Vienna Summer School Drug Design

# Programm 2021

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| Monday, 13.09.2021 | |
|---|---|
| **8:15-8:30** | **Welcome** |
| **8:30-9:00** | **Thierry Langer – University of Vienna**<br>Adventures in Computer-Assisted Molecular Design |
| **9:00-9:30** | **Stefan Boresch – University of Vienna**<br>Setting up MD Simulations of Biomolecules |
| **9:30-10:00** | **Chris Oostenbrink – BOKU Vienna**<br>Applications of free energy calculations from molecular dynamics simulations |
| **10:00-10:30** | **Break** |
| **10:30-11:00** | **Andrea Cavalli – University of Bologna**<br>Dynamic docking and free energy estimation approaches to drug discovery |
| **11:00-11:30** | **Daria Goldmann – KNIME**<br>Predicting bioactivity in KNIME Analytics Platform |
| **11:30-12:00** | **Marcus Gastreich – BioSolveIT**<br>Navigating Septillion-Sized Chemical Spaces |
| **12:00-12:30** | **Matt Segall – Optibrium**<br>Multi-parameter Optimisation in Drug Discovery: Targeting compounds with a high chance of success |
| **12:30-13:30** | **Lunch Break** |
| **13:30-15:00** | **Workshops** (running in parallel)<br>BioSolveIT beginners, StarDrop beginners, KNIME beginners |
| **15:00-15:30** | **Break** |
| **15:30-17:00** | **Workshops** (running in parallel)<br>BioSolveIT advanced, StarDrop advanced, KNIME advanced |
| **17:00-17:30** | **Break** |
| **17:30-18:00** | **Virtual Vienna Tour** |

| Tuesday, 14.09.2021 | |
|---|---|
| **8:30-9:00** | **Gerhard Ecker – University of Vienna**<br>Integrated approaches for toxicity prediction |
| **9:00-9:30** | **Andrea Volkamer – Charité Universitätsmedizin Berlin**<br>*In silico* Tools to Support Risk Assessment of Small Molecules |
| **9:30-10:00** | **Johannes Kirchmair – University of Vienna**<br>In silico prediction of drug metabolism |
| **10:00-10:30** | **Break** |
| **10:30-11:00** | **Manuel Pastor – Universitat Pompeu Fabra**<br>Application of knowledge-based computational methods in Toxicology |
| **11:00-11:30** | **Philipp Jäger – Boehringer-Ingelheim**<br>Integrative data approaches for smart PROTAC designs |
| **11:30-12:00** | **Gunther Stahl – OpenEye**<br>Virtual Screening - from small to LARGE scale - from local to the cloud |
| **12:00-12:30** | **Stephan Ehrlich – Schrödinger**<br>Structure-based screening of large chemical libraries |
| **12:30-13:30** | **Lunch Break** |
| **13:30-15:00** | **Workshops** (running in parallel)<br>Schrödinger beginners, Open Eye, eTransafe Flame |
| **15:00-15:30** | **Break** |
| **15:30-17:00** | **Workshops** (running in parallel)<br>Schrödinger advanced, Open Eye |
| **17:00-17:30** | **Break** |
| **17:30-19:00** | **Career Session** (Panel discussion)<br>Margot Ernst (Medical University of Vienna), Daria Goldmann (KNIME), Alexander Hillisch (Bayer AG), Martin Kotev (Evotec), Floriane Montanari (Bayer AG), Doris Schütz (IRIC - University of Montreal), Alžběta Türková (Uppsala University); Moderation: Gerhard Ecker (University of Vienna) |

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| Wednesday, 15.09.2021 | |
|---|---|
| **8:30-9:00** | **Margot Ernst – Medical University of Vienna**<br>Homology modeling in the gray zone of low sequence similarity |
| **9:00-9:30** | **Wolfgang Sippl – Martin Luther University of Halle-Wittenberg**<br>Structure based design of selective ligands for epigenetic targets |
| **9:30-10:00** | **Gerhard Wolber – Freie Universität Berlin**<br>In silico pharmacology: Pyrod and dynophores as powerful computational microscopes to decode receptor function |
| **10:00-10:30** | **Break** |
| **10:30-11:00** | **Barbara Zdrazil – University of Vienna**<br>Deciphering the molecular basis of ligand-recognition and selectivity in hepatic Organic Anion Transporting Polypeptides |
| **11:00-11:30** | **F. Javier Luque – University of Barcelona / Pharmacelera**<br>From simple solvation models to applications in target druggability and screening of drug-like compounds |
| **11:30-12:00** | **Sharon Bryant – Inte:Ligand**<br>De-Risking Compound Structures for Neurotoxicity: The NeuroDeRisk Inte:Ligand Profiler |
| **12:00-12:30** | **Andrew Henry – Chemical Computing Group**<br>MOEsaic: Guiding Multi-Parameter Optimization in Ligand-Based Design |
| **12:30-13:30** | **Lunch Break** |
| **13:30-15:00** | **Workshops** (running in parallel)<br>CCG, Ligand:Scout beginners, Pharmacelera |
| **15:00-15:30** | **Break** |
| **15:30-17:00** | **Workshops** (running in parallel)<br>Ligand:Scout advanced, CCDC |
| **17:30** | **Poster Session 1**<br>Posters 1-36 |

