

# Workshop on Modeling Biomolecular Systems in Cellular Environments

Oct.31 (Thu.) – Nov.1 (Fri.), 2013, Kyoto University, JAPAN

## Scientific Program

### October 31 (Thursday)

#### Session 1: Structure and dynamics of nucleus/nucleoid

- 09:30 – 10:10      **Koby Levy** (Weismann Institute of Science)  
Dynamics of DNA search under in vivo conditions: A molecular perspective.
- 10:10 – 10:40      **Tsuyoshi Terakawa** (Kyoto University)  
Transcription factor dynamics in nucleus studied by coarse-grained simulations.
- 10:40 – 11:10      **Wei Wang** (Nanjing University)  
Atomistic simulations on conformational fluctuations of TFIIIA zinc-finger in recognizing DNA/5S RNA.
- 11:10 – 11:30      << Coffee Break >>
- 11:30 – 12:10      **Remus Dame** (Leiden Institute of Chemistry)  
Unravelling the role of chromatin proteins in prokaryotic nucleoid organization.

#### Session 2: Cellular Imaging and Modeling

- 12:10 – 12:40      **Masayoshi Nakasako** (Keio University)  
Coherent X-ray diffraction imaging of non-crystalline particles with sub-micrometer dimensions.
- 12:40 – 14:30      << Lunch Break and Poster Presentation >>

- 14:30 – 15:10 **Peer Bork** (European Molecular Biology Laboratory)  
Systemic analysis of human-associated microbes: Lessons from a tiny bacterium and a large community.
- 15:10 – 15:40 **Masaki Sasai** (Nagoya University)  
Time and spatial scales of eukaryotic gene regulation.
- 15:40 – 16:00 << Coffee Break >>
- 16:00 – 16:30 **Kazuhiro Maeshima** (National Institute of Genetics)  
Chromatin structure and dynamics in living mammalian cells.
- 16:30 – 17:00 **Sachihiro Matsunaga** (Tokyo University of Science)  
Subnuclear dynamics and cell dynamics in root morphogenesis.
- 17:00 – 17:30 **Michael Feig** (Michigan State University)  
Cellular-scale simulations at atomistic resolution.
- 18:00 – 20:00 << Banquet >>

## November 1 (Friday)

### Session 3: Imaging of Macromolecular Complexes by new technique

- 09:00 – 09:30 **Florence Tama** (RIKEN)  
Structural modeling from low resolution experimental data.
- 09:30 – 10:00 **Mitsunori Ikeguchi** (Yokohama City University)  
Combination of Molecular Dynamics Simulations and Small-angle X-ray Scattering Experiments to Explore Protein Dynamics.
- 10:00 – 10:30 **Yasumasa Joti** (JASRI/SPring-8), **Kazuhiro Maeshima** (National Institute of Genetics)  
Chromosome Structure Revealed by SAXS and Simulation Studies.
- 10:30 – 10:50 << Coffee Break >>

#### Session 4a: Macromolecular Crowding

- 10:50 – 11:30      **Rebecca Wade** (Heidelberg Institute for Theoretical Studies)  
Simulation of protein diffusion in crowded environments.
- 11:30 – 12:00      **Masataka Kinjo** (Hokkaido University)  
Quantitative Analysis of the Dimer Formation of Transcription Factors in the Living Cell using Fluorescence Cross-Correlation Spectroscopy.
- 12:00 – 12:30      **Hideki Taguchi** (Tokyo Institute of Technology)  
Global analyses of protein aggregation, chaperone effects and in vivo protein dynamics.
- 12:30 – 14:30      << Lunch Break and Poster Presentation >>

#### Key Note Speech by Director of RIKEN QBiC

- 14:30 – 15:10      **Toshio Yanagida** (RIKEN QBiC)  
Towards the Whole Cell Modeling.

#### Session 4b: Macromolecular Crowding

- 15:10 – 15:50      **Joanna Trylska** (University of Warsaw)  
Brownian dynamics simulations of macromolecules.
- 15:50 – 16:20      **Koichi Takahashi** (RIKEN)  
Molecular crowding effects on biochemical reactions and signaling.
- 16:20 – 16:40      << Coffee Break >>
- 16:40 – 17:10      **Yutaka Itoh** (Tokyo Metropolitan University)  
In situ observation of protein structure and dynamics by in-cell NMR.
- 17:10 – 17:40      **Yuji Sugita** (RIKEN)  
Macromolecular crowding affects protein stability, hydration, and diffusion.