20th EuroQSAR

Confirmed Speakers

Keynote Lectures

Hansch Awardee: Lessons Learned from Chemical and Biological Data - Scientifically, and Personally

Prof. Andreas BENDER
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

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 - The Use of Open Data for in silico Models

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 - (Q)SAR, the Lifelong Learning for my Research Career

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

Computational Toxicology – An Essential Part of Drug Safety

Dr Catrin HASSELGREN
(UNIVERSITY OF NEW MEXICO, Albuquerque, United States)

Chemical Informatics Applied to Health and Drug Safety

Confirmed Speakers

Dr John OVERINGTON
(THE EUROPEAN BIOINFORMATICS INSTITUTE, London, United Kingdom)

Ensemble-Based Drug Design, Combining Protein Structures and Simulations

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

EU's Framework Programme for Research and Innovation Horizon 2020: Cooperation Opportunities (tentative)

Mrs Maria PUTSELEVA
(DELEGATION OF THE EUROPEAN UNION TO RUSSIA, Russia)

Opportunities and Challenges in Therapeutics Discovery and Development

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

eTOX: Integrative Strategies for Predicting Drug Toxicities

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

Closing Lecture - 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)

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

Confirmed Speakers

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

Molecular Design of Bivalent and Dual Action Drugs

Prof. Nikolay S. ZEFIROV
(INSTITUTE OF PHYSIOLOGICALLY ACTIVE COMPOUNDS, 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

Dr Isidro CORTES
(INSTITUT PASTEUR, Paris, France)

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)

EU-Openscreen? A Pan-European Resource and Infrastructure to Support chemical Biology Research

Dr Ronald FRANK
(FMP, Berlin, Germany)

When is Software Accepted by Medicinal Chemists? SEESAR: a Lead Optimization Example

Dr Marcus GASTREICH
(BIOSOLVEIT, St. Augustin, Germany)

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

Confirmed Speakers

Prof. INDIRA GHOSH
(SCIS, JNU, Kolkata, 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)

Performance Evaluation of Common Virtual Screening Tools on Selected Representatives of Different Target Classes

Mrs Teresa KASERER
(UNIVERSITY OF INNSBRUCK, Innsbruck, Austria)

“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)

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

Dr Alexey LAGUNIN
(INSTITUTE OF BIOMEDICAL CHEMISTRY, Moscow, Russia)

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

Prof. 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)

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

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

Structural and Functional Interpretation of QSAR Models

Dr Pavel POLISHCHUK
(A.V. BOGATSKY PHYSICO-CHEMICAL INSTITUTE, Olomouc, Czech Republic)

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

Prof. Jean-Louis REYMOND
(SCS DMCCB & 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

Dr Larisa SOLDATOVA
(BRUNEL UNIVERSITY OF LONDON, Uxbridge, United Kingdom)

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

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

Chemical Data Visualization and Modeling: Big Data Challenge

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