

TrEnCa2024 21st-22nd of November 2024, Benicassim, Spain

21st of November

9:23 – 9:30 Opening session.

Chair: Vicent Moliner

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

“De novo design of hydrolytic enzymes”

10:00 – 10:30 **Juan Mangas**. Universidad de Oviedo. Oviedo.

“Organocatalysed hydration of activated alkynes”

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

“Región-directed immobilization of enzymes through structure-guide surface engineering”

11:00 – 11:30 Coffee-Tea break

Chair: Maite Roca

11:30 – 12:00 **Gerardo Andres Cisneros**, University of Texas at Dallas. USA.

“QM/MM Simulations with Advanced Polarizable Potentials: The case of HRP catalysis”

12:00 – 12:30 **Xabi López**. Euskal Erriko Unibertsitatea.(UPV/EHU) and DIPC. Donostia.

“Intrinsically disordered peptides and regions: the importance of the conformational ensemble revealed by atomistic simulations.”

12:30 – 13:00 **Susana Carregal Romero**. CIC biomaGUNE. Donostia.

“Catalytic therapies using metal oxide nanoparticles as enzyme mimic”

12:00 – 12:30 **Silvia Osuna**. IQCC. Universitat de Girona. (Spain)

“Decoding Nature’s Catalysts for Rational Enzyme Design”

13:30 – 15:00 Lunch

Chair: Sergio Marti

15:00 – 15:30 **Marco De Vivo**. Istituto Italiano di Tecnologia. Italy.

“Cutinase proteins to process non-natural polyesters”

15:30 – 16:00 **Victor Guallar**. Barcelona Supercomputer Center. Barcelona.

“Got Plurizymes? Calm your thirst of cool enzymes “

16:00 – 16:30 **Miguel Alcalde**. Institute of Catalysis, CSIC. Madrid.

“When directed evolution met ancestral enzyme resurrection”

16:30 – 17:00 Coffee-Tea break

Chair: Raquel Castillo

17:00 - 17:30 **Jesús Jiménez-Barbero**. CICbioGUNE. Derio, Spain.

“Breaking the limits in understanding glycan recognition by NMR”

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

“The importance of conformations in enzymatic plastic degradation”

18:00 - 18:30 **Marcin Drag**. Wroclaw University of Science and Technology. Poland

“In search of perfection - the phenomenon of unnatural amino acids”

18:30 - 19:00 **Marc van der Kamp**. University of Bristol. United Kingdom.

Efficient multiscale simulations to aid enzyme engineering: methods, tools and applications”

20:30 – 24:00 Dinner

22nd of November

Chair: Katarzyna Świderek

09:30 – 10:00 **Gerard Roelfes**. Stratingh Institute for Chemistry. University of Groningen. The

Netherlands.

“Designer enzymes featuring abiological catalytic sites “

10:00 – 10:30 **Agnieszka Dobrzyń**. Nencki Institute of Experimental Biology, PAS. Poland.

“Stearoyl-CoA Desaturase – Friend or Foe in Developing Regenerative Medicine Applications for Diabetes Treatment”

10:30 - 11:00 **Masayuki Oda**. Kyoto Prefectural University. Japan.

“Structural dynamics of the Ca²⁺-regulated cutinase and its structure-based improvement of PET degradation activity“

11:00 – 11:30 Brunch break

Chair: Vicent Moliner

11:30 – 12:00 **Qiang Cui**. Boston University. USA

“Exploring effects of distant mutations and enzyme engineering with molecular simulations?”

12:00 – 12:30 **Petra Imhof**. Friedrich-Alexander-Universität, Erlangen-Nürnberg. Germany.

“Can we understand specificity from enzyme-substrate interactions?”

12:30 – 13:00 **Patrick Aloy** Institute for Research in Biomedicine (IRB). Barcelona.

“Blending biology, chemistry and AI to enable systems pharmacology“

13:00-13:15 **I. López-Carregal** CIC biomaGUNE. Donostia.

"Histories of a small world"

13:15 – 13:22 “Concluding remarks”

13:30 - 15:00 Lunch at Cafeteria