

## Junior postdoc in computer-aided drug design

### Offer Description:

- We are seeking a scientist with a solid background in molecular simulations eager to pursue a career in structure-based drug discovery.
- The work involves the discovery of druggable binding sites using mixed-solvent molecular dynamics, hit identification by means of virtual screening, and the development of confirmed hits into effective PROTAC molecules.
- Potentially, the candidate will also perform experimental testing with biophysical methods. Previous experience with these techniques will be a plus.
- You will be part of a multidisciplinary team including biophysicists, medicinal chemists, and virologists.

### Lab Description:

You will work in the Barril's lab (<http://www.ub.edu/bl>), in close collaboration with Galdeano's lab (<https://www.ub.edu/tpdlab>), both at the Faculty of Pharmacy, University of Barcelona.

### Essential Requirements:

The ideal candidate holds a PhD, has a solid understanding of molecular recognition, demonstrated experience in the use of molecular dynamics and has a strong interest in drug discovery. Advanced analytical and critical problem-solving skills are essential, as is the ability to deal with multiple tasks simultaneously, delivering results in a timely manner.

The following specific computational chemistry skills are considered essential:

- Molecular dynamics
- Molecular docking (protein-ligand)
- Command of shell scripting, python programming and the use of high-performance computing environments.

### Additional Competencies:

While not essential, the ideal candidate will also have experience in the execution of biophysical experiments. Surface plasmon resonance and isothermal titration calorimetry are particularly relevant for this project.

Knowledge of one or more of these specific areas is an important advantage:

- Bioinformatics
- Targeted protein degradation
- Chemoinformatics
- Programming and/or scripting skills
- Advanced MD methods (e.g. free energy calculations, MSM analysis)

### We Offer:

- Full time contract (1 year). Opportunities for contract extension will exist. This contract is linked to the project ref. 202135-30 funded by La Fundació La Marató de TV3.
- Stimulating, interdisciplinary research in a high-quality international scientific environment.
- Excellent working environment.
- Opportunities to acquire transferable skills (project management, people management, entrepreneurship,...)
- Flexible working conditions.

### To apply:

Interested candidates should send a letter of motivation and CV (including two potential referees) to [xbarril@ub.edu](mailto:xbarril@ub.edu), indicating as reference "La Marato project" as soon as possible and no later than 03/10/2021