21st EuroQSAR

Programme

Sunday September 4, 2016

15:00 **Registration**

17:00 **Opening Ceremony**

Prof. Andrea CAVALLI (UNIVERSITY OF BOLOGNA AND IIT, Bologna, Italy)
Prof. Gabriele COSTANTINO (UNIVERSITY OF PARMA, Parma, Italy)

17:30 **PL01 - Calculating Ligand-Protein Unbinding Rates**

Prof. Michele PARRINELLO
(ETH ZURICH, Lugano, Switzerland)

18:15 **Welcome drink**

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Monday September 5, 2016

08:00 **Registration**

09:00 **Welcome word**

Dr Henning STEINHAGEN
(APTUIT, Verona, Italy)

Session 1: Big Data Analysis and Precision Medicine

Session Chair

Prof. Modesto OROZCO
(INSTITUTE FOR RESEARCH IN BIOMEDICINE (IRB), Barcelona, Spain)

09:05 **PL02 - Informatics Methods for Understanding Drug Binding and Action**

Prof. Russ B. ALTMAN
(STANFORD UNIVERSITY, Stanford, United States)

09:50 **KL01 - Multi-Scale Structure-Based Drug Discovery**

Prof. Rommie AMARO
(UNIVERSITY OF CALIFORNIA, San Diego, United States)

10:20 **OC01 - Biosignature Based Drug Design: Impacts of a New Paradigm from a Pharma Perspective**

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

10:40 **OC02 - Chemical Reactions Mining: Big Data Challenge**

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

11:00 **Coffee break**

Session 2: QSAR Tools and Applications

Session Chair

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

11:25 **PL03 - QSAR and Environmental Toxicology - From Chemical Structure to Environmental Hazard: Exploiting QSAR for Screening, Prioritization and Safer Alternative's Design**

Prof. Paola GRAMATICA
(INSUBRIA UNIVERSITY, Varese, Italy)

12:10 **KL02 - A Method for Incorporating Proprietary SAR Information to Improve (Q)SAR Models without Disclosing Underlying Compounds**

Dr Catrin HASSELGREN
(LEADSCOPE, Columbus, United States)

12:40 **OC03 - A Cheminformatics Story Behind 141,000,000$ Molecule**

Prof. Artem CHERKASOV
(UNIVERSITY OF BC, VANCOUVER PROSTATE CENTRE, Vancouver, Canada)

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13:00 **OC04 - How Much Does a Molecule Cost? Molecular Statistics Explains the Big Data Problem In QSPR**
Prof. Jaroslaw POLANSKI
(UNIVERSITY OF SILESIA, Katowice, Poland)

13:20 **OC05 - How To Increase the Concordance of the Experimental Data for QSAR Modeling: Case Study for HIV-1 Reverse Transcriptase Inhibitors**
Dr Olga TARASOVA
(IBMC, Moscow, Russia)

13:40 **Lunch and Poster session**

14:10 - Workshop organised by OpenEye (75 min)

Session 3: Molecular Dynamics Simulations and Related Methods

Session Chair
Prof. Andrea CAVALLI
(UNIVERSITY OF BOLOGNA AND IIT, Bologna, Italy)

15:40 **PL04 - Exploring Protein Dynamics for Ligand Design**
Prof. Rebecca WADE
(HEIDELBERG UNIVERSITY AND HITS, Heidelberg, Germany)

16:25 **KL03 - Mechanistic and Inhibition Studies of the ARP2/3 Complex Using Computational Techniques**
Dr Zoe COURNIA
(BIOMEDICAL RESEARCH FOUNDATION ACADEMY OF ATHENS, Athens, Greece)

16:55 **Coffee break**

17:25 **OC06 - Hybrid Modeling Approach to Investigate Antibody Dynamics**
Dr Michal VIETH
(ELI LILLY & CO, Indianapolis, United States)

17:45 **OC07 - Finding a Way Toward Binding: A MD Biasing Potential Leading to the Protein-Ligand Complex**
Dr Walter ROCCHIA
(FONDAZIONE ISTITUTO ITALIANO DI TECNOLOGIA, Genova, Italy)

19:00 **City Tour for participants**

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Tuesday September 6, 2016

Session 4: Computational Biology and Quantum Enzymology

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

09:00 **PL05 - Biomolecular Simulations to Assay Enzyme Activity, Ligand Binding and Drug Resistance**
Prof. Adrian J MULHOLLAND
(UNIVERSITY OF BRISTOL, Bristol, United Kingdom)

09:45 **KL04 - The Bitter Taste of Molecules: Characterization, Prediction and Connection to Genetic Variants of Human Taste Receptors**
Prof. Masha NIV
(THE HEBREW UNIVERSITY, Rehovot, Israel)

