phosphate (PLP) is an important co-factor for proteins involved in many kinds of metabolic pathways, especially amino acid metabolism. Although homology-based methods predicts many PLP-dependent proteins so far, there are limitations with this approach. To predict novel PLP-binding proteins in homology-independent manner, we constructed a machine learning model with residue-wise features such as PLP-binding propensity, surface geometry, and site conservation. Our model showed better prediction performance for PLP-binding residues compared with other methods including template-based and deep learning-based methods. Furthermore, our model showed higher sensitivity in detecting PLP-binding proteins than the template-based method.

20446P Formation of chromatin remodeler Chd1-ADP-Pi analogues ternary complexes which mimic transient states in ATPase cycle

MD Noor A Alam, Sadakane Kei, Maruta Shinsaku (*SOKA UNIVERSITY*)

Chromatin remodeler Chd1 is one of the ATP driven motor protein moving along DNA to promote gene transcription. However, the motor mechanism at molecular level is still obscure. In this study, we analyzed the properties of the Chd1-ADP-Pi analogues ternary complexes which mimic transient states in ATPase cycle in order to clarify how ATP chemical energy transduced to motor activity. The catalytic domain of yeast CHD1 was expressed by using E.coli expression system. This catalytic domain shows DNA stimulated ATPase activity. In the presence of Pi analogues (AlF4-,BeFn, Vi) the Chd1-ADP-Pi analogues ternary complexes were formed. And the stability of the complexes was monitored with fluorescently labelled ADP analogue, Mant-ADP or NBD-ADP.

20447P 細胞イメージングへの応用のための蛍光増強アプタマーの開発
Development of fluorescence enhancement aptamers of dye for cell imaging applications

Tomoyuki Koike[1], Takashi Kubo[1], Kenjiro Hanaoka[2], Mitsuyoshi Ueda[3], Koichi Kuroda[3], Naoto Nemoto[1] ([1]*Graduate School of Science and Engineering, Saitama University.*, [2]*Graduate School of Pharmaceutical Sciences, The University of Tokyo.*, [3]*Graduate School of Agriculture, Kyoto University.*)

Although fluorescent proteins widely used for cell imaging as a fusion protein, they may affect the function of its fused protein due to their large molecular weight (~ 30 kDa). Further, it takes time to form the chromophore, which makes it difficult to observe the protein expression in real time. In a previous study, fluorescent labeling technologies such as FlAsH have been developed. One of these technical features is the fluorescence property change by binding of small molecules such as a pair of a peptide aptamer and a dye. Therefore, in this study, we focused to develop a novel fluorescent probe, a small molecule such as a dye that acts as a fluorescence quencher, with a peptide aptamer that changes the fluorescence property of the dye by binding to the dye.

20448P* マルチタスク学習を用いたタンパク質-リガンド結合部位の統合的な予測
Integrated prediction of protein-ligand binding sites using multi-task learning

Haruka Nakashima, Yoshitaka Moriwaki, Tohru Terada, Kentaro Shinizu (*Dept. of Biotechnol., Grad. Sch. of Agri. and Life Sci., Univ. of Tokyo*)

The prediction of protein-ligand binding sites is important for understanding cellular mechanisms and functions, and is useful for drug discovery and design. In this study, we developed a new prediction method using a multi-task learning approach to predict binding sites of multiple types of ligands. In the multi-task learning, the tasks which are related to each other are learned jointly; they share the common network architectures. It enables to improve prediction accuracy for ligands that are difficult to predict with conventional machine learning-based methods due to the small number of data. We present the results when applying the multi-task learning to multiple types of mono nucleotide ligands.

20449P 電顕フィッティング計算のための高速な原子モデルの GMM への変換：PCA ボックスダウンサンプル法
Fast calculation of Gaussian mixture models for atomic models to fit them on electron microscopy map: PCA-box down-sampling method

Takeshi Kawabata, Haruki Nakamura, Genji Kurisu (*IPR, Osaka U.*)

Gaussian mixture model (GMM) is useful to approximate an atomic model and a 3D electron microscopy map for fast fitting calculation. However, the standard EM algorithm requires a large computation time to convert many voxels or atoms into GMM. For quick map-to-GMM conversion, we have proposed a down sampling method by merging neighboring voxels. We developed a similar down sampling method for quick atoms-to-GMM conversion. Atoms are grouped by chains or secondary structures, then further divided into subgroups by rectangular boxes defined by PCA axes. Each atomic subgroup is represented by one anisotropic Gaussian function. The algorithm has been implemented in gmfit program, users can quickly fit atomic models on a map without performing gmconvert program.

20450P* GPCR オリゴマーに影響を及ぼすがん関連ホットスポット変異の予測
Prediction of cancer associated hotspot mutations that affect GPCR oligomerization

Sakie Shimamura[1], Vachiranee Limviphuvadh[2], Hiroyuki Toh[3], Wataru Nemoto[1] ([1]*Dept. Sch. & Tech., Tokyo Denki Univ.*, [2]*A*STAR, BII.*, [3]*Sch. of Sci. & Tech., Kwansei Gakuin Univ.*)

Oligomers of G Protein-Coupled Receptors (GPCRs) are closely related to their biochemical and biological functions and have been conserved during the course of molecular evolution. The mechanisms of GPCR interactions, and the reason why GPCRs interact between themselves, have remained unclear. In addition, some GPCRs are associated with diseases. We have developed a support vector machine-based method to predict interacting pairs for GPCR oligomerization, by integrating the structure and sequence information (GGIP) [Nemoto et al. Proteins. 2016]. In this work, we have applied GGIP to predict cancer associated hotspot mutations that affect GPCR oligomerization by comparing the results for a wild type sequence pair and a pair including at least one mutated sequence.

20451P Remodelers exploit spontaneous nucleosome fluctuations to reorganize chromatin

Giovanni Brandani, Shoji Takada (*Kyoto University, School of Science*)

Chromatin remodelers are molecular machines that consume ATP to slide nucleosomes along the genome, and modify the organization of chromatin. Their activity is essential for the regulation of gene expression, but their mechanism remains poorly understood. We performed all-atom MD simulations to reconstruct the pathway of DNA sliding in the absence of active remodeler. Preliminary results show that sliding involves the formation of twist-defect deformations similar to those observed in a recent cryo-EM structure of a nucleosome-remodeler complex. Our results suggest a model where remodelers reorganize chromatin by exploiting the spontaneous fluctuations of the nucleosome structure.

20452P 電顕画像と立体構造情報との照合による膜タンパク質ファミリーの判別技術開発
Development of membrane protein family identifier by collating EM images and atomic coordinate data

Ryuji Shinozaki[1], Masami Ikeda[2], Chikara Sato[3], **Makiko Suwa**[1] ([1]*College of Sci. and Eng., Aoyamagakuin Univ.*, [2]*AIRC, AIST*, [3]*Health med., AIST*)

Membrane proteins play important roles such as transporting signals while interacting with each other. We aim to develop a method that infers the protein family from EM (electron density microscope) images on the cell surface by comparing pseudo-EM images with the actual EM images. The 1,375 PDB structures were converted to the pseudo-EM images. Based on them, we developed three kinds of family identifiers using atom density, structural feature, and deep learning. Their discrimination accuracies for known EM images were evaluated by the correct/incorrect threshold based on the Youden's index, and the sensitivity. The best method is atom density matching, that can identify families from actual EM images with a probability of 87.8% if this shows score above the threshold.

20453P Analysis of Genetic Variants Through Protein and Residue Sociability

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Protein-protein interactions are essential for many biological processes, and the alteration of their binding properties can be critical for life. We have maintained a protein-protein interaction database PISITE (Protein Interaction SITE) and introduced a concept of protein- and residue-level “sociability” by counting the number of different interacting partners. Here we employ PISITE to understand the effect of recently identified human variants from the viewpoint of protein interactions and residue sociability. It was confirmed that proteins or interfacial residues with high sociability seemed to be more crucial, as the pLoF (LOEUF) scores of sociable proteins were higher than non-sociable ones and less non-synonymous variants were mapped onto sociable residues.

20454P* タンパク質機能部位予測に適切な相同配列群選択手法の構築
Construction of a set of appropriate homologous sequences to predict functional regions of a protein

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Evolutionary information depends on the set of sequences in multiple sequence alignment (MSA). We previously developed an index to evaluate the appropriateness of the set of sequences for functional region prediction by quantifying spatial autocorrelation of conservation scores [Nemoto & Toh, BMC Struct Biol, 2012]. The set of homologous sequences with the maximum index was adopted for the prediction among the candidate sequence sets. The candidate sets were constructed by gradually adding distantly-related sequences to the set including closely-related sequences without considering the topology of a phylogenetic tree. In this study, we have improved the way to construct the candidate sets by considering the topology of a phylogenetic tree.

20455P* 転写翻訳系とゲノムが同種の無細胞ゲノム転写翻訳系の確立
In vitro genome transcription-translation system using Escherichia coli systems

Yukino Matsui, Tatsuki Deyama, Nobuhide Doi, Kei Fujiwara (*Dept. Biosci. Info., Keio univ.*)

Reconstitution of a living cell from biomolecules is one of the challenging subjects in synthetic biology. Our previous study showed that in vitro transcription-translation (TX-TL) system can work with a bacterial genome by synthesizing the several proteins encoded in the genome, whereas the TX-TL system and the genome were derived from the different organism from each other. This study aims to reconstitute a cell-like transcriptome and proteome from the extracted or purified components of the E. coli using its genome as a DNA template. We successfully detected the synthesis of RNA and proteins encoded in the E. coli genome both in vitro and in liposomes. The details of the results and further challenges to realize the reconstitution of a living cell will be discussed.

20456P A comparative study of external morphology and phylogeny in the two species of earthworms

Hayato Endou (*Oyama Highschool*)

Protect the richness of land" is one of the 17 Sustainable Development Goals (SDGs). Earthworms are extremely important animals for protecting the richness of land. Here, we focused on the taxonomy of two species, Metaphire hilgendorfi and Amynthas yunoshimensis. These species are orthotopically inhabited and morphologically similar. We collected 22 earthworms from a site in Nikko in the Tochigi Prefecture and analyzed them based on their external morphology and the nucleotide sequences of the COI gene of their mitochondrial DNA. The morphological analysis showed that they were divided into 3 groups, whereas the nucleotide sequence analysis showed that they were divided into 4 groups, suggesting that M. hilgendorfi and A. yunoshimensis are reproductively isolated.

20457P Protein-Protein interaction patterns distinguish the hearing-loss phenotype between syndromic and non-syndromic types

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Many variations of human genes are related to hearing loss. The type of hearing related-diseases can be categorized into syndromic and non-syndromic according to the appearance with other abnormalities besides hearing loss. Notwithstanding the clinical description, the distinction of the genotypic characteristics between syndromic and non-syndromic diseases remains uncertain. In this study, we report that the syndromic hearing-loss related proteins interact with a broad spectrum of proteins compared to non-syndromic proteins. The non-syndromic hearing-loss related proteins tend to be involved in specific biological processes, whereas the syndromic proteins are ubiquitously expressed and involved in much broader biological processes related to both hearing and others.

20458P* PLA2 産生に関与する遺伝子と経路の同定
Identification of the genes and pathways responsible for PLA2 production

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We iterated NTG-based mutagenesis in Streptomyces lividans 1326 to obtain ten mutant strains with increase in PLA2 production. Their genome sequences were analyzed to identify mutant genes involved in efficient PLA2 production. We tried to identify how these mutations were involved in the efficient production using the KEGG pathway. However, 80% of the mutations were not assigned to any genes corresponding to the proteins on the pathways. We integrated KEGG pathways with the protein-protein interaction network in STRING. As a result, 98.2% of the mutated genes were assigned to a node on the pathways. We observed the accumulation of the mutations to genes corresponding to enzymes on these pathways, or to genes corresponding to proteins that interact with those enzymes.

20459Q 栄養構造を持つ 12 種微生物の人工生態系における確率現象
Stochastic phenomena in synthetic ecosystems of 12 microbial species with a trophic structure

Kazufumi Hosoda[1], Naomi Murakami[1], Shigeto Seno[2], Yutaka Osada[3], Hideo Matsuda[2], Chikara Furusawa[4], Michio Kondoh[5] ([1]*ITGP, Osaka univ.*, [2]*IST, Osaka univ.*, [3]*FRA*, [4]*Sci, Univ. Tokyo / BDR, Riken*, [5]*Life sci, Tohoku univ.*)

Stochastic phenomena in ecosystems are important to humanity. In this study, we investigated probabilistic phenomena of synthetic ecosystems composed of 12 microbial species with a trophic structure. We observed some probabilistic phenomena due to factors that are important also in natural ecosystems, such as the discreteness of the population of a keystone species, and a complex oscillation that was not reproduced by each of the two species. Our experimental system is reproducible and controllable, and we can test 10,000 ecosystems at the same time. The system will contribute to understanding not only stochasticity but also various aspects of biological dynamics, as an experimental system that includes multiple hierarchical levels, from molecules to ecosystems.

20460Q 蝶の模様の多様性と複雑性は、やわらかい要素やかたい要素を組み合わせて進化してきた
Combinations of flexible and fixed components facilitate colorful divergence and complexity in butterflies

Takao Suzuki (*Grad. Sch. Sci., Univ. Tokyo*)

How diversity and complexity of morphological structures have arisen is one of the fundamental questions of evolving living systems. Previous studies focused on how structures are decomposable into subcomponents: however, little attention has been paid to how such subcomponents are assembled. Here we used a large-scale data of butterfly wing patterns (275 species within the whole of a subfamily), and revealed that combinatorial logic in the evolution of wing patterns. Notably, flexible components facilitate species diversity of color patterns, whereas hierarchically-fixed components increase complexity of color patterns. Our studies have begun to reveal a combinatorial building logic in the evolution of morphological structures.

20461Q 大阪府の石川における外来のアメリカツノウズムシの繁殖生態
The breeding ecology of the invasive alien Planaria, Girardia dorotocephala, in the middle reaches of the Isikawa river in Osaka Pref

Sakura Takahashi (*Osaka Pref. Tondabayashi H.S.*)

The breeding ecology of the invasive alien Planaria, Girardia dorotocephala, in Japan is unknown, so I conducted a study on it in the middle reaches of the Isikawa river in Osaka Prefecture. I researched the population, body structure, and spawned eggs, from winter to summer of 2020. I found individuals created by asexual reproduction during this whole period, but I did not confirm the breeding season for primarily sexual reproduction. When I observed asexual reproduction in captive breeding, their tails separated from their bodies, and the separated tails did not move until the eyes were formed. I thought this improved the survival rate. I will continue to conduct field research to find out about and share information on the breeding ecology of this species in Japan.

