



領域会議プログラム

5月12日(木) 13:00-16:00

時間	タイトル	講演者
13:00-13:10	今後のプロジェクトの方針について	岩田 想 (領域代表)
13:10-13:30	質疑応答	
13:30-14:00	新公募班自己紹介*	
14:00-14:20	光で病態を検出・制御する機能性分子の開発研究	永澤 秀子 (岐阜薬科大学)
14:20-14:40	温度ジャンプ法による分子動画解析の技術開発	南後 恵理子 (東北大学)
14:40-15:00	シミュレーションによる XFEL 生体高分子動的構造解析の精密化	宮下 治 (理化学研究所)
15:00-15:20	マイクロ流路デバイスを用いた顕微分光法によるタンパク質の反応機構解析	木村 哲就 (神戸大学)
15:20-16:00	総合討論・アドバイザーコメント	

※対象の方には、別途詳細をご連絡します。

領域関係者のみ参加可、ハイブリッド開催

発表言語：日本語

講演 12分 + 質疑応答 5分 + 入替 3分



2019-2023 MEXT Grant-in-Aid for Scientific Research on Innovative Areas

“Non-equilibrium-state molecular movies
and their applications (Molecular Movies)”

Molecular Movies International Symposium 2022

International Symposium Program

12th / May 5:00pm- 9:10pm JST (CET 12th/May 10:00am- 2:10pm, CST 12th/May 4:00pm- 8:10pm)

	Speaker	Affiliation	Title	Session chair
17:00-17:10	Prof. So Iwata	Kyoto University	Opening Remarks	-
17:10-17:50	Prof. Ilme Schlichting	MPI for Medical Research	Mechanism and dynamics of fatty acid photodecarboxylase	Iwata
17:50-18:30	Dr. Alke Meents	DESY	Fixed target serial crystallography for studying protein dynamics	Yamamoto
18:30-19:10	Prof. Helmut Grubmüller	MPI for Multidisciplinary Sciences	Three routes to molecular movies	Miyashita
19:10-19:50	Prof. Erik Lindahl	Stockholm University	Resolving gating and allosteric modulation in ion channels through simulations and small-angle neutron scattering	Miyashita
19:50-20:30	Prof. Peng Chen	Peking University	Bioorthogonal Protein Activation in Space and Time	Kiyonaka
20:30-21:10	Prof. Petr Klán	Masaryk University	Visible/near-infrared-light photorelease: How far can we go with one-photon absorption?	Furuta

30min presentation + 10min Q&A



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“Non-equilibrium-state molecular movies
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Molecular Movies International Symposium 2022

13th / May 8:00am-12:05pm JST (CDT 12th/May 6:00pm-10:05pm, EDT 12th/May 7:00pm-11:05pm)

	Speaker	Affiliation	Title	Session chair
8:00-8:40	Prof. Dirk Trauner	New York University	Controlling the Fate and Function of Proteins with Proximity Photopharmacology	Kiyonaka
8:40-9:20	Prof. Marius Schmidt	University of Wisconsin- Milwaukee	Mix-and-Inject Serial Crystallography	Nango
9:20-10:00	Prof. Eriko Nango	Tohoku University	Time-resolved serial femtosecond crystallography of microbial rhodopsins	Iwata
10:00-10:40	Prof. Qiang Cui	Boston University	Classical and QM/MM simulations of “molecular movies” for understanding the functions of biomolecular machines	Miyashita
10:40-11:20	Dr. Junichi Ono	Waseda University	Unification of molecular movies and large-scale quantum molecular dynamics	Iwata
11:20-12:00	Prof. Shinya Tsukiji	Nagoya Institute of Technology	SLIPT: a chemical approach for controlling protein localization and cell signaling	Kiyonaka
12:00-12:05	Prof. So Iwata	Kyoto University	Closing Remarks	-