10:15 **OC08 - Rigorous Free Energy Calculations Applied to Protein Homology Models**
Dr Daniel CAPPEL
(SCHRÖDINGER, Mannheim, Germany)

10:35 **Coffee break**

11:05 **OC09 - Antagonist Binding of Human Adenosine Receptor in Nearly Physiological Conditions**
Prof. Giulia ROSSETTI
(RWTH UNIVERSITY AND FZJ, Juelich, Germany)

11:25 **OC10 - Integrating Molecular Dynamics and Molecular Interaction Fields: A Way to Enhance Structure-Based Virtual Screening**
Dr Francesca SPYRAKIS
(UNIVERSITY OF TURIN, Torino, Italy)

11:45 **OC11 - Optimization Algorithms for Chemoinformatics and Material-Informatics**
Prof. Hanoch SENDEROWITZ
(BAR-ILAN UNIVERSITY, Ramat Gan, Israel)

12:05 **OC12 - New Insight into the Catalytic and Inhibition Mechanism of the Human Acyl Protein Thioesterase**
Dr Martina AUDAGNOTTO
(EPF LAUSANNE, Lausanne, Switzerland)

12:25 **OC13 - Structure-Based Design of Riboswitch Ligands**
Prof. Ruth BRENK
(UNIVERSITY OF BERGEN, Bergen, Norway)

12:45 **Lunch and Poster Session**

Session 5: Ligand-Based and Structure-Based Approaches to Drug Design

Session Chair
Prof. Andrew R. LEACH
(GSK, Hinxton, United Kingdom)

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14:45 **PL06 - Computer-Aided Drug Discovery Approaches Applied to Hit-Generation**
Dr Johanna JANSEN
(NOVARTIS, Emeryville, United States)

15:30 **KL05 - Finding Drug Targets in 3D**
Prof. Ruben ABAGYAN
(UNIVERSITY OF CALIFORNIA, La Jolla, United States)

16:00 **Sponsor's presentation - QuaSAR3D: An Integrated Platform for 3D QSAR Analysis**
Mr Andrew HENRY
(CHEMICAL COMPUTING GROUP, Cambridge, United Kingdom)

16:15 **Coffee break**

16:45 **OC14 - Mappability of Drug-Like Space: Towards a Polypharmacologically Competent Map of Drug-Relevant Compounds**
Dr Dragos HORVATH
(CNRS , Strasbourg, France)

17:05 **OC15 - Novel Gridless Program SOL-P for Flexible Ligand Docking with Moveable Protein Atoms**
Dr Vladimir SULIMOV
(LOMONOV MOSCOW STATE UNIVERSITY, Moscow, Russia)

17:25 **OC16 - The Astex Fragment Network**
Dr Richard HALL
(ASTEX THERAPEUTICS, Cambridge, United Kingdom)

17:45 **OC17 - QSAR Models for Prediction Of Drug-Induced Liver Injury in Human Using Decision Forest Algorithm And a Large Set of FDA-Approved Drugs**
Dr Huixiao HONG
(US FDA, Jefferson, United States)

18:05 **OC18 - Pharmacophores: From a Static Concept to a Dynamic One**
Prof. Thierry LANGER
(UNIVERSITY OF VIENNA, Vienna, Austria)

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Wednesday September 7, 2016

Session 6: ADME Prediction and Computational Toxicology

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

09:00 **PL07 - Prediction of Toxic Endpoints: Fact or Fantasy?**
Prof. Gabriele CRUCIANI
(UNIVERSITY OF PERUGIA, Perugia, Italy)

09:45 **KL06 - *In Silico* ADME-PK in Modern Industrial Drug Discovery**
Dr Fabio BROCCATELLI
(GENENTECH INC., San Francisco, United States)

10:15 **OC19 - Prediction Of Cytochrome P450 Mediated Metabolism Using Molecular Dynamics**
Ms Mira KUUSISTO
(UNIVERSITY OF JYVÄSKYLÄ, University of Jyväskylä, Finland)

10:35 **OC20 - Mixtures, Metabolites, Ionic Liquids: A New Measure to Evaluate Similarity Between Complex Chemical Systems**
Prof. Roberto TODESCHINI
(UNIVERSITY OF MILANO-BICOCCA, Milano, Italy)

10:55 **Coffee break**

Session 7: Hansch Session

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

11:25 **PL08 - Hansch Fujita Awardee - Chemical Space Networks and SAR Visualization**
Prof. Jürgen BAJORATH
(UNIVERSITY OF BONN, Bonn, Germany)

