

Sunday September 22, 2024

- 15:00

Registration
- 17:00

Opening Ceremony

Prof. Jordi MESTRES
(UNIVERSITY OF GIRONA, Girona, Spain)

Fujita Award Lecture

Session Chair

Prof. Rebecca WADE
(HEIDELBERG UNIVERSITY AND HITS, Heidelberg, Germany)
- 17:20

Fujita Award Lecture 2024

Intelligence Aplification is much better than Artificial Intelligence (AL01)

Prof. Gabriele CRUCIANI
(UNIVERSITY OF PERUGIA, Perugia, Italy)
- 18:15

Welcome drink

24th EuroQSAR

Preliminary Programme

Monday September 23, 2024

- 08:00** **Registration**
- 09:00** **Session 1 - QSAR without Borders**
- 09:00** **Session Chair**
Prof. Alexander TROPSHA
(UNIVERSITY OF NORTH CAROLINA, Chapel Hill, United States)
- 09:05** **Plenary Lecture to be announced (PL01)**
- 09:45** **Session Lecture 01**
- 10:15** **Oral Communication 1**
- 10:35** **Coffee break**
- 11:05** **Session 2 - Generative models**
- 11:05** **Session Chair**
Dr Patrick ALOY
(INSTITUTE FOR RESEARCH IN BIOMEDICINE (IRB), Barcelona , Spain)
- 11:10** **Applying ML/AI to drug design (PL02)**
Dr Ola ENKVIST
(ASTRAZENECA, Mölndal, Sweden)
- 11:50** **Session Lecture 02**
- 12:20** **Oral Communication 2**
- 12:40** **Lunch, Exhibitions & Poster Session**
- 13:00** **Company Workshop**
- 14:10** **Session 3 - Protein Design**
- 14:10** **Session Chair**
Dr Silvia OSUNA
(UNIVERSITY OF GIRONA, Girona, Spain)

Preliminary Programme

- 14:15** **De Novo Protein Design: Expanding Sequence & Structure Space, Engineering Dynamics, and Building Synthetic Cellular Signaling (PL03)**
Prof. Tanja KORTemme
(UNIVERSITY OF CALIFORNIA SAN FRANCISCO, San Francisco, United States)
- 14:55** **Active Learning Processes in Biomolecular Modelling (SL03)**
Prof. Victor GUALLAR
(BARCELONA SUPERCOMPUTING CENTER, Barcelona, Spain)
- 15:25** **Oral Communication 3**
- 15:45** **Coffee break**
- 16:15** **Session Chair**
- 16:15** **Session 4 - Hall of Fame**
- 16:20** **Title to be announced (SL04)**
Dr Yvonne C. MARTIN
(ABBVIE, North Chicago, IL, United States)
- 16:50** **From LogP to Early Human Dose Projections (SL05)**
Dr Ingo MÜGGE
(ALKERMES, Waltham, MA, United States)
- 17:20** **Poster Session**

Tuesday September 24, 2024

- 09:00** **Session 5 - Ultra-Large Chemical Spaces**
- 09:00** **Session Chair**
Dr Barbara ZDRAZIL
(EMBL-EBI, Hinxton, United Kingdom)
- 09:05** **Chemical Space from First Principles (PL04)**
Prof. Jean-Louis REYMOND
(UNIVERSITY OF BERN, Bern, Switzerland)
- 09:45** **Title to be announced (SL05)**
Prof. Francesco GENTILE
(UNIVERSITY OF OTTAWA, Ottawa, Canada)
- 10:15** **Oral Communication 4**
- 10:35** **Coffee break**
- 11:05** **Session 6 - New Drug Modalities**
- 11:05** **Session Chair**
Dr Albert A. ANTOLIN
(CATALAN INSTITUTE OF ONCOLOGY - IDIBELL, Barcelona, Spain)
- 11:10** **Modelling a (New) Modality: Computational Tools for Peptide Design (PL05)**
Dr Thomas FOX
(BOEHRINGER INGELHEIM PHARMA GMBH & CO KG, Biberach, Germany)
- 11:50** **Session Lecture 07**
- 12:20** **Oral Communication 5**
- 12:40** **Lunch, Exhibitions & Poster Session**
- 13:00** **Company Workshop**
- 14:10** **Session 7 - Synthetic Data**
- 14:10** **Session Chair**
Dr Roger ESTRADA-TEJEDOR
(IQS SCHOOL OF ENGINEERING - URL, Barcelona, Spain)
- 14:15** **Plenary Lecture to be announced (PL06)**

