# Vienna Summer School Drug Design

Program 2013

## Sunday, September 15.

16:00 Registration
18:00 Welcome & Introduction (G. Ecker)
18:15 Computer-assisted Drug Discovery in the 21st Century: Ready For Success? (T. Langer)
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(GB)SA 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
15:00 *Workshops:* Schrödinger, InteLigand

## 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. Tsareva)
12:45 Lunch
14:00 H2O Friend or Foe? – Revisited (D. Cappel)
14:40 Coffee Break
15:00 *Workshops:* Schrödinger, InteLigand
17:00 Poster Session

## 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 miner alocorticoid 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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