Program, Workshop in Hünfeld, April 20-21, 2018
"COMPUTER SIMULATION AND THEORY OF MACROMOLECULES"

Friday, April 20, 2018	
11:00 – 13:00	Arrival, registration and lunch
13:00 – 13:05	Welcome
13:05 – 13:30	**Oskar Klaja** (Free University of Berlin) ***Force field for the photo-switchable lipid molecule***
13:30 – 13:55	**Hossein Batebi** (University of Berlin) ***A Mechanistic Study of the Enzymatic Excision Mechanism in AP Endonuclease (APE 1)***
13:55 – 14:20	**Mark Abraham** (Royal Technical University of Stockholm) ***Physical validation of molecular dynamics simulations***
14:20 – 14:45	**Danial Pourjafar Dehkordi** (Technical University of Munich) ***Phsphorylation of Rab8a Interrupts Its Activation by the Guanine Nucleotide Exchange Factor Rabin8***
14:45 – 15:10	**Mahdi Bagherpoor Helabad** (Free University of Berlin) ***Protein-DNA Dynamic and Recognition Rule in DNA Binding Specificity of Androgen and Glucocorticoid Receptors***
15:10 – 15:25	Coffee break
15:25 – 15:50	**Aljaz Godec** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Thermal Noise and the Single Molecule: A Theoretical Perspective***
15:50 – 16:15	**Matteo Aldeghi** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Predictions of Ligand Binding Affinity Changes Upon Protein Mutation Using Non-Equilibrium Free Energy Calculations***
16:15 – 16:40	**Eko Aditya Rifai** (Free University of Amsterdam) ***Binding Affinity Prediction Using an LIE Approach with Reliability Estimation***
16:40 – 17:05	**Steffen Wolf** (Albert Ludwigs University of Freiburg) ***Langevin Modeling of Targeted Molecular Dynamics: A Novel Approach to Calculate Equilibrium Free Energies from Non-Equilibrium Simulations***
17:05 – 17:30	**Hendrik Goeddeke** (Ruhr University Bochum) ***Atomistic Mechanism of Large-Scale Conformational Transition in a Heterodimeric ABC Exporter***
17:30 – 17:55	**Stephan Nicolás Schott Verdugo** (Heinrich Heine University Düsseldorf) ***Calculated Dimerization Free Energy Profile and Equilibrium of the Phospholipase PlaF from Pseudomonas aeruginosa***
18:00 – 19:00	Dinner
19:30 –	Poster Session / Beer

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Saturday, April 21, 2018	
8:00 – 8:50	Breakfast
8:55 – 9:20	**Sehee Na** (Albert Ludwigs University of Freiburg) ***Thermodynamic Integration Network Approach to Ion Transport through Protein Channels: Perspectives and Limits***
9:20 – 9:45	**Julian Tim Brennecke** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Mechanism of Mechanosensitive Gating of the TREK-2 Potassium Channel***
9:45 – 10:10	**Esam Abualrous** (Free University of Berlin) ***Understanding The Structural Dynamics of TCR-pMHC Interactions by Molecular Dynamics Simulations and Markov State Models***
10:10 – 10:45	Coffee break
10:45 – 11:10	**Sebastian Stolzenberg** (Free University of Berlin) ***PySFD: A General, Big Data Python Framework to Analyze Significant Features Differences among MD-Simulated Ensembles***
11:10 – 11:35	**Benjamin Lickert** (Albert Ludwigs University of Freiburg) ***Long Time Dynamics from Short MD Simulations: a comparison of Markov State and Langevin Modeling***
11:35 – 12:00	**Lars V Bock** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Thermodynamic Control of Ribosomal Frameshifting Efficiencies***
12:00 – 13:00	Lunch
13:00 – 13:25	**Anela Ivanova** (Sofia University St. Kliment Ohridskit) ***Interactions of Targeting Ligands with a Receptor Embedded in a Multilipid Bilayer***
13:25 – 13:50	**Alexander Götz** (Technical University of Munich) ***What Does the Dynamic Heterogeneity of Its Substrates Tell us About γ-Secretase's Role in the Cell Membrane?***
13:50 – 14:15	**Christian Blau** (University of Stockholm) ***Molecule Mechanics from cryo-EM Images and Multiple Reconstructed Densities***
14:15 – 14:40	**Gabor Nagy** (Max Planck Institute for Biophysical Chemistry, Göttingen) ***Molecular Modeling of Intrinsically Disordered Proteins: Structure and Interactions***
14:40 – 15:05	**Nicola Salvi** (Institute of Structural Biology, Grenoble) ***Combining Molecular Dynamics Simulations with NMR Relaxation to Capture the Dynamics of Intrinsically Disordered Proteins***
15:05 – 15:20	Coffee break
15:20 – 15:45	**Ana Herrera** (Heidelberg Institute for Theoretical Studies) ***Towards Spider Silk Proteins Self-Assembly Under Uniform Flow***
15:45 – 16:10	**Kashif Sadiq** (Heidelberg Institute for Theoretical Studies) ***Modeling Reaction-Triggered Oligomerization of Envelope Membrane Glycoproteins During HIV-1 Maturation***
16:10 – 16:35	**Thomas McManus** (University of Bath) ***Simulating Proteins as Mechanical Networks - FRODA***
16:35 – 17:00	**Penelope Pesara** (Ruhr University Bochum) ***The Protein Recycling Machine of the Cell - Interactive Integrative Modeling From In Vivo to In Situ***
17:00 – 17:30	Poster prize, final remarks
18:00	Dinner / Departure