Vienna Summer School Drug Design

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Program 2019

Sunday, 15.09.2019	
16:00	**Registration**
18:00	**Welcome & Introduction**
18:15	**Johannes Kirchmair – University of Bergen** In silico prediction of drug metabolism
19:00	**Get-together Party**

Monday, 16.09.2019	
09:00	**Thierry Langer – University of Vienna / Inte:Ligand** Adventures in Computer-Assisted Molecular Design
09:30	**Claire Colas – University of Vienna** Structure, Function and Ligand Discovery for Solute Carrier Transporters
10:00	**David Machalz – Freie Universität Berlin (Europin)** Targeting Cytochrome P450 4Z1 as Novel Cancer Target
10:15	**Jennifer Hemmerich – University of Vienna (Europin)** Cover: Conformational OVERsampling of toxicological datasets for deep learning
10:30	**Coffee break**
11:00	**Dušanka Janežič – University of Primorska** Protein interaction atlas for prediction of genetic variations involved in drug interactions and disease development
11:30	**Matt Segall – Optibrium** Multi-parameter Optimisation in Drug Discovery: Targeting compounds with a high chance of success
12:00	**Gunther Stahl – OpenEye** Virtual Screening – do I REAL-ly need large scale?
12:30	**Lunch**
14:00	**Stephan Ehrlich – Schrödinger** Hydrogens Matter - Considering Tautomers and Protomers in Drug Discovery
14:30	**Coffee break**
15:00	**Workshops:** OpenEye, Optibrium, Schrödinger
17:00	**Poster session 1** Beer and Pretzel

Tuesday, 17.09.2019	
09:00	**Gerhard Ecker – University of Vienna** Computational Toxicology - from models to workflows
09:30	**Doris Schütz – University of Montreal** Integrating Interaction Hotspots of the Ras/SOS Complex to Rationalize Small Molecule Design
10:00	**Floriane Montanari – Bayer AG** Deep learning for computational chemistry: compound representation, ADMET profiles and automatic optimization
10:30	**Coffee break**
11:00	**Martyna Pawletta - KNIME** Cheminformatics in the open-source KNIME Analytics Platform
11:30	**Daniela Digles – University of Vienna** Accessing public databases with KNIME
12:00	**Daniela Dolciami – University of Perugia (Europin)** Virtual Screening Campaigns for the Identification of New Immunomodulatory Drugs Targeting AhR
12:15	**Szymon Pach – Freie Universität Berlin (Europin)** Design of novel NS2B-NS3 flaviviral protease inhibitors
12:30	**Lunch**
14:00	**Andrea Cavalli – University of Bologna / BiKi Technologies** Thermodynamics and Kinetics of Drug-Target Binding via Molecular Simulations
14:30	**Coffee break**
15:00	**Workshops:** BiKi Technologies, KNIME, Schrödinger
17:00	**Zoe Cournia - Biomedical Research Foundation Athens** Women at the Interface of Computational Chemistry and Drug Discovery

Wednesday, 18.09.2019	
09:00	**Margot Ernst – Medical University of Vienna** Ligand bound proteins – the underestimated skill of template choice and analysis in homology based approaches
09:30	**Wolfgang Sippl – Martin Luther University of Halle-Wittenberg** Design of selective histone deacetylase inhibitors - lessons learned from X-ray crystallography and molecular modelling
10:00	**Gerhard Wolber – Freie Universität Berlin** Exploring dynamic 3D interaction patterns for mechanistic understanding of protein-ligand binding
10:30	**Coffee break**
11:00	**Zoe Cournia - Biomedical Research Foundation Athens** Lessons learned from protein-ligand complex prediction and lead optimization with FEP in the D3R Challenge
11:30	**Barbara Zdrazil – University of Vienna** Intertwining Data Science and Computational Molecular Design – Recent Examples from Modeling Hepatic Uptake Transporters
12:00	**Stefanie Kickinger – University of Vienna (Europin)** Structural and molecular aspects of GABA transporter subtype selectivity
12:15	**Nguyen Trung Ngoc – Freie Universität Berlin (Europin)** Dihedral angle dynamics of GPCR activation hotspots
12:30	**Lunch**
14:00	**Sharon Bryant – Inte:Ligand** Advanced 3D-Pharmacophores and Their Use In Drug Discovery Research
14:30	**Coffee break**
15:00	**Workshops:** BioSolveIT, KNIME, LigandScout
18:00	**Poster session 2** Beer and Pretzel

Thursday, 19.09.2019	
09:00	**Stefan Boresch – University of Vienna** Setting up MD Simulations of Biomolecules
09:30	**Chris Oostenbrink - BOKU Vienna** Applications of free energy calculations from molecular dynamics simulations
10:00	**Eva Hellsberg – University of Vienna (Europin)** Computational studies of molecular interactions in the human serotonin transporter
10:15	**Chiara Luise – Martin-Luther University of Halle-Wittenberg (Europin)** Computer-based approaches for the search of new Spindlin1 inhibitors
10:30	**Coffee break**
11:00	**Anna Weinzinger – University of Vienna** Computational studies on ion channels
11:30	**Alexander Hillisch – Bayer AG** Bayer's "Next Generation Library Initiative": Selected Examples of Computational Compound Design
12:00	**Alžběta Türková – University of Vienna (Europin)** Multiscale Computer-based Studies to Identify Ligand Interactions and Selectivity Among Hepatic Organic Anion Transporting Polypeptides
12:15	**Florentina Troger – University of Vienna** Combining structure- and ligand-based methods for toxicity prediction linked to human mitochondrial respiratory complex I inhibition and *in vitro* validation
12:30	**Lunch**
14:00	**Marcus Gastreich – BioSolveIT** Chemical Space Navigation — A Journey to 10^{20} Possibilities
14:30	**Coffee break**
15:00	**Workshops:** BioSolveIT, LigandScout, ProBiS
17:00	**Hugo Kubinyi** Reflections on Discovery in Science
19:00	**Congress Dinner at Heuriger**

Friday, 20.09.2019	
09:00	**Peter Ettmayer – Boehringer-Ingelheim** PROTACs - a New Therapeutic Modality
09:30	**Arthur Garon – University of Vienna** Novel Graph Representation of 3-D Pharmacophore Models Extracted from Molecular Dynamics Simulation
10:00	**Klaus-Jürgen Schleifer – BASF** Computational Chemistry @ BASF
10:30	**Coffee break**
11:00	**Eva-Maria Plessl – University of Vienna** Structure-activity relationship of the hERG activator ICA-105574
11:30	**Philipp Schmalhorst – Boehringer-Ingelheim** Extracting hidden design opportunities from protein structure ensembles
12:00	**Gerhard Hessler – Sanofi** Efficient Mining of Chemical Space
12:30	**Lunch**
14:00	**Europin application talks**