20th EuroQSAR

Programme

Thursday August 28, 2014

August 28-30, 2014
School-seminar on Computer-Aided Drug Design held on the basis of Saint-Petersburg State Chemical-Pharmaceutical Academy (Prof. Popov str., Bldg. 14, Saint-Petersburg, Russia)

Programme

Sunday August 31, 2014

Excursion Tour 1 - Peterhof (until 14:00)

Excursion Tour 2 - Pavlovsk and Pushkin (until 15:00)

Excursion Tour 3 - Hermitage (until 16:00)

Registration

Excursion Tour 4 - Boat Trip (until 16:30)

Session Chair:
Prof. Vladimir POROIKOV
(INSTITUTE OF BIOMEDICAL CHEMISTRY, Moscow, Russia)

Opening Ceremony

Opening Lecture - (Q)SAR, the Lifelong Learning for my Research Career
Prof. Toshio FUJITA
(KYOTO UNIVERSITY, Kyoto, Japan)

Welcome drink

Programme

Monday September 1, 2014

Registration

Session 1 - Chemical-Biological Space: Representation, Visualization and Navigation

Session Chair

Dr Marc NICKLAUS
(NATIONAL CANCER INSTITUTE, Frederick, United States)

Navigation in Chemical Space Towards Biological Activity

Dr Peter ERTL
(NOVARTIS INSTITUTE FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

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)

Chemical Data Visualization and Modeling: Big Data Challenge

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

Large-Scale SAR-Mining and Visualization in Pharmaceutical Research

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

Coffee Break - sponsored by SciFinder - Chemical Abstracts Service (CAS) & Exhibition

Session 2 - Chemo- and Bioinformatics Approaches to Multi-Target (Q)SAR

Session Chair

Prof. Gabriele COSTANTINO
(UNIVERSITY OF PARMA, Parma, Italy)

Opportunities and Challenges in Therapeutics Discovery and Development

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

Protein Active Site Comparison with Sitehopper: Phylogeny to Polypharmacology

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

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)

Molecular Field Topology Analysis (MFTA) as a Tool For Multi-Target QSAR

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

Programme

Lunch

Workshop organised by OpenEye (lunch served in auditorium for workshop attendees)

Poster Session & Exhibition

Session 3 - Modeling of Protein-Ligand Interactions: Structure, Function and Dynamics

Session Chair
Dr Uko MARAN
(UNIVERSITY OF TARTU, Tartu, Estonia)

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)

Importance of Conformations in Ligand-Based Drug Discovery Approaches
Dr Daniel CAPPEL
(SCHRÖDINGER, Mannheim, Germany)

Predicting Dynamically Dominated Allostery from Constraint Network Analysis
Prof. Holger GOHLKE
(HEINRICH-HEINE-UNIVERSITY DÜSSELDORF, Düsseldorf, Germany)

Coffee Break - sponsored by SciFinder - Chemical Abstracts Service (CAS) & Exhibition

Ensemble-Based Drug Design, Combining Protein Structures and Simulations
Dr Will PITT
(UCB PHARMA, Slough, United Kingdom)

City Tour for participants

Programme

Tuesday September 2, 2014

Session 4 - Assessing Ligand Binding Kinetics

Session Chair

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

Lead Discovery and Optimisation by Use of Interaction Kinetic Analysis

Prof. Helena DANIELSON
(UPPSALA UNIVERSITY, Uppsala, Sweden)

Session 4b - QSAR/Modelling Methods and Applications

Session Chair

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

Which Distance For Similarity/Diversity Analysis?

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

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

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

Identification of Mechanism of Action of DNA-Topoisomerase II Inhibitors By Molecular Modeling Studies

Prof. Esin AKI-YALCIN
(ANKARA UNIVERSITY, Ankara, Turkey)

Coffee Break & Exhibition

Session 5 - Computational Toxicology in Drug and Chemical Safety Assessment

Session Chair

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

Computational Toxicology – An Essential Part of Drug Safety

Dr Catrin HASSELGREN
(UNIVERSITY OF NEW MEXICO, South San Francisco, CA, United States)

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 Systems Biology Identification of Drug Targets Related with Cardiovascular Adverse Effects

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

Programme

Active QSAR Modelling for Evironmental Toxicity Prediction of Chemical Substances

Prof. Yoshimasa TAKAHASHI
(TOYOHASHI UNIVERSITY OF TECHNOLOGY, Toyohashi, Japan)

Lunch

Company Workshop organised by BIOVIA (formerly Accelrys) (lunch served in auditorium for workshop attendees)

Poster Session & Exhibition

Session 6 - Translational Bioinformatics: From Genomes to Drugs

Session Chair

Prof. Anna LINUSSON
(UMEA UNIVERSITY, Umea, Sweden)

The Impact of Large-Scale Genetic Data on Drug Targets

Dr Josef SCHEIBER
(BIOVARIANCE GMBH, Munich, Germany)

Applications of Proteochemometrics – From Species Extrapolation to Cell Line Sensitivity Modelling

