23rd EuroQSAR

Programme

Monday September 26, 2022

14:30 **Registration**

15:00 **Schrödinger workshop: "QSAR Expert in a Box: Automated Machine Learning for ADMET properties"**

Dr Anna BOCHICCHIO (SCHRÖDINGER GMBH, München, Germany)
Dr Stephan EHRLICH (SCHRÖDINGER GMBH, Mannheim, Germany)

16:30 **Opening Ceremony**

Prof. Rebecca WADE
(HEIDELBERG UNIVERSITY AND HITS, Heidelberg, Germany)

Award Lectures 2020

Session Chair

Prof. Andrea CAVALLI (UNIVERSITY OF BOLOGNA AND IIT, Bologna, Italy)
Prof. Tudor I. OPREA (ROIVANT SCIENCES INC., San Diego, CA, United States)

16:45 **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)

17:30 **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)

18:15 **Welcome drink**

Programme

Tuesday September 27, 2022

08:00 **Registration**

Session 1 - QSAR Without Borders

09:00 **Session Chair**
Prof. Alexander TROPSHA
(UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)

09:05 **Visualizing Data at Scale: Complex Science, Unruly Users, and the Vitruvian Triad (PL01)**
Dr Dimitris AGRAFIOTIS
(PFIZER, Philadelphia, United States)

09:45 **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)

10:15 **3D Pride Without 2D Prejudice: Bias-Controlled Multi-Level Generative Models for Structure-Based Ligand Design (OC01)**
Dr Carl POELKING
(ASTEX PHARMACEUTICALS, Cambridge, United Kingdom)

10:35 **Coffee break**

Session 2 - Chemical Space Annotation and Expansion

11:05 **Session Chair**
Prof. Andrew R. LEACH
(EMBL-EBI, Hinxton, United Kingdom)

11:10 **Cheminformatics for Next Generation Make-on-Demand Compound Catalogs (PL02)**
Prof. Matthias REREY
(UNIVERSITY OF HAMBOURG, Hamburg, Germany)

11:50 **Integrating Toxicity and Metabolism Prediction (SL02)**
Prof. Johannes KIRCHMAIR
(UNIVERSITY OF VIENNA, Vienna, Austria)

12:20 **Chemography Concept in Chemical Space Analysis (SL03)**
Prof. Alexandre VARNEK
(UNIVERSITY OF STRASBOURG, Strasbourg, France)

12:50 **Lunch, Exhibition & Posters**

13:00 **WuXi AppTec workshop : "Introduction to Self-Service DNA-Encoded libraries (DELs)"**
Dr Alex SATZ
(WUXI APPTEC, Basel, Switzerland)

Session 3 - Network Medicine

Programme

14:20 **Session Chair**

Prof. Rob RUSSELL
(HEIDELBERG UNIVERSITY, Heidelberg, Germany)

14:25 **Combining Multi-Omics and Network Knowledge to Study Diseases and Therapies (PL03)**

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

15:05 **Disentangling Host and Microbiome Contributions to Drug Pharmacokinetics and Toxicity (SL04)**

Dr Maria ZIMMERMANN
(EMBL, Heidelberg, Germany)

15:35 **Multi-Target QSAR Modeling for the Identification of Novel Inhibitors Against Alzheimer's Disease (OC02)**

Mr Vinay KUMAR
(JADAVPUR UNIVERSITY, Kolkata, India)

15:55 **Coffee Break**

Session 4 - In Memoriam - Peter Goodford

16:25 **Session Chair**

Prof. Rebecca WADE
(HEIDELBERG UNIVERSITY AND HITS, Heidelberg, Germany)

16:30 **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)

17:00 **40 years of Molecular Interaction Fields (SL06)**

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

17:30 **Meeting in courtyard for group picture**

17:40 **Poster Session 1 - odd numbers**

Programme

Wednesday September 28, 2022

Session 5 - Challenges in GPCR Drug Design

09:00 **Session Chair**
Prof. Federico GAGO
(UNIVERSITY OF ALCALA, Alcala de Henares, Spain)

09:05 **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)

