Vienna Summer School
Drug Design

Program 2017

Sunday, 17.09.2017	
16:00	**Registration**
18:00	**Welcome & Introduction**
18:15	**Peter Nussbaumer** Drug Discovery: a Constant Challenge
19:00	**Get-together Party**

Monday, 18.09.2017	
09:00	**Thierry Langer** Adventures in Computer-Aided Molecular Design
09:45	**Johannes Kirchmair** Computational Prediction of Drug Metabolism
10:30	**Coffee break**
11:00	**Gerhard Wolber** Addressing challenging targets using 3D pharmacophores
11:30	**Gerhard Ecker** Predicting drug residence time - its all about how long you stay
12:00	**Stephan Ehrlich** Computational Prediction of Compound Stability for Pharmacological Formulations
12:30	**Lunch**
14:00	**Sharon Bryant** Innovative molecular design and decision support in drug discovery research
14:40	**Coffee break**
15:00	**Workshops:** **Schroedinger, IL**

Tuesday, 19.09.2017	
09:00	**Andrea Cavalli** Thermodynamics and kinetics of drug-target binding via molecular simulations
09:45	**Stefan Boresch** MD Simulations of Proteins: Practical Hints and Pitfalls to Avoid
10:30	**Coffee break**
11:00	**Anna Weinzinger** Towards a structural view of drug binding to the hERG K+ channel
11:30	**Chris Oostenbrink** Applications of free energy calculations from molecular dynamics simulations
12:00	**Eleni Kotsampasakou** Computational Toxicology: Current Practices and Challenges in Industry
12:15	**Donatella Callegari** Ranking Short and Long Residence-Time Inhibitors of Cyclin-Dependent Kinase 8 with Metadynamics Simulations
12:30	**Lunch**
14:00	**Matt Segall** Multi-parameter Optimisation in Drug Discovery: Targeting compounds with a high chance of success
14:40	**Coffee break**
15:00	**Workshops:** **IL, BIKI**
17:00	**Poster session** **Beer and Pretzel**

Wednesday, 20.09.2017	
09:00	**Matthias Frech** Residence Time- The why and when
09:45	**Maurizo Botta** Small molecule inhibitors of DDX3 as potential broad-spectrum antiviral agents
10:30	**Coffee break**
11:00	**Andreas Goeller** ADMET in the Real World: Opportunities and Challenges for Off-target Modeling in the Pharmaceutical Industry
11:30	**Knut Baumann** Predictive Modelling in Computational Medicinal Chemistry - The Do's and Don'ts in Model Development
12:00	**Barbara Zdrazil** How popular is my scaffold? - A trend analysis of scaffold properties over time
12:30	**Lunch**
14:00	**Gunther Stahl** Sampling molecular alignment space: how much is enough?
14:40	**Coffee break**
15:00	**Workshops:** **OpenEye, Optibrium, ProBiS**

Thursday, 21.09.2017	
09:00	**Wolfgang Sippl** Structure-guided optimization of epigenetic inhibitors - impact of protein flexibility
09:45	**Peter Ettmayer** Hit and Lead Generation Strategies – where do our Drugs come from?
10:30	**Coffee break**
11:00	**Gabriele Cruziani** Lipidomics in pharmaceutical research and drug design
11:30	**Dusanka Janezic** New computational tools at the molecular scale for protein-ligand binding in drug discovery
12:00	**Alexandra Nass** PTP1B Selectivity – Exploring the world of protein ligand interactions beyond hydrogen bond counts in static structures
12:15	**Francesco Greco** Unveiling Hidden Motifs of Substrate Binding to IDO1
12:30	**Lunch**
14:00	**Marcus Gastreich** Correlation vs. Causility: Don't Get Lost in Sigma Holes
14:40	**Coffee break**
15:00	**Workshops:** **BIT, Open eye, ProBiS**
17:00	**Hugo Kubinyi** Reflections on Discovery in Science
19:00	**Congress Dinner at Heuriger Schuebl-Auer**

Friday, 22.09.2017	
09:00	**Matthias Rarey** Dealing with Protein Structures for Molecular Design: From Geometric Searching to Ensemble Generation
09:45	**Alexander Hillisch** Design of BAY1217224, a Neutral, Non-Prodrug Thrombin Inhibitor with Good Oral Pharmacokinetics
10:30	**Coffee break**
11:00	**Gerhard Hessler** Peptide-based drug discovery
11:45	**Klaus-Jürgen Schleifer** Digitalization in R&D
12:30	**Lunch**
14:00	**Europin application talks**

univie: summer schools
europin
Computational Life Sciences
BASF We create chemistry
SANOFI
BAYER
BIKI TECHNOLOGIES
BioSolve
inte:ligand
OpenEye
optibrium
ProBiS
SCHRÖDINGER.