Dr Isidro CORTES
(INSTITUT PASTEUR, Paris, France)

“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)

Coffee Break & Exhibition

Chemical Informatics Applied to Health and Drug Safety

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

Programme

Wednesday September 3, 2014

Session 7 - Non-Traditional Applications of QSAR & Modeling (Cosmetics, Food Supplements, Drug Delivery, Materials- and Nano-Informatics)

Session Chair

Dr David T MANALLACK
(MONASH UNIVERSITY, Parkville, Australia)

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)

QSPR Modeling of Chemical And Physical Stability of Pharmaceuticals

Dr Yuriy ABRAMOV
(PFIZER, Groton, United States)

Recent Trends in QSAR Modeling of Chemical Mixtures

Dr Eugene MURATOV
(UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)

Material-Informatics: Chemoinformatics and Combinatorial Material Science for the Design of Novel Photovoltaic Cells

Prof. Hanoch SENDEROWITZ
(BAR-ILAN UNIVERSITY, Ramat Gan, Israel)

Coffee Break & Exhibition

Session 8 - Hansch Session - Grand Challenges for QSAR

Session Chair

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

On the Nature of Non-Classical Hydrogen Bonds and Aromatic Interactions

Prof. Anna LINUSSON
(UMEA UNIVERSITY, Umea, Sweden)

Molecular Design of Bivalent and Dual Action Drugs

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

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

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

Lunch & Exhibition

Programme

Company Workshop organised by Chemical Computing Group (lunch served in auditorium for workshop attendees)

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

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

Excursion Tour 5 - Hermitage (until 19:00)

Excursion Tour 6 - Boat Trip (until 17:30)

Banquet

Programme

Thursday September 4, 2014

Session 9 - Emerging QSAR and Modeling Methods

Session Chair

Prof. Antonia TAVARES DO AMARAL
(UNIVERSITY OF SÃO PAULO, São Paulo, Brazil)

Integrating Pharmacometrics into Drug Development

Dr Roberta BURSI
(GRÜNENTHAL, Aachen, Germany)

META-QSAR

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

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

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

Structural and Functional Interpretation of QSAR Models

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

Coffee Break & Exhibition

Closing Lecture - Large-Scale Chemogenomics in Pharma - Definition, Benchmarking, and Application

Dr Joerg Kurt WEGNER
(JOHNSON & JOHNSON, Beerse, Belgium)

Session Chair

Prof. Vladimir POROIKOV
(INSTITUTE OF BIOMEDICAL CHEMISTRY, Moscow, Russia)

4 poster presentations selected by the committee (5 minutes each)

Session Chair

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

Closing Ceremony

Lunch

Session Seminar/Roundtable: (Q)SAR-Related European Initiatives

Moderators

Prof. Gerhard ECKER (UNIVERSITY OF VIENNA, Vienna, Austria)
Prof. Ferran SANZ (UNIVERSITY POMPEU FABRA, Barcelona, Spain)

14:00 **EU-Openscreen? A Pan-European Resource and Infrastructure to Support chemical Biology Research**

Programme

Dr Ronald FRANK
(FMP, Berlin, Germany)

14:20 **eTOX: Integrative Strategies for Predicting Drug Toxicities**

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

14:40 **Open PHACTS - The Use of Open Data for in silico Models**

Prof. Gerhard ECKER
(UNIVERSITY OF VIENNA, Vienna, Austria)

15:00 **When is Software Accepted by Medicinal Chemists? SEESAR: a Lead Optimization Example**

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

15:20 **EU's Framework Programme for Research and Innovation Horizon 2020: Cooperation Opportunities (tentative)**

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

15:35 **Roundtable**

Session Hot Topics: Modern Techniques in Computer-Aided Drug Discovery

Session Chair

Prof. Tudor I. OPREA
(UNIVERSITY OF NEW MEXICO, Albuquerque, United States)

14:00 **Cosmo Sigma-Surfaces and Local Sigma-Profiles as Extremely Robust Descriptors for Alignment, 3D-Similarity and 3D-QSAR**

Prof. Andreas KLAMT
(COSMOLOGIC, Leverkusen, Germany)

14:20 **Structural Sensitivity Analysis Using Matched Molecular Pairs**

Dr Robert D. CLARK
(SIMULATIONS PLUS, INC, Lancaster, United States)

14:40 **QDB: From Static to Dynamic Nature of Published QSAR-S**

Dr Uko MARAN
(UNIVERSITY OF TARTU, Tartu, Estonia)

15:00 **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)

15:20 **Semi-quantitative SAR Using Bayesian Modelling on Activity Cliffs**

Dr Mark MACKEY
(CRESSET BIOMOLECULAR DISCOVERY LIMITED, Cambridgeshire, United Kingdom)

15:40 **Surflex QMOD: Protein Pocket Modeling for Affinity Prediction**

Dr Alexander STEUDLE
(CERTARA, München, Germany)

16:00 **Might Template COMFA Integrate Structure-Based and Ligand-Based Design?**

Dr Richard CRAMER
(TRIPOS, Santa Fe, United States)