

ELEGANCE: machine Learning for integrated multi-parametric enzyme and bioprocess design

DC4: ML-guided evolution of peroxygenases for selective C-H oxygenation reactions

Organization

The **Spanish National Research Council (CSIC)** is the largest public research performing organisation (RPO) in Spain, the fourth most relevant public institution in the European Union, and the sixth in the world. Attached to the Ministry of Science and Innovation, with independent legal personality, the CSIC plays a key role in scientific and technological policy in Spain and around the world. Its aim is “the promotion, coordination, development and dissemination of multidisciplinary scientific and technological research to contribute to the advancement of knowledge and economic, social, and cultural development, as well as the training of personnel and advice to public and private entities in these fields”. CSIC carries out research, innovation, and training activities in all fields of knowledge – from the most basic or fundamental aspects of science to the most complex technological developments – distributed in three global areas: Life, Society, and Matter. These areas include human and social sciences, food science and technology, biology, biomedicine, physics, chemistry, and materials, natural resources or agricultural sciences, among others.

The doctoral candidate (DC) will work at the Institute of Catalysis and Petrochemistry (ICP) (<https://icp.csic.es/es/>), within the Department of Biocatalysis, in Madrid, Spain. ICP is a leading research centre within CSIC, dedicated to advancing sustainable chemical technologies. Its mission focuses on the development of advanced catalysts—both inorganic and enzymatic—to drive progress in energy, environmental protection, and selective chemical synthesis, following the principles of “green chemistry”. The ICP combines fundamental research and technological innovation to contribute to cleaner industrial processes, resource efficiency and circular economy goals.

in 2021.

The central research of Miguel Alcalde laboratory (<https://miguelalcaldelab.eu/>) at the Institute of Catalysis and Petrochemistry (ICP-CSIC) primarily focuses on the engineering of enzymes by directed molecular evolution and computational approaches for a wide range of biotechnological purposes; the development of screening tools and genetic methods for library construction and exploration, as well as synthetic biology studies for environmental, energy and industrial applications. Some of the highlighted scientific contributions of this group are the development of a plethora of library creation methods based on the *Saccharomyces cerevisiae* in vivo machinery, the conjunction of directed evolution with ancestral sequence reconstruction protocols, and the creation of dozens of evolved enzymes for different biotechnological purposes (ranging from pharma synthesis to the design of biomedical devices or bioremediation strategies). In a multi-disciplinary environment, the group stands out for its innovative research efforts and dynamic international collaborations.

Roles and responsibilities

The PhD will be carried out in 3 years at the **Institute of Catalysis and Petrochemistry** (ICP-CSIC, Madrid, Spain) under the supervision of **Prof. Miguel Alcalde** in the Directed Enzyme Evolution group, at the Department of Biocatalysis. During the PhD studies, it is expected that three research stays (2-3 months) will be conducted in the Czech Republic, France and the Netherlands. The Horizon Europe Marie Skłodowska-Curie Action (MSCA) doctoral network (DN) project starts in January 2026. The date of recruitment and state of the PhD project is planned for June 2026 and latest by December 2026. The PhD degree will be awarded based on successful completion of the research work at ICP-CSIC. The PhD student will also be required to participate in the training events organized by the DN and is expected to contribute with the dissemination of the PhD results via social media and public engagement.

The PhD project will focus on:

- Set up a machine-learning-assisted directed evolution platform (with unsupervised and supervised PLMs) for unspecific peroxygenases (UPOs).
- Generation of a portfolio of new-to-nature peroxygenases (both modern but also ancestral counterparts) with modified selectivities and improved stabilities for the production of pharmaceuticals, flavours and fragrances.
- Understanding the principles of mutational epistasis underlying the directed UPO evolution campaigns.

Main supervisor: Miguel Alcalde and David González, Institute of Catalysis and Petrochemistry, CSIC, Madrid, Spain

Co-supervisor 1: Stanislav Mazurenko, Faculty of Science, RECETOX, Loschmidt Laboratories, Czech Republic

Co-supervisor 2: Frédéric Cadet, Artificial Intelligence, PEACCEL, France

Co-supervisor 3: Frank Hollmann and Marieke Klijn, Dept. of Biotechnology, Delft University of Technology, The Netherlands

Qualifications:

