ELEGANCE: machinE LEarning for inteGrated multi-parAmetric eNzyme and bioproCess dEsign

DC7: Engineering conformational dynamics and mechanism in oxygenases

Organization
The **University of Girona** (UdG), located in the city of Girona, has been part of the Catalan public university system since 1992. The UdG is devoted to excellence in both teaching and research, and it seeks to contribute to society's progress and development through the creation, dissemination, transference, and knowledge review related to Sciences, Technology, Humanities, and Arts. Over 100 research groups, distributed in 24 departments and 12 research institutes, comprise the University's rich and varied investigation landscape. A considerable part of this research is conducted in international contexts, where the UdG has gained wide experience in the management and coordination of international and European grants. UdG actively participates in European and international projects, with a strong focus on interdisciplinarity, cross-border cooperation, and global talent development. UdG is a member of the ACROSS European University Alliance, recognized by the European Commission, and actively contributes to cross-border knowledge sharing and regional development. Its UdG2030 strategy reinforces its commitment to the SDGs, digital transformation, gender equality, and climate resilience.

The doctoral candidate (DC) will work at Osuna group at the Institute of Computational Chemistry and Catalysis (IQCC) within the Department of Chemistry (http://iqcc.udg.edu/). IQCC is formed by world leaders in sustainable catalysis and computational chemistry and has extensive experience in heading and participating in large European research consortia. The vision of the institute to be aligned with EU initiatives is that scientific activities that impact in production and recycling methods at a molecular scale are called to be the main contributors in the transition towards a circular economy, and green energy for a more sustainable world for our future generations. Prof. Dr. Osuna's research group (https://www.osunalab.com/) offers a multicultural, inclusive and interdisciplinary research environment that integrates computational chemistry and synthetic biochemistry. The team maintains strong national and international collaborations (both academic and industrial) focusing on the computational design of enzymes for industrially and medically relevant targets. Their work centres on the computational modelling and design of new stable and active enzymes based on the application of conformation and correlation-based (Shortest Path Map, SPM) tools in combination with coevolutionary information.

Roles and responsibilities
The PhD will be carried out in 3 years at **the University of Girona** (UdG, Spain) under the supervision of **Prof. Dr. Sílvia Osuna** in the Department of Chemistry at the Institute of Computational Chemistry and Catalysis (IQCC). Within this time, it is expected that three research stays (2-3 months) will be conducted, two in academic groups in Germany and Czechia and one industrial stay in France. 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. Your PhD degree will be awarded based on successful completion of the research work at UdG. You will also be required to participate in the training events organized by the DN and you are expected to contribute with the dissemination of your PhD results via social media and public engagement.

The PhD project will focus on:
- Interdisciplinary project on bioinformatics, biocatalysis, and chemistry
- Development of physics- and data-based approaches for rationally generating new oxygenases
- Application of this methodology to rationally identify the subset of positions and potential amino acid replacements that will be experimentally validated
- Cloning, expression, and elucidation of enzyme promiscuity of selected candidates,
- Computational evaluation of the best hits found experimentally to identify key dynamic/structure descriptors and generate new variants with enhanced oxygenase activity
- Structural and mechanistic investigations of selected enzymes

Main supervisor: Sílvia Osuna, University of Girona, Spain
Co-supervisor 1: Josef Sivic, Czech Technical University in Prague, Czechia
Co-supervisor 2: Cecilia Clementi, Free University Berlin, Germany
Co-supervisor 3: Juliette Martin, Protéus, SEQENS, France

Qualifications:
- An outstanding M.Sc. degree in Chemistry, Biological chemistry, Biochemistry, or related field
- Eligible as a graduate student at the University of Girona (Spain)

- Research experience in computational modelling of biomolecular systems (bioinformatics, machine learning, molecular dynamics, quantum mechanics, python programming).
- Ability to work in an international team,
- Inter- and multidisciplinary thinking,
- High motivation,
- An integrative and cooperative personality with excellent communication and social skills,
- Fluency in English – written and oral.

Preferred qualifications but not mandatory:
- Experience in organic chemistry, analytical methods (HPLC, GC, MS, NMR etc.), enzyme purification and assays, experience in molecular biology (molecular cloning) is a plus
- Experience with automation and coding in Python or other programing language

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 Chemistry UdG PhD program. For information about our enrolment requirements and the general planning of the PhD study programme, please see ttps://www.udg.edu/en/ed.

We offer
UdG is a leading university globally recognized for the excellence of its research, education, innovation and scientific advice. We offer a rewarding and challenging job in an international environment. We strive for academic excellence in an environment characterized by collegial respect and academic freedom tempered by responsibility.

Salary and appointment terms
The preferred starting date is 1st June 2026 or according to mutual agreement. The position is full time. The average yearly salary is 3.310,84€ gross per month (Living and Mobility). We offer you in accordance with the Conveni col·lectiu PDI, el que estableix la Llei 17/2022 de 5 de setembre, per la que es modifica la Llei 14/2011 de 1 de juny, de la Ciència, la Tecnologia i la Innovació, art. 21 https://www.udg.edu/en/coneix/treballa-a-la-udg/personal-docent-i-investigador/legislacio. The period of employment is 3 years. The conditions of employment: https://www.udg.edu/en/coneix/treballa-a-la-udg/Pla-acollida-pdi and https://www.udg.edu/ca/investiga/hr-excellence-in-research/genere

Further information
Further information may be obtained from Sílvia Osuna: silvia.osuna@udg.edu
Website about MSCA doctoral network ELEGANCE: https://elegance.dtu.dk/
Google Scholar profile: https://scholar.google.com/citations?user=rHtokY4AAAAJ&hl=ca
OsunaLab group: https://www.osunalab.com/
More information about UdG IQCC: http://iqcc.udg.edu/
More information about UdG: https://www.udg.edu/en/

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 click 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.

All interested candidates irrespective of age, gender, disability, race, religion or ethnic background are encouraged to apply. The University of Girona strives to be a university in which students and staff are respected and feel at home, regardless of differences in background, experiences, perspectives, and identities. We believe that working on our core values of inclusion and equality are a joint responsibility and we are

constructively working on creating a socially safe environment. Diversity among students and staff members enriches academic debate and contributes to the quality of our teaching and research. We therefore invite applicants from underrepresented groups in particular to apply. Our selection procedure follows the HRS4R, https://guia-investigador.udg.edu/recerca-i-innovacio-responsable/hrs4r-estrategia-europea-de-rrhh/
European Commission's European Code of Conduct for recruitment of researchers, https://euraxess.ec.europa.eu/jobs/charter/code