23rd EuroQSAR

Confirmed Speakers

A. Award Lectures

Fujita Award Lecture 2022 (AL04)
Consulting the Experiment: Are our Currently Applied Computational Drug-Design Tools Comprehensive Enough

Prof. Gerhard KLEBE
(PHILIPPS-UNIVERSITY MARBURG, Marburg, Germany)

Fujita Award Lecture 2020 (AL02)
Set-Theoretic Analysis of Ligand-Target Datasets - An Intuitionistic Fuzzy Set Approach
Prof. Vogt will stand in for Prof. Maggiora, awardee of the Fujita Award 2020.

Prof. Gerald M. MAGGIORA
(UNIVERSITY OF ARIZONA, Tucson, United States)

Dr Martin VOGT
(UNIVERSITY OF BONN, Bonn, Germany)

Hansch Award Lecture 2020 (AL01)
Multi-scaling the CRISPR-Cas Revolution from Gene Editing to Viral Detection

Dr Giulia PALERMO
(UNIVERSITY OF CALIFORNIA RIVERSIDE, Riverside, United States)

Hansch Award Lecture 2022 (AL03)
Data-Driven Methods for Active Compound Design and Risk Assessment

Prof. Andrea VOLKAMER
(SAARLAND UNIVERSITY, Saarbrücken, Germany)

B. Plenary Lectures

Visualizing Data at Scale: Complex Science, Unruly Users, and the Vitruvian Triad (PL01)

Dr Dimitris AGRAFIOTIS
(PFIZER, Philadelphia, United States)

Mesoscale Simulations Reveal Unseen Vulnerabilities of Viral Glycoproteins (PL06)

Prof. Rommie AMARO
(UNIVERSITY OF CALIFORNIA, San Diego, United States)

Enhanced Sampling Atomistic Simulations for The Estimation of Drug Binding Kinetics (PL11)

Confirmed Speakers

Prof. Paolo CARLONI
(FORSCHUNGSZENTRUM JÜLICH, Jülich, Germany)

Towards Machine Learning-Driven Drug Development (PL09)

Prof. Olivier ELEMENTO
(CORNELL UNIVERSITY, New York, United States)

Efficient Computational Strategies for Increasingly Accurate Representations of Metastable Conformational States of G Protein-Coupled Receptors and their Kinetic Relations (PL04)

Prof. Marta FILIZOLA
(ICAHN SCHOOL OF MEDICINE AT MOUNT SINAI, New York, United States)

Promiscuity of Ligand Binding: From Off-target Prediction to Fragment-based Design (PL08)

Prof. Oliver KOCH
(UNIVERSITY OF MÜNSTER, Münster, Germany)

Can Humans Learn from Machine Learning in Drug Discovery? (PL12)

Prof. Tudor I. OPREA
(ROIVANT SCIENCES INC., San Diego, CA, United States)

Cheminformatics for Next Generation Make-on-Demand Compound Catalogs (PL02)

Prof. Matthias REAREY
(UNIVERSITY OF HAMBOURG, Hamburg, Germany)

Insights into the Passive Membrane Permeation Process of Cyclic Peptides (PL07)

Prof. Sereina RINIKER
(ETH ZÜRICH, Zurich, Switzerland)

Enhancing Confidence in Computational Methods for the Evaluation of Drug Safety (PL05)

Dr Alessandra RONCAGLIONI
(MARIO NEGRI INSTITUTE FOR PHARMACOLOGICAL RESEARCH, Milano, Italy)

Combining Multi-Omics and Network Knowledge to Study Diseases and Therapies (PL03)

Prof. Julio SAEZ-RODRIGUEZ
(HEIDELBERG UNIVERSITY, Heidelberg, Germany)

Exploring Alchemical Binding Free Energy Calculations in Drug Discovery (PL10)

Confirmed Speakers

Dr Gary TRESADERN
(JANSSEN, Beerse, Belgium)

C. Session Lectures

Deep Docking - Deep Learning Based QSAR Approach for Augmenting Structure-Based Drug Discovery (SL01)

Prof. Artem CHERKASOV
(UNIVERSITY OF BC, VANCOUVER PROSTATE CENTRE, Vancouver, Canada)

40 years of Molecular Interaction Fields (SL06)

Prof. Gabriele CRUCIANI
(UNIVERSITY OF PERUGIA, Perugia, Italy)

Structure-Activity Relationships from Drug-Receptor Complexes Using the Comparative Binding Energy (Combine) Method (SL05)

Prof. Federico GAGO
(UNIVERSITY OF ALCALA, Alcala de Henares, Spain)

Quantifying GPCR Signaling in an Oligomeric Context (SL07)

Dr Jesús GIRALDO
(AUTONOMOUS UNIVERSITY OF BARCELONA, Bellaterra, Spain)

Neural Networks Learning Computational Chemistry (SL16)

