

Position Offered: UNIVERSITY GRADUATE

Project: *Automated Discovery of Biocatalysts through Artificial Intelligence for the Production of Compounds of Pharmaceutical Interest*

Technological and scientific fields: Artificial Intelligence, Biotech, Computational Biology, Data Analysis and Integration, New Drug Design

Location: Zaragoza, Aragón, ISQCH, <http://isqch.unizar-csic.es/ISQCHportal>

Research Group/PI: The Alegre Group, Juan V. Alegre Requena, <https://thealegregroup.com>

PROJECT SUMMARY

This project will advance basic knowledge in digital biocatalysis, as well as promote the use of artificial intelligence protocols to design new biocatalysts and synthesize high-value chemicals such as pharmaceuticals. The ability to design biocatalysts through computational approaches not only increases the efficiency of their discovery, but also opens the door to performing complex chemical transformations that were previously considered unattainable. This advanced methodology promises to offer greener and more economical solutions for the synthesis of chemical products that are attractive to the chemical and pharmaceutical industries.

PROFESSIONAL PROFILE

Minimum requirements:

- Licenciante or Graduate and MSc in Chemistry
- Proficiency in English

Merits to be considered:

- Knowledge of chemical machine learning and computational chemistry
- Experience with Python
- Proficiency in Gaussian

WHAT IS OFFERED

- 160 ECTS including bibliographic work, carrying out the proposed research, writing articles, and conference presentations
- 60 ECTS in research stays at the University of Girona and international institutions
- 120 ECTS in learning to code, familiarizing with computational chemistry programs, conducting data analysis and interpretation, and developing predictive artificial intelligence models, among other digital competencies
- 40 ECTS in scientific dissemination and supervision of junior group members

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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