

9:23 – 9:30 Opening session.

Chair: Vicent Moliner

9:30 – 10:00 **Donald Hilvert**. ETH Zurich, Switzerland.

“Adventures with AI-guided enzyme design “

10:00 – 10:30 **Stephan Hammer**. Bielefeld University. Germany.

“New catalytic reactions by enzyme engineering”

10:30 – 11:00 **Fernando López-Gallego**. CIC biomaGUNE. Donostia

“Lipase-driven alcoholysis of polyether polyurethanes towards a closed-loop plastic recycling”

11:00 – 11:30 Coffee-Tea break

Chair: Sergio Marti

11:30 – 12:00 **Joelle Pelletier**. University of Montreal. Canada.

“From a binding domain to the emergence of a catalyst conferring intrinsic antibiotic resistance “

12:00 – 12:30 **Andrea Cavalli**. CECAM-EPFL, Lausanne, Switzerland.

“Towards Fully Dynamical Docking via Molecular Dynamics and Related Methods“

12:30 – 13:00 **Sam Hay**. University of Manchester, United Kingdom.

“Deciphering the mechanism of new photoenzymes“

13:00 – 15:00 Lunch

Chair: Raquel Castillo

15:00 – 15:30 **Johan Åqvist**. Uppsala Universitet. Sweden.

“Computational Design of the Temperature Dependence of Enzyme Reactions”

15:30 – 16:00 **Ferran Feixas**. Universitat de Girona. Girona.

“Decoding the principles of long-range regulation in enzymatic catalysis and evolution”

16:00 – 16:30 **Maria José Hernaiz**. Universidad Complutense de Madrid. Madrid

“Biocatalysis as a Green Approach for the Preparation of Multivalent Glyco-Carbon Platforms with Therapeutic Potential “

16:30 – 17:00 Coffee-Tea break

Chair: Maite Roca

17:00 - 17:30 **Angela Casini**. Technical University of Munich. Germany.

“Organometallic catalysis in cells for medicinal applications: a new era in drug discovery “

17:30 - 18:00 **Per-Olof Syrén**. KTH Royal Institute of Technology. Stockholm. Sweden.

“Cascade depolymerization of polyurethanes“

18:00 - 18:30 **Marcin Drag**. Polish Academy of Sciences, Poland

“Unnatural amino acids - perfection at its best”

20:30 – 24:00 Dinner

Chair: Katarzyna Świderek

09:30 – 10:00 **Ania Fryszkowska**. Novartis AG, Basel, Switzerland

“Biocatalysis in sustainable drug discovery and development – evolving perspective from pharmaceutical industry“

10:00 – 10:30 **Miguel Alcalde**. Institute of Catalysis, CSIC. Madrid.

“Engineering peroxygenases on the route”

10:30 - 11:00 **Damien Laage**. École normale supérieure – PSL, Paris. France

“A molecular picture of allosteric communication in dihydrofolate reductase“

11:00 – 11:30 Brunch break

Chair: Vicent Moliner

11:30 – 12:00 **Ashwin Chari**. Max-Planck Institute for Multidisciplinary Sciences.
Göttingen. Germany.

“High-precision, high-accuracy macromolecular crystallography“

12:00 – 12:30 **Adrian J. Mulholland**. University of Bristol. United Kingdom.

“Evolution of natural and designer enzymes: simulations to guide biocatalyst design and engineering“

12:30 – 13:00 **Lorenzo Casalino**. University of California San Diego. USA.

“Multiscale Computational Microscopy of Viral Glycoproteins“

13:00 – 13:07 “Concluding remarks”