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Objectives

We are pleased to announce the first BSC workshop on Computational Enzyme Bioprospecting and Engineering, which is being organized as part of the European projects FuturEnzyme (https://www.futurenzyme.eu/) and Oxipro (https://www.oxipro.eu/). This event will provide a comprehensive overview of the principles and techniques used in this exciting field, including the latest advancements and techniques in protein engineering using computational methods such as bioprospecting, molecular simulations, and artificial intelligence.

Our aim is to equip attendees with the knowledge and tools necessary to design and engineer proteins with enhanced properties, whether they are seasoned researchers or new to the field. The workshop will feature talks from leading experts, including Dr. Pablo Pérez García from the University of Hamburg, who will discuss the discovery of new enzymes with HMM-based bioprospecting, Dr. Sergi Rodà Llordés from Nostrum Biodiscovery, who will present AsiteDesign, a semi-rational algorithm for automated enzyme design, and Dr. Hein J Wijma from the University of Groningen, who will introduce FRESCO, a rapid computational protocol for enhancing protein stability.

Our objectives for the workshop include promoting interdisciplinary thinking and collaboration between different fields, highlighting the real-world applications of computational protein engineering, introducing participants to the leading software for computational protein engineering, and promoting the importance of computational protein engineering in advancing our understanding of biological systems and developing new solutions for global challenges.

Please stay tuned for more information on the dates and registration for this exciting event.

Check the program of the event.

This workshop has been organized with the support of FuturEnzyme (DOI 10.3030/101000327) and Oxipro (DOI 10.3030/101000607) projects, as well as the collaboration of M. Ferrer (supported by MICINN and AEI (DOI 10.13039/501100011033) and the "NextGenerationEU/PRTR"; PID2020-112758RB-I00, PDC2021-121534-I00, TED2021-130544B-I00). We are grateful for their contributions to the success of this workshop.

Objectives

- 1. Comprehensive understanding of the principles and techniques used in computational protein engineering.
- 2. Introduce participants to the leading software for computational protein engineering.

- 3. Real-world applications of computational protein engineering.
- 4. Encourage interdisciplinary thinking and collaboration between different fields.
- 5. Promote the importance of computational protein engineering in advancing our understanding of biological systems and developing new solutions for global challenges.

Presenters

Albert Cañellas Solé

Rubén Muñoz Tafalla

Ruite Xiang

Ana Robles Martín

Martin Floor Pilquil

Chairs

Martin Floor Pilquil

Victor Guallar Tasies

Invited talks

Dr. Pablo Pérez García (University of Hamburg), Discovering New Enzymes with HMM-Based Bioprospecting

Dr. Sergi Rodà Llordés (Nostrum Biodiscovery), AsiteDesign: A semi-rational algorithm for automated enzyme design

Dr. Hein J Wijma (University of Groningen), FRESCO: A Rapid Computational Protocol for Enhancing Protein Stability



Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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