Sunday 19/9/2010

18:30-19:00 Opening Ceremony

Chair persons: Bernard Testa

19:00-20:00 **Inaugural Lecture**
The long road from QSAR to virtual screening
Hugo Kubinyi

21:00- Welcome reception

Monday 20/9/2010

Chemical Space navigation and virtual screening

Chair persons: Tudor Oprea -

8:45-9:30 **Plenary Lecture**
Charting biologically relevant chemical space.
Herbert Waldmann
Max Planck Institute, Dortmund, Germany

9:30-9:50 **Oral Presentation**
Qsearch: A new method for de novo ligand design
Tanja Schulz-Gasch
Hoffmann-La Roche, Basel, Switzerland

9:50: -10:10 **Oral Presentation**
LigandScout: More accuracy for pharmacophore-based virtual screening
Gerhard Wolber
InteLigand, Innsbruck Austria

10:10-10:30 **Oral Presentation**
Recovering design strategies of GPCRs modulators from explorations of the chemical space
Antonio Macchiarulo
University of Perugia, Italy

10:30-11:00 Coffee Break

Targets-Transporters-Antitargets

Chair persons: Emmanuel Mikros-

11:00-11:45 **Plenary Lecture**
Ligand- and structure-based approaches for targeting drug transporter
Gerhard Ecker
University of Vienna, Austria

11:45-12:05 **Oral Presentation**
Stereoselective interaction of benzopyrano[3,4-b][1,4]oxazines with p-glycoprotein
Ishrat Jabeen
University of Vienna, Austria

12:05-12:25	**Oral Presentation** *Identification and application of antitarget activity hotspots to guide compound optimization* Gerhard Hessler Sanofi-Aventis, Frankfurt, Grmany
12:25-12:45	**Oral Presentation** *Biophysics-based library design: Discovery of 'non-acid' inhibitors of S1 DHFR* Veerabahu Shanmugasundaram Pfizer, USA
12:45-14:00	*Lunch*
14:00-16:00	**Poster session I**

Cheminformatics in drug design

Chair persons: Dimitris Agrafiotis

16:00-16:45	**Plenary Lecture** *Information theory and QSAR* Anthony Nicholls OpenEye Scientific Software, USA
17:45-17:05	**Oral Presentation** *Local correspondence concept in bio- and cheminformatics* Dimitri Filimonov Russian Academy of Medical Sciences, Moskow, Russia
17:05-17:30	***Coffee***
17:30-17:50	**Oral Presentation** *Using local models to improve QSAR predictivity* Fabian Buchwald Technische Universität München, Germany.
17:50-18:10	**Oral Presentation** *The use of design of experiments to develop efficient arrays for SAR and property exploration* Chris Luscombe GlaxoSmithKline Research Medicines Centre, U.K.
18:10-18:30	**Oral Presentation** *Analysis and comparison of 2D fingerprints: Insights into database screening performance using eight fingerprint methods* Duan Jianxin Schrodinger GmbH

Tuesday 21/9/2010

Molecular descriptors in QSAR

Chair persons: Synthia Selasie- Dimitra Hadjipavlou

8:45-9:30	**Plenary Lecture** *Hydrogen bonding and molecular design* Peter Kenny
9:30-9:55	**Key Note Lecture** *Tautomerism, the forgotten molecular descriptor* Yvonne Martin Martin Consultant, USA
9:55-10:15	**Oral Presentation** *Robust sparse feature/descriptor selection for QSAR.* Frank Burden CSIRO Molecular and Health Technologies Australia
10:15-10:35	**Oral Presentation** *The pKa distribution of screening compounds Application to drug discovery* David Manallack Monash University, Australia
10:35-11:00	*Coffee Break*

In Silico PhysChem Profiling and ADMET

Chair persons: Raimund Mannhold – Panos Macheras

11:00-11:45	**Plenary Lecture** *Real – time in silico physchem and ADMET support using autoQSAR* Han van de Waterbeemd
11:45—12:05	**Oral Presentation** *Understanding the Blood Brain Barrier: Optimization strategies for CNS penetration and distribution* Mario Lobell Bayer Schering Pharma, Wuppertal, Germany
12:05-12:25	**Oral Presentation** *Multi-pH QSAR: regression analysis sensitive enough to determine the transition-state pKa of human buccal absorption* Robert Scherrer BIOpKa, USA
12:25-12:45	**Oral Presentation** *Multi-parameter optimization and in silico modeling in lead optimization* Hua Gao Pfizer, USA