20462Q マミズクラゲの無性世代の 2 つの芽体を決める生息条件について
The habitat conditions determined two types of sprout formation of the asexual generation of Freshwater jellyfish, Craspedacusta sowerbii

Yuki Tanino, Yuta Hirayama, Sota Moriyama (*Osaka Pref.Tondabayashi H.S.*)

Freshwater jellyfish, Craspedacsta sowerbii, inhabits freshwater ponds and has two generations: sexual and asexual. The asexual generation of this species has two types of sprout formation: predatory polyps and non-predatory frustules. We hypothesized polyps may form frustules and move when their habitat becomes poor because they don't move. We focused on feeding conditions and observed sprout formation under different feeding frequencies. We found, at a higher frequency, polyps proliferated and formed colonies, but at a lower frequency, frustules were formed and began to move. This result suggests they may form frustules that help them to move if the habitat conditions deteriorate. We want to conduct experiments under different water quality conditions in future.

20463Q 金剛山地(大阪府)におけるヨツワクガビルの生息環境について
The Habitat of the Orobdella whitmani Oka in the Kongo Mountains (Osaka pref.)

Yuya Uenishi (*Osaka pref. Tondabayshi H.S.*)

Gastrostomobdellidae is large leeches which can grow up to about 30cm long. It`s difficult to spot it and much behavior is shrouded in mystery except its dietary habit of eating worms. Therefore, in order to find the area where they live, I went to many points throughout the Kongo Mountains where it is believed they can , and surveyed the vegetation, the soil of the forest floor and distances from streams to their homes. I found Orobdella whitmani Oka under a stone nearby a waterfall in a broadleaf forest at an elevation of about 600 m. I also found worms at nearby sites. The illuminance was low and the humidity was high at this point. Based on the above, their food source and other conditions may be closely related to the habitat of this species.

20464Q 大阪府で初めて繁殖を確認したイワナ Salvelinus leucomaenis の生態とその由来の研究
The study of the ecology and origin of Salvelinus leucomaenis that has been confirmed to breed for the first time in Osaka prefecture

Kanato Nakamura, **Kaito Oana** (*Osaka pref. Tondabayashi H.S.*)

The genus Salvelinus is a fish that inhabit cold regions of the world. We found Salvelinus leucomaenis in the Chihaya River which is at an altitude of about 600 meters in the Kongo Mountain (Osaka Pref.). Because we found them freshly hatched, it is highly probable that they are breeding there. In Japan, they disperse through rivers at high altitudes by getting left behind. There is also the possibility that they naturally dispersed, but it is also possible that they escaped from a downstream fishing pond. This is the first time it has been confirmed that the genus Salvelinus breeds in Osaka Prefecture. It is worth studying their ecology and origin in the southernmost parts of the world. Hereafter, we plan to do DNA analysis in addition to fieldwork.

20465Q 三面コンクリート張り水路でゲンジボタルが生息できる理由
Reasons why Japanese Firefly, Luciola cruciate, can inhabit in a three-sided concrete channel

Takumi Matsuo, Tomoki Ikegawa (*Osaka Pref. Tondabayashi H.S.*)

Every year, we can observe the luminescence of the Japanese Firefly, Luciola cruciate, in the Hatada channel, in spite of its three-sided concrete channel. We tried to determine how this species lives in the concrete channel, where habitat conditions are considered to be poor. We investigated the shape of the concrete unit, water flow velocities, and sediment deposition, as well as the larvae of this species. The velocity of the channel was relatively high, but the velocity was reduced in the wider units, and sediment was deposited there, allowing this species to inhabit it. Based on the above, it is suggested that a mechanism for water flow deceleration and sediment deposition is necessary to create a habitat for this species in concrete channels.

20466Q 海浜植物のハマヒルガオが浜辺で生育できる理由
Reasons why the beach plant, Calystegia Soldanella, can grow on the beach

Kei Yanazawa (*Osaka Pref. Todabayashi H.S.*)

We observed, the water plant, Egeria Densa, the vegetable lettuce, Lacyuca Sativa, the beach plant, Calystegia Soldanella, and the seaweed, Ulva Ulva in four different salt solutions. E.Densa and L.Sativa became softer and weighed less, while C.Soldanella and U.Ulva showed no change in consistency. There was no change in the epidermal cells of C.soldanella, but the cells inside its epidermis became smaller when they were immersed in salt solutions. Thus, while plants other than U.Ulva are damaged to by salt solutions with the reduction of cell size, we consider that the C.Soldanella was protected by an epidermis that was not affected by salt solutions. This led us to conclude that this plant could grow in a place where it gets splashed with seawater.

20467Q ドジョウの繁殖行動を誘発するトリガーについて
Triggers that trigger breeding behavior in loaches, Misgurnus anguillicaudatus,

Yohei Okugawa (*Osaka Pref. Tondabayashi H.S.*)

It is known that loaches, Misgurnus anguillicaudatus, migrates to wetlands during rising waters to spawn, but the trigger for migrating is unknown, so I conducted this study to try to determine it. Once a month, I tried to collect samples of this species in an agricultural canal that branches off a river. The channel was separated from the main stream until May, and many loaches could be collected, but in June it was connected to the rising main stream, and few loaches could be collected. I placed the mature loaches and dry soil in the tank and observed their subsequent behavior. They were active immediately after adding soil, but did not spawn. it is possible that changes in water quality caused by river rising and soil inputs may be a trigger for breeding behavior.

20468R Fisher 情報量による ERK リン酸化ダイナミクスの熱力学的性質の解明
The Fisher information of time reveals the thermodynamic property of ERK phosphorylation dynamics

Keita Ashida[1], Yohei Kondo[2,3,4], Kazuhiro Aoki[2,3,4], Sosuke Ito[1,5] ([1]*Universal Biology Institute, The University of Tokyo*, [2]*Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Science*, [3]*National Institute for Basic Biology, National Institutes of Natural Sciences*, [4]*Department of Basic Biology, School of Life Science, SOKENDAI*, [5]*JST, PRESTO*)

It is important to understand the thermodynamic property of biological systems. Here, we introduce information geometry to investigate the thermodynamic property of the extracellular signal-regulated kinase (ERK) activation dynamics. Information geometric analysis revealed that cell density affected activation and inactivation dynamics of the pulsatile ERK activation, and both thermodynamic cost and transition velocity were higher under the condition of higher cell density. Moreover, the cost and velocity of the activation were higher than those of the inactivation regardless of cell density. Our information geometric approach is useful to understand the thermodynamic aspects of signaling dynamics.

20469R Life-logger, 1000 匹の線虫の寿命時間スケールでの行動動態を計測するためのビデオ撮影装置の開発
Life-logger, a video-recorder of crawling motion of 1,000 *C. elegans* individuals during their lifespan

Yukinobu Arata, Peter Jurica, Yasishi Sako (*Cellular Informatics Laboratory, Riken*)

Animals age and eventually die. Many theories proposed the causes of aging, but have not been tested experimentally. To test aging hypotheses, we developed Life-logger, a video-recording device for crawling motion of more than 1,000 *C. elegans* adults during their lifespan (about one month). From the behavioral time series obtained by Life-logger, we found that the average velocity of the crawling motions continuously decayed and the decay curves fit with an exponential function. Our result supports a model that aging process in *C. elegans* is driven by a simple reaction where molecular or cellular elements in the body are disrupted irreversibly and in one step, such as by an irreversible gene distruption due to the translocation of transposons.

20470R 度数情報だけで再訪性を判断するエージェントのネットワーク探索
A Random walk model on the Scale-Free Network with the Cognitive Biases

Koji Takashima, Tomoko Sakiyama (*Soka University*)

Most networks are scale-free networks with many edges on a few nodes. Since the scale-free network has a complicated structure, random walk models have been developed for the exploring method for paths between specific nodes. The self-avoiding walk model is one of these models for network exploring method. The self-avoiding walk model is a model in which the agent cannot revisit a node for a certain period after it visited that node. However, the self-avoiding model has a problem that the agent cannot return to a hub node immediately, which may lead the agent to staying within a part of the network. In this paper, we propose the self-selection walk model that changes revisit property of the agent according to the degree of the current node.

20471R* 遺伝子発現レベルの情報から ErbB シグナルの動態を予測する数理モデリング基盤の開発
Model-based prediction of ErbB signaling dynamics solely from the information about gene expression levels

Hiroaki Imoto, Marie Maeda, Suxiang Zhang, Mariko Okada (*IPR, Osaka Univ.*)

We developed a novel computational platform to predict the signaling dynamics solely from the information about gene expression levels. We first developed an ODE model describing early transcriptional regulation trigged by ErbB receptor activation. Then, we use gene expression data obtained from the Cancer Cell Line Encyclopedia as an input and trained model parameters against several breast cancer cell lines. After parameter optimization, the model accurately predicted the quantitative behavior of ErbB signals in another cell line. Overall, our work revealed that gene expression level related to ErbB network governs signaling dynamics and might play a key role in determining subsequent cell fate.

20472R Approximation of transition density of the conductance based neuronal model with noise

Takanobu Yamanobe (*Sch. Med., Hokkaido Univ.*)

We derive an approximation of the transition density of the conductance-based neuronal model with noise. The theory of the asymptotic expansion of stochastic processes can apply to approximate the transition density. However, since the gating variables of the stochastic Morris-Lecar model are in [0, 1], the asymptotic expansion does not apply directly. To avoid difficulty, we use the equivalent potential, which transforms grating variables in [0,1] to potentials in R (Kepler et al. 1992). Using the Morris-Lecar model with a diffusion term that approximates synaptic current, we show that the approximated transition density can reproduce the original one with reasonable accuracy.

20473R 人工トリペプチドからなる自己集合性ナノファイバーの進行波による力発生
Force generation by a propagating wave of artificial tripeptide-based fibrous assemblies

Ryou Kubota[1], Masahiro Makuta[2], Ryo Suzuki[3], Masatoshi Ichikawa[2], Motomu Tanaka[3], Itaru Hamachi[1,4] ([1]*Grad. Eng., Kyoto Univ.*, [2]*Grad. Sci., Kyoto Univ.*, [3]*Inst. Adv. Stud., Kyoto Univ.*, [4]*JST ERATO*)

Spatiotemporal patterns that arise from out-of-equilibrium biochemical reactions generate forces in living cells. Despite considerable recent efforts, rational design of spatiotemporal patterns in artificial molecular systems remains at an early stage of development. Here, we describe force generation by a propagating wave of artificial tripeptide-based self-assembled nanofibers. Real-time confocal microscopic imaging visualizes the propagating wave based on spatiotemporally coupled generation and collapse of nanofibers. Moreover, we succeeded to measure the force of this propagating wave, which can move nanobeads along the wave direction.

20474R Quantifying expressive power of gene regulatory systems

Yohei Kondo[1,2], Kazuhiro Aoki[1,2,3] ([1]*ExCELLS*, [2]*SOKENDAI*, [3]*NIBB*)

A gene regulatory system represents a function that transforms environmental signals into gene expression pattern. Thus, it might be reasonable to hypothesize that living organisms have evolutionary optimized functional richness, or expressive power, of their gene regulatory systems. Here we employed learning-theoretic complexity measures such as Vapnik-Chervonenkis (VC) dimension in order to quantify the expressive power. We investigated small feedforward networks with Hill-type activation, and found that the expressive power correlate highly with the information-theoretic efficacy explored in previous studies. This means that high expressive power and information-transmission efficacy could have been acquired as a by-product of the other through evolution.

20475R 質量保存を満たす反応拡散系にみられる相分離的な挙動
Phase-separation like behavior in mass-conserved reaction diffusion systems

Michio Tateno, Shuji Ishihara (*Shuji Ishihara Lab., Graduate School of Arts and Sciences, The University of Tokyo*)

Mass conservation of chemical spices is known as a factor to bring about coarsening of bistable Turing patterns. Recent studies on reaction-diffusion systems with conserved variables (MCRDs) point out that the interfacial curvature between the two states contributes to the coarsening, which is reminiscent of phase separation. Yet, as MCRDs do not presuppose a variational principle and thus, whether description of surface tension is operative for MCRDs or not is largely unknown. Here, we demostrate that droplet patterns forming in MCRDs obey the Young-Laplace equation and coarsen following the evaporation-condensation mechanism. This suggests that in the presence of conserved variables, a surface-tension like quantity nontrivially emerges in reaction-diffusion systems.

20476R Investigation of related genes in the development of atopic dermatitis by geometric feature extraction from gene expression patterns

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Atopic dermatitis (AD) is one of inflammatory skin diseases caused by abnormal immune system genes and less skin barrier function. In this study, we aimed to clarify the co-expression (CX) mechanism of related genes causing AD by discriminant analysis (DA) using geometrically extracted data. As a method, we used DA for comparing similarity ratio of triangle with three randomly chosen differentially expressed genes (DEGs) as vertices between AD patients and healthy people. As a result of DA by using DEGs with high expression significance (top 250), F-measure was 92.6%, improved by about 7.9% compared to only expression data. From the extraction of genes contributed to the accurate discrimination, the CX of genes involved in cell adhesion and glucose import was suggested.

20477R 脳神経系の可塑的結合力学系モデルにおける自己組織的ネットワーク
Self-organized network structures in coupled dynamical system with connection plasticity inspired by cerebral nervous system

Amika Ohara, Masashi Fujii, Akinori Awazu (*Dept. of math. and life sci. Hiroshima univ.*)

Living systems contain various networks and the topological properties of them encode their functions. Additionally, these networks involve the plasticity that changes in the topology of networks through the development, learning, and evolution. The study of coupled dynamical systems with the connection plasticity provides rich insights to reveal the universal aspects of biological networks. In this study, we focused on the network structure formations of a globally coupling map system with the coupling plasticity that reflects STDP in the nervous system. We focus on the formations of various hierarchical networks as observed in cerebral nervous systems. We also reveal the relationship between formed network topology and dynamical property of each element.

20478R ディープラーニング及びオートエンコーダーを用いた乳癌組織中の DEGs からの特徴抽出と予後予測
Feature extraction and prognosis prediction from DEGs in breast cancer tissue using Deep learning and Autoencoder

Yusuke Mizukoshi[1], Masahiro Sugimoto[2], Takanori Sasaki[1] ([1]*Fac. Adv. Math. Sci., Meiji Univ.*, [2]*RDCMIT, Tokyo Med. Univ.*)

Differential Expressed Genes (DEGs) are detected in various cancer tissues with each prognosis and stage, and useful for prediction of those prognosis and stage by machine learning. But, since there are several hundreds of DEGs as feature values, effective feature extraction is needed. In this study, we performed feature engineering from expression data of breast cancer for accurate prognosis prediction by deep learning (DL). Actually, feature extraction by hierarchical clustering (k=20) and Autoencoder was performed on 334 DEGs from 147 breast cancer tissues. As a result, the accuracy of the prediction was reached 91% by DL. Also, clusters and their biological functions involved in cancer progression were predicted by analyzing the weights which connect nodes in DL.

20479R Determination of the interacting time between KaiA and KaiB during clock oscillation

Risa Mutoh[1], Takahiro Iida[1], Mino Hiroyuki[2] ([1]*Faculty of Sci. Fukuoka Univ.*, [2]*Grad. Sch. of Sci., Nagoya Univ.*)

Cyanobacterial circadian clock is composed of three clock proteins, KaiA, KaiB, and KaiC. These proteins interact each other, and the size and stoichiometry of Kai protein complex change during circadian cycle. We previously revealed by electron spin resonance (ESR) analysis that the KaiB directly interacted with KaiA. We prepared 15 Cys-substituted mutants of KaiB with spin labels. ESR results show that one of KaiB -Cys mutants interacted with KaiA C-terminal domain proteins, but not reacted with full length KaiA. By monitoring of the interaction, we observed the spectral change in the mixture of three Kai proteins. and found KaiA-KaiB interaction around 10 h period.

