

Postdoctoral position at the Computational Chemistry Group

The Computational Chemistry Group led by [Dr. Gonzalo Jiménez-Osés](#) at CIC bioGUNE in Bilbao, Spain, seeks a highly skilled and motivated Postdoctoral candidate to develop multidisciplinary and highly collaborative projects in the interphase between Chemical Biology, Computation and Artificial Intelligence. Such projects are focused on drug design and development in collaboration with pharma companies, with strong emphasis on molecular docking, molecular dynamics, free energy calculations and machine learning. Skills in programming (Python) will be highly appreciated. In addition, he/she will participate in project management and planning, including the supervision of Ph.D. students.

The Computational Chemistry Group (CCG) constitutes a solid platform for the theoretical prediction of chemical reactions for Biorthogonal Chemistry, design and simulation of therapeutic peptides and proteins, and understanding Glycochemistry processes. A strong emphasis is made on the Computer-Aided Enzyme Design and Directed Evolution. The CCG tightly collaborates with leading national and international experimental labs with a particular interest in site-selective protein modification, whole-cell catalysis and laboratory evolution of enzymes for unnatural reactions.

Characteristics of the position

- A renewable **one-year contract (12 months)** is offered.
- It is desirable that the PhD degree was obtained not earlier than **5 years** at the time of application (for specific cases and exceptions, please contact us).

Characteristics of the position

- PhD degree in chemistry, biochemistry, computer science, or a related discipline.
- Strong hands-on skills on molecular dynamics, docking, bioinformatics and machine learning.
- Knowledge in chemistry and biochemistry basics, computer programming (Python), mathematical modeling and deep neural networks is strongly desired.
- A strong first-author publication record in the fields of Computational Chemistry and/or Bioinformatics.

Applications should contain the following documents

- An abbreviated curriculum vitae (four pages maximum) highlighting computational and machine learning training, particularly in the field of drug discovery.
- A brief letter (one page maximum) describing past research experience and future interests, as well as motivations for joining the group.
- Two signed reference letters explicitly detailing the candidate's skills and development and their professional experience with the candidate.

Candidates should submit their CV, a cover letter and the name and contact details of, at least, 2 references using the following [form](#) and indicating **44671** as reference.

