# Symposium List

# [Satellite Symposium]

# 24(Wed), November

13:30-16:00

# 50 years of the Protein Data Bank and the frontier of the Structural Biology in Asia

Organizers : Genji Kurisu (Osaka Univ.), Toshimichi Fujiwara (Osaka Univ.) Summary :

In 1971, the structural biology community established the single global archive for 3D macromolecular structure data: the Protein Data Bank (PDB). Approximately one fourth of the entire PDB data originated from Asia. In 2000, Protein Data Bank Japan (PDBj) started on-site data processing as a newly founded Asian hub for PDB data resource. Since 2001, PDBj has provided our newly developed online Data-out services available freely and publicly through our own web site (https://pdbj.org), which we have enhanced through the years. With the establishment of the worldwide PDB in 2003, we have served as one of its regional data centers, collaborating on Data-in and Data-out activities on a global scale. In 2021, we are celebrating the 50th anniversary of our single global archive, especially this time in Asia, and want to discuss the frontier of the Structural Biology in Asia.

# [Symposium]

# 25(Thu), November

# 9:00-11:30

# Japan-US symposium on cytoskeletal motor proteins and their associated proteins

Organizers : Kumiko Hayashi (Tohoku Univ.), Shinsuke Niwa (Tohoku Univ.)

# [Pick up speakers from the students and post-doctoral fellows]

## Summary :

Speakers in this symposium are recognized internationally as experts in the field of cytoskeletal motor proteins such as kinesin and dynein, and their associated proteins. We are planning to prepare enough time to have a deep and detailed discussion among the speakers and audience on these subjects. The symposium topics cover multidisciplinary applications of genetics, bio-engineering, bio-chemistry, medical science, and physics, which will give us new insights into the intracellular transport and motor proteins, as well as interesting applications of existing single-molecule techniques.

## 9:00-11:30

# Dawn of Molecular System Engineering for Chemical AI

Organizers : Taro Toyota (The Univ. of Tokyo), Shogo Hamada (Tohoku Univ.) Summary : C. Elegance has a brain consisting of 302 cells, which controls all the behaviors of the organism. The neurons in its brain are classified into three levels, and they are connected by about 6000 synapses. On what principle do these "wet" information processing systems operate? At least, such systems must be constructed by the power of chemistry. A new methodology of "how to assemble individual molecules and molecular devices into complex functional systems" is attracting attention as "molecular systems engineering". In Grant-in-Aids for transformational research "Molecular Cybernetics" (2020-2024), we will investigate principles of the molecular systems engineering. Specifically, designed molecules that function as sensors, processors, and actuators will be assembled in a micrometer-sized compartment (artificial cell) such as a liposome. The resulting artificial cells can then be further combined with each other to construct higher-order functional systems. In this symposium, we will discuss the design principles and practice of such artificial cells and other issues related to the construction of chemical artificial intelligence (AI).

### 9:00-11:30

# Recent progress in biometal sciences: synergy between theory and experiments

Organizers : Yasuteru Shigeta (Univ. of Tsukuba), Takehiko Tosha (RIKEN) Summary :

Various metallic and semi-metallic elements, which are present in very small amounts in living organisms (defined as biometals), are essential for all living organisms. Their functions range from signal transduction and electron transfer to enzymatic reactions for the production and metabolism of substances. It is mystery that these trace amounts of biometals are programmed into life besides the central dogma. In this symposium, the latest researches on biological reactions and structures involving biometals and their kinetic analysis will be presented from both theoretical and experimental approaches.

### 9:00-11:30

# Structural and Functional Dynamics of Biomolecules: Interplay between Single Molecule Measurement and Molecular Simulation

Organizers : Tadaomi Furuta (Tokyo Inst. of Tech.), Kiyoto Kamagata (Tohoku Univ.) Summary :

Currently, the qualitative and quantitative developments of experimental and computational methods have made it possible to directly observe important structural and functional dynamics of various biomolecules. Recently, there have been many reports that lead to further understandings of biological phenomena by integrating information obtained from these experiments and simulations. In view of this situation, the theme of this symposium is at the stage where it should be promoted further. Therefore, in this symposium, several researchers on the experimental side, simulation side, and integrated researches will present the latest research results and general remarks, which would be clues leading to profound understandings of biological phenomena.

