**Program 2013**

**Sunday, September 15.**

16:00  Registration  
18:00  Welcome & Introduction (G. Ecker)  
19:15  Get-together Party

**Monday, September 16.**

09:00  Discovering interaction patterns: A closer look at 3D pharmacophore perception and virtual screening (G. Wolber)  
09:45  Stepping stones for protein-ligand interaction prediction: Small fragments make beautiful mosaics (C. de Graaf)  
10:30  Coffee break  
11:00  Three different approaches to target the T315I mutation: ATP-competitive, ATP-non-competitive and 14-3-3 inhibitors (M. Botta)  
11:30  Surflex QMOD: Physically Meaningful QSAR (A. Steudle)  
12:00  Short lectures by Europin students: Application of MM-PB(G)BSA and QM/MM-GBSA rescoring approaches for predicting biological activities of novel PRK1 kinase inhibitors (I. Slynko)  
A structural analysis of functional selectivity in serotonin receptors using molecular dynamics simulations (M. Marti)  
12:30  Lunch  
14:00  tba (S. Bryant)  
14:40  Coffee Break

**Tuesday, September 17.**

09:00  Steered Molecular Dynamics as a Tool to Map Receptor Unbinding Pathways. Application to the Glucocorticoid Receptor (G. Costantino)  
09:45  Drug Metabolism (H. Kubinyi)  
10:30  Coffee break  
11:00  Prodrugs and Soft Drugs (H. Kubinyi)  
11:45  Combined metabolism and reactive toxicity prediction for safety assessment of chemicals (C. Schwab)  
12:15  Short lectures by Europin students: Ligand-based pharmacophores of TRPV1 antagonists derived from open data sources (D. Tsevara)  
12:45  Lunch  
14:00  tba (D. Cappel)  
14:40  Coffee Break

**Wednesday, September 18.**

09:00  Protein-ligand docking and binding free energy calculation - how useful are they in drug discovery projects? (W. Sippl)  
09:45  What you ever wanted to know about Cheminformatics (M. Rarey)  
10:30  Coffee break  
11:00  Using water and semi-continuum solvent to guide Drug Design (P. Hawkins)  
11:30  tba (F. Klepsch)  
12:00  Short lectures by Europin students: Molecular Modeling and Virtual Screening Studies on Sirtuin-5 (M. Scharfe)  
Approaching a protein without a face: Investigating the molecular basis of GAT-1 inhibition (A. Jurik)  
12:30  Lunch  
14:00  Rationalization and Visualization of Non-bonded Interactions (M. Kossner)  
14:40  Coffee Break  
15:00  Workshops: OpenEye, Chemical Computing Group

**Thursday, September 19.**

09:00  Computational Approaches for BASF Crop Protection (K. Schleifer)  
09:45  Discovery of BAY 94-8862: a nonsteroidal antagonist of the minera locorticoid receptor for the treatment of cardiorenal diseases (A. Hillisch)  
10:30  Coffee break  
11:00  Making Safer Drugs: Past Lessons and Future Possibilities (S. Boyer)  
11:30  Exploration of chemical space using multiple similarity methods (A. Bergner)  
12:00  How to tackle challenging targets (C. Lemmen)  
12:30  Lunch  
14:00  A novel platform for integrated data-driven drug discovery (G. Ecker)  
14:40  Coffee Break  
15:00  Workshops: OpenEye, Chemical Computing Group, BioSolveIT, OpenPHACTS  
17:00  Integrative approaches in pharmaceutical R&D (F. Sanz)  
19:00  Dinner at Heuriger “Das Schreiberhaus”

**Friday, September 20.**

09:00  Impact of New Crystal Structures on Drug Discovery and Ligand Design (G. Hessler)  
09:45  Open Data in Pharmacoinformatics – Do they improve our models? (G. Ecker)  
10:30  Coffee break  
11:00  ChemSpider and drug discovery (C. Batchelor)  
11:30  Surfing at the Interface of Chemistry and Biology (C. Lemmen)  
12:00  How to deal with open access bioassay data? (B. Zdrazil)  
12:30  Fast and Accurate Prediction of Substrate Binding Affinities for Cytochrome P450s (R. Vosmeer)  
12:45  Lunch  
14:00  Europin students progress reports  
15:30  Coffee Break  
15:50  Europin application talks  
17:00  Discussion and farewell party

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