20480R オンチップ単一細胞培養システムによる 3 細胞系心筋ネットワークの拍動同期過程の観察
Observation of synchronized beating cycles of cardiomyocytes during three cell network formation in on-chip single cell measurement assay

Yoshitsune Hondo[1], Kazufumi Sakamoto[1], Rikuto Sekine[2], Yuhei Tanaka[1], Haruki Watanabe[1], Kenji Shimoda[1], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*)

To elucidate how cardiomyocyte select a given stimulus and beat on a single cell level, we investigated beating before and after synchronization constructing a network of spontaneous and non-spontaneous beating cells. We placed two spontaneous beating cells and one non-beating cell on microfabricated agarose patterns and connected them step-wisely and examined their beating interval change before and after the synchronization. We found the non-spontaneous beating cell was synchronized to the network of the two spontaneous beating cells without any influence on the previous network's beating and their fluctuation. The results indicate the addition of non-spontaneous beating cardiomyocyte doesn't contribute to the stability improvement of synchronized beating intervals.

20481R Active Inference of Gradient in Reward-oriented Behavior

WeiQing Chen[1], Naoki Honda[1,2] ([1]*Grad. Sch. Bio., Univ. Kyoto*, [2]*Theoretical Biology Research Group, Exploratory Research Center on Life and Living Systems (ExCELLS), National Institutes of Natural Sciences, Okazaki, Aichi, Japan.*)

In natural environments, animals face uncertainty that the underlying state cannot be directly observed. Thus, animals must constantly take actions to estimate the information of latent state from partial observations, while make a decision for reward. However, how the animals balance between such information- and reward-oriented behaviors remains elusive. We addressed this issues by focusing on C. elegans thermotaxis. When worms are cultivated at a constant temperature with food, they associates temperature with food such that they migrate to that temperature on thermal gradients. We modeled their decision making process by Bayesian-based free energy principle. We showed how the actions are selected by balancing between the information and reward in their behaviors.

20482R 膜タンパク質のクラスター形成機構の数理的研究
A Mathematical study on the mechanism of cluster formation of membrane proteins

Hiroaki Takagi (*Sch. Med., Nara Med. Univ.*)

We have previously performed spatial statistical analysis of the positional data of cAR1 (GPCR) in Dictyostelium cells measured by PALM, and found that the spatial density of cAR1 within 100 nm scale is higher than that of spatially homogeneous distribution, and the cluster size of the number of cAR1 shows power-law like distributions. To explore the mechanism of such spatial distributions of membrane molecules and their functional significance, we mathematically studied models of cluster formation in spatial point processes and their extensions. We examined the conditions for various statistical properties to be realized, and will discuss the possible relationship between the spatial distribution of receptors and the spatial distribution of membrane lipids ("field").

20483R ES 細胞分化初期における染色体動態
The dynamics of chromosomes on early differentiation stage from ES cell

Tetsushi Komoto, Masashi Fujii, Akinori Awazu (*Hiroshima univ. Grad. Sch. Integrated Sciences for Life*)

The genomic activities of mammalian X chromosomes (X chrs) are mutually suppressed to make only one X chr is active in each cell. Such X chromosome inactivation (XCI) enables X chrs number compensation of gene expression level. In mouse embryo, one of two X chrs is inactivated in inner clump of cells on blastocyst stage. The experiment of mouse ES cell suggested that mutual spatial approach of X chrs and localization of X chrs at the nuclear envelope occur after induction of differentiation. On the other hand, the mechanism how X chrs could search their homologous pair in mouse nucleus containing 40 chromosomes is still unclear. In this study, we developed the coarse-grained models of chromosome in mouse ES cell and simulated to unveil this mechanism.

20484R* Inferring domain of Interactions among Dictyostelium discoideum colony from the Ensemble of Trajectories of cells

Udoy S. Basak[1,2], Sulimon Sattari[1], Md. Motaleb Hossain[1], Kazuki Horikawa[3], Tamkiki Komatsuzaki[1] ([1]*Hokkaido University*, [2]*Pabna University of Science and Technology*, [3]*Tokushima University*)

An information-theoretic scheme is proposed to estimate the underlying domain of interactions and the timescale of the interactions for many-particle systems. Based on ensemble data of trajectories of the Vicsek model system, it is shown that using the interaction domain significantly improves the performance of classification of leaders and followers compared to the approach without utilizing knowledge of the domain. Given an interaction timescale estimated from an ensemble of trajectories, the first derivative of transfer entropy averaged over the ensemble with respect to the cut-off distance is presented to serve as an indicator to infer the interaction domain. This approach can also be used to infer the interaction domain of a Dictyostelium discoideum colony.

20485R 栄養の枯渇が引き起こす酵母の解糖系振動現象
Glycolytic Oscillation in Yeast Induced by Nutrient Depletion

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Products in glycolysis of yeast, such as NADH, ATP, GAP, and pyruvate, show concentration oscillations when yeast cells in the stationary phase experience the starvation. In this study, we have investigated effects of the depletion of glucose on the oscillation using yeast cells in lag, log, and stationary phases of the growth curve. Yeast cells in the log phase show the oscillations only after long starvation, whereas they in the stationary phase show the oscillations even after short starvation. Thus, the oscillations in the glycolysis is triggered by the depletion of glucose. We analyze the effect of glucose concentration on the oscillations by theoretical model developed by Wolf and Heinrich, and reveal roles of the glycolytic oscillations in the bacterial life.

20486R ミトコンドリア呼吸鎖エナジェティクスの速度論的解析
Kinetic analysis of energetics in mitochondrial respiratory chain

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Mitochondria synthesize ATP effectively using electrochemical reactions. The other part of energy, which was not used for the ATP synthesis, can drive the series of the electrochemical reactions and can dissipate as a heat finally. We aim to understand the energetic mechanisms in the electrochemical system in mitochondria using both of the model calculations and experiments. We have firstly modeled an electrochemical reaction circuit including redox potentials at each active site in addition to the reaction velocities. The energetic analysis using the model semi-quantitatively represents the efficiency of ATP synthesis and the largest heat production was observed in a complex I. The effects of the decrease in O2 concentration were also analyzed by the model.

20487R Chromatin dynamics in Hox-mediated animal body development

Yoshifumi Asakura[1], Naoki Honda[1,2] ([1]*Grad. Sch. Biostudies, Univ. Kyoto*, [2]*ExCELLS, NINS*)

Hox genes are core factors for animal development of axial body plan. They are linearly arrayed on the genome and expressed in a sequential manner along the body. In spite of the importance of Hox genes, it has been unclear how continuous upstream signals are converted into the discontinuous Hox gene expression. To address that, we mathematically developed a model of the chromatin dynamics coupled with gene expression regulation. We modeled the genome DNA as a series of particles with discrete states corresponding to the epigenetic marks. Our model showed a discontinuous gene expression as observed in Hox genes expression. Therefore, our approach would be powerful to understand the role of chromatin dynamics in the gene regulation of the Hox genes cluster.

20488R エピジェネティック修飾の変化の影響を考慮した EM 遷移のシミュレーション
A model on the effects of epigenetic modification on epithelial-mesenchymal transitions (EMT)

Kenichi Hagiwara, Masaki Sasai (*Dept.Appl.phys.,Nagoya Univ.*)

Epigenetic modifications including histone modifications and DNA methylation are crucial for gene regulation, but their quantitative effects are still unclear. We studied the effects of epigenetic modifications on the epithelial-mesenchymal transitions (EMT), which play a critical role in cancer metastasis. We extended a gene network model of Jolly et al. (Phys Biol 2019) by introducing two new variables that represent histone modifications and DNA methylation. The simulated results showed that the intermediate state of EMT is destabilized and the metastable E or M state is stabilized through the positive feedback of epigenetic modifications. We analyze how the dynamical fluctuations of EMT are affected by the rates and cooperativity in epigenetic dynamics.

20489R Length scale-dependent relaxation in chromatin with and without the transcription factory

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The relationship between genome organization and gene regulation plays a central role in molecular biology. Using single nucleosome tracking data from live cells, it was inferred that chromatin is possibly organized in the form of domains with liquid-like order. Further, it was demonstrated that nucleosome dynamics in the interphase nucleus is enhanced when transcription is suppressed, suggesting that interactions of transcriptionally active RNAPII with droplets/clusters of transcription factors/cofactors, globally constraint chromatin movement. We use a simple toy model of nucleosome-domain organization to calculate the structure factor to understand length-scale dependent relaxations, which we use to infer dynamics at domain length scales during transcription.

20490R 出芽酵母の DNA 二本鎖切断時における染色体動態の数理モデル
A mathmatical model of chromosomal dynamics in budding yeast during DNA double strand break

Shinjiro Nakahata, Akinori Awazu, Masashi Fujii (*Hiroshima univ. Grad. Sch. Integrated Sciences for Life*)

Genome DNA plays important roles of cellular activities, but they are damaged by various stresses frequently. Most serious DNA damage is double-strand-break (DSB) by the radiations. Since the damaged DNA involves the potentials to induce cancer or unproper gene expressions, living organisms have developed various mechanisms to recognize and repair such damages. Recent studies reported various intranuclear behaviors of damaged DNA, for example the damaged DNA site by DSB tends to move to and locate at nuclear periphery in budding yeast. However, the mechanism of such phenomena is still unclear. In this study, we constructed and simulated the mathematical models of normal and damaged genome of budding yeast to reveal the mechanism of such observed DNA repair processes.

20491R Quantifying the length- and time-scales of influence of cells in collective motion

Sulimon Sattari[1], Udoy Basak[1], Md. Hossain Motaleb[1], Kazuki Horikawa[2], Tamiki Komatsuzaki[1] ([1]*Hokkaido University Research Institute for Electronic Science*, [2]*Tokushima Unviersity, Institute of Biomedical Sciences*)

Dictyostelium Discoideum (DD) cells communicate via a chemoattractant called cyclic-AMP (cAMP). Upon starvation, cells signal to one another by emitting a spike in cAMP. In response nearby cells move towards the cAMP gradient and release an additional cAMP spike, resulting in a feedback effect and a spiral wave cAMP pattern. In this study, we analyze the influence of individual cells to interpret the length- and time-scales of interaction using the Morse Potential from molecular dynamics as an example. We apply information-theoretic techniques to identify direct causal relationships between cells and to quantify the timescales, length-scales, and strength of these relationships, and propose a similar scheme to quantify influence in DD cells.

20492R Circular probability currents and correlation functions for gene switching coupled with epigenetic dynamics

Bhaswati Bhattacharyya, Masaki Sasai (*Department of Applied Physics, Graduate School of Engineering, Nagoya University*)

The gene activity in eukaryotes is controlled by binding/unbinding of transcription factors (TFs) and also by epigenetic mechanism like histone modifications. Here, histone modification is affected by the TF binding, which constitutes a feedback loop in self-regulating gene circuits. We investigate the effects of these coupled processes for fast and slow histones/TF switches. Starting from a model involving discrete state changes of histones and TF binding status, we analyze the probability landscapes of a set of continuous parameters related to the histone and TF states. The circular flow of probability on the landscape and a cross-correlation function indicate that the histone state changes prior to the change in the state of TF in the self-regulating circuits.

20493R 植物のストレス応答を担う植物ホルモン時空間動態の数理モデル
Mathematical model of spatiotemporal dynamics of plant hormones responsible for plant stress response

Mariko Arimoto, Akinori Awazu, Masashi Fujii (*Grad. Sch. Sci., Univ. Hiroshima*)

Plants developed the excellent autotrophic and stress responsive systems evolutionally that are regulated by the metabolic and signaling processes of plant hormones and the interaction among them. For example, recent live imaging studies of Arabidopsis thaliana reported that salicylic acid and jasmonic acid, which are an antagonistic relationship, form a concentric pattern on the same leaf in the response to a biotic stress like disease that causes cell death. However, the mechanism and physiological roles of such pattern were still unknown. In this study, we developed a mathematical model of the spatiotemporal dynamics of SA and JA, and our simulation results suggested the importance of the balance of SA and JA mutual inhibitions for SA-JA pattern formation.

20494R 協同的に振る舞う遺伝子発現制御ネットワークの定量的解析
Quantitative analysis of cooperative network from sloppy gene expression dynamics

Masayo Inoue[1], Kunihiko Kaneko[2] ([1]*IMS, Meiji Univ.*, [2]*Univ. of Tokyo*)

Gene expression dynamics satisfying given input-output relationships were investigated by evolving the networks for an optimal response. We had reported that three different types of networks and corresponding dynamics evolved depending on the sensitivity of gene expression dynamics. We also showed the cooperative networks composed with many sloppy and unreliable genes were more functional in terms of robustness and unforeseen challenge. In this presentation, we quantitatively study how and why the cooperative networks achieve the advantages by means of data analysis techniques; principal component analysis with dynamic mode decomposition and dynamics similarity evaluation with dynamic time warping.

20495R ヒトゲノム中の 3 塩基リピート配列周辺エピゲノムとクロマチン構造のゲノムワイドな解析
Genome-wide analysis of epigenetic and chromatin-structural features around triplet repeat sequences in human genome

Kenji Ojima[1], Yuudai Hirose[2], Masashi Fujii[1], Akinori Awazu[1] ([1]*Department of Mathematical and Life Sciences, Graduate School of Integrated Sciences for Life, Hiroshima University*, [2]*Department of Mathematical and Life Sciences, Graduate School of Science, Hiroshima University*)

Human genome consists of around 30 Gbps DNA but contains less than 1.5% regions as protein coding regions. Around 45% regions of the human genome are occupied by various repetitive sequences as typical noncoding DNA regions. Triplet Repeat Sequences (TRS) are simple repetitive sequences consisting of the repeats of a set of 3 base pairs DNA. TRS is classified to 10 types by considering the complementarity of DNA sequences, but the physiological roles of the most of them were still unknown. In this study, we performed the genome-wide analysis of epigenetic and chromatin structural features of/around TRSs in human genome using comprehensive publicly available ChIP-seq, MNase-seq and Hi-C data to unveil the novel functional roles of TRSs.

20496R バクテリアの集団運動による走性の変化
Enhanced bacterial taxis by collective movement

Tatsuro Kai, Takahiro Abe, Shuichi Nakamura, Seishi Kudo, Shoichi Toyabe (*Department of Applied Physics, Graduate School of Engineering, Tohoku University*)

Bacteria modulate "run" and "tumbling" frequencies for realizing taxis, that is, the response to, for example, the chemical, thermal, or photo stimuli. It is known that bacteria cells interact with other cells and exhibit diverse phenomena driven by collective motion. However, it has not been studied extensively how collective motion affects the taxis response. We examined the effect of collective motion on the tactic behavior under a local temperature gradient created by LASER irradiation. We analyzed each cell by tracking it and examining its speed and tumble frequency. We found that the tactic efficiency increased with the cell density, suggesting the enhancement of the taxis by cellular interaction.

