20th EuroQSAR

Confirmed Speakers

Keynote Lectures

From QSAR to MQSPR and Beyond: Predictive Materials Informatics Using a Blend of Heuristic and Physics-Based Methods

Prof. Curt BRENEMAN
(RENSSELAER EXPLORATORY CENTER FOR CHEMINFORMATICS RESEARCH, Troy, United States)

Integrating Pharmacometrics into Drug Development

Dr Roberta BURSI
(GRÜNENTHAL, Aachen, Germany)

Lead Discovery and Optimisation by Use of Interaction Kinetic Analysis

Prof. Helena DANIELSON
(UPPSALA UNIVERSITY, Uppsala, Sweden)

Open PHACTS

Prof. Gerhard ECKER
(UNIVERSITY OF VIENNA, Vienna, Austria)

Navigation in Chemical Space Towards Biological Activity

Dr Peter ERTL
(NOVARTIS INSTITUTE FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

Opening Lecture - SAR, the Lifelong Learning for my Career

Prof. Toshio FUJITA
(KYOTO UNIVERSITY, Kyoto, Japan)

Computational Toxicology – An Essential Part of Drug Safety

Dr Catrin HASSELGREN
(ASTRAZENECA, Mölndal, Sweden)

Chemical Informatics Applied to Health and Drug Safety

Dr John OVERINGTON
(EMBL-EBI, Cambridgeshire, United Kingdom)

Ensemble-Based Drug Design, Combining Protein Structures and Simulations

Dr Will PITT
(UCB PHARMA, Slough, United Kingdom)

Confirmed Speakers

Closing Lecture - Opportunities and Challenges in Therapeutics Discovery and Development

Dr John C. REED
(F. HOFFMAN-LA-ROCHE, Basel, Switzerland)

eTOX: Integrative Strategies for Predicting Drug Toxicities

Prof. Ferran SANZ
(UNIVERSITY POMPEU FABRA, Barcelona, Spain)

Large-Scale Chemogenomics in Pharma - Definition, Benchmarking, and Application

Dr Joerg Kurt WEGNER
(JOHNSON & JOHNSON, Beerse, Belgium)

Hansch Session

On the Nature of Non-Classical Hydrogen Bonds and Aromatic Interactions

Prof. Anna LINUSSON
(UMEA UNIVERSITY, Umea, Sweden)

The Road Ahead: New Challenges for Computational Forecasts

Prof. Tudor I. OPREA
(UNIVERSITY OF NEW MEXICO, Albuquerque, United States)

Molecular Design of Bivalent and Dual Action Drugs

Prof. Nikolay S. ZEFIROV
(MOSCOW STATE UNIVERSITY, Moscow, Russia)

Oral Communications

QSPR Modeling of Chemical And Physical Stability of Pharmaceuticals

Dr Yuriy ABRAMOV
(PFIZER, Groton, United States)

Identification of Mechanism of Action of DNA-Topoisomerase II Inhibitors By Molecular Modeling Studies

Prof. Esin AKI-YALCIN
(ANKARA UNIVERSITY, Ankara, Turkey)

Importance of Conformations in Ligand-Based Drug Discovery Approaches

Dr Daniel CAPPEL
(SCHRÖDINGER, Mannheim, Germany)

Structural Sensitivity Analysis Using Matched Molecular Pairs

Dr Robert D. CLARK
(SIMULATIONS PLUS, INC, Lancaster, United States)

Applications of Proteochemometrics – From Species Extrapolation to Cell Line Sensitivity Modelling

Mr Isidro CORTES
(INSTITUT PASTEUR, Paris, France)

Confirmed Speakers

Might Template COMFA Integrate Structure-Based and Ligand-Based Design?

Dr Richard CRAMER
(TRIPOS, Santa Fe, United States)

Cross-Mining in 3D-2D-1D, the PDB, Chemical Libraries and Structure Activities to Extract Shared Modes of Binding for PDB Ligand Substructures

Mr François DELFAUD
(MEDIT, Palaiseau, France)

Novel Method for Multi Target Selective Pharmacophore Design Using Complementary Interaction Field at the Active Sites of Acid Proteases, in Search of Anti Malarial

Prof. INDIRA GHOSH
(SCIS, JNU, New Delhi, India)

Predicting Dynamically Dominated Allostery from Constraint Network Analysis

Prof. Holger GOHLKE
(HEINRICH HEINE UNIVERSITY DÜSSELDORF, Düsseldorf, Germany)

Protein Active Site Comparison with Sitehopper: Phylogeny to Polypharmacology

Dr Paul HAWKINS
(OPENEYE SCIENTIFIC SOFTWARE, Santa Fe, United States)