### 9:00-11:30

# New perspectives on cells provided by single cell analyses

Organizers : Yuichi Taniguchi (Kyoto Univ.) , Shinya Kuroda (The Univ. of Tokyo) Summary :

Single cell biology is a growing field to quantitatively understand the nature of individual cells that inherently have large heterogeneity. This growth is supported by progresses in a variety of single-cell approaches such as DNA/RNA sequencing, optical imaging, mass spectroscopy, high-throughput measurement, theory and informatics. In this symposium, we invite several single-cell biology scientists who conduct cutting-edge research using different approaches, aiming at discussing what single cell biology will bring towards understanding of life phenomena.

### 9:00-11:30

# New concepts in GPCR research and implications for drug discovery

Organizers : Kota Katayam (Nagoya Inst. of Tech.), Ryoji Suno (Kansai Medical Univ.)

## [Pick up speakers from the students and post-doctoral fellows]

Summary :

The recent trend in the field of structural studies of G-protein-coupled receptors (GPCRs) using cryoelectron microscopy (Cryo-EM) and 3D reconstruction techniques supported by biophysical, computational and advanced biochemistry have facilitated GPCRs research towards drug discovery. These techniques contributed significantly to our understanding about GPCRs functions, ligand recognition, pharmacological targets in biomedicine. This symposium will highlight the latest developments in GPCR structure/function, ligand discovery and design, intracellular signalling pathways and their impact on modern drug discovery.

## 16:00-18:30

# India-Japan joint symposium: Various challenges on biophysical research

Organizers : Miyuki Sakaguchi (Saitama Univ.), Ken H. Nagai (JAIST)

## Summary :

To promote the exchange between the Indian Biophysical Society (IBS) and the Biophysical Society of Japan (BSJ), this joint symposium focusing on energetic young scientists was planned. Four up-andcoming researchers are nominated by IBS, and they will give talks in a wide range of fields like protein function during embryogenesis, super-resolution imaging with DNA, morphogenesis in an active-polar gel, and the physical basis on self-reproducing catalytic RNAs. From BSJ, three leading researchers in related fields will also give talks. In the symposium, we will share the problems at the forefront, and exchange cutting-edge technologies and knowledge.

## 16:00-18:30

# Water dynamics and biological functions: Revisit

Organizers : Masahiko Imashimizu (AIST), Hiroshi Murakami (QST)

[Pick up speakers from the students and post-doctoral fellows]

Summary :

Extensive studies of hydration water dynamics show that they occur from the picosecond to nanosecond timescales. We, however, consider from recent studies that much slower dynamics of water may play critical roles in expressing biological functions. Such studies include findings of glass-like water in a model of cells and glassy behaviors of cytoplasm, and of nonthermal effects on slow biomolecular dynamics and reactions by the externally applied alternating electromagnetic field with terahertz frequency. In this symposium, we will attempt to discuss new directions that connect the physicochemical studies of hydration to biological functions through water relaxation processes in a wide temporal range.

## 16:00-18:30

## Trends in the research field of thermo-sensation

Organizers : Kunitoshi Uchida (Univ. of Shizuoka), Yuichiro Fujiwara (Kagawa Univ.) Summary :

Since TRPV1 channel, the world's first mammalian thermo-receptor, was uncovered in 1997, several thermo-receptors have been elucidated, and the biological meaning of thermo-sensation are becoming clearer. In this symposium, we will introduce the recent works aimed to evaluate the measurement and manipulation techniques of temperature in living matter, and to elucidate the gating mechanisms of thermo-receptors by temperature changes and physiological roles of thermo-sensation. We will also discuss the biological significances and future perspectives of thermo-sensation.

### 16:00-18:30

## **Recent Advances in Origins of Life and Protocell Research**

Organizers : Tony Z. Jia (Tokyo Inst. of Tech.), Yutetsu Kuruma (JAMSTEC)

### [Pick up speakers from the students and post-doctoral fellows]

### Summary :

One of the major questions in ancient and modern science is the question of our own creation. How did life emerge on Earth? What were the structures and functions of the first cells? Recent technological advances in biophysics, especially in Japan, are now allowing researchers in a variety of fields such as synthetic biology, evolutionary biology, and biochemistry to finally begin to answer these questions. This symposium highlights recent advances in Origins of Life and Protocell research by biophysicists from Japan and around the world. We hope to inspire other biophysicists, especially young researchers, to also consider studying these very difficult (but important) unanswered questions.

### 16:00-18:30

# Toward understanding biological functions: atomic-level characterization of structures and dynamics of biomolecules

Organizers : Osamu Miyashita (RIKEN), Eriko Nango (Tohoku Univ.)

