EUROPIN Summer School on Drug Design

September 14 - 19, 2025

Josef-Holaubek-Platz 2, 1090 Vienna, Lecture Hall 7

Sunday, September 14

Time	Speaker	Title / Activity
16:00	—	**Registration**
18:00	**Gerhard Ecker** University of Vienna	Welcome & Introduction
18:15	**Johannes Kirchmair** University of Vienna	Methods and Strategies for Tackling Assay Interference Caused by Small Molecules
18:00	—	**Welcome Get-Together**

Monday, September 15

Time	Speaker	Title / Activity
09:00	**Thierry Langer** University of Vienna	Next Generation Pharmacophore Modeling: Recent Success Stories
09:30	**Mehran Jalaie** Pfizer	Beyond the Lead Identifications: HPK1 (Hematopoietic Protein Kinase 1 HPK1/MAP4K1)
10:00		**Coffee Break**
10:30	**Barbara Zdrazil** EBI	The ChEMBL Database in 2025 - Towards AI-ready Data
11:00	**Matthias Rarey** University of Hamburg	Cheminformatics and Structure-Based Design - Shaping the Framework for Machine Learning
11:30	**Julia Kandler** University of Vienna	Investigating Developmental Neurotoxicity: Integrated Models of Thyroid Function Disruption
11:45	**Christian Fellinger** University of Vienna	Binding Affinity Estimation using GRADE
12:00		**Lunch Break**
14:00	**Sharon Bryant** Inte:Ligand	Addressing Challenging Targets in Drug Discovery: Recent Applications of LigandScout
14:30	**Workshops**	Chemical Computing Group 1 (2D 313) // Inte:Ligand 1 (2F 363) // KNIME basics (2D 404)
16:30		**Coffee Break**

Time	Speaker	Title / Activity
17:00	**Palle Steen Helmke** University of Vienna	Refining Cholestasis and Steatosis Prediction: An Explainable Model
17:15	**Hosein Fooladi** University of Vienna	Bridging Islands in Chemical Space: Evaluating and Enhancing ML Generalization for Drug Discovery
17:30		**Poster Session**

Tuesday, September 16

Time	Speaker	Title / Activity
09:00	**Stefan Boresch** University of Vienna	Setting up MD Simulations of Biomolecules
09:30	**Stefan Boresch** University of Vienna	An Introduction to Alchemical Free Energy Simulations
10:00		**Coffee Break**
10:30	**Martin Lepšík** IOCB Prague	Semiempirical Quantum Mechanical Scoring in Structure-based Drug Design
11:00	**Anna Weinzinger** University of Vienna	Ion Channels in Health and Disease: From Mechanistic Understanding to Therapeutic Solutions
11:30	**Peter Ettmayer** Boehringer Ingelheim	Case Study: Discovery of BI 1810631 - A HER2 Selective, EGFR Sparing, Irreversible Tyrosine Kinase Inhibitor
12:00		**Lunch Break**
14:00	**Daniel Cappel** Schrödinger	A Novel Workflow for the In Silico Identification and Prioritization of Potential Allosteric Binding Sites Based on Mixed Solvent Simulations and SiteMap
14:30	**Workshops**	Inte:Ligand 2 (2F 363) // KNIME for Drug Discovery (2D 404) // Schrödinger 1 (2D 313)
16:30		**Coffee Break**
17:00	**Vincent-Alexander Scholz** University of Vienna	Modelling the Dissipation Kinetics of Small Molecules
17:15	**Valerij Talagayev** Freie Universität Berlin & AIIffinity	Identification and Optimization of Toll-like Receptor 8 Modulators Using Pharmacophores and Molecular Dynamics Simulations
17:30	**Mireille Krier** OpenEye, Cadence Molecular Sciences	Shape and Color: A Unifying Principle for Modeling Molecules

Wednesday, September 17

Time	Speaker	Title / Activity
09:00	**Klaus-Jürgen Schleifer** BASF	Calcium Channel Inhibitors: Can Small Drugs and Large Toxins Use the Same Principle?
09:30	**Hanoch Senderowitz** Bar-Ilan University	Addressing Global Food Security via a Combined Experimental / Agroinformatics Approach
10:00		**Coffee Break**
10:30	**Stefanie Kickinger** Boehringer Ingelheim	Potential and Limitations of Free-Energy Calculations in Lead Optimization of KRAS Inhibitors
11:00	**Francesca Grisoni** Eindhoven University of Technology	De Novo Drug Design with Chemical Language Modeling
11:30	**Sara Tkaczyk** University of Vienna	Free Energy Calculations with Machine Learning Potentials
11:45	**Thi Ngoc Lan Vu** University of Vienna	Assessing the Role of Machine Learning-Based Pose Sampling in Virtual Screening
12:00		**Lunch Break**
14:00	**Marcus Gastreich** BioSolveIT	0D, 2D, and 3D Navigation of Zetta-Sized On-Demand Chemical Spaces
14:30	**Workshops**	BioSolveIT 1 (2D 404) // OpenEye 1 (2F 363) // Schrödinger 2 (2D 313)
16:30		**Coffee Break**
17:00	**Karin Grillberger** University of Vienna	Leveraging Consensus Docking Strategies at Mitochondrial Complexes I & III
17:15	**Niklas Piet Doering** Freie Universität Berlin	MDPath: Unraveling Allosteric Communication Paths through Molecular Dynamics Simulations
17:30		**Poster Session**