“Walking Toxic Pathways” - Changes in Gene Regulation Circuits Predict Human Toxicity of Chemical Compounds after Repeated Dose Inhalation Exposure

Dr Alexander KEL
(GENEXPLAIN GMBH, Wolfenbuettel, Germany)

Cosmo Sigma-Surfaces and Local Sigma-Profiles as Extremely Robust Descriptors for Alignment, 3D-Similarity and 3D-QSAR

Prof. Andreas KLAMT
(COSMOLOGIC, Leverkusen, Germany)

A Strategy Towards Ligand-Protein Association via Computational Chemogenomics

Dr Maria KONTOYIANNI
(SOUTHERN ILLINOIS UNIVERSITY EDWARDSVILLE, Edwardsville - Illinois, United States)

Chemical Systems Biology Identification of Drug Targets Related with Cardiovascular Adverse Effects

Dr Alexey LAGUNIN
(V.N.OREKHOVICH INSTITUTE OF BIOMEDICAL CHEMISTRY OF RUSSIAN ACADEMY OF MEDICAL SCIENCES, Moscow, Russia)

Ligand Promiscuity and Conformational Specificity in the Aryl Hydrocarbon Receptor (AHR): The Case of L-Tryptophan Metabolites

Dr. Antonio MACCHIARULO
(UNIVERSITY OF PERUGIA, Perugia, Italy)

Semi-quantitative SAR Using Bayesian Modelling on Activity Cliffs

Dr Mark MACKEY
(CRESSET BIOMOLECULAR DISCOVERY LIMITED, Cambridgeshire, United Kingdom)

QDB: From Static to Dynamic Nature of Published QSAR-S

Dr Uko MARAN
(UNIVERSITY OF TARTU, Tartu, Estonia)

Recent Trends in QSAR Modeling of Chemical Mixtures

Dr Eugene MURATOV
(UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)

Confirmed Speakers

Conformational Energies of Small-Molecule Ligands in Protein-Ligand Complexes: A Quantum-Chemical Analysis of PDB Structures

Dr Marc NICKLAUS
(NATIONAL CANCER INSTITUTE, Frederick, United States)

Molecular Field Topology Analysis (MFTA) as a Tool For Multi-Target QSAR

Dr Vladimir A. PALYULIN
(M.V.LOMONOSOV MOSCOW STATE UNIVERSITY, Moscow, Russia)

Structural and Functional Interpretation of QSAR Models

Dr Pavel POLISHCHUK
(A.V. BOGATSKY PHYSICO-CHEMICAL INSTITUTE, Odessa, Ukraine)

In Silico Prediction of Aqueous Solubility, from Random Global Model Forward Individual Local Regression for Each Chemical of Interest

Mr Oleg RAEVSKY
(INSTITUTE OF PHYSIOLOGICALLY ACTIVE COMPOUDS, Moscow, Russia)

Nanoparticles Properties Prediction: Physico-Chemical, Toxicological and Pharmacological Assessment

Dr Bakhtiyor RASULEV
(JACKSON STATE UNIVERSITY, Jackson, United States)

Interactive Visualization of Large Databases In 2D And 3D Using the Chemical Space Mapplet and Its Application to Drug Discovery

Prof. Jean-Louis REYMOND
(UNIVERSITY OF BERN, Bern, Switzerland)

The Impact of Large-Scale Genetic Data on Drug Targets

Dr Josef SCHEIBER
(BIOVARIANCE GMBH, Munich, Germany)

Material-Informatics: Chemoinformatics and Combinatorial Material Science for the Design of Novel Photovoltaic Cells

Prof. Hanoch SENDEROWITZ
(BAR-ILAN UNIVERSITY, Ramat Gan, Israel)

Large-Scale SAR-Mining and Visualization in Pharmaceutical Research

Dr VEER SHANMUGASUNDARAM
(PFIZER, Groton, CT, United States)

META-QSAR

Larisa SOLDATOVA

Surflex QMOD: Protein Pocket Modeling for Affinity Prediction

Dr Alexander STEUDLE
(CERTARA, München, Germany)

Active QSAR Modelling for Evironmental Toxicity Prediction of Chemical Substances

Prof. Yoshimasa TAKAHASHI
(TOYOHASHI UNIVERSITY OF TECHNOLOGY, Toyohashi, Japan)

Which Distance For Similarity/Diversity Analysis?

Prof. Roberto TODESCHINI
(UNIVERSITY OF MILANO-BICOCCA, Milano, Italy)

Alerting About Single Alerts: Bridging SAR and QSAR Approaches for Flagging or Avoiding Compounds with Undesired Toxicity Profiles

Confirmed Speakers

Prof. Alexander TROPSHA
(UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL, Chapel Hill, United States)

Chemical Data Visualization and Modeling: Big Data Challenge

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