Summary :

Information on the structures and dynamics of biological molecules plays a critical role in understanding their functional mechanisms and possible medicinal applications. Time-resolved serial femtosecond crystallography (TR-SFX) using X-ray free electron laser (XFEL) is a state-of-art technique that can provide 3D structures of the molecules following the time-development of reactions. Furthermore, integrative analyses combining TR-SFX data with other approaches could provide more detailed information on dynamic structures and energetics. This symposium will focus on recent updates on TR-SFX experiments and applications, as well as recent developments of other experimental techniques and computational approaches, aiming to advance our understanding of biomolecular functions through integrative research.

### 16:00-18:30

# Bridging biophysics/soft-matter physics and medical science

Organizers : Hiroshi Fujisaki (Nippon Medical School), Komura Shigeyuki (Tokyo Metro. Univ.) Summary :

Research towards tailor-made and precision medicine is accelerating, and this requires mathematical and physical approaches in addition to empirical medical traditions. Medical physics has been established as a field that links medicine and physics, and recently, AI has been used for pathological imaging diagnosis and particle therapy. On the other hand, biological phenomena have various hierarchies, starting from the molecular level to cells, organs, individuals, and populations, and with the advancement of computers, highly precise simulations of these phenomena are now becoming possible. In this symposium, we will explore the possibility of medical applications, including therapeutic methods, from the standpoint of biophysics and soft matter physics. The main purpose of this symposium is to have a lively discussion among medical scientists, biophysicists, and physicists about the awareness of problems in the field of medicine and how to deal with them in theory and calculations.

## 16:00-18:30

## Approaches to diverse biological phenomena produced by singularity cells

Organizers : Hiroko Bannai (Waseda Univ.), Ken-ichi Wakabayashi (Tokyo Inst. of Tech.) Summary :

In multicellular systems, there are many phenomena that result in dramatic changes in morphology and dynamics caused by a small number of cells. In this symposium, we will introduce challenging research to find rare cells, i.e. "singularity cells", which are the driving force of dramatic changes in diverse biological phenomena such as algal behavior, stem cell differentiation, organogenesis, and neurological diseases. Elucidating the mechanism by which "singularity cells" significantly change the entire system requires new perspectives and methodologies. By sharing this approach with members, we aim to spread a new methodology of biophysics and a new academic field "Singularity Biology".

### 16:00-18:30

## Information biophysics of gradient sensing in organisms

Organizers : Akihiko Ishijima (Osaka Univ.), Yasushi Okada (RIKEN/The Univ. of Tokyo)

[Pick up speakers from the students and post-doctoral fellows] Summary : Biological sensory systems, such as chemotaxis, phototaxis, gradient sensing and so on, are functions that are widely available in the biological world. For example, bacterial chemotaxis is one of the most well-studied areas from both theoretical and experimental perspectives. Various methods have been used in experiments, including genetics, biochemistry, and imaging. Theories have been discussed from various perspectives such as Ising model, information theory, and efficiency. In this symposium, we would like to gather theoretical and experimental researches to promote mutual integration from the viewpoint of information biophysics.

# 26[Fri], November

#### 9:00-11:30

# Technical Development and Sharing of High-Resolution Cryo-Electron Microscopes

Organizers : Haruki Nakamura (Osaka Univ.), Masahide Kikkawa (The Univ. of Tokyo), Takeshi Murata (Chiba Univ.)

#### Summary :

So far, high-end cryo-electron microscopes (EMs) have been installed along with the BINDS (Basis for Supporting Innovative Drug Discovery and Life Science Research) program since 2017, and 8 more cryo-EMs are going to be introduced in 2021 at several laboratories in Japan. Recent technological progresses including development of new grids and methods for on-line usage will surely provide higher-resolution, higher-throughput structural analysis, by sharing the cryo-EM devices among researchers in Japan. In this symposium, we will review the results of single particle analysis, tomography, and micro-ED by cryo-EMs, and will introduce the issues to be overcome by the recent technologies. Finally, we will discuss the future development including the scope of the next BINDS program, which is expected to start in 2022.

#### 9:00-11:30

# Biophysical basis for understanding the protein-protein interaction involved in essential cellular process

Organizers : Risa Mutoh (Fukuoka Univ.), Takumi Koshiba (Fukuoka Univ.)

### [Pick up speakers from the students and post-doctoral fellows]

Summary :

Protein-protein interactions are essential biological reactions occurring at inter- and intra-cellular levels. The analysis of their mechanism is generally required in order link to understand their various cellular functions. Recent biophysical methodologies provide us useful tools for investigating protein-protein interactions, especially in live cells. In this symposium, we invite domestic young investigators and discuss on new techniques (e.g. IP-MS, lipid mixing assay, bioluminescence) that explore a new study of protein-protein interaction and membrane protein complexes involved in essential cellular processes.

