

## Workshop

# "The Relationship of Numerical Simulations and Experimental methods"

May 26-28, 2011, Warsaw, Poland

#### **Organizers:**

- Sławomir Filipek, University of Warsaw, Faculty of Chemistry, Warsaw, Poland
- Helmut Grubmüller, Max-Planck-Institut für Biophysikalische Chemie, Göttingen, Germany

### **Invited speakers:**

- Georg Büldt, Research Centre Jülich, Institute of Complex Systems, Jülich, Germany
- Jerzy Czaplewski, Institute Of Pharmacology And Structural Biology, CNRS, Toulouse, France
- Volker Dötsch, Center For Biomolecular Magnetic Resonance, Goethe University, Frankfurt/Main, Germany
- Andreas Engel, Case Western Reserve University, USA and Biozentrum, University of Basel, Switzerland
- Kris Palczewski, Department of Pharmacology, Case Western Reserve University, Cleveland, Ohio, USA
- Eva Pebay-Peyroula, Institut De Biologie Structurale, University Joseph Fourier, Grenoble, France

The workshop is intended for PhD students and postdocs interested in understanding how numerical simulations and other computational techniques can aid experiment and provide visualization of processes at molecular level.

### **Experimental methods discussed:**

NMR, crystallography, AFM, cryo-electron microscopy.

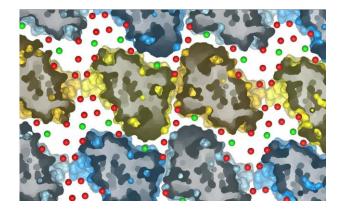
### Theoretical methods:

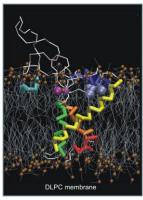
all-atom and coarse-grained molecular dynamics simulations, ligand docking, protein structure modeling, steered molecular dynamics.

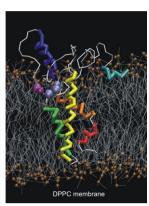
The last day of the workshop will be devoted for practical exercises on computer workstations using programs for modeling, visualizations and simulations.

Please see the website of the workshop: <a href="http://www.chem.uw.edu.pl/simul0511/">http://www.chem.uw.edu.pl/simul0511/</a> where you can find the most up to date program, hotels, transportation, and a registration page.

The workshop is free for SBMPs ITN participants.







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