09:45 **Quantifying GPCR Signaling in an Oligomeric Context (SL07)**
Dr Jesús GIRALDO
(AUTONOMOUS UNIVERSITY OF BARCELONA, Bellaterra, Spain)

10:15 **Opportunities and Challenges in GPCR SBDD: Finding the Sweet Spots (SL08)**
Dr Pierre MATRICON
(SOSEI HEPTARES, Cambridge, United Kingdom)

10:45 **Coffee break**

Session 6 - Modelling Drug Safety

11:15 **Session Chair**
Prof. Klaus-Jürgen SCHLEIFER
(BASF, Ludwigshafen, Germany)

11:20 **Enhancing Confidence in Computational Methods for the Evaluation of Drug Safety (PL05)**
Dr Alessandra RONCAGLIONI
(MARIO NEGRI INSTITUTE FOR PHARMACOLOGICAL RESEARCH, Milano, Italy)

12:00 **Machine Learning for Early Toxicity Detection at Bayer (SL09)**
Dr Floriane MONTANARI
(BAYER AG, Berlin, Germany)

12:30 **Translational Safety Meets Pharmacovigilance (SL10)**
Prof. Jordi MESTRES (IMIM HOSPITAL DEL MAR MEDICAL RESEARCH INSTITUTE, Girona, Spain)
(SANOFI-AVENTIS DEUTSCHLAND GMBH)

13:00 **Lunch, Exhibition & Posters**

13:15 **Workshop: "Orienting your career compass" (1h)**
Organisers: Giulia Paiardi and Giulia D'Arrigo (HITS, Heidelberg)
Prof. Andrew R. LEACH (EMBL-EBI, Hinxton, United Kingdom)
Dr Friedrich RIPPMANN (MERCK HEALTHCARE KGAA, Darmstadt, Germany)

Session 7 - Molecular Dynamics and Kinetics

14:30 **Session Chair**

Programme

Prof. Andrea CAVALLI
(UNIVERSITY OF BOLOGNA AND IIT, Bologna, Italy)

14:35 **Mesoscale Simulations Reveal Unseen Vulnerabilities of Viral Glycoproteins (PL06)**
Prof. Rommie AMARO
(UNIVERSITY OF CALIFORNIA, San Diego, United States)

15:15 **Free Energy Predictions Using Deep Learning in Combination with Targeted Free Energy Perturbations (OC03)**
Ms Soo Jung LEE
(UNIVERSITY OF BASEL, Basel, Switzerland)

15:35 **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)

15:55 **Coffee break**

Session 8 - Modelling Drug Transport Mechanisms

16:25 **Session Chair**
Dr Ulrike UHRIG
(EMBL, Heidelberg, Germany)

16:30 **Insights into the Passive Membrane Permeation Process of Cyclic Peptides (PL07)**
Prof. Sereina RINIKER
(ETH ZÜRICH, Zurich, Switzerland)

17:10 **Contextualizing Ligand-Transporter Interactions with Data-Driven Approaches (SL11)**
Dr Barbara ZDRAZIL
(EMBL-EBI, Hinxton, United Kingdom)

17:40 **Derivation of Molecular Substructures Enhancing Drug Activity in Gram-Negative Bacteria (OC05)**
Mr Dominik GURVIC
(UNIVERSITY OF DUNDEE, Dundee, United Kingdom)

18:00 **Poster Session 2 - even numbers**

Programme

Thursday September 29, 2022

Session 9 - Predicting Off-Target Pharmacology

09:00 **Session Chair**
Prof. Fred HAMPRECHT
(HEIDELBERG UNIVERSITY, Heidelberg, Germany)

09:05 **Promiscuity of Ligand Binding: From Off-target Prediction to Fragment-based Design (PL08)**
Prof. Oliver KOCH
(UNIVERSITY OF MÜNSTER, Münster, Germany)

09:45 **Assessing the Suitability of 3D QM-Derived Atomic Hydrophobicity Patterns for Ligand-Target Interactions (SL12)**
Prof. F. Javier LUQUE
(UNIVERSITY OF BARCELONA, Barcelona, Spain)

10:15 **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)

