Program for the Hünfeld Workshop 2005

"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES 2005"

Friday, April 22th, 2005	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Paul Strodel** (German Cancer Research Institute, Heidelberg) *Understanding the mechanims of color tuning and photoisomerization in retinal proteins with QM/MM methods: a challenge for theory*
13:30 – 13:55	**Nicoleta Bondar** (IWR, University Heidelberg) *Computer simulations on the early steps of the bacteriorhodopsin photocycle*
13:55 – 14:20	**Lars Schäfer** (MPI for biophysical Chemistry, Göttingen) *QM/MM simulations accelerated by chemical flooding*
14:20 – 14:45	**Friedemann Reinhard** (MPI for biophysical Chemistry, Göttingen) *Calculation of solvent entropies from MD simulations*
14:45 – 15:10	**Riccardo Baron** (ETH-Zurich) *Estimating the configurational entropy of β-peptides in solution from molecular dynamics simulations: Anharmonicity and correlation corrections to the quasi-harmonic approximation*
15:10 – 15:45	Coffee break
15:45 – 16:10	**Zoe Cournia** (IWR, University of Heidelberg) *Cholesterol in Membrane Simulations*
16:10 – 16:35	**Jan Saam** (Charite Berlin) *Identification of Oxygen Channels in Proteins by Molecular Dynamics*
16:35 – 17:00	**Danilo Roccatano** (International University Bremen) *Insights into the dynamics of nucleosome core particle by molecular dynamics simulations*
17:00 – 17:25	**Harshad Joshi** (MPI for biophysical Chemistry, Göttingen) *Molecular mechanism of sugar degrading processive enzymes - A molecular dynamics study*
17:25 – 17:50	**Vlad Cojocaru** (MPI for biophysical Chemistry, Göttingen) *The snRNP 15.5K protein folds its cognate RNA. A combined theoretical and biochemical study*
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

Saturday, April 23th, 2005	
8:00 – 8:30	Breakfast
8:30 – 8:55	**Daniel Wüstner** (Max-Delbrück Center for Molecular Medicine, Berlin) *A new chain breakage/closure algorithm for efficient atomistic Monte Carlo simulation of phospholipids*
8:55 – 9:20	**Verena Schultheis** (University of Munich) *Extracting Markov models of peptide conformational dynamics from simulation data*
9:20 – 9:45	**Kei Moritsugu** (University of Heidelberg) *Langevin model of protein dynamics*
9:45 – 10:10	**Thorsten Erdmann** (MPI for Colloid and Interfaces) *Stochastic dynamics of adhesion clusters under force*
10:10 – 10:45	Coffee
10:45 – 11:10	**Michel Cuendet (**ETH Zurich) *Association free energy profile of the TCR-p-MHC complex determined by steered molecular dynamics*
11:10 – 11:35	**Razif Gabdoulline (**EML Research gGmbH, Heidelberg) *Simulation of diffusional association of proteins with electrostatic and hydrophobic interactions*
11:35 – 12:00	**Alexander Spaar** (Saarland University) *Free energy of protein-protein association resulting from Brownian Dynamics*
12:00 – 13:00	Lunch
13:00 – 13:25	**Alessandra Villa** (University of Frankfurt /Main) *Interactions within coiled-coils: A MD study*
13:25 – 13:50	**Martina Stork** (University of Munich) *Molecular dynamics simulations indicate a possible role of parallel beta-helices in seeded aggregation of poly-Gln*
13:50 – 14:15	**Yungki Park** (Saarland University) *Structure prediction of polytopic membrane proteins using sequence conservation patterns*
14:15 – 14:40	**Thomas Steinbrecher** (University of Freiburg) *A Multi Step Approach to Structure based Drug Design: Studying Ligand Binding at the Human Neutrophil Elastase*
14:40 – 15:05	**Christian Gossens** (Swiss Federal Institute of Technology EPF Lausanne) *Binding of organoruthenium anticancer drugs to DNA*
15:05 – 15:30	Coffee
15:30 – 15:55	**Astrid Klingen** (University of Bayreuth) *Which mechanistic events are coupled to the reduction of cytochrome bc1 complex*
15:55 – 16:20	**Hao Fan** (University of Groningen) *SC3 Hydrophobin: Modeling and interface experiments*
16:20 – 16:45	**Bojan Zagrovic** (ETH Zurich) *Studying the long-range structure of flexible polypeptides by small-angle X-ray scattering and molecular dynamics*
18:00	Dinner/Departure