12:45-14:00	*Lunch*
14:00-16:00	**Poster session II**

Assessing Drug Safety and Efficacy through ADME predictions

Chair persons: Han van de Waterbeemd-

16:00-16:45	**Plenary Lecture** *The biochemistry of drug metabolism - Which are the important reactions and enzymes?* Bernard Testa University Hospital Centre, Lausanne, Switzerland
16:45-17:05	**Oral Presentation** *Combined in silico approaches for drug design and pharmacokinetic optimization of a set of carnosine analogues as potent and selective carbonyl quenchers* Giulio Vistoli University of Milan, Italy
17:05-17:25	*Coffee*
17:25- 18:10	**Plenary Lecture** *Computational-regulatory developments in the prediction of oral drug absorption* Panos Macheras University of Athens, Greece
18:10-18:30	Oral Presentation *Is predicting active transport necessary to predict bioavailability?* Albin Kristl University of Ljubljana, Slovenia
20:30-	**Cultural event**

Wednesday 22/9/2010

QSAR in the era of Biological Complexity

Chair persons: Eric Martin,

8:45-9:30	**Plenary Lecture** *Disease Systems Chemical Biology and Toxicogenomics* Søren Brunak Technical University of Denmark
9:30-9:50	**Oral Presentation** *Target identification for behavioral screening hits using a chemical similarity method* Christian Laggner University of California, USA

9:50-10:10	**Oral Presentation** *Characterization and Mapping of Ligand-Binding Cavities in Proteins* Anna Linusson Umeå University, Sweden
10:10-10:30	**Oral Presentation** *In Silico Approaches, And In Vitro And In Vivo Mutagenicity Assays: Alternatives To The Carcinogenicity Bioassay* Romualdo Benigni Istituto Superiore di Sanità, Italy
10:30-10:50	*Coffee Break*

Predictive Toxicology and Risk Assessment

Chair persons: Haralambos Sarimveis,- Vladimir Palyulin

10:50-11: 35	**Plenary Lecture** *Rodent Toxicity Studies On Perfluorinated Chemicals For Reach* Paola Gramatica University of Insubria, Italy
11:35-12.00	**Key Note Lecture** *Novel approaches to chemical toxicity prediction that rely on the entire structure-in vitro-in vivo data continuum* Alex Tropsha University of North Carolina, USA
12:05-12:30	**Key Note Lecture** *Assessing reactive metabolite risk in drug discovery using a weight-of-evidence approach* Scott Boyer AstraZeneca, Sweden
12:30-12:50	**Oral presentation** *Evaluation of the OECD QSAR application toolbox for predicting the biodegradability of chemicals* James Devillers Centre de Traitement de l'Information Scientifique, France
12:50-13:10	**Oral Presentation** *Classification and Regression-based QSAR of acute chemical rodent toxicity* Oleg Raevsky-Vladimir Poroikov Russian Academy of Sciences, Moscow, Russia
13:15-14:15	*Lunch (standing buffet)*
14:30	**Excursion**

Thursday 23/9/2010

Pharmacoinformatics and pharmacophores

Chair persons: Angelo Carotti- Gerhard Ecker

8:45-9:30	**Plenary Lecture** *Integrative phamacoinformatics approaches in the prediction of clinical outcomes of drugs* Ferran Sanz IMIM - Universitat Pompeu Fabra, Barcelona, Spain
9:30-9:55	Key Note Lecture *Pharmacophores - Versatile tools to bridge the gap between structure-based and ligand based approaches* Thierry Langer Prestwick Chemical, Inc.
9:55-10:15	**Oral Presentation** *From activity cliffs to target-specific scoring models and pharmacophoric hypothesis* Birte Seebeck University of Hamburg, Germany
10:15-10:35	**Oral Presentation** *Template-Constrained Fragment Alignment (TCFA)* Richard Cramer Tripos Int.USA
10:35-11:00	*Coffee Break*

