First BSC workshop on Computational Enzyme Bioprospecting and Engineering

Day 1 - 22nd May, 2023

Introduction

9:00 - 9:30: Registration and Welcome

- Participants check-in at the BSC hall and receive a brief welcome and introduction to the workshop.

9:30 - 10:00: Session 1 - Introduction and Key Concepts

- Protein Engineering introduction and its importance.
- Key concepts and theories, including the machine learning revolution in biocatalysis, are covered.

In silico Bioprospecting

10:00 - 10:50: Session 2 - High throughput *in silico* Bioprospecting

- An introduction to computational bioprospecting and its relevance for enzyme discovery and engineering.

10:50 - 11:10: Coffee Break

11:10 - 11:50: Session 3 - Discovering New Enzymes with HMM-Based Bioprospecting. Invited Speaker: Dr. Pablo Pérez García

11:50 - 12:30: Session 4 - The potential of machine learning in bioprospecting

- EP-Pred for the bioprospecting of promiscuous ester hydrolases.
- Generative adversarial networks (GANs) as an infinite source of synthetic protein sequences.

12:30 - 14:15: Lunch Break

- Informal presentation and discussion with the Coordinators of FUTURENZYME, Dr. Manuel Ferrer, and OXIPRO, Dr. Gro Bjerga (remote connection).

14:15 - 14:45: Session 5 - Bioexcel building blocks and workflow theory

- Discussion of the importance and benefits of using building blocks in scientific workflows for computational modeling and simulation.

14:45 - 18:00: Session 6 - Hands-on (I)

- Participants engage in a practical, hands-on activity related to the workshop sessions of Bioprospecting.

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Day 2 - 23rd May, 2023
Protein Engineering

9:00 - 9:40: Session 7 - System Preparation for Protein Simulations

- Selection and preparation of the protein structure for simulations, including protonation states, water molecules…
- Overview of recommended tools and software.

9:40 - 10:20: Session 8 - AsiteDesign: A semi-rational algorithm for automated enzyme design. Invited Speaker: Dr. Sergi Rodà Llordés

10:20 - 10:40: Coffee Break

10:40 - 11:20: Session 9 - Multiobjective optimization for Protein Engineering

11:20 - 12:00: Session 10 - Protein Energy Landscape Exploration (PELE) software

- Theory and methodology of PELE software for simulating protein-substrate binding affinity with high accuracy and efficiency.
- Applications of PELE in protein engineering for industrial biotechnology.

12:00 - 12:45: Session 11 - FRESCO: A Rapid Computational Protocol for Enhancing Protein Stability. Invited Speaker: Dr. Hein J Wijma

12:45 - 14:00: Lunch Break

14:00 - 18:00: Session 12 - Hands-on (II)

- Participants engage in a practical, hands-on activity related to the workshop sessions of Protein Engineering.

Acknowledgments

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.

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