





# JOB OPENING AT IRB BARCELONA

# Postdoctoral Fellow (ref. PD/24/02)

IRB Barcelona is a world-class research centre devoted to understanding fundamental questions about human health and disease. It was founded in October 2005 by the Government of Catalonia (Generalitat de Catalunya) and the University of Barcelona (UB), and is located at the Barcelona Science Park (Parc Científic de Barcelona).

The Institute's missions include conducting multidisciplinary research of excellence at the unique interface between biology, chemistry and medicine, providing high-level training in the biomedical sciences to staff, students and visitors, driving innovation through active technology transfer to the benefit of society, and actively participating in an open dialogue with the public through a series of engagement and education activities.

IRB Barcelona seeks a talented Postdoctoral Fellow to join our structural bioinformatics team in the Molecular Modeling and Bioinformatics group (Structural Bioinformatics Program), under the framework of the "XNA-Hub" initiative, co-funded by the Instituto de Salud Carlos III. The project pursues the creation of a platform to ease the development of therapies based on xeno-nucleic acids, and implies the use of molecular dynamics (MD) tools in a high-throughput (HT) regime and the development of automated tools for the parameterization of nucleic acids derivatives. The candidate will work in a wide consortium including companies and experimental groups and should be ready to interact with experimental biophysicists and molecular biologists.

#### **DUTIES**

We are looking for a candidate to work on theoretical computational studies of nucleic acids, involving programing new algorithms and scientific workflows, using all kinds of classical and quantum mechanics methods (MD, QM, QM/MM), and applying bio-statistics and artificial intelligence (AI) to obtain and refine new modified oligonucleotide parameters.

### EXPERIENCE, KNOWLEDGE, SKILLS & SELECTION CRITERIA

### Must Have - Required

- Bachelor degree or higher in Chemistry, Physics, Mathematics, Computational Sciences, Bioinformatics, or similar.
- PhD in Chemistry, Physics, Computational Sciences, Bioinformatics, Biotechnology, Biomedicine or similar.
- Experience in computational Molecular Dynamics (MD) technique: simulations and analysis (AMBER, GROMACS, OpenMM) and visualization (VMD, PyMol), ideally on nucleic acids.
- Experience in **High Performance Computing** infrastructures: workload managers (Slurm), remote connections (ssh), file transfer (scp, rsync).
- Experience in shell and scripting languages (Bash, CSH, Perl, Python, R).
- Excellent Linux OS skills.
- Fluent English and good teamwork skills.



IRB BARCELONA endorses the Requirements and Principles of the European Charter for Researchers, the Code of Conduct for the Recruitment of Researchers and Open, Transparent, Merit-based recruitment promoted by the European Commission and follows Equal Opportunities policies.







# Knowledge of the following technologies is advisable

- Experience in computational Quantum Mechanics (QM) technique: simulations and analysis (Gaussian, GAMESS).
- Programming languages C, Fortran, Perl
- Environment Modules (HPC)
- Experience in Version-control systems:Git (GitHub, GitLab)

# **WORKING CONDITIONS & ENTITLEMENTS**

- Employed in compliance with Spanish legislation and regulations under a full-time contract. Employees receive the benefits of the Spanish Social Security system covering sickness, maternity/paternity leaves and injuries at work.
- The unique opportunity to work within an international consortium that brings together the most prominent European researchers in the field of computational biology.
- The unique opportunity to work closely with a High Performance Computing (HPC) centre as the Barcelona Supercomputing Centre (BSC), with one of the most powerful supercomputers in Europe (Marenostrum IV), and recently selected by EuroHPC to host one of the largest European supercomputers (Marenostrum V).
- The possibility to work in multiple state-of-the-art platforms, such as Cloud infrastructures,
   Docker containers or HPC supercomputers.
- The unique opportunity to work in a multidisciplinary group which is currently involved in several National and European projects related to computational biology.
- Salary commensurate with experience and qualifications.

### **HOW TO APPLY & SELECTION PROCESS**

Applications for the above opening should include Full CV, Motivation Letter and references and should apply on https://recruitment.irbbarcelona.org/, Reference: PD/24/02

- Deadline for applications: 31/03/2024
  When the applicants do not fit the requirements, the deadline will be able to be extended.
- Number of positions available: 1
- Selection process
  - Pre-selection: Will be based on CV, motivation letter, experience, management of research and innovation.
  - Interviews: Short-listed candidates will be interviewed.
  - Offered Position: Job Offer will be sent to the successful candidate after the interview.

For more information please visit our website at: www.irbbarcelona.org

Note: The strengths and weaknesses of the applications will be provided upon request.



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If you, as an applicant, have any suggestion or wish to make a complaint regarding the selection process, please contact us at the following email address: <a href="mailto:irrecruitment.suggestions@irbbarcelona.org">irbbarcelona.org</a> You will receive a response within a month.



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