10:35 **Coffee break**

Session 10 - Artificial Intelligence in Drug Discovery

11:05 **Session Chair**
Prof. Tudor I. OPREA
(ROIVANT SCIENCES INC., San Diego, CA, United States)

11:10 **Towards Machine Learning-Driven Drug Development (PL09)**
Prof. Olivier ELEMENTO
(CORNELL UNIVERSITY, New York, United States)

11:50 **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)

12:20 **Fragment-Based and Pocket-Focused Library Design by Protein-Applied Computer Vision and Deep Generative Linking (OC07)**
Dr Didier ROGNAN
(CNRS, Illkirch, France)

12:40 **Lunch & Exhibition**

13:05 **QCMS General Meeting (Open to all attendees)**

Session 11 - New Modes of Target Interaction

Programme

14:10 **Session Chair**

Prof. Christian KLEIN
(HEIDELBERG UNIVERSITY, Heidelberg, Germany)

14:15 **Exploring Alchemical Binding Free Energy Calculations in Drug Discovery (PL10)**

Dr Gary TRESADERN
(JANSSEN, Beerse, Belgium)

14:55 **Covalent Reversible Inhibition of Rhodesain; A Key Player in African Sleeping Sickness (SL14)**

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

15:25 **In Silico Design of Tubulin Activity Modulators (OC08)**

Dr Dragos HORVATH
(CNRS , Strasbourg, France)

15:45 **Coffee break**

Session 12 - New Trends in Quantum Mechanics

16:15 **Session Chair**

Prof. Frauke GRÄTER
(HEIDELBERG UNIVERSITY & HITS, Heidelberg, Germany)

16:20 **Enhanced Sampling Atomistic Simulations for The Estimation of Drug Binding Kinetics (PL11)**

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

17:00 **QRNN: Transferable Neural Network for Potential Energy Surfaces of Closed-Shell Organic Molecules Including Ions (OC09)**

Dr Stephan EHRLICH
(SCHRÖDINGER GMBH, Mannheim, Germany)

17:20 **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)

17:45 **Erasmus public seminar: An Intuitive Drug Design Suite of Web Applications for Ligand-Based and Structure-Based Studies – Part 1 (1h15)**

Prof. Rino RAGNO
(SAPIENZA ROME UNIVERSITY, Roma, Italy)

20:00 **Symposium Banquet**

Programme

Friday September 30, 2022

Session 13 - The Challenges Ahead

09:00 **Session Chair**
Dr Friedrich RIPPMANN
(MERCK HEALTHCARE KGAA, Darmstadt, Germany)

09:05 **Can Humans Learn from Machine Learning in Drug Discovery? (PL12)**
Prof. Tudor I. OPREA
(ROIVANT SCIENCES INC., San Diego, CA, United States)

09:45 **Neural Networks Learning Computational Chemistry (SL16)**
Dr Olexandr ISAYEV
(CARNEGIE MELLON UNIVERSITY, Pittsburgh, United States)

10:15 **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)

10:35 **Coffee break**

Session 14 - Award Lectures 2022

11:05 **Session Chair**
Prof. Andrea CAVALLI (UNIVERSITY OF BOLOGNA AND IIT, Bologna, Italy)
Prof. Tudor I. OPREA (ROIVANT SCIENCES INC., San Diego, CA, United States)

11:10 **Hansch Award Lecture 2022 (AL03)**
Data-Driven Methods for Active Compound Design and Risk Assessment
Prof. Andrea VOLKAMER
(SAARLAND UNIVERSITY, Saarbrücken, Germany)

11:55 **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)

12:40 **Closing Ceremony**
Prof. Rebecca WADE (HEIDELBERG UNIVERSITY AND HITS, Heidelberg, Germany)
Prof. Jordi MESTRES (IMIM HOSPITAL DEL MAR MEDICAL RESEARCH INSTITUTE, Girona, Spain)

13:00 **Erasmus public seminar: An Intuitive Drug Design Suite of Web Applications for Ligand-Based and Structure-Based Studies – Part 2 (1h)**
Prof. Rino RAGNO
(SAPIENZA ROME UNIVERSITY, Roma, Italy)