Program, Workshop in Hünfeld, May 7-9, 2004
"Computer Simulation and Theory of Macromolecules 2004"

Friday, May 7th, 2004	
12:00 – 13:30	Arrival, registration and lunch
13:30 – 14:00	**Edda Kloppmann** (University of Bayreuth) *The role of electrostatics in the opsin shift*
14:00 – 14:30	**Durba Sengupta** (Heidelberg University) *Understanding the energetics of helical peptide orientations in the membrane*
14:30 – 15:00	**Tihamer Geyer** (Saarland University) *Large scale brownian dynamics simulations of proteins in cell compartments: achievements and open questions*
15:00 – 15:30	**Alexander Spaar** (Saarland University) *Trajectory analysis of protein-protein encounter studied by brownian dynamics simulations*
15:30 – 16:00	Coffee break
16:00 – 16:30	**Francesco Rao** (University of Zürich) *The conformation space network model for folding*
16:30 – 17:00	**Wei Gu** (Saarland University) *Solvation free energies and transfer free energies for amino acids from hydrophobic solution to water solution from a very simple residue model*
17:00 – 17:30	**Volker Knecht** (University of Groningen) *Interpreting experiments on Langmuir lipid monolayers by molecular dynamics simulations*
17:30 – 18:00	**Iris Antes** (Max Planck Institut für Informatik, Saarbrücken) *Target specific scoring functions: Parameter optimization using ensemble Methods*
18:00 – 19:00	Dinner
19:00 – 19:30	**Wolfgang Wenzel** (Forschungszentrum Karlsruhe) *Reproducible folding of a three-helix protein in an all-atom forcefield*
19:30 –	Poster Session / Beer

Saturday, May 8th, 2004	
8:00 – 9:00	Breakfast
9:00 – 9:30	**Eduard Schreiner** (Ruhr-University Bochum) *Temperature dependent conformational transitions and hydrogen bond dynamics of the elastin-like octapeptide GVG(VPGVG): a molecular dynamics study*
9:30 – 10:00	**Emil Mittag** (University of Hamburg) *Thermodynamic properties of proteins in the Wang-Landau framework*
10:00 – 10:30	**Lars Meinhold** (Heidelberg University) *Protein collective motions, X-ray diffuse scattering*
10:30 – 11:00	Coffee
11:00 – 11:30	**Vandana Kurkal** (Heidelberg University) *Towards understanding the origin of the Boson peak in proteins*
11:30 – 12:00	**Philippe Hünenberger** (ETH Zürich) *Stabilization of biomolecules by the disaccharide trehalose*
12:00 – 13:00	Lunch
13:00 – 13:30	**Rainer Böckmann** (University of Zürich) *Differential peptide dynamics is linked to MHC polymorphism*
13:30 – 14:00	**Wolfgang Fischer** (University of Oxford) *Modelling viral membrane proteins: Vpu from HIV-1*
14:00 – 14:30	**Ulrich Kleinekathöfer** (Technical University of Chemnitz) *Molecular dynamics simulations of isolated β-subunits of F_1-ATPase*
14:30 – 15:00	**Phuong Nguyen** (Johann Wolfgang Goethe University Frankfurt) *Structure of a bicyclic peptide in explicit solution: a replica-exchange molecular dynamics simulations study*
15:00 – 15:30	Coffee
15:30 – 16:00	**Martin Stumpe** (MPI for biophysical Chemistry, Göttingen) *Structural characterization of urea/water solutions*
16:00 – 16:30	**Frauke Meyer** (Shanghai Institute of Materia Medica) *Tension-induced titin kinase activation studied by force-probe molecular dynamics simulation*
16:30 – 17:00	**Marco Klähn** (Ruhr-University Bochum) *Intrinsic GTPase Process of Ras p21: MD simulation with QM-MM Force Field*
17:00 – 17:30	**Jörg Grunenberg** (Technical University Braunschweig) *Compliance constants from density functional theory for hydrogen bonds in biomolecules*
17:30	Departure