- An outstanding M.Sc. degree in Biotechnology, Biochemistry, Biology, Chemistry, Molecular Biology, or related fields
- Experience with molecular biology techniques (PCR, mutagenesis, plasmid handling and cloning), microbial cultivation (*E. coli*, *S. cerevisiae* and *P. Pastoris*), and analytical techniques commonly used in biocatalysis
- Basic knowledge about directed evolution and/or protein engineering
- Bioinformatics (it will be an added value to have knowledge about machine learning and protein language models applied to protein engineering)
- Ability to work in a multidisciplinary and international team environment
- Interdisciplinary thinking, problem-solving orientation, and autonomy in the laboratory
- An integrative and cooperative personality with strong communication and social skills
- A high level of written and oral English is expected. English proficiency must be documented and verifiable

Preferred qualifications, but not mandatory:

- Experience in organic chemistry, spectroscopy, chromatography and other analytical techniques (HPLC, GC-MS, UV-Vis, and enzyme purification)
- Experience with high and ultrahigh-throughput screening, experimental design and data analysis
- Familiarity with bioinformatics tools and protein structural modeling. Basic programming is optional but valuable

Conditions of employment

You must have a master's degree (60 ECTS points).

Approval and Enrolment

The scholarship for the PhD degree is subject to academic approval, and the candidate will be enrolled in the Biomolecular Sciences or Microbiology PhD program at Universidad Autónoma de Madrid (UAM). For information about our enrolment requirements and the general planning of the PhD study programme, please see <https://www.uam.es/EscuelaDoctorado/Home.htm>

For more information about UAM's enrolment requirements, please visit: [https://www.uam.es/EscuelaDoctorado/\(es_ES\)-Acceso/1446832643299.htm](https://www.uam.es/EscuelaDoctorado/(es_ES)-Acceso/1446832643299.htm)

We offer

We are a dynamic research group committed to scientific excellence, innovation, and the advancement of cutting-edge biotechnology. We offer an engaging and stimulating position within a highly international and collaborative environment. Our workplace culture values integrity, openness, and teamwork, fostering both professional growth and personal development. In addition, candidates will have the opportunity to participate in a highly competitive and frontline research project, joining a community that promotes scientific ambition, creativity, and responsibility in equal measure.

Salary and appointment terms

The preferred starting date is 1st June 2026 or according to mutual agreement. The position is full time. The period of employment is 3 years. The gross monthly salary is **3,495.59 €**, including Living and Mobility allowances (Family allowances will be added if applicable). Payment will be made in 12 monthly installments, including pro-rated extra/bonus payments. We offer you in accordance with the internal policies of the CSIC and the Marie Skłodowska-Curie Actions (MSCA) Doctoral Networks, fully complying with applicable Spanish labor regulations. This ensures that all compensation meets the minimum legal requirements, as well as the standards set by MSCA for living allowance, mobility, and other relevant allowances. For more information about the salary calculations, visit: https://www.euraxess.es/system/files/2025-02/Guide%20on%20salary%20calculations%20for%20MSCA%20fellowships%20in%20Spain_0.pdf

Further information

Further information may be obtained from Miguel Alcalde: malcalde@icp.csic.es

Website about the MSCA doctoral network ELEGANCE: <https://elegance.dtu.dk/>

Google Scholar profile: <https://scholar.google.com/citations?user=mir4lawAAAAJ&hl=es>

Directed Enzyme Evolution group: <https://miguelalcaldelab.eu/>

More information about ICP-CSIC: <https://icp.csic.es/>

More information about CSIC: <https://www.csic.es/es>

More information about UAM: <https://www.uam.es/uam/inicio>

If you are applying from abroad, you may find useful information on working in Spain and at CSIC at:
<https://www.csic.es/es/internacional/aterrizar-en-el-csic>

Application procedure

Your complete online application must be submitted no later than **January 31st 2026 (23:59 Spanish time)**. Applications must be submitted as **one PDF file** containing all materials to be given consideration.

To apply, please open the link "Apply now", fill out the online application form, and attach **all your materials in English in one PDF file**. The file must include:

- A letter motivating the application (cover letter)
- Curriculum vitae
- Grade transcripts and BSc/MSc diploma (in English), including official description of grading scale

You may apply prior to obtaining your master's degree, but cannot begin before having received it.

Applications received after the deadline will not be considered.

The ICP and CSIC are committed to creating a research environment in which all staff and students are respected, valued, and feel welcome, irrespective of differences in background, experiences, perspectives, or identities. We consider inclusion, diversity, and equality to be a shared responsibility and actively work to foster a socially safe and supportive environment. Diversity among researchers enriches scientific discussion and contributes to the excellence and impact of our research. Our recruitment procedures follow the CSIC policies and the principles of the HRS4R initiative, in line with the European Commission's European Code of Conduct for the Recruitment of Researchers (<https://www.euraxess.es/spain/services/human-resources-strategy-researchers-hrs4r>).