

# Post-doctoral Position Computational Chemistry, Bilbao



The Computational Chemistry Group led by [Dr. Gonzalo Jiménez-Osés](#) at CIC bioGUNE in Bilbao, Spain, seeks a highly skilled, open-minded, imaginative 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 the computational design and understanding of engineered enzymes subjected to natural and laboratory evolution, with strong emphasis on computational and experimental mutagenesis, multiscale molecular dynamics, big data analysis and machine learning. In addition, he/she will participate in project management and planning, including the supervision of Ph.D. students.

The Computational Chemistry Group (CCG) aims to create 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.

## Requirements of the ideal candidate:

- PhD degree in chemistry, biochemistry, computer science, engineering, physics or a related discipline.
- Strong hands-on skills on molecular dynamics, docking, bioinformatics and machine learning.
- Knowledge in chemistry and biochemistry basics, computer programming, mathematical modeling and artificial intelligence 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.
- A brief letter (one page maximum) declaring the reference number and 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.

Interested candidates should apply using the [form](#) and indicating [44672](#) as reference.