### 9:00-11:30

# A variety of photoreceptors and the frontiers of optogenetics.

Organizers : Satoru Tokutomi (Osaka Prefect. Univ.), Satoshi P Tsunoda (Nagoya Inst. Tech.) Summary :

Lives have acquired a variety of photoreceptors which absorb light in the UV to far red region during the evolution, such as many different types of rhodopsin, blue-light receptors, cryptochrome and phototropin, and red-far red-light reversible phytochromes. Researchers have adapted and utilized them for photobiological studies including optogenetics. The present Symposium introduces some leading results which includes channel rhodopsin in the trendy neuroscience, a novel function of mouse cryptochrome in circadian rhythm, use of a light-inactivated rhodopsin, peropsin, for vision restoration, photoregulation of protein kinase by phototropin, application of phytochrome-PIF and cryptochrome-CIB for optogenetics, and color tuning of cyanobacteriochrome.

### 9:00-11:30

# Biophysics on Genome DNA - Toward Understanding of Genome Modality -

Organizers : Masahiro Takinoue (Tokyo Inst. of Tech.), Shoji Takada (Kyoto Univ.),

Kazuhiro Maeshima (NIG)

### Summary :

The current trends in genome research, from genome sequencing to enome editing, have revolved based on the understanding of the informational aspects of genome, such as the replication and recombination of base sequences, and epigenetic regulation by histone modifications. However, the physical properties of genomic DNA as a polymer have not been fully elucidated yet, although it is an important property underlying all the phenomena caused on the genome. In this symposium, we will introduce a research area "Genome Modalities", which aims to reveal the true nature of genomes through understanding the physical properties of DNA, and discuss this issue with researchers inside and outside this area.

### 9:00-11:30

# An Integrated Multi-scale Approach for Studying Cyanobacterial Circadian Clock System

Organizers : Shuji Akiyama (CIMoS), Hironari Kamikubo (NAIST)

## [Pick up speakers from the students and post-doctoral fellows]

### Summary :

Circadian rhythms are self-sustained oscillations with a period of approximately 24 h, enabling organisms to adapt to daily alterations in the environment. So far, many studies have investigated the time-measuring mechanism in the circadian clocks from bacteria to mammals. However, it remains unknown how the period is implemented in clock oscillators and kept unaffected against temperature changes (temperature compensation). In this symposium, we will focus especially on cyanobacterial circadian clock as a model system and address these questions using a multidisciplinary approach including, biophysics, structural biology, chronobiology, molecular biology, and protein engineering.

### 9:00-11:30

# Advances in enhanced sampling methods for molecular simulations of protein systems

Organizers : Ayori Mitsutake (Meiji Univ.), Hisashi Okumura (ExCELLS)

## [Pick up speakers from the students and post-doctoral fellows]

### Summary :

In recent years, it has become possible to perform molecular simulations on time scales of the order of milliseconds using special-purpose system and massive parallel computers. However, sampling methods that is about 10 to 100 times more efficient than ordinary molecular simulations are still important to investigate binding simulations and longer simulations. Since about 25 years ago, various sampling methods have been energetically introduced and developed into protein systems in Japan. Currently, many enhanced sampling methods are widely introduced in protein softwares such as AMBER, CHARMM, GENESIS, GEMB, GROMACS, NAMD, and myPresto. In this symposium, researchers who have originally developed sampling methods and applied to protein systems will give their talks.

### 9:00-11:30

# New artificial approaches and biophysical communications to control function of biological membranes

Organizers : Ikuhiko Nakase (Osaka Prefect. Univ.), Yoshiaki Yano (Kyoto Univ.)

## [Pick up speakers from the students and post-doctoral fellows]

### Summary :

Biological membranes have a complex supermolecular bilayer structure composed of diverse biomolecules such as lipids, proteins, and sugars. It is well known that biomembranes contain receptor proteins to detect changes in external environments, and their ligand molecules are available for controlling cell functions. Moreover, alternative approaches are possible to artificially perturb function of biomembranes by e.g., changing their shape, permeability, and domain structures following molecular interactions with lipids. New approaches using hybrid/designed molecules, model membranes, ultrafast spectroscopy, and chemistry on/in cells, will be introduced to discuss complex membrane functions with biophysical communications and their usefulness for molecular sensing and controlling cell functions

# 27[Sat], November

#### 9:00-11:30

### **ASB-BSJ Joint Symposium**

Organizers : Kota Katayam (Nagoya Inst. of Tech.) , Matthew AB Baker (Univ. of New South Wales)

### Summary :

This symposium aims at highlighting the current main stream topics in protein science and biophysics and also searching for the collaboration and development in research filed of biophysics in the JapanAustralia region. The symposium includes three up-and-coming young researchers related to biophysics from the ASB and BSJ sides. With the rapid progress of science and technology in recent years, through this constructive discussion, we wish to keep the scientific activity, and to give a large impact to the community.