| Thursday, 16.09.2021 | |
|---|---|
| **8:30-9:00** | **Dušanka Janežič – University of Primorska**<br>Protein Binding Sites Tools for Innovative Drug Design |
| **9:00-9:30** | **Alexander Hillisch – Bayer AG**<br>Design and Preclinical Characterization Program Towards BAY 2433334, an Oral Factor XIa Inhibitor for the Prevention and |
| **9:30-10:00** | **Claire Colas – University of Vienna**<br>Structure based ligand discovery methods applied to Solute Carrier Transporters |
| **10:00-10:30** | **Break** |
| **10:30-11:00** | **Floriane Montanari – Bayer AG**<br>An introduction to explainable AI for small molecules |
| **11:00-11:30** | **Daniela Digles – University of Vienna**<br>Analysing Solute Carrier (SLC) substrates with KNIME |
| **11:30-12:00** | **Stuart Firth-Clark – Cresset**<br>Using Spark™ and Flare™ to design and prioritize novel molecules in a drug design project |
| **12:00-12:30** | **Lorena Zara – Discngine**<br>Learn how to navigate the vast and rich protein structural space with 3decision |
| **12:30-13:30** | **Lunch Break** |
| **13:30-15:00** | **Workshops** (running in parallel)<br>Cresset beginners, Discngine beginner 1, eTransafe UNIVIE Modeling Tools |
| **15:00-15:30** | **Break** |
| **15:30-17:00** | **Workshops** (running in parallel)<br>Cresset advanced, Discngine beginner 2 (group 1) |
| **17:00-17:30** | **Break** |
| **17:30** | **Poster Session 2**<br>Posters 37-72 |

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| Friday, 17.09.2021 | |
|---|---|
| **8:30-9:00** | **Abhik Mukhopadhyay – CCDC**<br>Ligand based virtual screening in Drug discovery |
| **9:00-9:30** | **Klaus-Jürgen Schleifer – BASF**<br>Learning from Ligands |
| **9:30-10:00** | **Gerhard Hessler – Sanofi**<br>Computational Design of macrocyclic compounds |
| **10:00-10:30** | **Break** |
| **10:30-10:45** | **Oliver Wieder – University of Vienna**<br>Improved lipophilicity and aqueous solubility prediction with composite graph neural networks. |
| **10:45-11:00** | **Theresa Noonan – Freie Universität Berlin** (EUROPIN Student)<br>Inhibiting Bacterial Ribosomal Assembly as a Novel Antibiotic Approach |
| **11:00-11:15** | **Theres Friesacher – University of Vienna**<br>Molecular Dynamic Simulations of Ion Channels: Investigating a Rare Disease Mutation through the Computational Microscope |
| **11:15-11:30** | **Dominique Sydow - Charité Universitätsmedizin Berlin**<br>KiSSim: Subpocket-Enhanced Kinase Similarity Assessment for Off-Target Prediction |
| **11:30-11:45** | **Barbara Füzi – University of Vienna** (EUROPIN Student)<br>Pathway and network studies of toxic compounds |
| **11:45-12:00** | **Doha Naga – Hofmann La Roche / University of Vienna**<br>Automated machine learning in drug discovery |
| **12:00-12:15** | **Stefan Kohlbacher – University of Vienna**<br>QPhAR: Quantitative Pharmacophore Activity Relationship |
| **12:15-12:30** | **Christian Permann – University of Vienna**<br>Greedy 3-Point Search (G3PS) - A novel algorithm for pharmacophore alignment |
| **12:30-13:30** | **Closing & Lunch Break** |
| **13:30-16:30** | **Presentations from EUROPIN Students & Applicants**<br>See agenda below |
| **16:30-18:00** | **Workshops**<br>Discngine beginner 2 (group 2) |

| Friday, 17.09.2021 – Presentations from EUROPIN students | |
|---|---|
| **13:30 - 13:45** | **Szymon Pach – Freie Universität Berlin**<br>Tracing interactions of SARS Cov2 spike protein in complex with animal ACE2 ortholgs |
| **13:45 - 14:00** | **Nguyen Trung Ngoc – Freie Universität Berlin**<br>ACE2-variants indicate potential SARS-CoV-2 susceptibility in animals: data analysis |
| **14:00 - 14:15** | **Pablo Rodríguez Belenguer – Pompeu Fabra University**<br>Combining machine learning models for improving their predictive quality and usefulness in biomedical applications |
| **14:15 - 14:30** | **Kristina Puls – Freie Universität Berlin**<br>Mechanistic investigation and development of tailored modulators of the Kappa opioid receptor |
| **14:30 - 14:45** | **Nejra Granulo – University of Vienna**<br>The macrocyclic landscape of SLCs |
| **14:45 - 15:00** | **Alexander Wolf – Freie Universität Berlin**<br>*In silico* modelling of human Cytochrome P450 enzymes |
| **15:00 - 15:15** | **Break** |
| **15:15 - 15:30** | **Aljoša Smajić – University of Vienna**<br>Decentralized machine learning approaches for toxicity predictions |
| **15:30 - 15:45** | **Francesca Galvani – University of Parma**<br>Multiscale simulations for the design of new drug-like compounds |
| **15:45 - 16:00** | **Jiahui Huang – University of Vienna**<br>Structure landscape analysis and functional mapping of mutations on SLC transporters |
| **16:00 - 16:15** | **Gian Marco Elisi – University of Parma**<br>Free-energy simulations on melatonin receptors ligands |
| **16:15** | **Closing** |

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