Vienna Summer School
Drug Design

Program 2015

Sunday, September 20	
16:00	Registration
18:00	Welcome & Introduction
18:15	Biophysics in Drug Discovery: A Game Changer for the Early Research Pipeline? **(M. Frech)**
19:00	*Get-together Party*

Monday, September 21	
09:00	Thermodynamics and kinetics of drug-target binding through molecular simulations **(A. Cavalli)**
09:45	HTMD: an environment for computer aided drug discovery, focus on simulations **(G. De Fabritiis)**
10:30	*Coffee break*
11:00	Ligand-protein binding and ligand-based virtual screening using maximum clique algorithm **(D. Janežič)**
11:45	Protein-Ligand Kinetics and Interactions by means of molecular dynamics simulations **(M. Grandits)**
12:15	Analysis of molecular features influencing HSP90 binding kinetics **(D. Schuetz)**
12:30	*Lunch*
14:00	Organizing 3D Project Data for Structure-Based Drug Design in MOE **(M. Kossner)**
14:40	*Coffee break*
15:00	WS: CCG, OpenEye, BiKi, OPS/KNIME

Tuesday, September 22	
09:00	Pharmacophores - The Current and The Future **(T. Langer)**
09:45	Structure-based design of selective histone deacetylase inhibitors - challenges and opportunities **(W. Sippl)**
10:15	Pharmacophoric descriptors from molecular dynamics simulations for predicting sulfotransferase activity **(C. Rakers)**
10:30	*Coffee break*
11:00	Allosteric Inhibitors Drug Design: Successful Examples in the Field of HIV and Cancer **(M. Botta)**
11:45	Exploring protein-ligand binding using three-dimensional pharmacophore patterns **(G. Wolber)**
12:15	Hunting parasite-killing histone deacetylase inhibitors by computer-based methods **(J. Melesina)**
12:30	*Lunch*
14:00	Sampling molecular alignment space: how much is enough? **(G. Stahl)**
14:40	*Coffee break*
15:00	WS: CCG, OpenEye, Inte:Ligand, OPS/KNIME
17:00	Poster Sessions

Wednesday, September 23	
09:00	MD Simulations of Proteins: Practical Hints and Pitfalls to Avoid **(S. Boresch)**
09:45	Applications of free energy calculations from molecular dynamics simulations **(C. Oostenbrink)**
10:30	*Coffee break*
11:00	Toxicological Predictions: The role of public, commercial and in-house data **(K.-J. Schleifer)**
11:45	Coupling enhanced sampling simulations with experimental techniques. Theory and case studies **(G. Costantino)**
12:15	Covalently Binding Fragments: Reaction-Driven Design of Viral Protease Inhibitors **(R. Schulz)**
12:30	*Lunch*
14:00	Innovative in silico approaches to hit finding, lead molecule design and drug hunting **(S. Bryant)**
14:40	*Coffee break*
15:00	WS: Inte:Ligand, OPS/ChemBioNavigator, ChEMBL

Thursday, September 24	
09:00	Drug Metabolism and Prodrugs **(H. Kubinyi)**
09:45	Predicting drug metabolism **(J. Kirchmair)**
10:30	*Coffee break*
11:00	A Direct Approach to Protein-Ligand Systems combining Cheminformatics, Specific Isotope-Labelling and NMR Spectroscopy **(R. Konrat)**
11:30	Elaboration of pharmacophore structure of new targets by molecular dynamics simulation - case study **(M. Baginski)**
12:00	Design of novel neuroprotective agents that inhibit endocannabinoids degradation **(L. Scalvini)**
12:15	Ligand- and structure-based methods to predict and understand BCRP inhibition **(F. Montanari)**
12:30	*Lunch*
14:00	Predicting binding affinity doesn't work — or does it? **(C. Lemmen)**
14:40	*Coffee break*
15:00	WS: BioSolveIT, OPS/ChemBioNavigator, Inte:Ligand
19:00	*Dinner at Heuriger Schuebl-Auer*

Friday, September 25	
09:00	Best of Both Worlds: Combining Pharma Data and State of the Art Modeling Technology To Improve in silico pKa Prediction **(A. Hillisch)**
09:45	Insights into the Polypharmacology of PARP Inhibitors **(A. Macchiarulo)**
10:30	*Coffee break*
11:00	QSAR applications in modern Drug Discovery **(G. Hessler)**
11:45	Computational methods to manage uncertainty in drug risk assessment **(S. Boyer)**
12:30	*Lunch*
14:00	Europin application talks
15:30	*Coffee break*
15:50	Europin progress reports
17:00	Discussion