20497R Fluctuation distribution of propagation time was conserved during excitation conduction in lined-up cardiomyocyte networks

Kazufumi Sakamoto[1], Yoshitsune Hondo[1], Kenji Yasuda[1,2] ([1]*Dept. Pure & Appl. Phys., Grad. Sch. Adv. Sci. & Eng., Waseda Univ.*, [2]*Dept. Pure & Appl. Phys., Sch. Adv. Sci. & Eng., Waseda Univ.*)

We examined whether the “faster firing regulation” can explain the excitation conduction in cardiomyocyte networks in geometrically controlled constructive environments. We measured the extracellular field potentials by multi-electrode assay and tracked local conduction time of cardiomyocytes in the lined-up cell networks with 100-300-μm wide agarose microstructures. The propagation time of conduction between two neighbor micro electrodes showed Gaussian distribution. The distribution maintained its form regardless of conduction distances up to 2.1 mm, meaning diffusion of propagation of excitation conduction did not occur. The results indicate that the “faster firing regulation” is not sufficient to explain the conserve of the propagation time distribution.

20498R Vector analysis of amoeba motion with respect to the propagation of chemoattractant cyclic-AMP
Vector analysis of amoeba motion with respect to the propagation of chemoattractant cyclic-AMP

Md. Motaleb Hossain[1,2], Sulimon Sattari[1], Udoy S Basak[1], Kazuki Horikawa[3], Tamiki Komatsuzaki[1] ([1]*Hokkaido University*, [2]*University of Dhaka*, [3]*Tokushima University*)

Dictyostelium Discoideum (DD) cells communicate via a chemoattractant called cyclic-AMP (cAMP). Upon starvation, cells signal to one another by emitting a spike in cAMP. In response nearby cells move towards the cAMP gradient and release an additional cAMP spike, resulting in a feedback effect and a spiral wave cAMP pattern. In this study, we use particle image velocimetry on blurred and unblurred fluorescent images of DD to quantify the effect of cAMP wave motion on the velocities of cells. Before the development of the spiral wave, cells move randomly, however after the wave has developed, cells move in a predictable pattern coherently and with higher speed against the direction of the wave as it is passing, and more slowly and randomly after the wave has passed.

20499R* 免疫系の記憶ダイナミクスにおける適応的な抗原の有害・無害識別
Adaptive Discrimination of Risk of Antigens in Immune Memory Dynamics

Kana Yoshido[1], Naoki Honda[1,2] ([1]*Grad. Sch. Biostudies, Univ. Kyoto*, [2]*ExCELLS, NINS*)

The immune system discriminates the risk of antigens to induce reactions with the proper intensity. Harmful antigens induce strong immune responses, whereas harmless ones do not lead to them to prevent unnecessary inflammation. However, how the immune system distinguishes countless antigens as harmful or harmless remains unclear. Towards this question, we developed a computational model of T cell population dynamics. The model simulation showed that the immune system discriminated harmful or harmless antigens based on their temporal dynamics and the discriminative ability can be modified by memory formation depending on the experience of antigens. Thus, our model shed light on the importance of temporal history of antigen exposure on immunological memory formation.

20500R* ERK シグナル伝達系の進化生化学
Evolutionary biochemistry of ERK signaling network

Masaya Mukai[1,2,3], Yohei Kondo[2,3], Kazuhiro Aoki[1,2,3] ([1]*Division of Quantitative Biol., NIBB*, [2]*Quantitative Biol. Group, ExCELLS*, [3]*Dept. of Basic Biol., Sch. of Life Sci., SOKENDAI*)

The Raf/MEK/ERK signaling network is essential for cell proliferation. Empirical perturbation and dynamical simulations suggested that the temporal dynamics of ERK activation is critical. However, it is still unknown what characteristic of the dynamics is important. We assumed that the important characteristic(s) must have been evolutionarily conserved and it is reflected by conservation of the biochemical parameters. We applied the genome comparison of Raf/MEK/ERK and found that, for example, the MEK-ERK binding site had mutations among vertebrates, implying those perturb the involved parameters and effect to the less important characteristic(s) of ERK activation. This approach is applicable to the rest of parameters.

20501S BSA における AQDS 結合サイトの光誘起電子電子二重共鳴(DEER)計測
Light-induced DEER measurement on the AQDS-binding site in Bovine Serum Albumin

Hiroki Nagashima, Lewis Antill, Kiminori Maeda (*Dep. Chem., Grad. Sch. Sci., Saitama University*)

The double electron-electron resonance (DEER) technique is one of the powerful EPR techniques employed to study protein structures, which measures distances between electron spin labels attached to the proteins. The light-induced DEER (LiDEER) technique uses a laser pulse instead of a microwave pulse, which resonate with the electron spin. Here, we applied the LiDEER technique to study the light-induced radical pairs formed in the AQDS and BSA complex to determine the location of the AQDS binding site. This technique can also be applied to other areas in interest, for example, clarifying drug binding sites in proteins and also elucidating structural changes accompanied by the charge separation and electron transfer in proteins, such as cryptochromes and photosystems.

20502S ヒト皮膚または培養皮膚に貼付したセラミド含有粘着性ゲルシートからのセラミド放出のマイクロ FT-IR 分光法による計測
Micro FT-IR Spectroscopic Study on Ceramide-release from Ceramide-Containing Adhesive Gel Sheet Affixed to Human Skin or Cultured Skin

Hiroshi Takahashi[1], Ryota Watanabe[2], Kenichi Nishimura[2], Taro Moriwaki[3] ([1]*Grad Sci Sci.&Tech., Gunma Univ.*, [2]*ALCARE Co., Ltd.*, [3]*JASRI/SPring-8*)

Ceramide, an intercellular lipid of the stratum corneum, is indispensable for the skin barrier function. Medical adhesive tape and sheets may damage the skin by repeatedly applying and removing them. The addition of ceramide molecules to the adhesive has been reported to reduce skin damage clinically. Here, by using synchrotron micro FT-IR spectroscopy, we examined whether ceramide is released from the sheet of UV-curable acrylic adhesive gel with added ceramide after affixing to real human skin or cultured skin for a specified period. The results showed that the release behavior of ceramide from the gel sheets was different between human skin and cultured skin. We will discuss the mechanisms by which different results were obtained in human and cultured skin.

20503S ウニの発生初期における核内染色体構造の動的および細胞特異的変化
Dynamic and cell specific changes in intranuclear chromosomal structures during early development of sea urchin

Yuhei Yasui, Ayaka Sugiyama, Naoaki Sakamoto, Akinori Awazu (*Integrated science for life, Hiroshima University*)

Recent imaging study for cell nucleus suggested that various intranuclear activities such as gene expression, DNA replications, and DNA repair are regulated by dynamic changes in chromosomal structures. On the other hand, intranuclear structural dynamics during the embryonic development are still unclear. In this study, we observed cell type and developmental stage dependent intranuclear structures of sea urchin embryo, one of typical model organisms for early embryonic development, using fluorescence in situ hybridization, immunofluorescence and image analysis. We specifically focused on the formation, shape and positioning of telomere, histone locus body, RNA polymerase II, and heterochromatin to characterize the developmental stage dependent intranuclear features.

20504S 伝導度計測を用いたペプチドのリン酸化の単一分子検出
Single-molecule detection of peptide phosphorylation using electrical conductance measurement

Takanori Harashima[1], Yoshiyuki Egami[2], Tomoya Ono[3], Tomoaki Nishino[1] ([1]*School of Science, Tokyo Institute of Technology*, [2]*Faculty of Engineering, Hokkaido University*, [3]*Department of Electrical and Electronic Engineering, Kobe University*)

We demonstrated a single-molecule detection of peptide phosphorylation based on an electrical conductance measurement. A scanning tunneling microscopy was utilized to measure conductance of a 7-amino-acid peptide. We found that the phosphorylated peptides exhibit a highly conductive signal because of the formation of the metal-phosphate-metal junction, which is absent for unphosphorylated counterpart. Calculations based on density-functional theory indicated that the high-conductivity of phosphate is due to the little energy difference between the HOMO of the phosphate and the Fermi level of the electrodes. The present study opens up the novel technique for ultrasensitive and rapid disease diagnosis.

20505S* イオン液体-スピン乾燥法で走査型電子顕微鏡の試料作製を容易にする
A simple and quick method to prepare biological specimens for scanning electron microscopy by an ionic liquid

Tatsuya Suehiro, Naoki Uemura, Saki Taguchi, Katsuya Shimabukuro (*Chem. Bio. Eng., NIT Ube College*)

We present an easy method to prepare a specimen for scanning electron microscopy (SEM) using ionic liquids (ILs). ILs are liquid salts with an electronic conductivity and low vapor pressure, possessing ideal physical properties for SEM imaging. Some applications of ILs to biological specimens have been reported so far, however, those application are limited to relatively large samples such as pollen. High viscosity of ILs prevents formation of a thin layer, making fine structures indistinct. To solve this, we remove an excess IL by spinning-dry and succeeded in observation of fine structures like eukaryotic flagella under conventional SEM. Because IL-coated samples do not require a metal spattering, our method will give an easy access to SEM for biological science.

20506S 短波赤外光を発する量子ドットによる無侵襲マウス脳表血管造影とその焦点合わせについて
Novel angiography for mouse cerebral vasculature using short-wave infrared light emitting quantum dots and its focusing

Tatsuto Iida[1], Hiro Yamato[1], Takashi Jin[2], **Yasutomo Nomura**[1,2] ([1]*Department of Systems Life Engineering, Maebashi Institute of Technology*, [2]*RIKEN Center for Biosystems Dynamics Research*)

Quantum dots emitting near-infrared light at 1100 nm were administered through the caudal vein of mice. Based on the anatomical properties reported previously, we focused 0.4 mm below the intact scalp surface. The intensity of clear fluorescence images which observed transiently under a microscope became very weak within several seconds. To investigate focus, photons exciting quantum dots at depths of 0.4 - 2.0 mm and emission photons were tracked in a Monte Carlo model including the scalp, skull, cerebrospinal fluid, and cortex. Based on the most near-ballistic photons emitted from quantum dots at 0.4 mm depth and specification of the microscope used, including numerical aperture and depth of field, the optimal focus plane was interpreted to be set suitably.

20507S Variogram/Correlogram 法を使った生物対流解析
Variogram and correlogram assay of cell motility: Bioconvection in harmful algae *Chattonella*

Mina Nakahara, Atsuto Kobayashi, **Shinji Kamimura** (*Dept. Biol. Sci., Fac. Sci. & Eng., Chuo Univ.*)

Chattonella are single-celled marine algae that causes harmful algal blooms (HAB). When collected in a shallow petri dish, they start gradual accumulation in a few minutes and forms specific patterns of nonhomogeneous distribution. This phenomenon of bioconvection is expected to be closely related to the formation of HAB in fields. In order to understand the mechanism of HAB development, we are executing the image analysis of collective swimming behavior of *Chattonella marina var. ovata* (Raphidophyceae) using spatial statistical techniques as well as high-speed-video microscopy. In the presentation, we will show examples to show novel quantitative descriptions of bioconvection with variogram or correlogram, an empirically useful tool in geostatics.

20508S 分裂期の染色体の 3D-AFM 像の理論予測と実測との比較
A theoretical prediction of 3D atomic force microscopy image of chromosomes in mitotic phase and its comparison with experiments

Takashi Sumikama[1], Keisuke Miyazawa[1,2], Makiko Meguro-Horike[3], Ryohei Kojima[2], Naoko Okano[2], Shin-ichi Horike[3], Adam S. Foster[1,4], Takeshi Fukuma[1,2] ([1]*Nano Life Sci. Inst. (WPI-NanoLSI), Kanazawa Univ.*, [2]*Grad. Sch. of Nat. Sci. and Tech., Kanazawa Univ.*, [3]*Div. of Func. Gen., Adv. Sci. Res. Center, Kanazawa Univ.*, [4]*Dept. of Appl. Phys., Aalto Univ.*)

Chromosomes are the long chain molecules coding genes. Several polymer models have been proposed to simulate chromosomes. In the previous model including condensin and topoisomerase II, it was shown that rod-like chromatids in the mitotic phase was formed. However, the resultant structure was different from the x-shape chromosome seen in the experiments. Here, we developed a model including cohesion in addition to the conventional model. Chromosome structure where two sister chromatids lie next to each other, as similar to the experiments, was formed in the simulation. To validate the simulation, we are planning to measure the three-dimensional atomic force microscopy (3D-AFM) image of chromosomes, which will be compared with the simulated 3D-AFM image.

20509S 原子間力顕微鏡の位相イメージングを用いた *Paracoccus denitrificans* 細胞に結合した膜小胞の解析
Analysis of bacterial extracellular membrane vesicles bound to *Paracoccus denitrificans* cell by atomic force microscopy phase imaging

Yousuke Kikuchi[1], Yuuki Ichinaka[1], Masanori Toyofuku[2,3], Nozomu Obana[3,4], Nobuhiko Nomura[2,3], Azuma Taoka[1,5] ([1]*Col. of Sci. and Eng., Kanazawa Univ.*, [2]*Life and Env. Sci., Tsukuba Univ.*, [3]*MiCS, Tsukuba Univ.*, [4]*Trans. Med. Res., Tsukuba Univ.*, [5]*WPI-NanoLSI, Kanazawa Univ.*)

Bacterial cells release nanometer-sized extracellular membrane vesicles (MVs) for transporting molecules to other cells. We measured physical properties of MVs bound to *Paracoccus denitrificans* living cell surfaces by high-speed atomic force microscopy (AFM) phase imaging. For observation of MVs binding to *P. denitrificans* cells, isolated MVs were added during AFM imaging of living *P. denitrificans* cells. We measured the physical properties of individual MVs and other cellular structures on cell surface by detecting phase shift value. The phase shift values of MVs were significantly decreased during AFM imaging, while those of the other structures were static. This result showed the dynamic changing of MVs' physical properties in bacterial cell surface.

20510S 神経細胞分化における細胞内温度の関与
Involvement of intracellular temperature in neuronal differentiation

Shunsuke Chuma[1], Kohki Okabe[2,3], Yoshie Harada[1,4] ([1]*IPR, Osaka Univ.*, [2]*Grad. Sch. Pharm. Sci., The Univ. Tokyo*, [3]*PRESTO, JST*, [4]*QIQB, OTRI, Osaka Univ.*)

Neural stem cells differentiate into neurons with neurite outgrowth, which is controlled by various intracellular and extracellular factors. Recent studies showed that neurite reacts to thermal stimulation from outside. However, the involvement of intracellular temperature in neuronal differentiation is elusive. To elucidate the involvement of intracellular temperature in neuronal differentiation, PC12 cells, which are model cells for neuronal differentiation, were used to analyze the intracellular temperature change during neuronal differentiation by fluorescence polymeric thermometer(FPT). We found that the intracellular temperature of PC12 cells increased by neurite differentiation. The generation of heat suggests involving transcription and translation.

