19th EuroQSAR

Confirmed Speakers

Inaugural Lecture

Inaugural Lecture: Myths and Fallacies about Exploring Chemical Space: SAR is the Medicinal Chemist's Retrospective Tool in Ligand Design

Christopher A. LIPINSKI
(MELIOR DISCOVERY, Waterford, United States)

Keynote Lectures

Pharmacophore Modeling in Early Drug Discovery

Karl-Heinz BARINGHAUS
(SANOFI, Frankfurt, Germany)

Closing Lecture - Is it Just Me or Did the Haystack Grow? Molecular Design in a Time of Data Abundance.

Niklas BLOMBERG
(ASTRAZENECA, Cambridgeshire, United Kingdom)

Open Innovation Applied to Agrochemical Discovery

Mark FORSTER
(SYNGENTA, Bracknell, United Kingdom)

How Valid are Popular Assumptions Applied in Computational Drug Design

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

Mining in Corporate Databases: What Can We Learn from our Historical Data

Jan M. KRIEGL
(BOEHRINGER-INGELHEIM, Biberach, Germany)

QSAR: Past Achievements, Present Problems and Future Directions

David LIVINGSTONE
(CHEMQUEST, Isle of Wight, United Kingdom)

New trends and Perspectives in QSAR Modelling

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

Fluorine Local Environment: From Screening to Drug Design

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Anna VULPETTI
(NOVARTIS, Basel, Switzerland)

Hansch Awardee - "My Struggle with Binding Data"

Renxiao WANG
(SHANGHAI INSTITUTE OF ORGANIC CHEMISTRY, Shanghai, China)

Why the Knowledge Required for Ligand Design of Transmembrane Protein Targets Goes Well Beyond the Binding Site

Harel WEINSTEIN
(CORNELL UNIVERSITY, New York, United States)

Hansch Session: "Grand Challenges for QSAR"

The Impact of QSAR on Medicinal Chemistry

Hugo KUBINYI
(UNIVERSITY OF HEIDELBERG, Weisenheim am Sand, Germany)

Activity cliffs, Information Theory, and QSAR

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

QSAR without Borders

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

Data Matters. The Discovery of New Knowledge

Wendy WARR
(WENDY WARR & ASSOCIATES, Cheshire, United Kingdom)

Oral Communications

OC02 - Receptor-Ligand Pharmacophores: A Novel Structure-Based Screening Weapon for Ligand Profiling and Discovery of Protein-Protein Interface Inhibitors

OC06 - Discovery of Ligands for ADP-Ribosyltransferases via Docking-Based Virtual Screening

David ANDERSSON
(UMEA UNIVERSITY, Umea, Sweden)

OC20 - The Power of Matched Pairs in Drug Design

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Jonas BOSTRÖM
(ASTRAZENECA, Mölndal, Sweden)

OC07 - MD Simulations and Conformational Sampling of Monomeric and Dimeric GPCRS

Agostino BRUNO
(UNIVERSITY OF PARMA, Parma, Italy)

OC08 - Community Structure-Activity Resource (CSAR) Benchmark Exercise 2011: Docking And Relative Ranking of a Blinded Congeneric Series of Compounds

Heather CARLSON
(UNIVERSITY OF MICHIGAN, Ann Arbor - Michigan, United States)

OC19 - Diverse Valid 3D-QSAR Models of Off-target Risks from Template CoMFA

Richard CRAMER
(TRIPOS, Santa Fe, United States)

OC11 - Efficient in Silico Scaffold Hopping for Lead Finding Considering Robust Chemical Reactions and Available Reagents

Andreas EVERS
(SANOFI-AVENTIS, Frankfurt am Main, Germany)

OC24 - Open Access Web-Services for Predicting Biological Activity

Dmitry FILIMONOV
(INSTITUTE OF BIOMEDICAL CHEMISTRY OF RAMS, Moscow, Russia)

OC10 - Recore ROX U.

Marcus GASTREICH
(BIOSOLVEIT, St. Augustin, Germany)

OC15 - In Defense of Cross-Validation

Martin GÜTLEIN
(ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG, Freiburg, Germany)

OC28 - Open Drug Discovery Intelligence: Open Phacts and SciBite

Lee HARLAND
(CONNECTED DISCOVERY, London, United Kingdom)

OC12 - The Fast and the Precious: Reaction Driven de Novo Design in the Chemical Space of Synthetically Accessible Compounds

Markus HARTENFELLER
(NOVARTIS PHARMA AG, Basel, Switzerland)

OC14 - Positive False Discovery Rate: A New Deal" for Shape Searching?"

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

OC05 - Consistent Handling of Flexible Interaction Sites for Efficient Structure-Based Virtual Screening

Angela HENZLER
(CENTER FOR BIOINFORMATICS, UNIVERSITY OF HAMBURG, Hamburg, Germany)

OC03 - Desigining Better Compounds Faster: the Tale of Discovering a Novel Class of CENP-E Inhibitors Using Structure-Guided Pharmacophore Methods in Combination With a New Visualization Tool

Confirmed Speakers

Mehran JALAIE
(PFIZER, San Diego, United States)

OC13 - Designing MHC-I Stabilizing Peptides by Multi-Model Cascaded Machine-Learning

Christian KOCH
(ETH ZÜRICH, Zürich, Switzerland)

OC18 - An Integrated Computational Strategy to Probe Ligand Promiscuity in the Human Cytochrome 3A4

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

OC25 - Using Public Data for Statistical Scoring Functions

Christian KRAMER
(NOVARTIS, Basel, Switzerland)

OC21 - A Chemogenomic Analysis of Ionization Constants

David T MANALLACK
(MONASH UNIVERSITY, Parkville, Australia)

OC17 - Towards in Silico Structure-Based Admet Prediction: Mechanistic Insights from Probing Small Molecule Binding to Metabolising Enzymes

Maria MITEVA
(INSERM, Paris, France)

OC23 - The Lilly Open Innovation Drug Discovery Program

Christos NICOLAOU
(ELI LILLY AND CO, Indianapolis, United States)

OC27 - Utopia Documents

Steve PETTIFER
(THE UNIVERSITY OF MANCHESTER, Manchester, United Kingdom)

OC16 - Structure-Based Design of Covalent Inhibitors: Reality or Wishful Thinking

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

OC26 - In Silico Prediction of the Target Space Relevant to Malaria

Andreas SPITZMÜLLER
(FUNDACIÓ INSTITUT MAR D'INVESTIGACIONS MÈDIQUES, Barcelona, Spain)

OC22 - Open Innovation at Openeye: A Decade of Practice

Bob TOLBERT
(OPENEYE SCIENTIFIC SOFTWARE, Santa Fee, United States)

OC09 - Generative Topographic Maps: Universal Tool for Data Visualization, Datasets Comparison and Structure-Activity Modeling

Alexandre VARNEK
(UNIVERSITY OF STRASBOURG, Strasbourg, France)

OC04 - Discovery of Novel Small Molecule Inhibitors of BRD4 Using a Structure-Based Virtual Screening Approach

Lewis VIDLER
(INSTITUTE OF CANCER RESEARCH, Sutton, United Kingdom)

OC01 - Improving 3D pharmacophore Perception and Virtual Screening by Increased Geometric Accuracy

Confirmed Speakers

Gerhard WOLBER
(FREIE UNIVERSITAET BERLIN, Berlin, Germany)