

### Sunday September 20, 2020

15:00     **Registration**

17:00     **Opening Ceremony**

17:15     **Opening Lecture - Deep Learning Approaches to Structural Bioinformatics**

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

18:00     **Welcome Drink**

### Monday September 21, 2020

**08:00**      **Registration**

#### Session 1 - QSAR Without Borders

**09:00**      **Session Chair**

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

**09:05**      **Title to be announced (PL01)**

Dr Dimitris AGRAFIOTIS  
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Cambridge MA, United States)

**09:45**      **Short Lecture 1**

**10:15**      **Short Lecture 2**

**10:45**      **Coffee break**

#### Session 2 - Network Medicine

**11:15**      **Session Chair**

Dr Patrick ALOY  
(INSTITUTE FOR RESEARCH IN BIOMEDICINE (IRB), Barcelona , Spain)

**11:20**      **Systems Pharmacology Merging Omics Data and Biological Knowledge (PL02)**

Prof. Julio SAEZ-RODRIGUEZ  
(HEIDELBERG UNIVERSITY, Heidelberg, Germany)

**12:00**      **Short Lecture 3**

**12:30**      **Short Lecture 4**

**13:00**      **Lunch, Exhibition & Poster Session**

**13:15**      **Workshops**

#### Session 3 - Molecular Dynamics and Kinetics

**14:30**      **Session Chair**

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

## Programme

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**14:35 Title to be announced (PL03)**  
Prof. Rommie AMARO  
(UNIVERSITY OF CALIFORNIA, San Diego, United States)

**15:15 Short Lecture 5**

**15:45 Oral Communication 1**

**16:05 Coffee Break**

**Session 4 - In Memoriam - Peter Goodford**

**16:30 Session Chair**  
Prof. Rebecca WADE  
(HITS, Heidelberg, Germany)

**16:35 Structure-Activity Relationships from Drug-Receptor Complexes Using the Comparative Binding Energy (Combine) Method (SL06)**  
Prof. Federico GAGO  
(UNIVERSITY OF ALCALA, Alcala de Henares, Spain)

**17:05 Short Lecture 7**  
Prof. Gabriele CRUCIANI  
(UNIVERSITY OF PERUGIA, Perugia, Italy)

**17:35 Poster Session**

### Tuesday September 22, 2020

#### Session 5 - Chemical Space Annotation and Expansion

**09:00 Session Chair**

Prof. Andrew R. LEACH  
(EMBL-EBI, Hinxton, United Kingdom)

**09:05 The ChEMBL Database: Past, Present and Future (PL04)**

Dr Anna GAULTON  
(EMBL-EUROPEAN BIOINFORMATICS INSTITUTE, Hinxton, United Kingdom)

**09:45 Short Lecture 8**

**10:15 Short Lecture 9**

**10:45 Coffee break**

#### Session 6 - Modelling Drug Safety

**11:15 Session Chair**

Prof. Manuel PASTOR  
( UNIVERSITY POMPEU FABRA , Barcelona, Spain)

**11:20 Enhancing Confidence in Computational Methods for the Evaluation of Drug Safety (PL05)**

Dr Alessandra RONCAGLIONI  
(MARIO NEGRI INSTITUTE FOR PHARMACOLOGICAL RESEARCH, Milano, Italy)

**12:00 Short Lecture 10**

**12:30 Short Lecture 11**

**13:00 Lunch, Exhibition & Poster Session**

**13:15 Workshop**

#### Session 7 - Challenges in GPCR Drug Design

**14:30 Session Chair**

Prof. Harel WEINSTEIN  
(CORNELL UNIVERSITY, New York, United States)

**14:35 Thermodynamics and Kinetics Properties of G Protein-Coupled Receptors from Combinations of Machine Learning and Enhanced Molecular Dynamics Methods (PL06)**

## Programme

Prof. Marta FILIZOLA  
(ICAHN SCHOOL OF MEDICINE AT MOUNT SINAI, New York, United States)

**15:15 Quantifying GPCR Signaling in an Oligomeric Context (SL12)**

Dr Jesús GIRALDO  
(AUTONOMOUS UNIVERSITY OF BARCELONA, Bellaterra, Spain)

**15:45 Oral Communication 2**

**Session 8 - Modelling Drug Transport Mechanisms**

**16:30 Session Chair**

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

**16:35 Title to be announced (PL07)**

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

**17:15 Short Lecture 13**

**17:45 Oral Communication 3**

**18:05 Poster Session**

### Wednesday September 23, 2020

#### Session 9 - Predicting Off-Target Pharmacology

- 09:00**    **Session Chair**  
Prof. Vladimir POROIKOV  
(INSTITUTE OF BIOMEDICAL CHEMISTRY, Moscow, Russia)
- 09:05**    **Off-target Prediction Based on Binding Site Similarity (PL08)**  
PD Dr Oliver KOCH  
(UNIVERSITY OF MÜNSTER, Münster, Germany)

**09:45**    **Short Lecture 14**

**10:15**    **Short Lecture 15**

**10:45**    **Coffee break**

#### Session 10 - Artificial Intelligence in Drug Discovery

- 11:15**    **Session Chair**  
Prof. Tudor I. OPREA  
(UNIVERSITY OF NEW MEXICO, Albuquerque, United States)
- 11:20**    **Towards Machine Learning-Driven Drug Development (PL09)**  
Prof. Olivier ELEMENTO  
(CORNELL UNIVERSITY, New York, United States)

**12:00**    **Short Lecture 16**

**12:30**    **Short Lecture 17**

**13:00**    **Lunch, Exhibition & Poster Session**

**13:15**    **Workshop**

#### Session 11 - New Modes of Target Interaction

- 14:30**    **Session Chair**  
Prof. Leonardo PARDO  
(AUTONOMOUS UNIVERSITY OF BARCELONA, Bellaterra, Spain)

**14:35**    **Title to be announced (PL10)**  
Dr Gary TRESADERN  
(JANSSEN, Beerse, Belgium)

## Programme

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**15:15      Short Lecture 18**

**15:45      Oral Communication 4**

**16:05      Coffee break**

### **Session 12 - New Trends in Quantum Mechanics**

**16:30      Session Chair**

Prof. Carme ROVIRA  
(UNIVERSITY OF BARCELONA, Barcelona, Spain)

**16:35      Studies on Enzyme-Catalysed Reactions (PL11)**

Prof. Maria Joao RAMOS  
(UNIVERSITY OF PORTO, Porto, Portugal)

**17:15      Short Lecture 19**

**17:45      Oral Communication 5**

**20:00      Conference Banquet**

### Thursday September 24, 2020

#### Session 13 - The Challenges Ahead

**09:00 Session Chair**

Dr Jordi MESTRES  
(IMIM HOSPITAL DEL MAR MEDICAL RESEARCH INSTITUTE, Barcelona, Spain)

**09:05 Can Humans Learn from Machine Learning in Drug Discovery? (PL12)**

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

**09:45 Short Lecture 20**

**10:15 Short Lecture 21**

**10:45 Coffee break**

#### Session 14 - Hansch & Fujita Awards

**11:15 Session Chair**

Prof. Andrea CAVALLI (UNIVERSITY OF BOLOGNA AND IIT, Bologna, Italy)  
Prof. Tudor I. OPREA (UNIVERSITY OF NEW MEXICO, Albuquerque, United States)

**11:20 Hansch Award Lecture**

**12:00 Fujita Award Lecture**

**12:40 Closing Ceremony**

Dr Jordi MESTRES  
(IMIM HOSPITAL DEL MAR MEDICAL RESEARCH INSTITUTE, Barcelona, Spain)