20511S 原子間力顕微鏡と多孔窒化シリコン薄膜を用いた生きた細胞表面の高分解能観察方法の開発
Development of high-resolution observation method of living cell surface in atomic force microscope using porous silicon nitride membrane

Takehiko Ichikawa[1], Taiki Kitamura[2], Dong Wang[1,3], Hiroko Oshima[3], Masanobu Oshima[1,3], Takeshi Fukuma[1,2] ([1]*NanoLSI, Kanazawa Univ.*, [2]*College of Science and Engineering, Kanazawa Univ.*, [3]*Cancer Research Institute, Kanazawa Univ.*)

Atomic force microscope (AFM) can observe single atom in crystal and single-molecule in liquid. However, nano-scale observation of living cell surface has been difficult probably because the living cell surface is soft and changes dynamically. In this study, to improve the resolution in AFM imaging of the surface of the living cell surface, we adopted a thin membrane with small holes used for a transmission electron microscope to make the cell surface flat and prevent the membrane fluctuation. We cultured cells on the silicon nitride membrane which has 5 μm holes and 200 nm thickness and found that stable observation is possible, and we could observe 10 - 20 nanometer-sized structures on living colon cancer cell surface.

20512S 自動イオンチャネル電流測定装置の開発
Development of a system for automated ionic current measurement

Minako Hirano[1], Masahisa Tomita[2], Chikako Takahashi[1], Nobuyuki Kawashima[2], Toru Ide[3] ([1]*Grad. Sch. Creation Photon Indust.*, [2]*SYSTEC Corporation*, [3]*Okayama Univ.*)

We have developed an automated system to measure ion-channel activities electrophysiologically. This system is based on a simple technique to make a lipid bilayer membrane containing ion channels, which we previously developed. It consists of ionic current-detecting system and a driving device, and the driving device controls a position of a probe on which channels are immobilized. We optimized the shape of the probe, chemical modification of the probe surface, and lipid compositions. By automatically controlling the optimized probe having channels, we could incorporate channels into the membrane at the same time as the bilayer membrane was stably formed at aqueous-oil interface. This system makes it possible to increase the measurement efficiency of channel activities.

20513S 上皮成長因子受容体癌変異への自動化 1 分子解析の薬理学的応用
Pharmacological application of automated single-molecule analysis for EGFR cancerous mutants

Michio Hiroshima[1,2], Daisuke Watanabe[3], Masahiro Ueda[1,3] ([1]*RIKEN BDR*, [2]*RIKEN CPR*, [3]*FBS, Osaka Univ.*)

Single-molecule analysis revealed that epidermal growth factor receptor (EGFR) shows phosphorylation dependent mobility on the plasma membrane. The quantitative property can be used as an index for ligand/drug efficacy on EGFR, leading to novel single-molecule drug screening as a pharmacological application. Recently we developed a fully automated imaging system with artificial intelligence and robotics to remove the inefficiencies in conventional single-molecule analysis, which prevents the application to large-scale drug screening. By using this system, EGFR molecules with structural deletions and cancerous mutations were shown that the behavior sensitively reflected the deleted structures and mutations, and quantitatively corresponded to tyrosine kinase inhibitors.

20514S 生細胞 1 分子超解像イメージングによるヒストンバリアントのナノスケール局在解析
Nano-scale localization analysis of histone variants in living cells using single-molecule super-resolution imaging

Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech*)

Histone variants have important roles in cellular process such as transcription beyond packaging DNA into the nucleosome. Although variants have been identified in specific gene loci, their distribution in the nucleus is still elusive. Here, we performed single-molecule super-resolution imaging to visualize the nano-scale distribution of histone variants. Localization analysis revealed that both canonical histone H3.1 and active gene-associated H3.3 formed cluster, but their size and clustering strength were different. Inhibition of histone deacetylation results in the reduction of the strength of H3.1 clustering, but not H3.3. These results suggest that the chromatin nano-scale distribution is regulated by the distinct mechanism through the epi-genomic modification.

20515S サブミリ秒光波面シェイピングシステムによる厚さ 2mm の鶏肉を通した光集束及び蛍光イメージング
Optical focusing and fluorescence imaging through a 2mm thick chicken tissue slice by submillisecond wavefront shaping system

Atsushi Shibukawa, Keiichi Kojima, Yuki Sudo (*Grad. Sch. of Med. Dent. Pharm. Sci., Okayama Univ.*)

Optical wavefront shaping (WFS) with a spatial light modulator has proved to give us the ability to implement optical focusing and imaging at the depth of more than 2mm in biological tissues. However, to exploit such the ability in a living mouse brain, the response speed of WFS system needs to be accelerated to the submillisecond order. We here aim to realize the submillisecond WFS system for the first time by developing an ultrafast 1D-spatial light modulator with ~20 MHz refresh rate. In the presentation, we will show that the proposed WFS system can achieve optical focusing and fluorescence imaging through a 2mm-thick chicken slice that mimics scattering responses of the living mouse brain.

20516S Development of continuous non-clogging cell fractionation technique using pillar arrangement and AC electric field

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To overcome the limitation of membrane filtration, we developed a continuous size fractionation technology exploiting a pillar array microfabrication. We placed the pillar array on a PDMS chip to form 11 degrees to solution flow with a 10 μm gap between the pillars. And we flowed different sized polystyrene beads in the chip with 0.5 Hz 4.5 Vpp AC field applied perpendicular to flow direction for preventing them clogging up at the pillars. We fractionated different size of polystyrene beads, 10 μm and 15 μm. The former beads passed through the pillars and flowed to one outlet. The latter clogged up at pillars and flowed to another outlet. For the technology which prevent clogging up, continuous size fractionation accomplished using the two sizes of model standard beads.

20517S Interaction of nicked-DNA with solid state nanopores

Shimba Ichino, Kento Lloyd, Takumi Yoshikawa, Ryoma Omori, Yuuta Moriyama, Toshiyuki Mitsui (*Aogaku Univ.*)

Solid state nanopores are expected to be a commercialized DNA sequencer as well. However, there are crucial issues to deal with relatively long DNA molecules, i.e. DNA clog at a pore. We have developed an instrument to visualize DNA translocation through a pore and investigating the cause of the clog. The clogging probability increases not only the length but the conformation, u-shaped or knotted, of DNA. To further investigate the conformation effects, we tested nicked DNA molecules, cleaving one strand. Interestingly, nicked DNA molecules also increased the clogging probability despite their flexibility. By using 3D FEM, we estimated the opposing flow via nanopore by osmosis and realized the presence of multiple DNA strands inside a pore directly cause the DNA clog.

20518S Simple precise flow speed measurement in an on-chip flow cytometer with simultaneous two-wavelength differential image analysis

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Precise and quick measurement of flow velocities of samples is essential for decision of cell sorting timing and reconstruction of acquired image-analyzed data. We have developed a simple technique for a single-shot measurement of the flow velocities of plurality of particles simultaneously flowing through a microfluidic pathway in an imaging flow cytometer. The speed was calculated from the difference in the elongation of the particles that appeared in the images of a bead for each wavelength when two wavelengths of light with different irradiation times were applied. We ran polystyrene beads and the velocity distribution was highest in the center of the flow channel, which was consistent with the expected velocity distribution of the laminar flow.

20519S 多次元デジタルバイオアッセイで明らかになった、インフルエンザウイルスにおける粒子ごとの薬剤応答の多様性
Multi-Dimensional (MD) Digital Bioassay unveils heterogeneous drug-susceptibility of influenza A virus in a single-virus resolution

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We developed a high-throughput bioassay system called Multi-Dimensional (MD) Digital Bioassay to evaluate the activities of individual bioparticles and biomolecules (viruses and enzymes, etc.) under multiple conditions. As a demonstration, we employed an influenza A virus (IAV) strain. Although the heterogeneous responses to the drugs among IAV strains are well known, whether a certain IAV strain has intrinsic heterogeneity in drug susceptibility remains unclear, despite its implication in the emergence of drug-resistant mutants. We quantitatively measured the activities of discrete IAV particles under multiple doses of an inhibitory drug. We revealed that the IAV strain has a certain heterogeneity in drug susceptibility.

20520S Ligand is not necessary for progress of engulfment in IgG-coated and non-coated mixture of antigen cluster

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FcGR-IgG bond is thought to be necessary to progress the cell membrane extension in phagocytosis. To examine whether the IgG coated surface is necessary for progress of engulfment, we fed a mixture of 4.5-μm IgG-coated and 2-μm non-coated polystyrene cluster as antigen to macrophage and observed its membrane extension during engulfment. Macrophage engulfed the whole cluster including 2-μm non-coated polystyrene part, indicating non-coated surface did not influence the progress of engulfment. In contrast, the cluster of pure non-coated polystyrene spheres was not engulfed. The results suggest (1) IgG-coated surface is needed for anchoring of phagocytosis, and (2) once the triggering is induced, phagocytosis can proceed even uncoated surface involved in the antigen.

20521S 光ファイバー型蛍光相関分光装置を用いたエクソソームの同定
Identification of exosome by using optical fiber based fluorescence correlation spectroscopy

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Exosome is an extracellular vesicle found in body fluid and contains proteins and nucleic acids. Exosome secreted from cancer cells has cancer-specific biomolecules, and detecting and quantifying the exosome would contribute to cancer diagnosis. In this study, we developed new FCS unit (Fiber-connected FCS; FC-FCS) by using optical fiber coupler. FC-FCS is much smaller and simpler than conventional FCS system and is expected to spread widely. FC-FCS measurement was performed using an exosome-specific fluorescently labeled antibody to compare the expression ratio of specific membrane proteins in exosome. Furthermore, we are planning to extend the devise to dual-color system for detecting co-expression of two types of proteins.

20522S 最大エントロピー法と変分ベイズクラスタリングを用いた 1 分子 FRET データ解析による細胞質中 RAF のダイマー化状態の検出
Dimer formation of cytosolic RAF detected by single-molecule FRET analysis based on maximum entropy and variational Bayes-culstering

Kenji Okamoto, Yasushi Sako (*RIKEN CPR*)

We have recently succeeded single-molecule measurements of cytosolic RAF proteins in living HeLa cells. Alternative Laser EXcitation (ALEX) technique enabled us to detect single diffusing molecules as fluorescent bursts and acquire single-molecular distribution of the Förster resonance energy transfer (FRET) efficiency, which indicated CRAFs in the open and the closed conformation co-existed in cells. In addition, analysis of burst intensities implied homodimer formation. We developed a new data analysis method using maximum entropy and variational Bayes-clustering, to elucidate monomeric/dimeric states of cytosolic RAF proteins. Results indicate that homodimers are actually formed in cells and dimerization inhibitory mutation does not work solely.

20523S Investigation of automatic single-molecule tracking method for large-scale single-molecule imaging analysis

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Single-molecule imaging allows direct observation of signaling molecules on the cell membrane in living cells. The automated in-cell single-molecule imaging system (AiSIS) performs large-scale single-molecule imaging analysis efficiently. However, an difficulty has still remains in an automatic single-molecule tracking, which limits an accurate estimation of reaction kinetics. I evaluated several single-molecule automatic tracking software by comparing the results to those obtained by manual tracking. The dissociation curves of PTEN in Dictyostelium discoideum showed the tracking by “TrackMate” was as accurate as the manual tracking. Further evaluation by using simulated trajectories and an application to the chemotactic signaling molecules will be discussed.

20524S* ヨーロッパモノアラガイの咀嚼神経系の蛍光 NO イメージング ー味覚嫌悪学習前後の NO 放出の比較
Fluorescence NO imaging for feeding nervous system of the pond snail-Comparison of NO release before and after taste-aversive conditioning

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Nitric oxide (NO) affects the initiation and modulation of the feeding behavior in the pond snail *Lymnaea stagnalis*. In the present study, we investigated NO release in the feeding nervous system, and compared it before and after taste aversive conditioning that is a form of classical conditioning. 24 hours after the conditioning, the feeding behavior decreased to over 40% in most cases and the long-term memory was formed. Then, we measured NO release mainly in the buccal ganglia using fluorescence NO imaging. The brain preparation was stained with an NO-sensitive dye, DAR-4M AM, the fluorescence intensity of which is irreversibly increased by NO adsorption. The stained preparation was illuminated by LED, and the fluorescence images were acquired through sCMOS camera.

20525S DNA ナノデバイスを用いた細胞の機械シグナルイメージング技術開発
Development of mechanical signal imaging technique using DNA nano-device

Hiroki Fukunaga[1], Takahiro Saito[1], Satiko Onishi[2], Mitsuhiro Iwaki[1,2] ([1]*FBS, Univ. Osaka*, [2]*BDR, Riken*)

Mechanical forces are integral to many biological processes, however, the technology for high-resolution imaging of the mechanical force is still quite limited. We have recently developed nano-device called “Nanospring” using DNA nanotechnology. This is a protein-sized coil-shape nano structure with high brightness, high-resolution force sensing and tunable spring constant. Our nanospring can be applicable to force-sensing in cells by monitoring the extension and retraction of fluorescently labeled nanospring. Here, we aim at incorporating optimized nanospring into cells and observing it using super resolution imaging techniques to measure the force.

20526S クロモセンター領域内外におけるヘテロクロマチンタンパク質 HP1α 動態の生細胞 1 分子イメージング定量解析
Dynamics of Heterochromatin protein 1α inside and outside chromocenter domain in living cells using single-molecule imaging

Masanori Nakano[1], Yuma Ito[1], Takahiro Maeda[1], Chikashi Obuse[2], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Inst. Tech.*, [2]*Biosci. Grad Sch Sci., Osaka Univ*)

Heterochromatin protein 1α (HP1α) regulates gene expression by compacting chromatin. This is supported by phosphorylation of HP1α N-terminal extension, which promotes the formation of liquid-liquid phase separation. We used single-molecule tracking analysis to determine the dynamics of wild-type HP1α and protein-binding-, dimerization- and chromatin-binding-deficient mutants. The tracking data were analyzed by dividing them into the inside and outside of the chromocenter, the dense heterochromatin region. The wild-type and the three mutants showed two motilities, bound and mobile states, both inside and outside the chromocenter domain. This analysis provides new insight how protein binding, dimerization and chromatin binding affect the motility of HP1α.

20527S 補償光学系を用いた 1 分子イメージングにおける収差補正のシミュレーション
Light field simulation of single-molecule imaging for aberration correction using adaptive optics

Xiang Zhou, Yuma Ito, Makio Tokunaga (*Sch. Life Sci. Tech., Tokyo Tech.*)

Single-molecule microscopy allows imaging with high spatial resolution, and now widely used for super-resolution microscopy. It owes to high-performance and high-numerical-aperture objectives, which have still some residual aberrations at the utmost periphery. Here, we implement an simulation framework to examine how much adaptive optics can correct the aberrations of high-numerical-aperture objectives. Not only the correction of point images at the focal plane but also the effects on defocused images at off-focal planes are to be estimated. Our simulation framework is useful for optimizing methods for practical utilization of adaptive optics for super-resolution microscopy as well as single-molecule imaging and three-dimensional tracking analysis in living cells.