Thursday, September 18

Time	Speaker	Title / Activity
09:00	**Sergey Sosnin** University of Vienna	Maps, Compasses, and Chemimanship: Visual Navigation in Chemical Space
09:30	**Dušanka Janežič** University of Primorska	ProBiS: Innovative Computational Tools for Protein Binding Site Prediction and Structure-Driven Drug Design
10:00		**Coffee Break**
10:30	**Maria Letizia Barreca** University of Perugia	Beyond Traditional Drug Design: Targeting Protein Folding with Small Molecules

Time	Speaker	Title / Activity
11:00	**Igor Tetko** Helmholtz Zentrum München	Which Modern AI Methods Provide Accurate Predictions of Toxicological Endpoints? Analysis of Tox24 Challenge Results
11:30	**Gian Marco Elisi** University of Parma	Discovery of Covalent Inhibitors of Adenosine 5'-Phosphosulfate Reductase
11:45	**Friederike Wunsch** University of Münster	Dynamics Shaping GPCRs' Functionality
12:00		**Lunch Break**
14:00	**Alexander Amberg** Sanofi	Application of In Silico Approaches and SAR for Regulatory Risk Assessment of N-Nitrosamine Impurities in Drugs
14:30	**Workshops**	Chemical Computing Group 2 (2D 313) // BioSolveIT 2 (2D 404) // OpenEye 2 (2F 363)
16:30		**Coffee Break**
17:00	**Mark Cronin** Liverpool John Moores University	Making the Most of Structure-Based Predictive and Computational Toxicology
19:00		**Congress Dinner**

Friday, September 19

Time	Speaker	Title / Activity
09:00	**Gerhard Wolber** Freie Universität Berlin	Design – Make – Test: From Computational Design to Bioactive Molecules
09:30	**Gerhard Hessler** Sanofi	Large Language Models in Drug Discovery for the Design of Novel Molecules
10:00		**Coffee Break**
10:30	**Barbara Füzi** Barcelona Supercomputing Center	Sex-specific Toxicological Outcomes in Preclinical Control Group Data
11:00	**Daniele Pala** Chiesi Farmaceutici	Hop to It! – The Discovery of a Novel Series of ROCK Inhibitors by Scaffold Hopping
11:30	**Anders Hogner** AstraZeneca	Integrating Computations and Experiments to Unlock Structure-Based Design of Small Molecules Targeting RNA

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EUROPIN Talks – Friday Afternoon, September 19

Time	Speaker	Title
14:00	**Marvin Taterra** University of Münster	Modulation of Allosteric Communication in Common Drug Targets (Introductory Talk)
14:10	**Tarik Cerimagic** University of Vienna	A Multi-Task Learning Approach for Data Imputation of Compound Bioactivity Values Across the SLC Transporter Superfamily (Introductory Talk)
14:20	**Uday Abu Shehab** University of Vienna	Towards Tailored Domain Adaptive Models in the Context of Natural Products Research (Introductory Talk)
14:30	**Matthias Welsch** University of Vienna	Representational Alignment in Cheminformatics (Introductory Talk)
14:40		**5 min Break**
14:45	**Paula Linh Kramer** Saarland University	Active Learning for Fragment-Based Kinase Inhibitor Design (Acceptance Talk)
15:00	**Floriane Odje** Saarland University	Integrating Structural and Morphological Fingerprints: Understanding Information for Pattern Identification and Better Toxicity Prediction (Acceptance Talk)
15:15	**Clemens Alexander Wolf** Freie Universität Berlin	Novel Cytochrome P450 4A11 Inhibitors to Counteract Metabolic Dysfunction-Associated Fatty Liver Disease (MAFLD) (Progress Report Talk)
15:30	**Francesca Galvani** University of Parma	Multivariate Analysis of HRMS Lipidomics Data Reveals a Role for Glycosphingolipids in Cancer Resistance (Progress Report Talk)

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