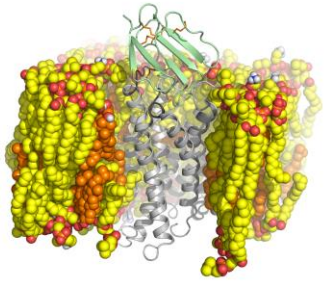
Shemyakin–Ovchinnikov
Institute of Bioorganic Chemistry
Russian Academy of Sciences,
Moscow, Russia (IBCh)
&
Joint Institute for Nuclear Research
Dubna, Moscow region, Russia (JINR)

7th Russian-Japanese International Workshop

Molecular Simulation Studies in Material and Biological Sciences

(MSSMBS'14)

SCIENTIFIC PROGRAM



21–22 September 2014

IBCh, Moscow

Host Institute:

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

Co-organizers:

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

Scientific program

September 21, Sunday

Arrival in “Astrus Hotel”, Moscow.

September 22, Monday. IBCh, Moscow

9^{00}–9^{30} Registration

9^{30}–10^{00} Opening ceremony

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

10^{00}–10^{30} **Yuko Okamoto** (Nagoya University, Japan)
Drug design by generalized-ensemble simulations

10^{30}–11^{00} **Roman Efremov** (IBCh, Russia)
Topography of molecular surfaces — a new computational tool to study structure-activity relationships for proteins and biomembranes

11^{00}–11^{30} **Mitsuhiro Matsumoto** (Kyoto University, Japan)
Lubrication mechanism in joints – Role of Biopolymers

11^{30}–11^{45} **Ilya Kovalenko** (Moscow State University)
Protein-protein interaction in photosynthetic electron transfer chain: computer simulation

11^{45}–12^{00} Coffee / tea break

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

12^{00}–12^{30} **Kenji Yasuoka** (Keio University, Japan)
1/f Noise in hydration dynamics on lipid membrane surfaces

12^{30}–13^{00} **Catherine Etchebest** (University Paris-Diderot, France)
New control mechanisms of water transport identified in AQP1 by combining molecular dynamics simulations and experiments

13^{00}–13^{15} **Grigory Smirnov** (JIHT, RAS, Moscow)
Phase diagram of methane and hydrogen hydrates from atomistic modeling

13^{15}–13^{30} **Andrey Kuznetsov** (IBCh & Moscow Institute of Physics and Technology, Russia).
Dimerization of glycophorin A transmembrane domain: the role of the environment

13^{30}–14^{45} Lunch break

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

14^{45}–15^{15} **Tomoyuki Yamamoto** (Waseda University, Japan)
Electronic structure of magnetic elements in dilute magnetic materials

15^{15}–15^{45} **Anton Chugunov** (IBCh, Russia)
Atomistic basis for unique physical properties of Archaeal-like membranes (discovered by computer simulations)

15^{45}–16^{00} **Katsufumi Tomobe** (Keio University, Japan)
Structural and hydration effects of pathogenic point mutation T188R in prion protein : a molecular dynamics simulation study

16^{00}–16^{15} **Eric Dushanov** (JINR, Dubna, Russia)
Difference of behavior of DNA and CPD in the reparing molecular system

16^{15}–16^{30} Coffee / tea break

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

16^{30}–17^{00} **Vladimir Palyulin** (Moscow State University)
QSAR and Molecular Modelling in the Design of Bioactive Compounds and Materials

17^{00}–17^{30} **Donguk Suh** (Keio University, Japan)
Simulations of Vapor-to-Liquid Nucleation on Various Solid Precursor Particle Configurations by Molecular Dynamics

17^{30}–17^{45} **Roman Eremin** (JINR, Dubna, Russia)
Solute-solvent interface peculiarities for mono-carboxylic acids organic solutions: Possible effect on small-angle neutron scattering data

17^{45}–18^{00} **Abdelouahab Kenoufi** (Scientific Consulting for Research and Engineering, Strasbourg, France)
Symbolic Regression of inter-atomic potentials via Genetic Programming

18^{00}–18^{15} **Tatiana Galochkina** (Moscow State University)
Molecular dynamics model of lipopolysaccharide molecule

18^{15}–21^{00} Welcome Party