September 4 (Wednesday)

10:20-10:30  Opening Remarks
Fumio Hirata (Toyota Physical and Chemical Research Institute, Japan)
Chair  Yuko Okamoto

10:30-11:00  Fumio Hirata (Toyota Physical and Chemical Research Institute, Japan)
Structural Fluctuation of Protein and Anfinsen’s dogma

11:00-11:30  Kazuyuki Akasaka (Kyoto Prefectural University of Medicine, Japan)
Warping to the Reality of Life through the World of Pressure

11:30-12:00  Masatake Sugita (Ritsumeikan University, Japan)
Developing a semi-analytical method for analyzing structural fluctuations of a molecule in solution phase by means of 3D-RISM theory

12:00-13:00  Lunch
Chair  Hirofumi Sato

13:00-13:30  Ryota Iino (Institute for Molecular Science, Japan)
Watching Dynamic Motions of Hydrolysis-Powered Protein Motors with Plasmonic Nanoprobes

13:30-14:10  Nancy Horton (The University of Arizona, USA)
The Mechanism of Activated DNA Cleavage by the Filament Forming Enzyme SgrAI

14:10-14:40  Masayuki Irisa (Kyushu Institute of Technology, Japan)
Role of Mg$^{2+}$ Ions in DNA Hydrolysis by EcoRV, Studied by the 3D-RISM and Molecular Dynamics

14:40-14:55  Coffee Break
Chair  Norio Yoshida

14:55-15:25  Nobuyuki Matubayasi (Osaka University, Japan)
Energetics of Cosolvent Effect on Structure Formation of Biomolecule Studied through Variational Principle

15:25-15:55  Makoto Suzuki (Tohoku University, Japan)
On the physicochemical origin of the driving force of actomyosin motor

15:55-16:25  Hirofumi Sato (Kyoto University, Japan)
Chemical Process in aqueous solution: Chemical Reaction, Excitation and Dynamics

16:25-16:40  Coffee Break
Chair 16:40-17:20 Masayuki Irisa

Ruchi Anand (IIT-Bombay, India)

Role of Allosteric Switches and Adaptor Domains in Long Distance Cross-Talk and Transient Tunnel Formation

Hideki Kandori (Nagoya Institute of Technology, Japan)

Panama Canal Model for Active Transport and One Exception

Norio Yoshida (Kyushu University, Japan)

Understanding biological processes in solution based on the statistical mechanics theory of liquids

18:30- Welcome Party

September 5 (Thursday)

Chair 9:30-10:10 Masatake Sugita

Thanyada Rungrotmongkol (Chulalongkorn University, Thailand)

In Silico and In Vitro Study on Drug Targets for Dengue and Zika Viruses

Saree Phongphanphanee (Kasetsart University, Thailand)

The selective adsorption of alkali ions on nanomaterials

10:50-11:05 Coffee Break

Chair 11:05-11:35 Koichi Kato

Kunihiro Kuwajima (IMS, Japan)

The Problem of Protein Folding

Mikio Kataoka (NAIST, Japan)

Effect of hydration on low-energy protein dynamics

12:05-13:00 Lunch

Chair 13:10-13:40 Kunihiro Kuwajima

Florence Tama (Nagoya University, Japan)

Molecular mechanisms involved in the regulation of the Circadian Clock

Yuji Goto (Osaka University, Japan)

Heating under agitation revealed the supersaturation-veiled amyloid fibrils of β2-microglobulin at neutral pH

14:10-14:40 Koichi Kato (IMS, Japan)

Dynamic Views of Structures and Interactions of Antibodies
14:40-14:55 Coffee Break
Chair Nobuyuki Matubayasi
14:55-15:35 Maxim V Fedorov (Skolkovo Institute of Science and Technology, Russia)
Exploration of properties of bioactive molecules from a vast chemical space by machine learning and molecular theories
15:35-16:05 Akio Kitao (Tokyo Institute of Technology, Japan)
Simulating Protein Complex Formation and Dissociation
16:20-18:10 Poster Presentation
18:30- Banquet

**September 6 (Friday)**

Chair John E. Straub
9:30-10:00 Ayori Mitsutake (Meiji University, Japan)
Stability and Dynamics Analysis of Protein-Folding Simulations using Relaxation Mode Analysis and 3D-RISM Theory
10:00-10:40 Ronald Levy (Temple University, USA)
Exploring free energy and fitness landscapes of proteins for alloster and binding
10:40-10:55 Coffee Break
Chair Akio Kitao
10:55-11:25 Yuji Sugita (Riken, Japan)
Free-Energy Calculations of Protein-Ligand Binding by Enhanced Conformational Sampling Methods
11:25-12:05 John E. Straub (Boston University)
Probing the principles governing protein assembly and amyloid aggregation
12:05-13:00 Lunch
Chair Fumio Hirata
13:00-13:30 Masataka Nagaoka (Nagoya University, Japan)
Toward Understanding Reaction Mechanism of Enzymatic Catalyzation: A Treatment using Red Moon Methodology
13:30-14:00 Yuko Okamoto (Nagoya University, Japan)
Enhanced Sampling Simulations for Water and Biomolecules
Poster Presentations September 5, 16:45-18:20

<P01> Shoichi Tanimoto (Kyushu University)
Effect of molecular orientational correlations on solvation free energy computed by reference interaction site model method

<P02> Tsuyoshi Yamaguchi (Nagoya University)
Dielectric Constant of 3D-RISM with Charge-Response Kernel

<P03> Yuki Yano (Kyushu Institute of Technology)
Cation and water distributions at the active site of BamHI–DNA complex calculated by 3D-RISM

<P04> Itaru Onishi (Kyushu Institute of Technology)
A QM/MM Metadynamics study of the DNA Hydrolysis by EcoRV Subsequent to Scissile-Phosphate Twist

<P05> Maho Yagi-Utsumi (Exploratory Research Center on Life and Living Systems)
NMR Study of Conformational Transition of Amyloid-β on Ganglioside Membrane

<P06> Methanee Hiranyakorn (Exploratory Research Center on Life and Living Systems)
NMR characterization of conformational dynamics of Lys48-linked ubiquitin chains

<P07> Takuya Hayashi (Nagoya University)
Identification of Structural Transitions of Proteins by Microcanonical Inflection-Point Analysis Method: Case of Helix-Coil Transitions

<P08> Arpita Srivastava (Nagoya University)
Conformational ensemble of a flexible loop in mitochondrial import protein Tim21

<P09> Ashutosh Srivastava (Nagoya University)
Structural and dynamical insights into functional divergence in mammalian cryptochromes

<P10> ASI Han (Nagoya University)
Ab Initio Modelling Using XFEL Diffraction Data

<P11> Kamonpan Sanachai (Chulalongkorn University)
Insights into binding recognition and susceptibility of tofacitinib toward Janus kinases: Molecular dynamics simulations and pharmacophore modeling

<P12> Kosuke Imamura (Kyoto University)
Dynamic Process of Nanocube Self-assembly using Coarse-grained Model