

## Confirmed Speakers

### Keynote Lectures

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



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

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



Prof. Curt BRENNEMAN  
(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, South San Francisco, CA, United States)

#### Chemical Informatics Applied to Health and Drug Safety

## Confirmed Speakers



Dr John OVERINGTON  
(THE EUROPEAN BIOINFORMATICS INSTITUTE, Oxford , 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, San Diego, CA, 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 COMPOUNDS, 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**

## Confirmed Speakers



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 Environmental 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)