20528S 核小体タンパク質の多色超解像 1 分子イメージング解析
Multicolor single-molecule imaging analysis of the nucleolar proteins

Supanut Sirisukhodom[1], Yuma Ito[1], Noriko Saitoh[2], Makio Tokunaga[1] ([1]*Sch. Life Sci. Tech., Tokyo Tech.*, [2]*Div. of Cancer Biol., The Cancer Inst. JFCR.*)

Nucleolus maintains its non-membrane bound structure by phase separation and is divided into three different compartments: FC, DFC, and GC. We examined the dynamics of molecules in these compartments using simultaneous multicolor single-molecule imaging. In contrast to the simple diffusion behavior of NPM1 protein in the outermost region GC, FBL protein in the intermediate region DFC slowly diffused and showed confined movement. In the presence of transcriptional inhibitor Actinomycin D (ActD), we observed distinct structural changes in the nucleoli. Single-molecule analysis showed slight changes in the dynamics of the GC regional protein NPM1. The result suggests that dynamic change in the inner region exerts a substantial influence on the outermost liquid-phase.

20529S Development of an enzyme-coupled fluorometric digital bioassay for ATPase

Hiroshi Ueno, Mayu Hara, Mio Sano, Hiroyuki Noji (*Dept. Appl. Chem., Grad. Sch. Eng., Univ. Tokyo*)

Digital bioassay using femtoliter (fL) reactor array is a powerful method that allows highly sensitive, quantitative analysis of biomolecules with single-molecule detection sensitivity. However, the current digital bioassay requires fluorogenic substrates for detection, which limits the applicability of this method. Here, to overcome this limitation, an enzyme-coupled fluorometric digital bioassay has been developed for ATPase that has no fluorogenic substrates. In this system, the non-fluorescent resazurin was converted to the fluorescent resorufin by using coupled reactions driven by ADP. The assay system performed well with F1-ATPase in bulk measurement, and now achieved the detection of the ATP hydrolysis reaction in fL reactors containing 10 molecules of F1-ATPase.

20530S 2 光子生体イメージングでみるインフルエンザウイルス感染肺
In vivo imaging of the cellular pathophysiology in influenza virus-infected mouse lung

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The cellular pathophysiology in influenza virus-infected lungs is poorly understood. Here, we established an in vivo imaging system that combines two-photon excitation microscopy and fluorescent influenza viruses of different pathogenicity. This approach allowed us to monitor and correlate several parameters and pathophysiological changes including the spread of infection, pulmonary permeability and perfusion speed, the number of pulmonary neutrophils, and neutrophil motion in the lungs of live mice. Our findings demonstrate the potential of this in vivo imaging system to provide novel information about the pathophysiological consequences of influenza virus infection and the immune response to it.

20531S Direct observation of force-induced release of SecM translation arrest

Zhuohao Yang[1], Ryo Iizuka[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. Pharm. Sci., The Univ. Tokyo.*, [2]*Dept. Biol. Sci., Grad. Sch. Sci., The Univ. Tokyo*)

SecM, an E. coli secretion monitor protein, contains an arrest sequence that interacts with the ribosomal tunnel to arrest its translation. It is considered that the pulling force of the Sec apparatus releases the translation arrest and resumes its translation. However, this release process has not been fully substantiated. Here, we developed a single-molecule force measurement system using magnetic tweezers. Using this system, we successfully applied force to the SecM-ribosome-mRNA arrested complexes and observed the resumed translation in real time. Our results indicate that applying a few pN force can release translation arrest in several minutes, while the translation arrest lasts for several hours without applying force.

20532S パッチクランプ AFM の開発に向けて
Toward the development of Patch Clamp Atomic Force Microscopy

Takeru Matsubara[1], Shinji Watanabe[2], Toshio Ando[2], Noriyuki Kodera[2] ([1]*Grad. Sch. NanoLS., Kanazawa Univ.*, [2]*WPI-NanoLSI, Kanazawa Univ.*)

The function and structure of ion channels have been studied separately by electrophysiological methods and structural biology methods (e.g., X-ray crystallography and cryo-EM). To simultaneously observe the channel activities (electrical flow) and the structural changes performed by ion channels in action, we have been developing a high-speed AFM (HS-AFM) system that can perform patch clamp analysis during HS-AFM observation. In this system, a patch pipette is used as a sample stage of HS-AFM. We demonstrated that the pipette end with an aperture size of ~100 nm can be observed by HS-AFM at sub-second temporal resolution. Currently, we are improving the scanning system and incorporating of a current measurement device into the system.

20533S* Biophysical analysis of pH-dependent conformational change of LDLR family members in ligand capture and release

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Low-density lipoprotein receptor (LDLR) is a cell-surface receptor that internalizes an LDL particle into the cell. The LDLR ectodomain is composed of ligand binding domain (LBD) and epidermal growth factor precursor homology domain (EGFPHD). The pH-dependent rearrangement of LBD with respect to EGFPHD is important for the regulation of ligand capture and release. Specifically, the ectodomain is presumed to be flexible to capture LDL particle at the cell surface with neutral pH. In contrast, LBD docks to EGFPHD and the entire ectodomain adopts a closed conformation to release LDL inside endosome with acidic pH. In this study, we attempted to examine whether or not the behavior of LDLR is affected by pH shift mainly by high-speed atomic force microscopy.

20534S* 客観的な生物物理学データ解析に向けた初期パラメータ設定を必要としない隠 れマルコフモデルフィッティング手法の開発
Development of a new hidden Markov model fitting algorithm without predefinition of parameters for objective biophysical data analysis

Hanjin Liu, Tomohiro Shima, Sotaro Uemura (*Sch. Sci., Univ. Tokyo*)

Hidden Markov model (HMM) is widely used to analyze biophysical chronological data with discrete states such as protein conformational changes. Despite its usefulness, the need to specify the number of states in advance has hindered the widespread application of HMM. For data with low signal/noise ratio, previously reported HMM pre-analyses do not provide enough accuracy for state-number estimation. Here, by combining a statistical step finding method and Gaussian mixture model clustering, we developed a fully automated HMM fitting algorithm. Simulation showed that our algorithm could detect state transitions accurately even with a small number of data points. We also demonstrated the applicability of our method to data of motor stepping and photobleaching.

20535S DNA motions near geometrically anisotropic nanopores

Takumi Yoshikawa, Ryoma Omori, Shimba Ichino, Yuuta Moriyama, Toshiyuki Mitsui (*Aogaku Univ.*)

The interaction between DNA molecules and nanoscale pores is likely affected not only by the pore materials but also by the pore structures since the pore diameter is in the range of DNA conformation in solution. Conventional DNA detection by a nanopore relies on ionic current through the pore. Therefore, the DNA motion under the influence of a nanopore, i.e. geometrically anisotropic nanopore, can not be investigated. Our home-build nanopore setup placed on an optical microscope allows to trace the DNA motion before DNA translocation. We prepared nanopores with various shapes such as circler, square and cross, and observed DNA motions near these pores. As a result, the clog probability of DNA depended on the shape and clogged DNA attached to the square and cross edge.

20536S* 統計的蛍光画像解析による濃度分布イメージング
Fluorescence Imaging for Concentration Based on Statistical Analysis

Ryosuke Fukushima[1], Johtaro Yamamoto[2,3], Masataka Kinjo[3] ([1]*Grad. Sch. of Life Sci., Hokkaido Univ.*, [2]*Health & Med. Res. Inst., AIST*, [3]*Fac. of Adv. Life Sci., Hokkaido Univ.*)

Fluorescence imaging reveals spatial localization and distribution of fluorescently labeled particles in living cell. However, it is challenging to quantify the concentration of labeled particles. Quantifying the concentration would give valuable information about molecular mechanism in cell. In this study, we developed a method based on maximum a posteriori (MAP) estimation. MAP estimation is a method utilizing prior distribution, and we constructed the prior distribution for a pixel by using information on the surrounding pixels. Our method estimated with an order of magnitude better precision than conventional method. Our method can be applied to wide field of fluorescence imaging and would contribute to understand dynamic processes on molecular mechanism in cell.

20537S* Hybrid Photon Counting (HPC)検出器の microED 法への応用
Hybrid Photon Counting (HPC) detector application for microED method

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MicroED gives us structural information from microcrystal samples (smaller than 1 microns) by electron diffraction. This availability is because with comparing with X-ray crystallography, electrons interact with samples much strongly than X-rays. Here we have developed a high-speed camera (over 100 frames/sec) for EM, that can detect single electrons. Its pixel size is larger than that of other latest camera, and the pixel number is less. Thus direct imaging is difficult to achieve. However, we suggested that this camera is suitable for high-throughput microED of smaller molecules. We took tilt-series of diffraction patterns for 90 degrees in about 2 minutes and successfully determined the 3D-structure of small molecules such as acetaminophen.

20538S* 環境の温度変化に対する RNA の状態変化を介した細胞応答の解明
Investigating cell response to environmental temperature change via RNA state changes

Hiroki Shibata[1], Kohki Okabe[1,2], Takashi Funatsu[1] ([1]*Grad. Sch. of Pharm. Sci., The Univ of Tokyo*, [2]*PRESTO, JST*)

Environmental temperature has a great impact on life. Living things have adapted to temperature change in the course of evolution by acquiring temperature-responsive systems including those at cellular level. However, the mechanism of response to the physiological temperature change inside cells has not been revealed. Here we show that physiological temperature changes affect intracellular mRNA dynamics. By culturing COS7 cells at moderately low temperature, we found that the diffusion of mRNA considerably decreased and mRNAs were localized around the nucleus. Moreover, artificial heating in these cells resulted in the suppressed temperature increase. These results suggested that cells can adapt to environmental temperature change by altering RNA dynamics.

20539S* 繊毛虫 *Tetrahymena* による遊泳軌跡の三次元定量
Three-dimensional analysis of the swimming trajectories of *Tetrahymena*

Akisato Marumo, Kyohei Matsuda, Masahiko Yamagishi, Mitsuhiro Sugawa, Junichiro Yajima (*Dept. Life Sci., Grad. Arts & Sci., Univ. Tokyo*)

Ciliates are organisms which swim in the water to obtain nutrients or to escape from threats and some of them swim over helical trajectories. For instance, *Paramecium* is known to swim over the left-handed helical trajectories through studies on the planer swimming. However, since ciliates swim in bulk water with responding to environments or stimulations in nature, three-dimensional quantifications of the trajectories are necessary to lead more successful discussion about ciliates swimming. In this work, we tracked the swimming of *Tetrahymena* in three dimensions. It revealed that it swims over right-handed helical trajectories with rotating in right direction. In addition, the shapes of trajectories across the axis of the helices were like ellipses rather than circles.

20540S 相関顕微鏡法（CLEM）による同一試料観察に向けた相関・位置合わせ精度の改善
Improvement of correlation and alignment accuracy toward the same sample observation by CLEM

Yuki Gomibuchi[1], Risa Ezoe[2], Hiroko Takazaki[1,3], Yasuhisa Honda[2], Yusuke V. Morimoto[1], Takuo Yasunaga[1] ([1]*Dept. of Phys. Info. Tech., Kyushu Inst. Tech*, [2]*Dept. of Biosci. Bioinfo., Kyushu Inst. Tech.*, [3]*IPR. Osaka Univ.*)

We can observe biomolecules by utilizing the characteristics of the LM and the EM. When observing the same samples in the same field, correlative light electron microscopy (CLEM) is useful in our research fields. Thus, we used fluorescent beads as a marker and determined coordinates in both of the LM and EM systems using SerialEM for alignment to evaluate the errors. We found that the better accuracy for alignment was, the more markers were selected around the target of interest. Typically, more than 20 particles gave us the accuracy within 5 μm, so that we can observe 10 μm-objects such as a cell. We are trying to develop a novel alignment system for CLEM and explore the better distributions of beads with different colors and sizes, which will improve the alignment.

20541S 画像解析システム Eos の次世代開発に向けて
Approach to the next generation of our developing image processing system, Eos

Takuo Yasunaga (*Comp. Sci and Sys. Eng., Kyutech*)

We have developed an image processing system for electron microscopic images, which we called Eos. Eos supplies more than four hundred of small processing tools such as smoothing, three-dimensional reconstruction and some applications with graphical user-interfaces. We are now challenging to develop the next generation of Eos as a more powerful image processing system. For examples, tiff-formated images can directly be used. More latest noise reduction filters and binarization for masking are supplied to identify target objects in the noisy 3d volumes. We here show some examples Eos processed.

20542S 高速原子間力顕微鏡データと分子シミュレーションのデータ同化によるミオシン V の動的構造解析
Dynamic structure analysis of myosin V by data assimilation combining HS-AFM data and molecular simulations

Sotaro Fuchigami[1], Rie Koga[2], Shoji Takada[1] ([1]*Grad. Sch. of Science, Kyoto Univ.*, [2]*ExCELLS, NINS*)

The high-speed atomic force microscopy (HS-AFM) is a powerful technique to directly observe structural dynamics of a biomolecule at single-molecule level in real time. However, its spatiotemporal resolution is not enough to reveal atomic details. In the present study, we focus on a myosin V walking on an actin filament and aim to obtain detailed information about structural dynamics based on single-molecule measurement data by HS-AFM. We modeled the myosin V consisting of two heavy and twelve light chains and performed coarse-grained molecular dynamics simulation many times from various initial structures. Using obtained trajectories, we construct Markov state models describing walking dynamics of myosin-V and perform data assimilation using the experimental data.

20543S 水素化アモルファスシリコンと有機半導体で増強された分子薄膜を用いた揮発性 化合物のセンサシステム
A sensor system for volatile organic compound using molecular film enhanced by hydrogenated amorphous silicon and organic semiconductor

Hikaru Hatakeyama[1], Kisiro Seino[1], Shu Mugita[1], Kairi Shimazaki[1], Hiroshi Masumoto[2], Yutaka Tsujiuchi[1] ([1]*Material Science and Engineering, Akita University*, [2]*Frontier Research Institute for Interdisciplinary, Tohoku University*)

Photo-controlled film system, by using molecular film laminated on gels, organic semiconductor, hydrogenated amorphous silicon film, have been studied for the purpose of fabrication of functional biosensor. Firstly Langmuir Blodgett films of different fluorescent molecules and fatty acid, hydrogenated amorphous silicon films and organic semiconductor was prepared for exposure in volatile organic compound. An emission spectrum analysis of films, and conductivity measurement was conducted. Secondly enhancement of rectification properties in gel, emission properties of molecular film on hydrogenated amorphous silicon was analyzed. The result was that the system functioned for detection of volatile organic compound. Phenomena observed in the experiments are discussed.

20544S 水素化アモルファスシリコンの上に積層したバクテリオロドプシンの分子間相互作用と構造変化
Inter molecular interaction and structural change of bacteriorhodopsin film laminated on hydrogenated amorphous silicon film

Yutaka Tsujiuchi[1], Hikaru Hatakeyama[1], Koki Shimanaka[1], Hiroshi Masumoto[2] ([1]*Mat.Sci.AkitaUNIV*, [2]*Fris.TohokuUNIV*)

Molecular films contains bacteriorhodopsin (BR) and lipid film on retinoic acid film on hydrogenated amorphous silicon (a-Si:H) were prepared and analyzed by AFM and FTIR spectroscopy. FTIR reflection absorption spectrums of DMPC LB film above fatty acid film. DFM image of RetA3L+DMPC2L film and a structural model are discussed. DFM image obtained by measurement from an angle of 45, or, 90 degrees upon magnification indicates gradually protruding curved surface portions with a maximum height difference of 9 nm and width of approximately 200nm. Further, analysis data of inter molecular interaction between bacteriorhodopsin molecules are discussed.

