

# Position Offered: UNIVERSITY GRADUATE

## Project: *Using protein design AI-based methods for the development of bioenzymes with therapeutic applications*

**Technological and scientific fields:** Structural biology, computational protein design and modelling, artificial intelligence

**Location:** Madrid, Comunidad de Madrid, Institute of Physical Chemistry Blas Cabrera (IQF) <https://www.iqf.csic.es/en/>

**Research Group/PI:** Crystallography and Structural Biology <https://www.xtal.iqfr.csic.es/>.  
PI: Inmaculada Pérez Dorado (<https://jiperez3.wixsite.com/perezdorado-group>)

### PROJECT SUMMARY

This program aims to train a motivated researcher in cutting-edge digital skills to be applied in bioenzyme design with therapeutic application in infectious diseases and with a high impact on human health. The hired candidate will acquire in-depth experience and competencies in the use of computational approaches, from artificial intelligence (AI) algorithms applied to protein design to molecular docking and molecular dynamics methods, oriented to the computational design of enzymes. This training program is supported by a solid experience of the two host groups in structural and computational biology, as well as by a rigorous training program in computational methods, including AI and programming.

### PROFESSIONAL PROFILE

#### Minimum requirements:

- Academic qualifications: Graduate in Chemistry, Pharmacy, Biotechnology or related biosciences.
- Good proficiency in English

#### Merits to be considered:

- Knowledge in structural biology
- Knowledge in Linux and Python

### WHAT IS OFFERED

We offer a training plan of 289 ECTS, to be completed along the 4 years of contract, and to be conducted by the groups of Dr. I. Pérez-Dorado (CSIC) and Prof. F. Gago (Universidad de Alcalá). This training plan will allow the candidate to acquire in-depth knowledge in computational approaches from a general perspective, as well as focused on R+D in biosciences and structural biology. This program ranges from training in the application and use of AI and other computational techniques applied to the study and design of proteins, to programming languages used in AI, and the creation of advanced software based on AI and machine learning, through the following objectives:

1. Training in advanced in silico approaches for structural validation of bioenzymes
2. Training in state-of-the-art digital competencies for bioenzyme design
3. Training in in silico and in vitro approaches to validate the activity of synthetic bioenzymes

The training program includes a 3-months stay in the group of Prof. Gago's and a master in AI, as well as additional training in the form of courses and workshops in computational structural biology, AI and programming.

#### 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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