Preliminary Programme

14:55	Session Lecture 08
15:25	Oral Communication 6
15:45	Coffee break
16:15	Session 8 - New Trends in Molecular Dynamics
16:15	Session Chair Prof. Giovanni BOTTEGONI (UNIVERSITY OF URBINO, Urbino, Italy)
16:20	Enzyme Mechanism and Dynamics in Drug Resistance, Evolution and Catalyst Design (PL07) Prof. Adrian J MULHOLLAND (UNIVERSITY OF BRISTOL, Bristol, United Kingdom)
17:00	Title to be announced (SL09) Dr Gianni DE FABRITIIS (ACELLERA, Barcelona , Spain)
17:30	Oral Communication 7
17:50	Poster Session

Wednesday September 25, 2024

- 09:00** **Session 9 - Artificial Intelligence in Drug Discovery**
- 09:00** **Session Chair**
Prof. Tudor I. OPREA
(ROIVANT SCIENCES INC., Albuquerque, United States)
- 09:05** **The CACHE Computational Hit Finding Initiative: Latest Results and Learnings (PL08)**
Dr Matthieu SCHAPIRA
(UNIVERSITY OF TORONTO, Toronto, Canada)
- 09:45** **Session Lecture 10**
- 10:15** **Oral Communication 8**
- 10:35** **Coffee break**
- 11:05** **Session 10 - Translational Safety**
- 11:05** **Session Chair**
Dr Scott BOYER
(CHEMOTARGETS, Barcelona, Spain)
- 11:10** **Title to be announced (PL09)**
Dr Thomas B. KNUDSEN
(US EPA, Madison, WI, United States)
- 11:50** **Session Lecture 11**
- 12:20** **Oral Communication 9**
- 12:40** **Lunch, Exhibitions & Poster Session**
- 13:00** **Company Workshop**
- 14:10** **Session 11 - Multiscale Modelling**
- 14:10** **Session Chair**
Prof. Andrea CAVALLI
(UNIVERSITY OF BOLOGNA AND IIT, Bologna, Italy)
- 14:15** **Plenary Lecture to be announced (PL10)**

Preliminary Programme

- 14:55** **Session Lecture 12**
- 15:25** **Oral Communication 10**
- 15:45** **Coffee break**
- 16:15** **Session 12 - Target-Oriented Drug Discovery**
- 16:15** **Session Chair**
Prof. Harel WEINSTEIN
(CORNELL UNIVERSITY, New York, United States)
- 16:20** **Targeting the Active Site of Splicing Machines (PL11)**
Dr Marco DE VIVO
(ITALIAN INSTITUTE OF TECHNOLOGY, Genova, Italy)
- 17:00** **Understanding Molecular Recognition and Protein-Ligand Binding (SL13)**
Prof. William L. JORGENSEN (YALE UNIVERSITY, New Haven, United States)
(SOPLVIAS AG (WAS FUJIFILM))
- 17:30** **Title to be announced (Oral Communication 11)**
Dr Maria-José FALAGUERA
(EMBL-EBI, Hinxton, United Kingdom)
- 20:00** **Conference dinner**

Thursday September 26, 2024

- 09:00** **Session 13 - The Challenges Ahead**
- 09:00** **Session Chair**
Prof. Jordi MESTRES
(UNIVERSITY OF GIRONA, Girona, Spain)
- 09:05** **Title to be announced (PL12)**
Dr John OVERINGTON
(EXSCIENTIA, Oxford , United Kingdom)
- 09:45** **Title to be announced (SL14)**
Dr Alex ALIPER
(INSILICO MEDICINE, Abu Dhabi, United Arab Emirates)
- 10:15** **Oral Communication 12**
- 10:35** **Coffee break**
- 11:05** **Hansch Award Lectures**
- 11:05** **Session Chair**
Prof. Rebecca WADE
(HEIDELBERG UNIVERSITY AND HITS, Heidelberg, Germany)
- 11:10** **Hansch Award Lecture 2024**
Combining MD Simulations and Machine Learning for the Study of Biomolecular Systems (AL02)
Prof. Sereina RINIKER
(ETH ZÜRICH, Zurich, Switzerland)
- 11:50** **Hansch Award Lecture 2024 (AL03)**
Prof. Philippe SCHWALLER
(ECOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE (EPFL), Lausanne, Switzerland)
- 12:30** **Closing Ceremony**
Prof. Jordi MESTRES
(UNIVERSITY OF GIRONA, Girona, Spain)