

Confirmed Speakers

Plenary Lectures

Title to be announced (PL01)



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

Title to be announced (PL03)



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

Title to be announced (PL07)



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

Towards Machine Learning-Driven Drug Development (PL09)



Prof. Olivier ELEMENTO
(CORNELL UNIVERSITY, New York, United States)

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



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

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



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

Off-target Prediction Based on Binding Site Similarity (PL08)



PD Dr Oliver KOCH
(UNIVERSITY OF MÜNSTER, Münster, Germany)

Can Humans Learn from Machine Learning in Drug Discovery? (PL12)



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

Studies on Enzyme-Catalysed Reactions (PL11)

Confirmed Speakers



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

Enhancing Confidence in Computational Methods for the Evaluation of Drug Safety (PL05)



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

Systems Pharmacology Merging Omics Data and Biological Knowledge (PL02)



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

Title to be announced (PL10)



Dr Gary TRESADERN
(JANSSEN, Beerse, Belgium)

In Memoriam Lectures - Peter Goodford

Short Lecture 7



Prof. Gabriele CRUCIANI
(UNIVERSITY OF PERUGIA, Perugia, Italy)

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)

Session Lectures

Quantifying GPCR Signaling in an Oligomeric Context (SL12)



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