Program, Workshop in Hünfeld, April 26-27, 2013
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

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Friday, April 26, 2013	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Balder Lai** (University of Natural Resources and Life Sciences, Vienna) ***Interpreting Protein-Ligand Binding Free Energies, Enthalpies and Entropies***
13:30 – 13:55	**Stepan Timr** (Institute of Organic Chemistry and Biochemistry AS CR, Prague) ***Accurate Determination of Orientational Distribution of a Fluorescent Molecule in a Model Membrane by Molecular Simulations and Polarization Microscopy***
13:55 – 14:20	**Zhou Beifei** (Heidelberg Institute for Theoretical Studies) ***Pre-Stress Tunes Stability of Regulatory Protein Disulfide Bonds***
14:20 – 14:45	**Falk Hoffmann** (Research Center Jülich) ***Protein Structure Prediction Using Basin-Hopping With NMR Chemical Shift Restraints***
14:45 – 15:10	**Guillermo Pérez-Hernández** (Free University Berlin) ***Slow Coordinate Detection in Small Peptides***
15:10 – 15:25	Coffee break
15:25 – 15:50	**Isaure Chauvot de Beauchêne** (Ecole Normale Supérieure de Cachan) ***Description of Allosteric Communications Through Protein Network Based on Molecular Dynamics Simulations***
15:50 – 16:15	**Béla Voß** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Structural Determinants of Conformational Flexibility and Long-Range Allostery of the CRM1 Export Complex***
16:15 – 16:40	**Kristyna Pluhackova** (University Erlangen-Nuremberg) ***InitraM ↔ Martini; A Powerful Tool for Reverse Transformation from Martini to UA and AA Force Fields***
16:40 – 17:05	**Servaas Michielssens** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Computational Biotechnology: Design of Selective Ubiquitin***
17:05 – 17:30	**Sarah Rauscher** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Structural Ensembles of Intrinsically Disordered Nucleoporins Depend on Force Field***
17:30 – 17:55	**Laura Orellana** (University of Barcelona/Institute for Research in Biomedicine, Barcelona) ***Oncogenic Residues Reveal Kinase Receptor Activation***
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, April 27, 2013	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Lars Skjaerven** (The European Molecular Biology Laboratory, Heidelberg) ***Accounting for Conformational Variability in Protein-Ligand Docking with NMR-Guided Rescoring***
9:20 – 9:45	**Po-Hsien Lee** (Saarland University, Saarbrücken) ***Coarse-Grained Brownian Dynamics Simulations of Protein Translocation Through Nanopores***
9:45 – 10:10	**Johannes Schöneberg** (Free University Berlin) ***ReaDDy - a Software for Particle Based Reaction Diffusion Dynamics in Crowded Cellular Environments***
10:10 – 10:45	Coffee break
10:45 – 11:10	**Johannes Wagner** (Heidelberg Institute for Theoretical Studies) ***Unclicking the Click: Quantum/Classical Calculations of How Force Triggers Chemical Triazole Opening***
11:10 – 11:35	**Timo Graen** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Fluorescent Dyes in Protein Simulations***
11:35 – 12:00	**Mithun Biswas** (University of Frankfurt) ***Effect of Azobenzene Isomerisation on DNA Stability***
12:00 – 13:00	Lunch
13:00 – 13:25	**Emiliano Brini** (Technical University Darmstadt) ***Hydrophilic Attraction and Hydrophobic Repulsion***
13:25 – 13:50	**Ana Vila Verde** (Max Planck Institute for Colloids and Interfaces, Potsdam) ***Coarse Grained Model of Bile Salts Reveals Structure and Mechanism of Microphase Separation***
13:50 – 14:15	**Moritz Wolf** (Karlsruhe Institute of Technoloy) ***All-Atom Modelling of Protein Folding and Aggregation***
14:15 – 14:40	**Musa Özboyaci** (Heidelberg Institute for Theoretical Studies) ***Adsorption of 3H-BLIP on a Gold Surface***
14:40 – 15:05	**Filip Leonarski** (University of Warsaw) ***Insight for a Design of Coarse-Grained Models for RNA Structure Prediction and Molecular Dynamics from Results of a Force Field Parameter Optimization Algorithm***
15:05 – 15:20	Coffee break
15:20 – 15:45	**Anna Kahler** (University of Erlangen-Nuremberg) ***Conformational Stability of Fibrillar Aβ-Oligomers: Unraveling the Growth Mechanism of Aβ-Fibrils***
15:45 – 16:10	**Vytautas Gapsys** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Phosphorylation Induced Dynamic Switch in a Serine/Arginine Repeat Peptide***
16:10 – 16:35	**Benjamin Lutz** (Karlsruhe Institute of Technology) ***Computational Analysis of Co-Transcriptional Riboswitch Folding***
16:35 – 17:15	Poster price, final remarks
18:00	Dinner / Departure