# 19th EuroQSAR

## Programme

### Sunday August 26, 2012

**14:00** **Registration**

**Session Chair**
Gerhard ECKER
(UNIVERSITY OF VIENNA, Vienna, Austria)

**17:00** **Opening Ceremony**

**17:30** **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)

**19:00** **Walking Dinner at the City Hall**

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## Programme

### Monday August 27, 2012

**Session 1 - Pharmacophore-based Screening and Design**

**Session Chair**
Thierry LANGER
(PRESTWICK CHEMICAL, Vienna, Austria)

**08:45** **Pharmacophore Modeling in Early Drug Discovery**
Karl-Heinz BARINGHAUS
(SANOFI, Frankfurt, Germany)

**09:30** **OC01 - Improving 3D pharmacophore Perception and Virtual Screening by Increased Geometric Accuracy**
Gerhard WOLBER
(FREIE UNIVERSITAET BERLIN, Berlin, Germany)

**09:50** **OC02 - Receptor-Ligand Pharmacophores: A Novel Structure-Based Screening Weapon for Ligand Profiling and Discovery of Protein-Protein Interface Inhibitors**

**10:10** **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**
Mehran JALAIE
(PFIZER, San Diego, United States)

**10:30** **Coffee Break**

**Session 2 - Molecular Docking - from Static to Dynamic Structures**

**Session Chair**
Gabriele COSTANTINO
(UNIVERSITY OF PARMA, Parma, Italy)

**11:15** **How Valid are Popular Assumptions Applied in Computational Drug Design**
Gerhard KLEBE
(PHILIPPS-UNIVERSITY MARBURG, Marburg, Germany)

**12:00** **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)

**12:20** **OC05 - Consistent Handling of Flexible Interaction Sites for Efficient Structure-Based Virtual Screening**
Angela HENZLER
(CENTER FOR BIOINFORMATICS, UNIVERSITY OF HAMBURG, Hamburg, Germany)

**12:40** **OC06 - Discovery of Ligands for ADP-Ribosyltransferases via Docking-Based Virtual Screening**
David ANDERSSON
(UMEA UNIVERSITY, Umea, Sweden)

**13:00** **Lunch and Poster Session**
**13:30: Accelrys Workshop - "Ligand Profiling Using Pharmacophores"**

## Programme

### Session 3 - Membrane Proteins - Structure, Dynamics and Integration of Ligand Information

**Session Chair**

Anna LINUSSON
(UMEA UNIVERSITY, Umea, Sweden)

**15:00** **OC07 - MD Simulations and Conformational Sampling of Monomeric and Dimeric GPCRS**

Agostino BRUNO
(UNIVERSITY OF PARMA, Parma, Italy)

**15:20** **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)

**15:40** **OC09 - Generative Topographic Maps: Universal Tool for Data Visualization, Datasets Comparison and Structure-Activity Modeling**

Alexandre VARNEK
(UNIVERSITY OF STRASBOURG, Strasbourg, France)

**16:00** **Coffee Break**

**16:45** **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)

## Programme

### Tuesday August 28, 2012

**Session 4 - Methods that will Rock you**

**Session Chair**
David LLOYD
(TRINITY COLLEGE DUBLIN, Dublin, Ireland)

**08:45** **Mining in Corporate Databases: What Can We Learn from our Historical Data**
Jan M. KRIEGL
(BOEHRINGER-INGELHEIM, Biberach, Germany)

**09:30** **OC10 - Recore ROX U.**
Marcus GASTREICH
(BIOSOLVEIT, St. Augustin, Germany)

**09:50** **OC11 - Efficient in Silico Scaffold Hopping for Lead Finding Considering Robust Chemical Reactions and Available Reagents**
Andreas EVERS
(SANOFI-AVENTIS, Frankfurt am Main, Germany)

**10:10** **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)

**10:30** **Coffee Break**

**Session 5 - From Patterns to Molecules - Translational Informatics and Machine Learning Techniques**

**Session Chair**
Gisbert SCHNEIDER
(ETH ZÜRICH, Zurich, Switzerland)

**11:15** **QSAR: Past Achievements, Present Problems and Future Directions**
David LIVINGSTONE
(CHEMQUEST, Isle of Wight, United Kingdom)

**12:00** **OC13 - Designing MHC-I Stabilizing Peptides by Multi-Model Cascaded Machine-Learning**
Christian KOCH
(ETH ZÜRICH, Zürich, Switzerland)

**12:20** **OC14 - Positive False Discovery Rate: A New Deal" for Shape Searching?"**
Paul HAWKINS
(OPENEYE SCIENTIFIC SOFTWARE, Santa Fe, United States)

**12:40** **OC15 - In Defense of Cross-Validation**
Martin GÜTLEIN
(ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG, Freiburg, Germany)

**13:00** **Lunch and Poster Session**
**13:30: BioSolveIT Workshop - "Visual Lead Optimisation"**

## Programme

### Session 6 - Proteins, Biologicals, Molecular Machines - Challenges and Prospects

**Session Chair**
Vladimir POROIKOV
(INSTITUTE OF BIOMEDICAL CHEMISTRY, Moscow, Russia)

**15:00** **OC16 - Structure-Based Design of Covalent Inhibitors: Reality or Wishful Thinking**
VEER SHANMUGASUNDARAM
(PFIZER, Groton, CT, United States)