30min presentation + 10min Q&A



Short talk Session Program

May 13th (Fri) 1:30pm -4:00pm

Room : Main Office Building Lecture Hall

Time	Name	Affiliation	Title
A01_Structural biology (Chair; Iwata)			
13:30-13:40	Shima Fumi	Kobe University	Elucidation of cancer signal transduction mechanism using photo-controllable Ras on an atomic scale.
13:40-13:50	Shimada Atsuhiko	Gifu University	The structures of catalytic intermediates of cytochrome c oxidase
13:50-14:00	Suga Michihiro	Okayama University	Extrapolated difference Fourier map is an illustrative method to analyze light-induced structural changes in a photosynthetic membrane protein
14:00-14:10	Cancel		
A01_Structural biology (Chair; Park)			
14:10-14:20	Ohashi Sayaka	Nagoya Institute of Technology	Strategic approach towards cone pigment structure determination
14:20-14:30	Katayama Kota	Nagoya Institute of Technology	Vibrational spectroscopic study of G protein-coupled receptor
14:30-14:40	Tanaka Ichiro	Ibaraki University	Reconsideration of hydrolysis reaction mechanism by lysozyme-NAG complex crystal structure analysis
(Break)			
A01_Chemical biology (Chair; Kiyonaka)			
14:50-15:00	Shimomura Takushi	National Institute for Physiological Sciences	Generation of photo-switchable potassium channels by incorporation of the azobenzene-based unnatural amino acid
15:00-15:10	Campbell Robert	The University of Tokyo	Next Generation Biosensors Enabled by High-speed Visualization of Dynamic Mechanisms
B01_Molecular Movie Platform Design (Chair; Yamamoto)			
15:10-15:20	Suzuki Akihiro	Hokkaido University	Reducing background noise of X-ray crystallography data through improved sample environment
15:20-15:30	Matsuura Hiroaki	RIKEN	Development of in-vacuum diffractometer for microcrystallography at SPring-8 (Online)



Room : YCU 2F Library

Time	Name	Affiliation	Title
C01_Computational Chemistry and Spectroscopy (Chair; Kubo, Kimura)			
13:30- 13:40	Kimura Tetsunari	Kobe University	Microspectroscopic systems for time-resolved measurements of protein microcrystals
13:40- 13:50	Mizuno Misao	Osaka University	Cis-trans reversion preceding reprotonation of the retinal chromophore in the schizorhodopsin photocycle (Online)
13:50- 14:00	Kubo Minoru	University of Hyogo	Time-Resolved Spectroscopy for Tracking DNA Repair by Photolyase
14:00- 14:10	Yagi Kiyoshi	RIKEN	Reaction dynamics of light-driven protein studied by non-adiabatic QM/MM molecular dynamics simulations
14:10- 14:20	Mizuno Yosuke	Nagoya Institute of Technology	Low-temperature UV-visible and FTIR spectroscopic studies on a UV sensitive visual pigment
(Break)			
C01_Computational Chemistry and Spectroscopy (Chair; Miyashita, Syouji)			
14:30- 14:40	Mitsutake Ayori	Meiji University	Analysis for Stability and Dynamics of Proteins using Molecular Dynamics Simulations
14:40- 14:50	Yokoi Shun	Meiji University	Molecular Dynamics Simulations for Determination of the Characteristic Structural Differences between Inactive and Active States of Wild-type and Mutants of the Orexin 2 Receptor (Online)
14:50- 15:00	Kitao Akio	Tokyo Institute of Technology	Analysis of free energy landscape and pathways of protein structural changes, dissociation and association
15:00- 15:10	Shoji Mitsuo	University of Tsukuba	Theoretical insights into the molecular mechanisms of dynamical biochemical reactions
15:10- 15:20	Hayashi Shigehiko	Kyoto University	Theoretical study on molecular mechanism of an activation process of aequorin bioluminescence (Online)

#Hybrid meeting with Zoom.

