



MARIE SKŁODOWSKA-CURIE POSTDOCTORAL FELLOWSHIPS 2022

EXPRESSION OF INTEREST IN HOSTING MARIE CURIE FELLOWS

HOST INSTITUTION

ITQB NOVA - MOSTMICRO

RESEARCH GROUP AND URL

Microbial & Enzyme Technology (MET) Laboratory / <https://www.itqb.unl.pt/research/biological-chemistry/microbial-enzyme-technology>

SUPERVISOR (NAME AND E-MAIL)

Lígia O Martins (lmartins@itqb.unl.pt)

SHORT CV OF THE SUPERVISOR

LO Martins is an Associate Professor and Principal Investigator of MET lab. Several oxidoreductive enzymes have been investigated by combining Microbiology, Molecular Biology, Biochemistry, Enzymology, and Structural Biology. Engineering methodologies, including rational, semi-rational, and directed evolution, were developed to improve the enzyme's performance and robustness and understand their functional properties. A toolbox of experimental approaches was mounted to explore biocatalysts in biodegradation and synthesis. LO Martins has coordinated six national projects and has been a team member of large EC-funded projects (SMARTBOX, ongoing). Currently, she coordinates the B-Ligzymes RISE-H2020 project (2019-2024). She has published 80+ papers (15 with 100+ citations, h-index = 39), three book chapters, and one patent. She has supervised 7 Post-docs and 11 Ph.D., 17 MSc, and 50+ graduate and undergraduate students. She has been a member of the Biocatalysis Board of the European Federation of Biotechnology since 2020.

5 SELECTED PUBLICATIONS

Brissos et al 2022. Distal mutations shape substrate-binding sites during evolution of a metallo-oxidase into a laccase *ACS Catal* 12: 5022

Rodrigues et al. 2021 Loops around the heme pocket have a critical role in the function and stability of BsDyO from *Bacillus subtilis*. *Int J Mol Sci*, 22:10862

Borges et al. 2020. Methionine-Rich loop of multicopper oxidase McoA follows open-to-close transitions with a role in enzyme catalysis. *ACS Catal* 10, 7162

Brissos et al. 2017. Engineering a Bacterial DyP-type Peroxidase for Enhanced Oxidation of Lignin-related Phenolics at Alkaline pH. *ACS Catal*. 7, 3454

Brissos et al. 2015 Turning a hyperthermostable metallo-oxidase into a laccase by directed evolution. *ACS Catal* 5: 4932

PROJECT TITLE AND SHORT DESCRIPTION

Title: Application of Computational Tools for Investigating Engineered Enzymes

Directed Evolution is the most recognized methodology for improving enzymes' properties. The characterization of engineered proteins allows the unveiling of key structure-function relationships such as details of catalytic mechanisms, protein stability, and substrate specificity. Furthermore the investigation of molecular changes underlying the optimization of enzyme function gives light to mechanisms enzyme evolution. These endeavors facilitate the future design of new protein functions.

Keywords: Computational biochemistry; Bioinformatics; Sequence and Network analysis; Quantum/Molecular mechanics; Molecular Dynamics; Monte-Carlo simulations.

SCIENTIFIC AREA WHERE THE PROJECT FITS BEST*

LIF – ENV - CHE

***Scientific Area where the project fits best** – Please select/indicate the scientific area according to the panel evaluation areas: Chemistry (CHE) • Social Sciences and Humanities (SOC) • Economic Sciences (ECO) • Information Science and Engineering (ENG) • Environment and Geosciences (ENV) • Life Sciences (LIF) • Mathematics (MAT) • Physics (PHY)