Program, Workshop in Hünfeld, April 17-18, 2015
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Friday, April 17, 2015	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Vytautas Gapsys** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Calculation of Relative Free Energies in Protein and Drug Design***
13:30 – 13:55	**Mazen Ahmad** (Max Planck Institute for Informatics, Saarbrücken) ***Enthalpy-Entropy Compensation upon Molecular Conformational Changes***
13:55 – 14:20	**Rosa Anneke Luirink** (Free University of Amsterdam) ***Towards Accurate Binding Free Energy and Binding Pose Prediction to Cytochrome P450 Enzymes***
14:20 – 14:45	**Florian Sittel** (University of Freiburg) ***Robust Density-Based Clustering to Identify Metastable Conformational States of Proteins***
14:45 – 15:10	**Guillermo Perez Hernandez** (Free University of Berlin) ***Analysis of Biomolecular Simulations via Markov State Models***
15:10 – 15:25	Coffee break
15:25 – 15:50	**Feliks Nueske** (Free University of Berlin) ***Variational Tensor Approach to the Rare-Event Kinetics of Macromolecular Systems***
15:50 – 16:15	**Floris Buelens** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Atomistic and Kinetic Modelling of the Reaction Network of Yeast Fatty-Acid Synthase***
16:15 – 16:40	**Silke Wieninger** (Institut Pasteur, Paris) ***Ensemble-based NMR Structure Determination - Classification and Weighting of exact NOE Restraints***
16:40 – 17:05	**Levin Brinkmann** (Georg-August-University of Göttingen) ***Structural Interpretation of Anisotropic Solution X-ray Scattering***
17:05 – 17:30	**Michal Walczak** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Bayesian Structure Determination from Sparse and Noisy Single Molecule X-ray Diffraction Images***
17:30 – 17:55	**Katrin Reichel** (Ruhr-University of Bochum) ***De Novo Prediction of Membrane Protein Structures Using CS-Rosetta With Sparse NMR Data***
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, April 18, 2015	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Sarah Rauscher** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Structural Ensembles of Intrinsically Disordered Proteins Using Molecular Dynamics Simulation***
9:20 – 9:45	**Christoph Wehmeyer** (Free University of Berlin) ***Optimal Combination of Umbrella Sampling and Unbiased Molecular Dynamics with TRAM***
9:45 – 10:10	**Alejandro Gil Ley** (Scuola Internazionale Superiore di Studi Avanzati, Trieste) ***Enhanced Conformational Sampling Using Replica Exchange with Collective-Variable Tempering***
10:10 – 10:45	Coffee break
10:45 – 11:10	**Andrea C. Vaiana** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Structural Determinants of Hybrid State Intermediates of the Bacterial Ribosome***
11:10 – 11:35	**Alexander Goetz** (Technical University of Munich) ***Investigating Dynamic Motifs in Amyloid Precursor Protein Mutants as Impact Factor for Alzheimer's Disease***
11:35 – 12:00	**Fabian Zeller** (Technical University of Munich) ***Adenylate Kinase: Interplay of Domain Motions and Ligand Binding***
12:00 – 13:00	Lunch
13:00 – 13:25	**Kalina Atkovska** (Georg August University of Göttingen) ***Energetics and Mechanism of Permeation across FNT Channels***
13:25 – 13:50	**Shreyas Kaptan** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***H95 is a pH Gate in AQP4***
13:50 – 14:15	**Stefan Gahbauer** (University of Erlangen-Nuremberg) ***In Silico Study of the Promiscuous Dimerization of CXCR4***
14:15 – 14:40	**Philipp Kynast** (Research Center Jülich) ***Evaluation of the OPEP Force Field for Protein-Protein Docking***
14:40 – 15:05	**Christina Schindler** (Technical University of Munich) ***Flexible Protein-Protein and Protein-Peptide Docking in ATTRACT***
15:05 – 15:20	Coffee break
15:20 – 15:45	**Tsjerk Wassenaar** (University of Erlangen-Nuremberg) ***The DAFT Approach: Landscapes of Protein Interactions***
15:45 – 16:10	**Olivier Fisette** (Ruhr-University Bochum) ***Protein Complexes from MD Simulations: the Rope-Pulling Game of Tapasin and Histocompatibility Molecules***
16:10 – 16:35	**Qinghua Liao** (Research Center Jülich) ***Development and Application of a Classical Cu2+ Model with Jahn-Teller Effect***
16:35 – 17:00	**Lars V. Bock** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Dynamic Contact Network between Ribosomal Subunits enables Rapid Large-Scale Rotation***
17:00 – 17:30	Poster prize, final remarks
18:00	Dinner / Departure