EUROPEAN WORKSHOP IN DRUG DESIGN 2024

UNIVERSITÀ DI SIENA 1240

SUNDAY – MAY 19

16:00 – 19:00 Registration
18:00 – 18:30 Coffee Break
19:30 – 20:30 Dinner
20:45 – 22:00 EWDD24 Opening Ceremony & Inauguration Lecture by **Gerd Folkers:** Creation – the USP of Chemistry – Drug Design, Evolution and Everything...

MONDAY – MAY 20

09:00 – 09:40 **Bruno Botta:** The chemistry of natural products: a forty-year journey
09:40 – 10:15 **Sharon D Bryant:** Advanced 3D-Pharmacophores for Bioactive Molecule Discovery and De-Risking Neurotoxicity
10:15 – 11:00 **Daniel Rauh:** Targeting Cancer
11:00 – 11:30 Coffee Break
11:30 – 12:10 **Wolfgang Sippl:** Structure-based Design of Subtype-selective Histone Deacetylase Inhibitors and PROTACs as Promising Anti-cancer Agents
12:10 – 12:50 **Mehran Jalaie:** Lead Identifications Across Therapeutic Areas
12:50 – 13:30 Poster Flash Presentations
13:30 – 14:30 Lunch Break
14:30 – 15:00 Poster Session (1)
15:00 – 16:30 Software Demonstrations | Case Studies (1)
inte:ligand & Optibrium & OpenEye
16:30 – 17:00 Coffee Break
17:00 – 18:30 Software Demonstrations | Case Studies (2)
inte:ligand & BioSolveIT & OpenEye
19:30 – 20:30 Dinner
20:30 – 21:30 Social Special Activity

TUESDAY – MAY 21

09:00 – 09:40 **Andrea Cavalli:** Computational Approaches to Drug Discovery in the Era of Precision Medicine
09:40 – 10:15 **Gianni DeFabritiis:** Relative binding free energies using machine learning potentials
10:15 – 11:00 **Klaus-Jürgen Schleifer:** Learning from Molecules
11:00 – 11:30 Coffee Break
11:30 – 12:10 **Edgar Jacoby:** The Use of Computational Chemistry in the Discovery of Novel DHODH Inhibitors for the Treatment of Acute Myelogenous Leukemia
12:10 – 12:50 **Hanoch Senderowitz:** Computational Studies in Green Pesticides
12:50 – 13:30 Poster Flash Presentations
13:30 – 14:30 Lunch Break
14:30 – 15:00 Poster Session (2)
15:00 – 16:30 Software Demonstrations | Case Studies (3)
inte:ligand & Schrödinger & Pharmacelera
16:30 – 17:00 Coffee Break
17:00 – 18:30 Software Demonstrations | Case Studies (4)
inte:ligand & Schrödinger & BioSolveIT
20:00 – 22:30 Social Dinner, Piazza del Campo, Siena

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WEDNESDAY – MAY 22

09:00 – 09:40 **Johannes Kirchmair:** Computational Approaches for Predicting Assay Interference
09:40 – 10:15 **Gerhard Ecker:** Prediction of Toxicity – It's All About Fingerprints
10:15 – 11:00 **Gerhard Hessler:** AI at work in industrial drug discovery
11:00 – 11:30 Coffee Break
11:30 – 12:10 **Anders Hogner:** Accelerating drug design with AI & simulation at AZ
12:10 – 12:50 **Gerhard Wolber:** Deciphering biological activity with next generation pharmacophore modeling and dynophores
12:50 – 13:30 Poster Flash Presentations
13:30 – 14:30 Lunch Break
14:30 – 15:00 Poster Session (3)
15:00 – 16:30 Software Demonstrations | Case Studies (5)
inte:ligand & BioSolveIT & Pharmacelera
16:30 – 17:00 Coffee Break
17:00 – 18:30 Software Demonstrations | Case Studies (6)
inte:ligand & OpenEye
19:30 – 20:30 Dinner
20:30 – 21:30 Social Special Activity

THURSDAY – MAY 23

09:00 – 09:40 **Rebecca Wade:** Protein dynamics and binding kinetics
09:40 – 10:15 **Martin Lepsik:** Semiempirical Quantum Mechanical Scoring in Structure-based Drug Design
10:15 – 10:45 Coffee Break
10:45 – 11:25 **Stefano Forli:** Slippery When Wet: Thermodynamic profiling of protein hydration sites
11:25 – 12:05 **Javier Luque:** Application of quantum mechanical 3D atomic models of hydrophobicity in virtual screening and drug design
11:05 – 12:30 Poster Award and Closing Ceremony
13:00 – 14:30 Farewell Lunch

EWDD24 is thankful for inte:ligand support provided by

BioSolveIT expect actives!
OpenEye SCIENTIFIC CADENCE MOLECULAR SCIENCES
optibrium
Pharmacelera
Schrödinger

