

## **Thursday Feb. 23rd**

12:00 - 14:00 Registration

14:00 - 14:10 Welcome address

### **1.) Structure and function of channels and transporters**

14:10 - 14:40

**Sychrová, Hana**

*Yeast as a tool to study cell membrane transporters*

14:40 - 15:10

**Schröder, Indra**

*K<sup>+</sup> channel selectivity filter gating correlates with site-specific ion occupation obtained from the same experiment*

15:10 - 15:30

**Elicharová, Hana**

*Potassium uptake systems in Candida species*

*15:30 - 16:00 Coffee Break*

16:00 - 16:30

**Zayats, Vasilina**

*Modulation of human ORAI1 channel: modeling and simulations*

16:30 - 16:50

**Atkovska, Kalina**

*Energetics and mechanism of permeation across the Formate-Nitrite Transporters (FNTs)*

### **2.) Protein folding and protein structural substate analysis**

16:50 - 17:20

**Hauser, Karin**

*Biomolecular dynamics studied with residue-specific resolution*

17:20-17:50

**Bednar, David**

*FireProt: Computational Design of Thermostable Proteins*

*18:00 - 19:00 Dinner*

19:30 - 19:50

**Andrea Schulze**

*Cooperation of Local Motions in the Hsp90 Molecular Chaperone ATPase Mechanism*

## **Friday Feb. 24th**

8:00 - 9:00 Breakfast

### **3.) Membrane receptors and their dynamic interactions**

9:00 - 9:30

**Schlierf, Michael**

*Watching Membrane Protein Folding in singulo*

9:30 - 10:00

**Böckmann, Rainer**

*Binding Pathway of S1P to the S1P1 Receptor and Activation Studied in Molecular Dynamics Simulations*

10:00 - 10:30

**Schneider, Bohdan**

*Interactions between interferon-gamma and extracellular portions of its two receptors R1 and R2*

10:30 - 11:00 Coffee Break

### **4.) New techniques A**

11:00 - 11:45

**Heberle, Joachim**

*The Grateful Infrared – Novel IR techniques to probe the functional changes of membrane proteins*

12:00 - 13:00 Lunch

### **5.) Lipid assemblies, dynamics and surface interactions with proteins**

13:00 - 13:30

**Keller, Sandro**

*Polymer-Bounded Nanodiscs for Membrane Biophysics*

13:30 - 13:50

**Subramanian, Madhumalar**

*Lipid nanodiscs with genetically engineered MSP1D1 for structural and functional studies*

13:50 - 14:20

**Coskun, Unal**

*Calcium directly regulates phosphatidylinositol 4,5-bisphosphate headgroup conformation and recognition*

14:20 - 14:40

**Martinez-Seara, Hector**

*Determinants of sodium and calcium adsorption onto neutral lipid bilayers and how the cell can use them to modulate hyaluronan–membrane interaction*

- 14:40 - 15:10      **Amaro, Mariana**  
*Impact of GM1 nanodomains in the oligomerization of membrane bound A $\beta$  monomers*
- 15:10-15:30      **Fallah, Mohammad**  
*Membrane interaction and conformational changes of  $\alpha$ -synuclein*
- 15:30 - 16:00 *Coffee Break*
- 16:00 - 16:30      **Vachá, Robert**  
*Anomalous Interactions of Amyloids with Surfaces*
- 16:30 - 16:50      **Hajiraissi, Roozbeh**  
*Adsorption and aggregation of hIAPP at different self-assembled monolayers*
- 16:50 - 17:20      **Cwiklik, Lukasz**  
*Tear Film Lipid Layer: a molecular-level view*
- 17:20 - 17:50      **Jungwirth, Pavel**  
*Cell Penetration and Membrane Fusion: Two Sides of the Same Coin*

*18:00 - 19:00 Dinner*

*19:00 Poster Session and Wine*

## **Saturday Feb 25th**

*8:00 - 9:00 Breakfast*

### **6.) Protein-protein interactions**

- 9:00 - 9:30            **Utrecht, Charlotte**  
*Lipid glue in clathrin adaptor assembly and new opportunities at XFELs*
- 9:30 - 10:00        **Hub, Jochen**  
*Detecting protein structures, ensembles, and dynamics in SAXS/WAXS data: combining MD simulations with Bayesian inference*
- 10:00 - 10:30      **Obsil, Tomas**  
*The 14-3-3 protein-dependent regulation of neutral trehalase Nth1*

*10:30 - 11:00 Coffee Break*

### **7.) Dynamics of protein solvent and ligand interactions**

- 11:00 - 11:30      **Fitter, Jörg**  
*Proteins in crowded environments*
- 11:30 - 12:00      **Hof, Martin**  
*Use of fluorescence spectroscopy in Synthetic Biology*
- 12:00 - 13:00 Lunch*
- 13:00 - 13:30      **Havenith, Martina**  
*THz Spectroscopy and Solvation Science*
- 13:30 - 13:50      **Novelli, Fabio**  
*Time-domain THz-Spectroscopy reveals coupled protein-hydration dielectric response in solutions of native and fibrils of human lysozyme*
- 13:50 - 14:10      **Sulmann, Stefan**  
*Differential Ca<sup>2+</sup>-sensing by GCAPs in rod and cone cells provide molecular basis of step-by-step regulation of retinal guanylate cyclase upon light activation*

## **8.) DNA structures and DNA-protein interactions**

14:10 - 14:40      **Seidel, Ralf**  
*Single-molecule insight into target recognition by CRISPR-Cas systems*

14:40 - 15:00      **Keller, Adrian**  
*On the stability and degradation of DNA origami nanostructures in urea and guanidinium chloride*

15:00 - 15:20      **Božíková, Paulína**  
*Annotation of DNA Structures by a Newly Formulated DNA Structural Alphabet*

*15:30 - 16:00 Coffee Break*

## **9.) New techniques B**

16:00 - 16:30      **Lazar, Josef**  
*No Need to FRET: Observing Membrane Protein Structure and Function by Polarization Fluorescence Microscopy*

16:30 - 17:00      **Huber, Thomas**  
*Novel chemical biology methods to study GPCRs one molecule at a time*

17:00 - 17:20      **Höfig, Henning**  
*Single-Molecule Studies on CFP-YFP-based biosensors*

17:20 - 17:40      **Schwieger, Christian**  
*Infrared Reflection Absorption Spectroscopy: a Potent Method to Study Membrane Binding (Macro)molecules*

17:40 - 18:00      **Rudack, Till**  
*From atom to cell: Integrating experimental results and user expertise into computational modeling*

*18:00 Dinner*

## **Sunday Feb 26th**

*8:00 - 9:00 Breakfast  
Departure*