Position Offered: UNIVERSITY GRADUATE

Project: *Revolutionizing Protein Drug Development - AI-driven Protein Engineering for Next-Generation Enzyme Therapy.*

Technological and scientific fields: Computational Biology; AI; Design of New Protein Drugs.

Location: Barcelona, Catalunya. Molecular Biology Institute of Barcelona, https://ibmb.csic.es/.

Research Group/PI: Synthetic Structural Biology, Ulrich Eckhard, https://bit.ly/UlrichEckhard. Protein Design and Modeling Lab, Enrique Marcos Benteo, https://bit.ly/EnriqueMarcos.

PROJECT SUMMARY

Enzymes are invaluable tools for biotechnology and medicine, but their structural complexity poses significant challenges for optimization and practical use. While directed evolution and structural bioinformatics can improve enzyme catalytic efficiency and specificity, these methods fall short for reducing structural complexity, increasing solubility, and enabling large-scale expression in bacteria. We plan to develop an AI-driven computational pipeline for enzyme design and optimization, integrating structural bioinformatics, deep learning-based protein structure prediction and design, high-performance computing, and experimental feedback. Our goal is to transform complex enzyme drugs, typically produced in costly mammalian systems, into robust proteins for high-yield production in bacterial systems, potentially revolutionizing the protein drug industry by providing sustainable biotechnological and medical solutions.

PROFESSIONAL PROFILE

Minimum requirements:

We are looking for a highly motivated scientist with initiative and strong motivation in combining computational techniques (protein design, docking, molecular dynamics) with experimental testing for protein drug development. The candidate must have studies in Biology, Biochemistry, Biotechnology, or related disciplines. Good English communication skills and basic computational experience is expected.

Merits to be considered:

Potential merits to be considered include: familiarity with AI-based methods for protein structure prediction; experience with molecular modelling tools; experience in protein expression, purification, and characterization techniques; strong motivation for combining computational and experimental approaches in enzyme design; documented research experience and publications.

WHAT IS OFFERED

We offer state-of-the art training in computational enzyme design, protein engineering, and high-throughput protein characterization. The candidate will be provided with extensive training on physics- and AI-based computational methods for protein modeling and subsequent experimental characterization through research, courses and short-stays abroad. The training encompasses a wide range of methods and programs for structure analysis, prediction, design, ligand docking, and molecular dynamics to assess protein flexibility. The candidate will receive training in programming languages such as Python and Bash, and will learn to utilize (inter)national supercomputing resources.

Contract conditions:

Indefinite contract for a University Graduate associated with the Momentum Project of 4 years' duration according to Spanish science law. Gross annual salary (37.000 € - 41.000 €).

Start of contract: before 31 December 2024

PRINCIPAL INVESTIGATOR CONTACT

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