

HOST INSTITUTE:

M.M. Shemyakin and Yu.A. Ovchinnikov
Institute of Bioorganic Chemistry,
Russian Academy of Sciences



CO-ORGANIZERS:

Waseda University, Japan
Nagoya University, Japan
Keio University, Japan
Dubna University, Russia



Shemyakin-Ovchinnikov Institute
of Bioorganic Chemistry,
Russian Academy of Sciences,
Moscow, Russia (IBCh)
&
Joint Institute for Nuclear Research
Dubna, Moscow region, Russia (JINR)

7th Russian-Japanese
International Workshop
MSSMBS'14 "Molecular
Simulation Studies in
Material and Biological
Sciences"

**INTERNATIONAL
WORKSHOP**

*21-22 September 2014
IBCh, Moscow*

**SCIENTIFIC
PROGRAM**

SCIENTIFIC PROGRAM



INTERNATIONAL WORKSHOP

September 21, Sunday

Arrival in “Astrus Hotel”, Moscow.

September 22, Monday (IBCh, Moscow)

9⁰⁰–9³⁰ **Registration**
9³⁰–10⁰⁰ **Opening ceremony**

Session I. Co-Chairs C. Etchebest & K. Yasuoka

10⁰⁰–10³⁰ **Yuko Okamoto** (Nagoya University, Japan)

“Drug design by generalized-ensemble simulations”

10³⁰–11⁰⁰ **Roman Efremov** (Shemyakin-Ovchinnikov IBCh, Russia)

“Topography of molecular surfaces — a new computational tool to study structure-activity relationships for proteins and biomembranes”

11⁰⁰–11³⁰ **Mitsuhiro Matsumoto** (Kyoto University, Japan)

“Lubrication mechanism in joints – Role of Biopolymers”

11³⁰–11⁴⁵ **Ilya Kovalenko** (Moscow State University)

“Protein-protein interaction in photosynthetic electron transfer chain: computer simulation”

11⁴⁵–12⁰⁰ *Coffee / tea break*

Session II. Co-Chairs T. Yamamoto & V. Palyulin

12⁰⁰–12³⁰ **Kenji Yasuoka** (Keio University, Japan)

“1/f Noise in hydration dynamics on lipid membrane surfaces”

12³⁰–13⁰⁰ **Catherine Etchebest** (University Paris-Diderot, France)

“New control mechanisms of water transport identified in AQP1 by combining molecular dynamics simulations and experiments”

13⁰⁰–13¹⁵ **Grigory Smirnov** (JIHT, RAS, Moscow)

“Phase diagram of methane and hydrogen hydrates from atomistic modeling”

13¹⁵–13³⁰ **Andrey Kuznetsov** (IBCh & Moscow Institute of Physics and Technology, Russia).

“Dimerization of glycophorin A transmembrane domain: the role of the environment.”

13³⁰–14⁴⁵ *Lunch break*

Session III. Co-Chairs Y. Okamoto & R. Efremov

14⁴⁵–15¹⁵ **Tomoyuki Yamamoto** (Waseda University, Japan)

“Electronic structure of magnetic elements in dilute magnetic materials”

15¹⁵–15⁴⁵ **Anton Chugunov** (Shemyakin-Ovchinnikov IBCh, Russia)

“Atomistic basis for unique physical properties of Archaeal-like membranes (discovered by computer simulations)”

15⁴⁵–16⁰⁰ **Katsufumi Tomobe** (Keio University, Japan)

“Structural and hydration effects of pathogenic point mutation T188R in prion protein : a molecular dynamics simulation study”

16⁰⁰–16¹⁵ **Eric Dushanov** (JINR, Dubna, Russia)

“Difference of behavior of DNA and CPD in the repairing molecular system”

16¹⁵–16³⁰ *Coffee / tea break*

Session IV. Co-Chairs M. Matsumoto & A. Chugunov

16³⁰–17⁰⁰ **Vladimir Palyulin** (Moscow State University)

“QSAR and Molecular Modelling in the Design of Bioactive Compounds and Materials”

17⁰⁰–17³⁰ **Donguk Suh** (Keio University, Japan)

“Simulations of Vapor-to-Liquid Nucleation on Various Solid Precursor Particle Configurations by Molecular Dynamics”

17³⁰–17⁴⁵ **Roman Eremin** (JINR, Dubna, Russia)

“Solute-solvent interface peculiarities for mono-carboxylic acids organic solutions: Possible effect on small-angle neutron scattering data”

17⁴⁵–18⁰⁰ **Abdelouahab Kenoufi** (Scientific Consulting for Research and Engineering, Strasbourg, France)

“Symbolic Regression of inter-atomic potentials via Genetic Programming”

18⁰⁰–18¹⁵ **Tatiana Galochkina** (Moscow State University)

“Molecular dynamics model of lipopolysaccharide molecule”

18¹⁵–21⁰⁰ *Welcome Party*