### 9:00-11:30

# Parametric biology based on translation rate regulatory mechanism

Organizers : Kohki Okabe (The Univ. of Tokyo), Yoshie Harada (Osaka Univ.) Summary :

Translation is not just a linear bridge between mRNA and protein, but is highly variable and characterized by a wide dynamic range (1,000 times that of transcription), local control within the cell, and reactions that consume up to 50% of the energy in the cell. This raises the possibility that translation is not controlled by 0 or 1 on/off control, but is subtly controlled by "rate variation" within a continuous reaction. Currently, we are beginning to create a translation parametric biology that focuses on the concept of "variable translation rate. This will elucidate its role in the flexible functional control of life.

### 9:00-11:30

# Protein hydration and its freezing phenomena -toward the application for cellfreezing and food frozen storage-

Organizers : Naoki Yamamoto (Jichi Medical Univ.), Hiroshi Nakagawa (J-PARC)

## [Pick up speakers from the students and post-doctoral fellows]

### Summary :

Protein hydration water is crucial for the activation of the dynamics related to the protein functional expression. We introduce recent progress on the understanding of the interplay between hydration water and protein in terms of the freezing of hydration water. Recent experimental results obtained by broadband dielectric spectroscopy and neutron scattering on proteins and tissues will be reported. Furthermore, present recent progress in the understanding the cell-freezing and food frozen storage will be represented. Especially, polymeric cryoprotectants, which have low toxicity and high protection capability, have been paid attention for those purposes, will be introduced and it physicochemical property will be discussed.

### 9:00-11:30

## Probing large-scale dynamics in protein through integrative approaches

Organizers : Tomohide Saio (Tokushima Univ.), Rintaro Inoue (Kyoto Univ.) Summary :

Large scale dynamics" (LS-dynamics) such as domain-domain correlation motion, often drives protein activity, but the scarcity of the information regarding them impedes the understanding of the mechanism. In other words, the LS-dynamics of protein is still a frontier in protein science. Everyone recognizes that, although state-of-the-art techniques provide the knowledge of various aspects of LS-dynamics, only a single method could not adequately cover the ranges of length and time scales

required for the LS-dynamics. Hence, agenda are how to integrate their results and build the full picture of LS-dynamics. In this symposium, young scientists from variety of scientific fields, solution scattering, NMR, cryo-EM, and computation, will lead to discuss about the integration of their methods aiming to unveil the biologically significant LS-dynamics.

#### 9:00-11:30

# Peptide-Membrane Biophysics: Current Biophysical Studies of Membrane-bound Antimicrobial Peptides and Amyloid Peptides

Organizers : Izuru Kawamura (Yokohama Natl. Univ.), Tomoyasu Aizawa (Hokkaido Univ.)

## [Pick up speakers from the students and post-doctoral fellows]

### Summary :

In the biophysical research field, the structure and dynamics of peptide and lipid molecules within complex biomolecular assemblies have been investigated for many years with a special focus on membrane-interaction of antimicrobial peptides (AMPs) and kinetics of amyloid fibril formation. In this symposium, current research topics on "peptide-membrane biophysics" by imaging, NMR, and computational methods will be presented. Additionally, advanced over-expression technology and deep learning for molecular design of AMPs will be presented.

### 9:00-11:30

# New Trends in Functional Omics Analysis Integrated with Live Cell Imaging

Organizers : Yoshitaka Shirasaki (The Univ. of Tokyo), Katsuyuki Shiroguchi (RIKEN)

# [Pick up speakers from the students and post-doctoral fellows]

Summary :

Cells change their function from time to time based on the alteration of their gene expression.

Live cell imaging is an excellent technique for tracking the cellular functions, though it has limited targets. On the other hand, omics analyses such as high-throughput sequencing and mass spectrometry have advantages for comprehensiveness on gene expression analysis, although they cannot obtain time-series information due to disruptive manipulations. In this symposium, we will focus on advanced single-cell technologies that bridge the gap between time-series and comprehensive information on dynamic cellular functions, and will discuss the future prospects of this field.