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

09:00 **Excursion Tour 1 - Peterhof (until 14:00)**

10:00 **Excursion Tour 2 - Pavlovsk and Pushkin (until 15:00)**

12:00 **Excursion Tour 3 - Hermitage (until 16:00)**

14:00 **Registration**

15:00 **Excursion Tour 4 - Boat Trip (until 16:30)**

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

17:00 **Opening Ceremony**

17:30 **Opening Lecture - (Q)SAR, the Lifelong Learning for my Research Career**
Prof. Toshio FUJITA
(KYOTO UNIVERSITY, Kyoto, Japan)

18:15 **Welcome drink**

Programme

Monday September 1, 2014

08:00 **Registration**

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

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

08:45 **Navigation in Chemical Space Towards Biological Activity**
Dr Peter ERTL
(NOVARTIS INSTITUTE FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

09:30 **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)

09:50 **Chemical Data Visualization and Modeling: Big Data Challenge**
Prof. Alexandre VARNEK
(UNIVERSITY OF STRASBOURG, Strasbourg, France)

10:10 **Large-Scale SAR-Mining and Visualization in Pharmaceutical Research**
Dr VEER SHANMUGASUNDARAM
(PFIZER, Groton, CT, United States)

10:30 **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)

11:15 **Opportunities and Challenges in Therapeutics Discovery and Development**
Dr John C. REED
(F. HOFFMANN-LA ROCHE, Basel, Switzerland)

12:00 **Protein Active Site Comparison with Sitehopper: Phylogeny to Polypharmacology**
Dr Paul HAWKINS
(OPENEYE SCIENTIFIC SOFTWARE, Santa Fe, United States)

12:20 **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)

12:40 **Molecular Field Topology Analysis (MFTA) as a Tool For Multi-Target QSAR**
Dr Vladimir A. PALYULIN
(LOMONOSOV MOSCOW STATE UNIVERSITY, Moscow, Russia)

Programme

13:00 **Lunch**

13:00 **Workshop organised by OpenEye (lunch served in auditorium for workshop attendees)**

14:30 **Poster Session & Exhibition**

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

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

15:30 **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)

15:50 **Importance of Conformations in Ligand-Based Drug Discovery Approaches**
Dr Daniel CAPPEL
(SCHRÖDINGER, Mannheim, Germany)

16:10 **Predicting Dynamically Dominated Allostery from Constraint Network Analysis**
Prof. Holger GOHLKE
(HEINRICH-HEINE-UNIVERSITY DÜSSELDORF, Düsseldorf, Germany)

16:30 **Coffee Break - sponsored by SciFinder - Chemical Abstracts Service (CAS) & Exhibition**

17:15 **Ensemble-Based Drug Design, Combining Protein Structures and Simulations**
Dr Will PITT
(UCB PHARMA, Slough, United Kingdom)

18:30 **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)

08:45 **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)

09:30 **Which Distance For Similarity/Diversity Analysis?**
Prof. Roberto TODESCHINI
(UNIVERSITY OF MILANO-BICOCCA, Milano, Italy)

09:50 **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)

10:10 **Identification of Mechanism of Action of DNA-Topoisomerase II Inhibitors By Molecular Modeling Studies**
Prof. Esin AKI-YALCIN
(ANKARA UNIVERSITY, Ankara, Turkey)

10:30 **Coffee Break & Exhibition**

Session 5 - Computational Toxicology in Drug and Chemical Safety Assessment

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

11:15 **Computational Toxicology – An Essential Part of Drug Safety**
Dr Catrin HASSELGREN
(UNIVERSITY OF NEW MEXICO, South San Francisco, CA, United States)

12:00 **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)

12:20 **Chemical Systems Biology Identification of Drug Targets Related with Cardiovascular Adverse Effects**
Dr Alexey LAGUNIN
(INSTITUTE OF BIOMEDICAL CHEMISTRY, Moscow, Russia)

Programme

12:40 **Active QSAR Modelling for Evironmental Toxicity Prediction of Chemical Substances**
Prof. Yoshimasa TAKAHASHI
(TOYOHASHI UNIVERSITY OF TECHNOLOGY, Toyohashi, Japan)

13:00 **Lunch**

13:00 **Company Workshop organised by BIOVIA (formerly Accelrys) (lunch served in auditorium for workshop attendees)**

14:30 **Poster Session & Exhibition**

Session 6 - Translational Bioinformatics: From Genomes to Drugs

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

15:30 **The Impact of Large-Scale Genetic Data on Drug Targets**
Dr Josef SCHEIBER
(BIOVARIANCE GMBH, Munich, Germany)

15:50 **Applications of Proteochemometrics – From Species Extrapolation to Cell Line Sensitivity Modelling**
Dr Isidro CORTES
(INSTITUT PASTEUR, Paris, France)

16:10 **“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)

16:30 **Coffee Break & Exhibition**

17:15 **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)

08:45 **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)

09:30 **QSPR Modeling of Chemical And Physical Stability of Pharmaceuticals**

Dr Yuriy ABRAMOV
(PFIZER, Groton, United States)

09:50 **Recent Trends in QSAR Modeling of Chemical Mixtures**

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

10:10 **Material-Informatics: Chemoinformatics and Combinatorial Material Science for the Design of Novel Photovoltaic Cells**

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

10:30 **Coffee Break & Exhibition**

Session 8 - Hansch Session - Grand Challenges for QSAR

Session Chair

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

11:15 **On the Nature of Non-Classical Hydrogen Bonds and Aromatic Interactions**

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

11:35 **Molecular Design of Bivalent and Dual Action Drugs**

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

11:55 **The Road Ahead: New Challenges for Computational Forecasts**

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

12:15 **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)

12:35 **Lunch & Exhibition**

Programme

12:35 **Company Workshop organised by Chemical Computing Group (lunch served in auditorium for workshop attendees)**

14:00 **Hansch Awardee: Lessons Learned from Chemical and Biological Data - Scientifically, and Personally**

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

15:00 **Excursion Tour 5 - Hermitage (until 19:00)**

16:00 **Excursion Tour 6 - Boat Trip (until 17:30)**

20:00 **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)

08:45 **Integrating Pharmacometrics into Drug Development**
Dr Roberta BURSI
(GRÜNENTHAL, Aachen, Germany)

09:30 **META-QSAR**
Dr Larisa SOLDATOVA
(BRUNEL UNIVERSITY OF LONDON, Uxbridge, United Kingdom)

09:50 **Performance Evaluation of Common Virtual Screening Tools on Selected Representatives of Different Target Classes**
Mrs Teresa KASERER
(UNIVERSITY OF INNSBRUCK, Innsbruck, Austria)

10:10 **Structural and Functional Interpretation of QSAR Models**
Dr Pavel POLISHCHUK
(A.V. BOGATSKY PHYSICO-CHEMICAL INSTITUTE, Olomouc, Czech Republic)

10:30 **Coffee Break & Exhibition**

11:15 **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)

12:00 **4 poster presentations selected by the committee (5 minutes each)**

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

12:25 **Closing Ceremony**

13:00 **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, San Diego, CA, 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)