12:10 **PL09 - Hansch Awardee**

12:55 **Lunch**

Session 8: Computationally-Driven Drug Discovery: Case Studies

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

14:25 **PL10 - Computationally Guided Discovery of Potent Enzyme Inhibitors**
Prof. William L. JORGENSEN
(YALE UNIVERSITY, New Haven, United States)

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15:10 **KL07 - Polypharmacology at Work – Examples from Pharmaceutical Industry**

Dr Gerhard HESSLER
(SANOFI-AVENTIS DEUTSCHLAND, Frankfurt am Main, Germany)

15:40 **OC21 - Navigating Genetic and Structural Landscapes of Human Protein Kinome in a System-Based Network Modeling of Kinases Binding and Drug Resistance: Leveraging Inhibitor-Induced Dimerization Mechanisms in Design of Targeted Anticancer Agents**

Prof. Gennady VERKHIVKER
(CHAPMAN UNIVERSITY AND UNIVERSITY OF CALIFORNIA SAN DIEGO, Orange, United States)

16:00 **Coffee break**

16:30 **OC22 - Prediction of Drug Efficiency: Our Experience in CNS Drug Design and Discovery**

Dr Alfonso POZZAN
(APTUIT, Verona, Italy)

16:50 **OC23 - Fusion Inhibitors of Tick-Borne Flaviviruses: Identification and Mode of Action Study**

Ms Evgenia DUEVA
(LOMONOSOV MOSCOW STATE UNIVERSITY, Moscow, Russia)

17:10 **OC24 - Discovery and Prediction of Novel Antimicrobial Using Large Scale Screening Data**

Dr Johannes ZUEGG
(CO-ADD, St. Lucia, Australia)

17:30 **OC25 - Computational Chemistry Input to the Development of Highly Potent Prevention of Activation (POA) MK2 Inhibitors**

Dr Emma EVERTSSON
(ASTRAZENECA, Mölndal, Sweden)

20:00 **Banquet**

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Thursday September 8, 2016

Session 9: Binding Kinetics in Drug Discovery

Session Chair
Prof. Stefano MORO
(UNIVERSITY OF PADOVA, Padova, Italy)

09:00 **PL11 - Looking Beyond Affinity: What Thermodynamics and Binding Kinetics Can Tell us About Drug Molecules**
Prof. Gerhard KLEBE
(PHILIPPS-UNIVERSITY MARBURG, Marburg, Germany)

09:45 **KL08 - Predicting Protein-ligand Binding and Ligand Residence Time Using Smoothed Molecular Dynamics**
Dr Pierre DUCROT
(INSTITUT DE RECHERCHES SERVIER, Croissy-sur-Seine, France)

10:15 **OC26 - Combining Accelerated Molecular Dynamics and Makov State Models to Disclose Hidden Protein States: Towards the Development of Selective Cyclophilin Inhibitors**
Dr Jordi JUÁREZ-JIMÉNEZ
(UNIVERSITY OF EDINBURGH, Edinburgh, United Kingdom)

10:35 **Flash Presentations**

FP01 - An Evaluation of the Epigenetic Target Space
Dr Vineet PANDE
(JANSSEN PHARMA. J&J, Beerse, Belgium)

FP02 - Evias Web Services: Cloud-Based Drug Discovery Platform
Dr Abdurrahman OLGAC
(GAZI UNIVERSITY FACULTY OF PHARMACY, Ankara, Turkey)

FP03 - Discovery of New Targets for the Development of Trypanocidal Drugs
Dr Paulino MARGOT
(FACULTAD DE QUIMICA - UDELAR, MONTEVIDEO, Uruguay)

FP04 - Cheminformatics Analysis of Polymeric Micelle-Based Delivery Systems
Dr Eugene MURATOV
(UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)

10:55 **Coffee break**

Session 10: Modelling of Biological Drugs

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

11:20 **PL12 - After 40 years of Structure-based Design, What Are We Missing?**
Dr Jeffrey BLANEY
(GENENTECH, SO. San Francisco, CA, United States)

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12:05 **KL09 - How Confident are you in your Predictions? Applications of Conformal Prediction and Teaching Schedules in Drug Discovery**

Dr Ernst AHLBERG
(ASTRAZENECA, Gothenburg, Sweden)

12:35 **OC27 - Modified Glycopeptides Targeting the Class II MHC DR4 Protein Associated with Rheumatoid Arthritis – Investigation of the Effect on T-Cell Response with MD Simulations**

Ms Cecilia LINDGREN
(UMEÅ UNIVERSITY, Umea, Sweden)

12:55 **Closing Ceremony**

Prof. Gabriele COSTANTINO (UNIVERSITY OF PARMA, Parma, Italy)
Prof. Andrea CAVALLI (UNIVERSITY OF BOLOGNA AND IIT, Bologna, Italy)