

## Programme

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### 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**

## Programme

### 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)

## Programme

- 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 CURNIA  
(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**

**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)

## Programme

- 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)

### 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, San Diego, CA, 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)

## Programme

- 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**

**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 Markov 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)



## Programme

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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)