

DC 8 | Halogenase engineering towards higher activities and halide promiscuity using AI-based computational tools

ORGANISATION

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 position we offer will be embedded in 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 main part of your PhD research (4 years in total) will be carried out at **the University of Girona** (UdG, Spain) under the supervision of **Prof. Silvia Osuna** in the Department of Chemistry at the Institute of Computational Chemistry and Catalysis (IQCC). Within these four years, an academic research stay (of 12 months) will take place at the **University of Groningen** (RUG, the Netherlands) under the supervision of **Prof. Sandy Schmidt**. Additionally, an industrial secondment at the company **Aminoverse** (the Netherlands) is foreseen. The Horizon Europe Marie Skłodowska-Curie Actions (MSCA) – Doctoral Network (DN) project starts in January 2026. The date of recruitment and start of the PhD project is planned for April 2026 and latest in December 2026. Your **PhD degree** (so-called double degree) will be awarded based on successful completion of the research work from **two universities (UdG, Spain and RUG, the Netherlands)**. You will also be required to participate in the training events and workshops organized by the DN- Joint Doctorates (JD) program. As a MSCA fellow, you are also expected to **contribute your time in the dissemination of your PhD project's result** through public engagement and other scientific platforms.

The PhD research will focus on:

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

Primary supervisor: Prof. Dr. Sílvia Osuna

Secondary supervisor: Prof. Dr. Sandy Schmidt

Recruiting institution: University of Girona (Girona, Spain)

Double degree awarding institution: University of Groningen (Groningen, the Netherlands)

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) and the University of Groningen (the Netherlands)
- Research experience in computational modelling of biomolecular systems (bioinformatics, machine learning, molecular dynamics, quantum mechanics, python programming). Additionally experience in organic chemistry, analytical methods (HPLC, GC, MS, NMR etc.), enzyme purification and assays, experience in molecular biology (molecular cloning) is a plus
- 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.

CONDITIONS OF EMPLOYMENT

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>

- a salary of 3.310,84€ gross per month (Living and Mobility)
- A PhD training programme is part of the agreement and the successful candidate will be enrolled in the Chemistry Sciences UdG PhD program.

The 1.0 FTE appointment is temporary for a specified period of four years. The preferred starting date is between April 1st and July 1st 2026. 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>

APPLICATION PROCEDURE

To apply for the position, kindly provide:

- (i) A letter of motivation including a statement of your research interests, relevant skills and experience and an explanation for the choice of position(s);
- (ii) A CV including publication list (if applicable);
- (iii) Names and contact details of up to three referees willing to write confidential letters of recommendation;
- (iv) Copies of relevant diplomas including explanation of international grades.

Please upload applications only according to instructions at <https://haloverse.eu/recruitment/>.

Address applications to: Prof. Dr. Sílvia Osuna

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/> and the [European Commission's European Code of Conduct for recruitment of researchers](#).

Unsolicited marketing is not appreciated.

APPLICATION DEADLINE

You may apply until 31st of December 2025 11:59pm / before 1st of January 2026 Central European Time (CET) for this position by means of the online application form (click on "Apply" below on the advertisement on the HaloVerse website).

MARIE SKŁODOWSKA-CURIE ACTIONS
Doctoral Networks (DN)



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