Program, Workshop in Hünfeld, April 16-18, 2010
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2010"

Friday, April 16th, 2010	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Tomasz Berezniak** (University of Heidelberg) *Conformational selection determines the activity of the Diels-Alderase Ribozyme*
13:30 – 13:55	**Mikolaj Feliks** (University of Bayreuth) *Molecular Modelling Study of Mechanisms of Enzymes Involved in the Anaerobic Degradation of Hydrocarbons - Acetylene Hydratase and 4-Hydroxyphenylacetate Decarboxylase*
13:55 – 14:20	**Farooq Kiani** (University of Heidelberg) *Catalytic mechanism of ATP hydrolysis in the Myosin molecular motor*
14:20 – 14:45	**Till Rudack** (Ruhr University Bochum) *Hydrolysis Mechanism of Ras Investigated by QM/MM Simulations*
14:45 – 15:10	**Fabian Burggraf (**Albert Ludwigs University Freiburg) *A non-heme iron complex is essential for charge transfer in the reaction center of Rb. sphaeroides: Theory and simulation*
15:10 – 15:45	Coffee break
15:45 – 16:10	**Jane Allison** (ETH Zurich) *Overcoming frustration with local elevation*
16:10 – 16:35	**Dirk Matthes** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Structure and dynamics of spontaneous steric zipper peptide aggregation*
16:35 – 17:00	**Martin Held** (Free University of Berlin) *Studying the Ensemble of Protein-Ligand Association Pathways*
17:00 – 17:25	**Hannes Kopitz** (Heinrich Heine University Düsseldorf) *Neither small nor unimportant, yet overlooked: How much unbound ligands contribute to the thermodynamic inhibition profile of thrombin inhibitors*
17:25 – 17:50	**Mazen Ahmad** (Saarland University, Saarbrücken) *Adhesive water networks facilitate binding of protein interfaces*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

Saturday, April 17th, 2010	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Piotr Setny** (Technical University of Munich) *Player or spectator? The role of water in cavity-ligand binding*
9:20 – 9:45	**Siti Azma Jusoh** (Saarland University, Saarbrücken) *Molecular Dynamic Simulation as an Alternative Approach to Study the Behavior of Charged and Polar Residues in the Transmembrane Domains of Envelope Glycoprotein of Flaviviridae Virus Family*

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9:45 – 10:10	**Veronica I. Dumit** (University of Bayreuth) *New Insights into Ferredoxin-NADP-Reductase Catalysis through Electrostatic Calculations*
10:10 – 10:45	Coffee break
10:45 – 11:10	**Paolo Mereghetti** (HITS gGmbH, Heidelberg) *Brownian Dynamics Simulations of Protein Solutions*
11:10 – 11:35	**Jens Krüger** (University of Paderborn) *Ion Permeation sampled by Steered Molecular Dynamics and Umbrella Sampling*
11:35 – 12:00	**Alexander Krah** (Max Planck Institute of Biophysics, Frankfurt) *Ion selectivity calculations for the rotor subunit of ATP synthases*
12:00 – 13:00	Lunch
13:00 – 13:25	**Bernhard Egwolf** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Free Energy Barrier for Extracellular Sodium Ion in the KcsA Selectivity Filter*
13:25 – 13:50	**Thomas Steinbrecher** (Karlsruhe Insitute of Technology) *The Thermodynamics of Charge Transfer in DNA Photolyase - New Perspectives from Free Energy Calculations*
13:50 – 14:15	**Daniel Seeliger** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Protein Thermostability Calculations using Alchemical Free Energy Simulations*
14:15 – 14:40	**Bettina Keller** (Free University of Berlin) *What stabilizes the 3_14-helix in beta3-peptides? A conformational analysis using molecular simulation*
14:40 – 15:05	**Christian Seifert** (HITS gGmbH, Heidelberg) *Force distribution analysis of the signal transduction in Hsp90*
15:05 – 15:25	Coffee break
15:25 – 15:50	**Alrun Koller** (Heinrich Heine University Düsseldorf) *Temperature-Jump MD Simulations of Trpzip2C for Comparison with Fast IR Spectroscopy*
15:50 – 16:15	**Eva-Maria Krammer** (University of Nancy) *High chloride concentration abolish the binding of ADP3- in the mitochondiral ADP/ATP carrier family*
16:15 – 16:40	**Nicole Doelker** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Squeezing through the Pore - Conformational Plasticity in Nuclear Import*
16:40 – 17:05	**Diana Garzon** (Max Planck Institute of Biophysics, Frankfurt) *Large-Scale Simulation Studies of Lipid-Antigen Presentation Mechanisms in the Human CD1 Family*
17:05 – 17:30	**Christian Blau** (Max Planck Institute for Biophysical Chemistry, Göttingen) *Modification induced changes in tRNA dynamics and base pairing*
18:00	Dinner/Departure