Title: Simulation and engineering of plastic-degrading enzymes

In tight collaboration with experiments, this proposal aims to develop a computational framework based on the combination of de-novo protein design by deep learning with advanced biomolecular simulations to build the next-generation of nature-inspired biotechnological catalysts for the depolymerization of high-crystallinity PET. The successful implementation of the project will open new avenues to plastic waste treatment & recycling toward a PET circular economy. By empowering circularity, it will enforce the protection of hydric and marine resources and prevent and control pollution.

We are a young and ambitious team that, with computer simulations as core technology, pursues highly interdisciplinary molecular research that ranges from computational molecular biophysics, plastic-degrading enzymes, to drug discovery and molecular evolution. We develop and apply molecular simulations approaches to impulse a paradigm shift in marine sciences based on the 3D and 4D (the 4th dimension being time) representation of biomolecular processes in the Ocean. Besides our headquarter at IQAC-CSIC, we have tight collaborations with experimental groups at the Institute of Marine Sciences (ICM-CSIC) and abroad, and we are embedded in an interdisciplinary network with excellent and infrastructures at our disposal.

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