**15:20** **OC17 - Towards in Silico Structure-Based Admet Prediction: Mechanistic Insights from Probing Small Molecule Binding to Metabolising Enzymes**
Maria MITEVA
(INSERM, Paris, France)

**15:40** **OC18 - An Integrated Computational Strategy to Probe Ligand Promiscuity in the Human Cytochrome 3A4**
Maria KONTOYIANNI
(SOUTHERN ILLINOIS UNIVERSITY EDWARDSVILLE, Edwardsville - Illinois, United States)

**16:00** **Coffee Break**

**16:45** **Fluorine Local Environment: From Screening to Drug Design**
Anna VULPETTI
(NOVARTIS, Basel, Switzerland)

## Programme

### Wednesday August 29, 2012

**Session 7 - Phys Chem Properties and Molecular Representations**

**Session Chair**
Anna TSANTILI-KAKOULIDOU
(UNIVERSITY OF ATHENS, Athens, Greece)

**08:45** **New trends and Perspectives in QSAR Modelling**
Roberto TODESCHINI
(UNIVERSITY OF MILANO-BICOCCA, Milano, Italy)

**09:30** **OC19 - Diverse Valid 3D-QSAR Models of Off-target Risks from Template CoMFA**
Richard CRAMER
(TRIPOS, Santa Fe, United States)

**09:50** **OC20 - The Power of Matched Pairs in Drug Design**
Jonas BOSTRÖM
(ASTRAZENECA, Mölndal, Sweden)

**10:10** **OC21 - A Chemogenomic Analysis of Ionization Constants**
David T MANALLACK
(MONASH UNIVERSITY, Parkville, Australia)

**10:30** **Coffee Break**

**Session 8 - Hansch Session - Grand Challenges for QSAR**

**Session Chair**
Tudor I. OPREA
(UNIVERSITY OF NEW MEXICO, San Diego, CA, United States)

**11:00** **QSAR without Borders**
Alexander TROPSHA
(UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)

**11:20** **Data Matters. The Discovery of New Knowledge**
Wendy WARR
(WENDY WARR & ASSOCIATES, Cheshire, United Kingdom)

**11:40** **Activity cliffs, Information Theory, and QSAR**
Gerald M. MAGGIORA
(UNIVERSITY OF ARIZONA, Tucson, United States)

**12:00** **The Impact of QSAR on Medicinal Chemistry**
Hugo KUBINYI
(UNIVERSITY OF HEIDELBERG, Weisenheim am Sand, Germany)

**12:20** **Lunch**
**12:45: OpenEye Workshop - "Ligand Design and Water Thermodynamics - SZMAP at Work"**

**14:15** **Hansch Awardee - "My Struggle with Binding Data"**

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

**15:15** **Excursions**

**19:30** **Buses leave for the Banquet**

## Programme

### Thursday August 30, 2012

**Session 9 - Open Innovation Stategies in Drug Discovery**

**Session Chair**
Bryn WILLIAMS-JONES
(CONNECTED DISCOVERY, London, United Kingdom)

**08:45** **Open Innovation Applied to Agrochemical Discovery**
Mark FORSTER
(SYNGENTA, Bracknell, United Kingdom)

**09:30** **OC22 - Open Innovation at Openeye: A Decade of Practice**
Bob TOLBERT
(OPENEYE SCIENTIFIC SOFTWARE, Santa Fee, United States)

**09:50** **OC23 - The Lilly Open Innovation Drug Discovery Program**
Christos NICOLAOU
(ELI LILLY AND CO, Indianapolis, United States)

**10:10** **OC24 - Open Access Web-Services for Predicting Biological Activity**
Dmitry FILIMONOV
(INSTITUTE OF BIOMEDICAL CHEMISTRY OF RAMS, Moscow, Russia)

**10:30** **Coffee Break**

**Session 10 - Poster Presentations**

**Session Chair**
Gerhard ECKER
(UNIVERSITY OF VIENNA, Vienna, Austria)

**11:15** **4 poster presentations selected by the committee (5 minutes each)**

**Session 11 - Late Breaking News**

**Session Chair**
Mark FORSTER
(SYNGENTA, Bracknell, United Kingdom)

**11:40** **OC25 - Using Public Data for Statistical Scoring Functions**
Christian KRAMER
(NOVARTIS, Basel, Switzerland)

**12:00** **OC26 - In Silico Prediction of the Target Space Relevant to Malaria**
Andreas SPITZMÜLLER
(FUNDACIÓ INSTITUT MAR D'INVESTIGACIONS MÈDIQUES, Barcelona, Spain)

**12:20** **OC27 - Utopia Documents**
Steve PETTIFER
(THE UNIVERSITY OF MANCHESTER, Manchester, United Kingdom)

## Programme

**12:40** **OC28 - Open Drug Discovery Intelligence: Open Phacts and SciBite**

Lee HARLAND
(CONNECTED DISCOVERY, London, United Kingdom)

**13:00** **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)

**13:30** **Farewell Lunch**
**14:00: Open Phacts Workshop - "Introducing Open PHACTS"**