POSTER SESSION

Omran	A Predictive Model for Interferon Gamma Release: Integrating Major Histocompatibility Complex and Peptide Sequences
Pecina	SQM2.20: universal physics-based scoring function for reliable protein-ligand affinity predictions
Biswas	An Automated System for Ranking Compounds Based on their Free Energy in Drug Discovery by Utilizing Docking and Molecular Dynamics
Barbieri	Insights into the linker domain in ABCB1/P-glycoprotein
Smajic	Data Exploration for Target Predictions using Proprietary & Publicly Available Data Sets
Grazzi	Development of a Coarse-Grained Molecular Dynamics (CG-MD) approach to explore tubulin-ligand binding
Cavalli	Machine learning scoring function for peptide docking
Llop Peiró	Enhancing Virtual Screening Strategies: Evaluating AutoDock Vina and Glide Methods for Predicting Conformations of Non-covalent Inhibitors Against SARS-CoV-2 Main Protease
Speroni	Development of a second generation of ArnT inhibitors: Abietane-type diterpenoids
Natale	Harnessing A Hybrid Approach to Dual Anti-Cancer Drug Discovery
Platella	Naphthalene diimide dimers designed as selective binders of G-quadruplex-G-quadruplex interfaces within telomeric DNA
Fellinger	Binding Affinity Estimation using X-GRADE
Garcia	Exploration of ultra-large chemical spaces in 3D
Mancino	Design, synthesis and biological evaluation of novel covalent kinase inhibitors to address mutant GIST
Pitasi	Computational alanine scanning and pharmacophore modelling to identify new potential elastase inhibitors with antiaging activity
Ferrara	Biotechnology-based approach for environmental bioremediation from toxic aldehydes using an Aldehyde Dehydrogenase endowed with broad substrate specificity
Minibaeva	Structure-based generation of synthetically feasible molecules
Kandler	A Structure-based View on Thyroid Peroxidase and the Sodium Iodide Symporter
Grillberger	Application of consensus docking and scoring for prioritization of compounds triggering a molecular initiating event at the human cytochrome bc1 complex
Meuser	A Quantum Algorithm for de novo Drug Design
Lombardo	Design of a robust S1R pharmacophore model via GBPM method
Ruberto	Assessment of Docking protocols for small molecules on Tubulin
Chiesa	LIT-AlphaFold: a new tool for multistate modelling
Chiesa	Function-based virtual screening using machine learning and single ligand dynamic interaction data
Mandalari	Molecular interaction between heparan sulfate mimetics and the recognition spike protein of SARS-CoV-2 virus
Roggia	Innovation in Virtual Screening: PyRMD2Dock's AI-Infused Approach
Krier	3D-QSAR meets ML for Binding Affinity Prediction

Schulte	Determination of Hyaluronidase Binding Free Energy using Advances Molecular Dyamic Methods
Gambacorta	Empowering Rare Disease Research and Toxicology Assessment through Public Web Platforms based on Explainable Artificial Intelligence
Vitale	Design of Lipid Nanoparticles (LNPs)for mRNA delivery through Molecular Dynamics simulation
Helmke	Predicting Drug-Induced Cholestasis with Enriched Biological Fingerprints
Aletayeb	Decoding RNA-protein Interaction Fingerprint by Molecular Dynamics Simulation, Binding Free Energy Calculation and Machine Learning Approach
Pacak	First steps in Sperm-Egg adhesion: Molecular Dynamics of JUNO-IZUMO1 complexation
Libouban	Exploring New Frontiers in Protein-Ligand Binding Affinity Prediction: Deep Learning with Molecular Dynamics Data Augmentation and Spatio-Temporal Methods
Scio'	Novel FtsZ inhibitors identified by virtual screening and Adaptive Steered Molecular Dynamics
Scarin	Design of pharmacological chaperones for the treatment of tyrosinemia type 1
Pieraccini	Modelling of short synthetic antifreeze peptides: insights into ice-pinning mechanism
Temml	Elucidating the Mechanism behind 15-LOX Activation with Homology Modeling and Molecular Docking
da Silva	Synthesis of new marinoquinoline derivatives with potential antimalarial activity and determination of their molecular target
Chen	Active learning approach for guiding site-of-metabolism measurement and annotation

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POSTER FLASH PRESENTATIONS

Pecina	SQM2.20: universal physics-based scoring function for reliable protein-ligand affinity predictions	*Monday*
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Fellinger	Binding Affinity Estimation using X-GRADE	*Monday*
Chiesa	LIT-AlphaFold: a new tool for multistate modelling // Function-based virtual screening using machine learning and single ligand dynamic interaction data	*Monday*
Roggia	Innovation in Virtual Screening: PyRMD2Dock's AI-Infused Approach	*Monday*
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Libouban	Exploring New Frontiers in Protein-Ligand Binding Affinity Prediction: Deep Learning with Molecular Dynamics Data Augmentation and Spatio-Temporal Methods	*Monday*
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