20545S 粒子フィルター MD シミュレーションによる高速 AFM の非斉時ビデオのデータ同化
Particle-filter MD simulations to assimilate asynchronous video data of high-speed AFM

Suguru Kato, Sotaro Fuchigami, Shoji Takada (*Kyoto University*)

High-speed (HS) atomic force microscopy (AFM) is useful for observing the structural dynamics of biomolecules. However, being a scanning microscopy, the AFM image has asynchronicity among pixels in each frame. To conquer this problem, we have employed the particle-filter molecular dynamics (MD) simulation in which the tip of AFM cantilever probes the surface sequentially pixel by pixel. In this study, we focused on the resampling schedule of our particle-filter simulation. We surveyed the reproducibility of the simulation trajectories while varying the resampling schedule in the case of synthetic HS-AFM data.

20546S HPD を用いた広視野蛍光 1 分子検出による局所環境変化のモニタリング
Local ambient condition monitoring by hybrid photo-detector (HPD)-based wide-field single-molecule fluorescence detection

Atsuhito Fukasawa[1], Gaku Nakano[1], Takayasu Nagasawa[1], Minako Hirano[2], Toru Ide[3], Hiroaki Yokota[2] ([1]*Hamamatsu Photonics K.K.*, [2]*Grad. Sch. Creation Photon Indust.*, [3]*Grad. Sch. Interdiscip. Sci. Eng. Health Sys.*)

We have presented that the Hybrid photo-detector (HPD) (Hamamatsu Photonics) consisting of a photocathode and an avalanche photodiode enables low-background wide-field single-molecule fluorescence detection with high temporal resolution. Here, we report an application of HPD to monitoring the ambient condition around single-molecule fluorophore. We have detected change in ambient condition as change in single-molecule fluorescence lifetime of a fluorophore whose image was simultaneously monitored by an EM-CCD. The HPD based time-resolved single-molecule fluorescence detection, which is unlike conventional single-molecule detection, provides us with a measurement method of local ambient condition.

20547S 多様な構造をもつタンパク質複合体の単粒子解析を改善する方法の調査研究
A survey and investigation on methods to improve single particle analysis of heterogeneous protein complexes

Kotaro Tanaka, Takuo Yasunaga (*Grad. Sch. Comp. Sci. Syst. Eng., Kyutech*)

Single particle analysis has now become one of the standard techniques for 3D protein structure determination. However, the technique is still not straightforward, especially for proteins with dynamic conformations or heterogeneous complex compositions. In such cases, researchers tend to have a hard time optimizing analysis workflows and their parameters by try-and-error. Also, the current algorithms for structure classification cannot resolve continuously changing conformations. We have been surveying and investigating methods to circumvent these difficulties, using our in-house heterogeneous dataset of GroEL-ES complexes as a testbed, with a main focus on machine-learning-based methods including deep-learning. We will share the results and knowledge in the poster.

20548S 生物発光共鳴エネルギー移動による発光バクテリアルシフェラーゼの高輝度化
Enhanced brightness of bacterial luciferase by bioluminescence resonance energy transfer

Tomomi Kaku, Megumi Iwano, Tetsuyuki Entani, Kenji Osabe, Takeharu Nagai (*The Institute of Scientific and Industrial Reseach, Osaka University*)

Light production in luminous bacteria is catalyzed by a reaction between luciferase and its substrate, luciferin. The use of bacterial luciferase gene as a luminous reporter has become a valuable tool for the study of biological events. However, many applications of bacterial luciferase-based imaging have been limited because of its low brightness. Here, we engineered the bacterial luciferase by fusion to Venus, a bright variant of yellow fluorescent protein, to enhance luminescence by bioluminescence resonance energy transfer (BRET). Our study demonstrated a ten-fold enhancement of luminescence intensity of the bacterial luciferase fused to the circularly permuted Venus. We believe the improved luciferase will broaden imaging applications.

20549S* Wash-free デジタルバイオ計測のための split enzyme の開発
Development of a split enzyme for wash-free digital bioassay

Yanbo Ma, Hiroshi Ueno, Hiroyuki Noji (*Department of Applied Chemistry, Graduate School of Engineering, University of Tokyo*)

Digital ELISA allows quantitative measurement in extremely low concentrations of biomolecules. However, the wash process in digital ELISA limits the simplification and miniaturization of the detection system for on-site diagnostics. To omit the wash process by generating a signal only when the target is present, a label-enzyme β-Glucuronidase (βGlu) was split into two inactive dimers that can be reactivated when placed in close proximity by target-protein interaction. To confirm the activation by the proximity, inactive dimers were cross-linked with an antibody. Cross-linked split βGlu showed an enhancement of its enzymatic activity in bulk measurement and also of single-molecule activity in digital bioassay, which suggests the potential for wash-free digital bioassay.

20550S Raman imaging for cancer diagnosis

Clement Jean-Emmanuel[1], Mochizuki Kenntaro[2], Fujita Katsumasa[3], Komatsuzaki Tamiki[1] ([1]*RIES Hokkaido University*, [2]*Kyoto University*, [3]*Osaka University*)

Raman imaging is becoming a promising technique to assist biomedical research. From single cells to tissue analysis, this label free and non-destructive method coupled with a Data Science pipeline is a powerful way to observe the metabolism of living systems and to deliver a new framework to diagnose diseases at the early stages. Indeed, not only this technology provides a spatial information, but also a rich chemical signature which embodies the biochemical composition of living systems. In that contribution we will show that Raman spectroscopy is able to detect metabolic alterations that occur in cancer cells. Lipid and redox alterations will be attentively explored and quantified by a machine learning framework.

20551T FRAP 法と遺伝子組換えを併用した反応拡散分子の細胞内動態解析
FRAP combined with genetic manipulation reveals the kinetics of actin-binding proteins in cells

Takumi Saito[1,2], Daiki Matsunaga[1], Tsubasa Matsui[1], Kentaro Noi[1], Shinji Deguchi[1] ([1]*Grad. Sch. Eng. Sci., Osaka uni.*, [2]*JSPS Research Fellow*)

Molecular transport is dominated not only by the diffusion but also by the molecular turnover. Such anomalous diffusion is particularly obstructed in cells. In this study, FRAP was combined with genetic manipulation to characterize the kinetics of reaction-diffusion proteins existing on stress fibers. The effective diffusion coef. measured by FRAP was increased compared with one of wild-type because the reaction disturbed the molecular transport according to the pure-diffusion depending on the molecular size. The pure-diffusion coef. and the equilibrium const. thus were estimated with the Stokes-Einstein eq. and reaction-diffusion equation respectively. In this framework, we can understand the reaction and diffusion kinetics as well as the conventional recovery rate.

20552T 高汎用性を目指した改良凝固ゲル中結晶化法の開発と評価
Development and evaluation of the high-strength hydrogel method for high versatility

Taichi Naruse[1], Mihoka Amano[1], Noriaki Kunimune[2], Tsuguo Nagasawa[2], Hiroaki Adachi[3], Yusuke Mori[4], Shigeru Sugiyama[5] ([1]*Grad. Sch. Sci., Kochi Univ.*, [2]*KUNIMUNE Inc.*, [3]*SOSHO Inc.*, [4]*Grad. Sch. Eng., Osaka Univ.*, [5]*Fac. Sci. & Tec., Kochi Univ.*)

Protein crystals grown in hydrogel allow us to prevent serious damage to the crystals caused by soaking in high-concentration organic solvents, producing crystals of complexes between the target protein and poor water-soluble compounds by soaking in it. We previously reported the high-strength hydrogel method (HSGM), but obstacles remain for general versatility. To overcome it, we developed and evaluated an improved HSGM for diffusing proteins into the pre-solidified hydrogel. It was found that the diffusion rate of protein into the hydrogel became slower as the molecular weight of the protein increased. Development of apparatus suitable for this method is currently under way to solve the problem.

20553T DNA オリガミによる人工 γ-TuRC
Artificial γ-TuRC made by DNA origami

Daisuke Inoue (*Kyushu University*)

Microtubules (MTs) are hollow cylindrical biopolymers commonly composed of 13 parallel tubulin protofilaments (PFs) and play essential roles in many cellular processes. The structures of microtubules are critical in how these seemingly disparate functions are accomplished. In living cells, the PF numbers and arrangements are tightly regulated by a template γ-tubulin ring complex (γ-TuRC). In contrast, the structure of in vitro MTs has been found to have a broad distribution of PF numbers and helicity. To study how MT structure affects its functions, well-defined assays are necessary, wherein the MT structures can be engineered. In this meeting, I am going to present recent progress for developing a DNA origami seeds to nucleate and control MT structures.

20554T 集光レーザービームによる動的微小管ネットワークの形成
Formation of dynamic microtubule networks by focused laser beam

Kei Takano[1], Takuya Takeshige[1], Humika Kiryu[1], Ryuzo Kawamura[1], Chi-shiun Wu[2], Shih Yang-Hshin[2], Seiichiro Nakabayashi[1], Teruki Sugiyama[2,3], Hiroshi Yoshikawa[1] ([1]*Grad. Chem., Saitama Univ.*, [2]*App. Chem., National Chiao Tung Univ.*, [3]*Mate. Sci., Nara Inst. Sci. Tech. Univ.*)

Microtubule is a fibrous assembly of αβ-tubulin proteins and forms dynamic networks with motor protein (kinesin). In this work, we introduce a unique method to form highly ordered, dynamic microtubule networks by using a focused laser beam. We found that radially and hemi-spherically aligned fibrous structures can be formed depending on laser irradiation conditions. Observation of the obtained structures by transmission electron microscopy revealed the formation of a hollow cylindrical fiber of 13 protofilaments with a diameter of 30 nm, which corresponds to microtubules. We expect that this method could be advantageous for the formation of a highly ordered microtubule network without template and molecular modification.

20555T Combination approach for identification of highly-active mutant of processive chitinase

Akasit Visootsat[1,2], Akihiko Nakamura[3], Tak-Wai Wang[4], Ryota Iino[1,2] ([1]*Department of Functional Molecular Science, School of Physical Sciences, The Graduate University for Advanced Studies*, [2]*Institute for Molecular Science*, [3]*Department of Applied Life Sciences, Faculty of Agriculture, Shizuoka University*, [4]*Chimie ParisTech*)

Serratia marcescens chitinase A (SmChiA) hydrolyzes chitin processively as linearly moves on the crystalline surface. We combined multiple sequence alignment of SmChiA and SmChiA-like proteins, site-saturation mutagenesis, and automated screening with a liquid-handling robot for hydrolytic activity improvement. Using the previous highly-active F232W/F396W mutant as a template, we identified the F232W/F396W/S538V mutant that shows further improved hydrolytic activity just by trying 8 different positions. Importantly, valine was not found in the alignment at the Ser538 site of SmChiA. Our method can screen highly-active mutants that cannot be identified only by the introduction of predominant amino acid residues in the alignment.

20556T Culture-independent method for screening macromolecule-degrading microbes using deformability-based microfluidic microdroplet sorting

Mikihisa Muta[1], Kai Saito[1], Ryo Iizuka[1], Wataru Kawakubo[2], Hyun Yoon Dong[3], Tetsushi Sekiguchi[3], Shuichi Shoji[2], Mei Ito[4], 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.*, [4]*Dept. of Life Sci. and Green Chem., Saitama Inst. of Technol.*)

We have developed a culture-independent method for screening macromolecule-degrading microbial cells using deformability-based microfluidic microdroplet sorting. In this method, microbial cells are encapsulated at the single-cell level in macromolecule-containing water-in-oil (W/O) microdroplets. The W/O microdroplets, where the macromolecules are degraded into smaller molecules, increase the deformability. The screening is achieved by using a microfluidic device that enables the sorting depending on the deformability of W/O microdroplets. Using this method, we successfully sorted the microdroplets in which agarose was hydrolyzed by single bacterial cells. The method can be used to screen a variety of macromolecule-degrading microbial cells.

20557T 方向性を持った運動をするアメーバ型分子ロボットの開発
Toward vector motion of the cell-sized motorized molecular

Noriki Fukami[1], Yuichi Hiratsuka[2], Ibuki Kawamata[1], Yuki Suzuki[1,3], Satoshi Murata[1], Shin-ichiro Nomura[1] ([1]*Department of Robotics, Graduate School of Engineering, Tohoku University, Sendai 980-8579, Japan.*, [2]*Japan Advanced Institute of Science and Technology*, [3]*Frontier Research Institute for Interdisciplinary Sciences, Tohoku University*)

Recently, we have constructed an amoeba-like molecular robot with a liposome body. The robot has functions to recognize specific signal molecules and control a force transfer of molecular actuators, which enable itself to switch between randomly shape change states and inactive states. In this study, we design the robot that can move like a crawler by binding to the front floor in the direction of movement following membrane deformation and dissociates at the rear surface. We use complementary DNAs to bind the robot to the floor and investigate the DNA binding force that the robot can roll and move. We hope the research will provide a platform for building molecular robots that can move in any direction with chemotaxis function.

20558U Topological Data Analysis of Large-scale Multicellular Networks

Suguru Shimomura[1], Satoru Iwasaki[1], Tadashi Nakano[2] ([1]*Graduate School of Information Science and Technology, Osaka University*, [2]*Institute for Datability Science, Osaka University*)

Topological data analysis (TDA) provides a method to compute topological features of a space at different spatial resolutions. In this study, we propose a TDA-based approach to analyze large-scale multicellular networks. Using the proposed approach, we can extract topological features from multicellular networks and relative relationships among cells that form networks, and understand what factors play an important role in the formation of multicellular networks. We analyzed microscopy images of large-scale multicellular networks that cells formed *in vitro*. Results show that the multicellular networks we analyzed are hierarchically structured. This approach is generic and applicable to the analysis of a wide variety of multicellular networks in biological systems.

20559U Observation of floating phenomenon of *Cyclotella meneghiniana* by direct microscope: Temperature dependence analysis using a heater

Yuki Ide[1], Yuji Matsukawa[1], Daisuke Miyashiro[1], Shigeki Mayama[2], Matthew L. Julius[3], Kazuo Umemura[1] ([1]*Tokyo Univ. Sci.*, [2]*Tokyo Gakugei Univ.*, [3]*St. Cloud State Univ.*)

Since some diatoms float near the water surface due to convection, studying the relationship between diatom floating and water temperature is a clue to understanding the photosynthetic mechanism. The inverted microscope (CKX53, OLYMPUS) was tilted 90 degrees and 1 ml of cell suspension was put into a glass chamber and mounted on a sample stage perpendicular to the ground surface. A temperature sensor was installed inside the chamber, and microscope observation was performed at room temperature, 30 degree Celsius, and 40 degree Celsius. As a result, floating speed of diatom cells was increased at 40 degree Celsius compared with that at room temperature. The effects of the medium temperature diatom floating could be visualized by the direct microscopic observation.