Dr Olexandr ISAYEV
(CARNEGIE MELLON UNIVERSITY, Pittsburgh, United States)

The Challenges Associated with Building Accurate Predictive Cytochrome P450 Inhibition Models Using Machine Learning Approaches (SL13)

Dr Petrina KAMYA
(INSILICO MEDICINE, Hong Kong, Hong Kong)

Integrating Toxicity and Metabolism Prediction (SL02)

Prof. Johannes KIRCHMAIR
(UNIVERSITY OF VIENNA, Vienna, Austria)

Assessing the Suitability of 3D QM-Derived Atomic Hydrophobicity Patterns for Ligand-Target Interactions (SL12)

Confirmed Speakers

Prof. F. Javier LUQUE
(UNIVERSITY OF BARCELONA, Barcelona, Spain)

Opportunities and Challenges in GPCR SBDD: Finding the Sweet Spots (SL08)

Dr Pierre MATRICON
(SOSEI HEPTARES, Cambridge, United Kingdom)

Translational Safety Meets Pharmacovigilance (SL10)

Prof. Jordi MESTRES
(IMIM HOSPITAL DEL MAR MEDICAL RESEARCH INSTITUTE, Girona, Spain)

(SANOFI-AVENTIS DEUTSCHLAND GMBH)

Machine Learning for Early Toxicity Detection at Bayer (SL09)

Dr Floriane MONTANARI
(BAYER AG, Berlin, Germany)

Covalent Reversible Inhibition of Rhodesain; A Key Player in African Sleeping Sickness (SL14)

Prof. Tanja SCHIRMEISTER
(UNIVERSITY OF MAINZ, Mainz, Germany)

Chemography Concept in Chemical Space Analysis (SL03)

Prof. Alexandre VARNEK
(UNIVERSITY OF STRASBOURG, Strasbourg, France)

Contextualizing Ligand-Transporter Interactions with Data-Driven Approaches (SL11)

Dr Barbara ZDRAZIL
(EMBL-EBI, Hinxton, United Kingdom)

Disentangling Host and Microbiome Contributions to Drug Pharmacokinetics and Toxicity (SL04)

Dr Maria ZIMMERMANN
(EMBL, Heidelberg, Germany)

D. Oral Communications

QRNN: Transferable Neural Network for Potential Energy Surfaces of Closed-Shell Organic Molecules Including Ions (OC09)

Confirmed Speakers

Dr Stephan EHRLICH
(SCHRÖDINGER GMBH, Mannheim, Germany)

Derivation of Molecular Substructures Enhancing Drug Activity in Gram-Negative Bacteria (OC05)

Mr Dominik GURVIC
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

In Silico Design of Tubulin Activity Modulators (OC08)

Dr Dragos HORVATH
(CNRS , Strasbourg, France)

Multi-Target QSAR Modeling for the Identification of Novel Inhibitors Against Alzheimer's Disease (OC02)

Mr Vinay KUMAR
(JADAVPUR UNIVERSITY, Kolkata, India)

Free Energy Predictions Using Deep Learning in Combination with Targeted Free Energy Perturbations (OC03)

Ms Soo Jung LEE
(UNIVERSITY OF BASEL, Basel, Switzerland)

The Use of Deep Neural Networks on Molecular Dynamics Simulations for the Prediction of Binding Affinities (OC06)

Mr Pierre-Yves LIBOUBAN
(INSTITUTE OF ORGANIC AND ANALYTICAL CHEMISTRY, Orléans, France)

Multiscale Molecular Dynamics: An Efficient Tool for Assessing the Affinity and Specificity of Covalent Inhibitors (OC10)

Dr Levente Márk MIHALOVITS
(RESEARCH CENTRE FOR NATURAL SCIENCES, Budapest, Hungary)

What Defines the Length of Drug-Target Residence Time of a Small-Molecule Inhibitor: Insights from Molecular Dynamics Simulations (OC04)

Dr Tatu PANTSAR
(UNIVERSITY OF EASTERN FINLAND, Kuopio, Finland)

3D Pride Without 2D Prejudice: Bias-Controlled Multi-Level Generative Models for Structure-Based Ligand Design (OC01)

Confirmed Speakers

Dr Carl POELKING
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

Fragment-Based and Pocket-Focused Library Design by Protein-Applied Computer Vision and Deep Generative Linking (OC07)

Dr Didier ROGNAN
(CNRS, Illkirch, France)

Privacy-Preserving Federated Learning at Unprecedented Scale Boosts Predictive Performance of Structure-Activity Modelling in Drug Discovery (OC11)

Dr Noé STURM
(NOVARTIS, Huningue, France)

Dr Wouter HEYNDRICKX
(JANSSEN PHARMACEUTICALS, Beerse, Belgium)

Dr Tobias MORAWIETZ
(BAYER AG, Wuppertal, Germany)

Dr Lewis MERVIN
(ASTRAZENECA, Cambridge, United Kingdom)