#Language: English

#5min presentation + 4min Q & A

Poster Session Program

May 13th (Fri) 4:00pm -6:00pm

名前	所属	ポスタータイトル
1 梅名 泰史	名古屋大学シンクロトン光研究センター	光アンテナ蛋白質フィコシアニンの光エネルギー移動の高速分子動画
2 大橋 沙也佳	名古屋工業大学大学院	Strategic approach towards cone pigment structure determination
3 小野 純一	早稲田大学	Hybrid in-silico drug discovery for covalent inhibitors against SARS-CoV-2 main protease
4 片山 耕大	Nagoya Institute of Technology	Vibrational spectroscopic study of G protein-coupled receptor
5 河村 高志	(公財)高輝度光科学研究センター	Drawing the structural dynamics information on Ras-mediated GTP hydrolysis out of freeze-trapped time-resolved SS-ROX data
6 Campbell Robert	東京大学大学院理学系研究科化学専攻	Next Generation Biosensors Enabled by High-speed Visualization of Dynamic Mechanisms
7 近藤 美欧	大阪大学大学院工学研究科	
8 島田 敦広	岐阜大学 応用生物科学部	The structures of catalytic intermediates of cytochrome c oxidase
9 下村 拓史	自然科学研究機構 生理学研究所	Generation of photo-sensitive ion channels by incorporation of the unnatural amino acid in <i>Xenopus</i> oocyte expression system
10 庄司 光男	筑波大学	Theoretical insights into the molecular mechanisms of dynamical biochemical reactions
11 鈴木 明大	北海道大学電子科学研究所	動的結晶構造解析の高感度化に向けた新規計測システムの開発
12 Srinivasaraghavan Sriram	RIKEN	Automated Density Extraction of Isomorphous Difference Map and Occupancy-estimation for Conformer Fitting
13 田中 伊知朗	茨城大学	Reconsideration of hydrolysis reaction mechanism by lysozyme-NAG complex crystal structure analysis
14 寺井 琢也	東京大学大学院理学系研究科化学専攻	Chemi-genetic indicators for metal ions using HaloTag self-labeling protein
15 Tran Duy	School of Life Science and Technology, Tokyo Institute of Technology	A hint to inhibit the hexamerization of the SARS-CoV-2 Nsp15 protein
16 Nuemket Nipawan	JASRI	Towards time-resolved serial femtosecond X-ray crystallography (TR-SFX) of human visual rhodopsin
17 橋本 佳奈	岡山大学	Extrapolated difference Fourier map is an illustrative method to analyze light-induced structural changes in a photosynthetic membrane protein
18 長谷川 颯人	国立大学法人鳥取大学持続性社会創生科学研究科	Diels-Alder 反応を行う酵素の時分割シリアルフェムト秒 X 線結晶構造解析に向けた変異体作製と結晶化
19 馬場 清喜	高輝度光科学研究センター	Non-cryogenic X-ray crystallography under various ambient conditions using the humid air and glue-coating (HAG) method
20 針尾 紗彩	東京大学大学院理学系研究科化学専攻	Development and applications of a series of genetically encoded GFP-based intracellular L-lactate indicators.
21 日野 智也	鳥取大学	高速分子動画でTRPチャネルの温度センサー部位を見極める
22 横野 義輝	神戸大学	Visualization of allosteric structural changes in Ras on GTP hydrolysis process using SACLA / SPring-8 / NMR
23 水野 陽介	名古屋工業大学大学院	Low-temperature UV-visible and FTIR spectroscopic studies on a UV sensitive visual pigment
24 光武 亜代理	明治大学	Dynamical Analysis for Protein Simulations Using Relaxation Mode Analysis
25 宮下 治	RIKEN Center for Computational Science	XFEL実験データを活用したハイブリッドモデリングアプローチ
26 村川 武志	大阪医科大学	シリアルフェムト秒結晶構造解析に基づく銅含有アミン酸化酵素の触媒機構の解明
27 八木 清	理化学研究所	非断熱QM/MM分子動力学計算による光駆動タンパク質の反応ダイナミクス
28 山口 一成	東京大学大学院理学系研究科化学専攻	Self-Complementing Split Fluorescent Protein-Based Biosensors for Calcium Ion
29 山田 大智	兵庫県立大学	Time-resolved microspectroscopic detection of a key intermediate in the UV-damaged DNA repair by (6-4) photolyase.
30 山元 淳平	大阪大学大学院基礎工学研究科	Kinetics of electron returns in successive two-photon DNA repair by (6-4) photolyase