20560U 矢が優れた飛び道具である理由ー自作風洞実験装置を用いた飛行する矢に働く力の分析ー
The reason why the arrow is superior flying tool - Analysis of forces acting on flying arrows by using a home-made wind tunnel device -

Haruto Tgawa, Akito Wada, Hinata Furuya, Ayumu Yamamori (*Osaka Pref. Tondabayashi H.S.*)

Based on last year's experiments results, our seniors suggested the existence of the lift force on the arrow. Therefore, we conducted an experiment using a handmade wind tunnel device to test their hypothesis. As a result, we confirmed the lift force, and it occurred mainly in the rear ends of the arrow blades. We thought the lift force on the arrow affects the flight posture and is an important factor in determining the trajectory and flight distance. When flight experiments were conducted by changing the size of the blades and the total length of the arrow, the degree of lift force and its effect on the flight posture changed. We think these are the characteristics of the arrow: "a flying tool with a structure that makes it easy to control distance and trajectory".

20561U 一本鎖 DNA を被覆した単層カーボンナノチューブと細胞膜間の力学的相互作用
Mechanical interaction between single-strand DNA wrapped single-walled carbon nanotubes and cell membrane

Daisuke Miyashiro[1,2], Ryo Hamano[1], Kazuo Umemura[1] ([1]*Tokyo University of Science*, [2]*ESTECH CORP.*)

Mechanical interaction between single strand DNA wrapped single-walled carbon nanotubes (ssDNA-SWCNTs) and cell membrane surface are important when applied to drug delivery, biosensor. In this study, we developed finite element model of the ssDNA- SWCNTs adhered to the cell membrane and analyzed the changes of natural frequency when ssDNA-SWCTNs freely vibrating adheres to the cell membrane in water. The vibration characteristics of ssDNA-SWCNT model were consistent with the experimental and Bernoulli-Euler beam theory. Since the lengths of SWCNTs are known to affect the permeation into the cell membrane, we report the mechanical interaction between ssDNA-SWCNTs with lengths of 25 to 200 nm and cell membrane.

20562U 二本鎖 DNA とカルボキシメチルセルロースで分散した単層カーボンナノチューブの吸光度特性
Absorption properties of single-walled carbon nanotubes dispersed with double-stranded DNA and carboxymethylcellulose

Ryo Hamano[1], Daisuke Miyashiro[1,2], Kazuo Umemura[1] ([1]*Tokyo Univ. Sci.*, [2]*ESTEC CORP.*)

We investigated the optical properties of SWNT bioconjugates with the stability of double-stranded DNA and the biocompatibility of carboxymethylcellulose. The bioconjugates can be applied to cell uptake by SWNTs. dsDNA/CMC-SWNT dispersions were prepared by mixing 1 mg/mL dsDNA and CMC solution at several different mixture ratios. Hydrogen peroxide (oxidant) was added to the dispersion, and catechin aqueous solution (antioxidant) was further added to measure the variation in near-infrared absorbance of SWNTs. The initial absorbance of dsDNA/CMC-SWNT dispersion of (10.00:0.00), (9.99:0.01), (9.90:0.10), (9.00:1.00) was 0.120, 0.125, 0.119, 0.130 and decreased to 0.108, 0.105, 0.095 and 0.102, and increased to 0.134, 0.133, 0.120 and 0.123 due to antioxidant activity.

20563U 空気の抵抗が雷の発生と発光に及ぼす影響
Effect of air resistance on the generation and lightning of thunderbolt

Shingo Iwasaki (*HatusibaTondabayasi H.S.*)

Thunderbolt is a phenomenon in which electricity flows through the air. I am interested in the mechanism of its lightning. I conducted the experiments in order to clarify the relationship between the discharge distance and the water vapor amount, or the lightning amount. I used a 16,000 V piezoelectric element to generate an aerial discharge between a needle and a sheet of aluminum. And I recorded the scene in the dark box and analyzed it. As a result, the discharge distance becomes shorter with the more water vapor amount, and the lightning amount becomes larger with the longer discharge distance. I think the discharge is less likely to occur because the resistance increases as the water vapor amount increases, while the lightning amount as the resistance increases.

20564U 基準振動解析を用いたロドプシンの動態予測と機能の連関
Relationship between function and dynamics of rhodopsin using normal mode analysis

Yukito Kaneshige[1], **Masashi Fujii**[1,2], Fumio Hayashi[3], Kenichi Morigaki[4], Hayato Yamashita[5], Akinori Awazu[1,2] ([1]*Dept. Math. Sci., Grad. Sch. Sci., Hiroshima Univ.*, [2]*Dept. Math. Sci., Grad. Integ. Sci. Life, Hiroshima Univ.*, [3]*Grad. Sch. Sci., Kobe Univ.*, [4]*Biosignal Research Center, Kobe Univ.*, [5]*Grad. Sch. Eng. Sci., Osaka Univ.*)

Rhodopsin (Rh) is a photoreceptor in the retina. The light-activated Rh activates the associated transducin (Gt) and begins the signal transduction. Rh mainly forms dimers on the cell membrane, and these Rh-dimers form row structures (Rh-cluster). As a functional significance of forming such Rh-cluster, the dynamic scaffold hypothesis has been proposed. However, such behavior has never been directly observed. In this study, we calculated the direction of fluctuation of dark-state Rh using normal mode analysis, and revealed that the fluctuation of dark-state Rh was highly correlated with the direction that promotes the transition of Gt to the adjacent Rh-dimer. In this presentation, we will discuss the methodology of normal mode analysis used in our analysis.

20565U Attempts at CA-type formal analysis of fibrous assembly of particles

Takashi Konno (*Math. Biol. Med. Univ. Fukui*)

In the framework of 2D and 3D cellular automata (CA), transition rules leading to fibrously assembled "structures" were constructed and analyzed. The elements could represent proteins in an abstractive form. The analysis in high dimensional CA systems could naturally be unexhaustive, but careful choice of the CA transition rules gave valuable insights into the physical reality. The rules could also be translated into the "energy" term. "Fibrous" pattern of a state in the CA lattice could directly be regarded as "fibers", but more abstractive definitions of "structure" were also challenged. This study is an initial step towards elucidating hidden logics unconsiously employed for recognizing "structures" in daily and/or scientific life.

20566U Formation of small G-protein Ras multimer induced by chemical modification of HVR domain

Rufiat Nahar[1], Maruta Shinsaku[2] ([1]*NAHAR RUFIAT*, [2]*SHINSAKU MARUTA*)

Previously we have shown that the chemical modification of the cysteine residues in the C-terminal hypervariable domain (HVR) of small G-protein H-Ras with hydrophobic thiol reactive reagents induces multimer formation of H-Ras. The multimerization may reflect the physiological conformational changes of Ras. SAXS and EM analysis revealed that the multimer exhibits pentamer of circular disk shape structure. In this study, we studied the conformational change of HVR domain accompanied by formation of Ras multimer. Ras.GDP state formed multimer by modification at HVR domain. Contrary GTP sate Ras (Ras.GTPγS) did not form. FRET analysis between Trp in HVR and Mant group in GTPase site showed that C-terminal of HVR domain in the GDP state Ras move to GTPase site.

20567U 模型飛行機の主翼長が滑空性能に与える影響
The Effect of Wing Length on Gliding Performance of Model Airplanes

Fumiya Yamanaka (*Osaka Pref. Tondabayashi H.S.*)

I was interested in the fact that the wings of a glider are very long and those of a fighter jet are much shorter,so I did research on the relationship between wing length and glide performance. I made three model planes with only the aspect ratio of the main wings differing, and glided them from a certain height and analyzed their performances on video. As a result, the model airplane with a high aspect ratio had a stable gliding attitude and increased gliding distance, whereas the airplane with a low aspect ratio tended to be unstable and had a large degree of deceleration, so it didn't fly as far. I thought that the form that could stabilize its gliding attitude and make it easier to glide as well as show the best gliding performance was the glider with long wings.

20568U 円環気流接合殺菌法によるウイルス感染ルートの遮断
Blocking virus infection routes by CARS-sterilizattion

Kuniaki Nagayama[1], Ryoichi Matsuda[2] ([1]*N-EM Labs.*, [2]*Grad. Sch. Sci., Tokyo Univ. Sci.*)

One of the authors (RM) suggested a new virus infection route through the fart airstream. There is no countermeasure against such a route as compared with that of the droplet or contact infection. Therefore, a measure for fecal-oral infection must be an urgent matter. We focused on the toilet and devised for rapidly sterilizing the infection source (1). For a toilet bowl, another sterilization space (sterilization box with UVC-LED) is provided, the both spaces are annularly air-flow joined with an air circulation by a blower. With this newly-developed Connected Air-flow Ring System (CARS), the sterilization efficiency can be arbitrarily set and quantified. The actual achievement of the CARS-sterilizer is to be reported. 1) K. Nagayama & R. Matsuda, Tokugan 2020-94964.

20569U* Self-Assembly of Flexible DNA Ring Motif

Shiyun Liu[1], Ibuki Kawamata[1,2], Satoshi Murata[1] ([1]*Grad. Sch. Eng., Univ. Tohoku*, [2]*Div. Natural Sci. Fac. Core Research, Univ. Ochanomuzu*)

The invention of DNA origami has expanded the geometric complexity and functionality of DNA nanostructures. Utilizing the DNA origami technology, we propose a joinable DNA ring motif, which consists of seven segments. The segments are linked by flexible hinges, allowing the motif to take various shapes. We can define the shape of the motif by fixing the flexible hinges in different locations. The motif can connect with each other by the self-complementary sequences, which are aligned symmetrically on segments. By adjusting the number and location of the connectable segments, the motif can self-assemble into different structures. We obversed the shape adjustment and the self-assembled structure by atomic force microscopy.

20570U 分子スウォームの自動制御のための DNA 反応回路の最適化
Optimization of the molecular circuit for automatic controlling movement of microtubules

Daiki Matsumoto[1], Ibuki Kawamata[1], Yuki Suzuki[1,2], Satoshi Murata[1], Jakia Jannat Keya[3], Akira Kakugo[3], Shin-ichiro Nomura[1] ([1]*Department of Robotics, Graduate School of Engineering, Tohoku University, Japan*, [2]*Creative Interdisciplinary Research Division,Frontier Research Institute for Interdisciplinary Sciences,Tohoku University*, [3]*Department of Chemistry, Faculty of Science, Hokkaio University*)

An active matter made of microtubules(MTs)/kinesin is called as a swarming molecular robot. Recently it is reported that the association/dissociation of the swarming of MTs can be performed by light irradiation or adding DNA. In this research, we aim to control the swarming of MTs automatically and continuously, by running a DNA molecular circuit at the same. We coordinated the condition such as concentration of DNA, ion and enzyme and succeeded in the association /dissociation cycle shorten from 24 hours to 3 hours. The reaction pathway of the DNA circuit was verified by computer simulation. The future of the study is expected to pave the way for the unified control of various molecular robots.

20571U 機械学習を用いた生物形態の定量化とその応用
Characterization of biological morphology by using machine learning

Masato Tsutsumi[1], Nen Saito[1,2], Chikara Furusawa[1,2,3] ([1]*Dept. of Physics,Grad School of Science, The Univ. of Tokyo*, [2]*Universal Biology Institute, The Univ. of Tokyo*, [3]*Center for Biosystems Dynamics Research, RIKEN*)

Morphology holds a lot of information about phenotypes, and its changes involve evolutionary and developmental processes. To understand morphological change, it is necessary to quantify the morphology itself. Geometric Morphometrics is one of the quantification methods. This method is based on the points called landmarks, but the setting of landmarks is different among researchers. To overcome this problem, we construct an unsupervised learning model with morphological images. We use mandibles from various species to train our model. We find that our model can extract features that distinguish the families to which species belong. We expect that our model will be applicable to species for which landmark is not known.

20572U Circularization in coding regions of Flaviviruses are crucial for viral fitness

Roland G. Huber (*A*STAR BII*)

RNA structures in Flaviviruses are crucial for viral replication in human and mosquito cells. Besides the well-known structures in the 5' and 3' UTR regions of flaviviral RNA, we identified and characterized a number of RNA structures in dengue and zika viruses that are necessary for proper replication of the viruses. We have characterized local and long-range interactions in the coding region of the viral genomes that are responsible for regulating viral transcription, genome replication and interact with host and viral protein components through combined chemical probing and structural modeling techniques.1 1. Huber, R. G. et al. Structure mapping of dengue and Zika viruses reveals functional long-range interactions. Nat. Commun. 10, 1408 (2019).

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。演題番号の末尾が 00 または 99 は，シンポジウムのオーガナイザーによる開会挨拶等を示しています。

Haering, Christian (Haering Christian) 20208G
Hagiwara, Kenichi (萩原 剣一) **20488R**
Hakamada, Kazuaki (袴田 一晃) 20141B
Hamachi, Itaru (浜地 格) 20473R
Hamada, Hiroshi (濱田 博司) 20242H
Hamakubo, Takao (浜窪 隆雄) 20054A
Hamamoto, Tatsuki (濱元 樹) 20288H
20291H
Hamano, Ryo (濱野 凌) 20561U
Hamano, Ryo (濵野 凌) **20562U**
Han, Huanwen (韓 煥文) 20096A
Hanai, Shunpei (華井 竣平) **20384M**
Hanaoka, Kenjiro (花岡 健二郎) **2S-7-7**
20447P
Hanayama, Rikinari (華山 力成) 2S-14-6
Hanazono, Yuya (花園 祐矢) 20154B
Hara, Mayu (原 舞雪) 20529S
Hara, Yuki (原 裕貴) **3S-5-6**
Harada, Ryuhei (原田 隆平) 20001A
20048A
Harada, Ryuichi (原田 龍一) 20093A
Harada, Yoshie (原田 慶恵) 20190G
20274H
20510S
Haraguchi, Takeshi (原口 武士) 20233G
Harashima, Takanori (原島 崇徳) **20504S**
Harusawa, Kanae (春澤 香苗) **20307I**
Haruyama, Takamitsu (春山 隆充) 20157B
Hase, Muneaki (長谷 宗明) 20024A
Hasebe, Mitsuyasu (長谷部 光泰) 2S-8-4
Hasebe, Takuya (長谷部 拓弥) **20476R**
Hasegawa, Taisuke (長谷川 太佑) 20405M
Hashimoto, Hidehiko (橋本 秀彦) **2S-3-2**
Hashimoto, Hideki (橋本 秀樹) 20401M
Hashimoto, Hiromichi (橋本 広道) 20264H
20266H
20273H
Hashimoto, Ken'ichi (橋本 賢一) 20053A
Hashimoto, Masanori (橋本 真典) **20049A**
Hasimoto, Hiromiti (橋本 広道) 20518S
Hatada, Yuji (秦田 勇二) 20556T
Hatakeyama, Hikaru (畠山 晃) **20543S**
20544S
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