Multi-target / Multi- objective QSAR

Chair persons: Ferran Sanz- Esin Sener

11:00-11:45	**Plenary Lecture** *Ligand-based approaches to in silico pharmacology: benchmarks and applications* Jordi Mestres IMIM - Universitat Pompeu Fabra, Barcelona, Spain
11:45-12:05	**Oral Presentation** *Enhancing molecular design via a multi-objective approach* Orazio Nicolotti Università di Bari, Italy
12:05-12:25	**Oral Presentation** *Prospectively validated proteochemometric models of HIV Reverse Transcriptase as a tool in lead optimization against multiple targets* Gerard van Westen LACDR, Leiden, The Netherlands
12:25-12:45	**Oral Presentation** *Computational drug design studies on antitumoral active heterocyclic compounds* Esin Aki Ankara University, Turkey

12:45-14:00	*Lunch*

Computational Strategies in Agrochemical Research

Chair persons: Ismail Yalcin - Klaus-Jürgen Schleifer

14:00-14:45	**Plenary Lecture** *Challenges in agrochemicals design* Klaus-Jürgen Schleifer BASF, Germany
14:45-15:05	**Oral Presentation** *New leads finding in agrochemistry: a computational chemistry challenge* Francesca Perruccio Syngenta Crop Protection, Switzerland
15:05-15:25	**Oral Presentation** *HYDE scoring of protein ligand complexes* Gudrun Lange Bayercropscience, Frankfurt, Germany
15:25-15:45	**Oral Presentation** *Inhibition of Eimeria tenella CDK-related Kinase 2: From target identification to lead compounds* Richard J. Marhöfer Intervet Innovation GmbH, Schwabenheim, Germany
15:45-16:05	*Coffee Break*

Database Mining

Chair persons: Alex Tropsha –

16:05-16:25	**Oral Presentation** *Back to the roots – Benefits and limitations concerning the in silico integration of natural products in drug discovery* Irene Kouskoumvekaki Technical University of Denmark Denmark
16:25-16:45	**Oral Presentation** *Capturing SAR-trends from chemogenomical spaces* Bernd Wendt Elara Pharmaceuticals GmbH, Heidelberg, Germany
16:45 – 17:05	**Oral Presentation** *Mining exhaustively the Protein Data Bank enables computational Fragment-Based Drug Design* Fabrice Moriaud Medit SA, France
17:05-17:40	**Short oral presentation of selected posters** 4 presentations (2 from Poster Session I +2 from Poster session II) 7 min each
17:40-18:30	**Tudor Oprea** Meeting of Cheminformatics and QSAR Society
21:00	**Gala Dinner**

Friday 24/9/2010

New Tools and Applications

Chair persons: Vladimir Poroikov-Thomas Mavromoustakos

9:00-9:45	**Plenary Lecture** *Iterative kinase Medium-Throughput Screening (ikMTS) with 2D profile-QSAR and 3D surrogate AutoShim Ensemble Docking* Eric Martin Novartis, USA
9:45-10:05	**Oral Presentation** *Investigation of the structural requirements for multi-kinase inhibition using GQSAR method* Subhash Ajmani NovaLead Pharma, India
10:05-10:25	**Oral Presentation** *Understanding the selectivity of organophosphorus inhibitors of serine esterases* Vladimir Palyulin Moscow State University, Russia
10:25-10:45	Oral Presentation *Structure-Activity Relationship of Arkadia ring finger E3 ubiquitin ligase through NMR spectroscopy* George Spyroulias University of Patras, Greece
10:45-11:05	*Coffee Break*

New avenues in QSAR

Chair persons: Thierry Langer- Yvonne Martin

11:05:11:50	**Plenary Lecture** *Ligand-receptor binding affinity predictions with Linear Response Methods and Free Energy Perturbation Calculation* Ruhong Zhou IBM, USA
11:50-12:15	**Key Note Lecture** *Visual (Q)SAR: SAR maps, scaffold trees, and R-cliffs.* Dimitris Agrafiotis Johnson and Johnson, USA
12:15-12:45	**Key Note Lecture** *Computer-Aided Drug Repurposing* Tudor Oprea University of New Mexico, USA
12:45-13:00	*Closing of the Symposium*
13:00-14:00	**Farewell party (standing buffet)**