

## JOB OPENING AT IRB BARCELONA

### POSTDOCTORAL FELLOW in BIOLOGICAL DATA SCIENCE (ref. PD/20/07)

Created in 2005 by the Generalitat de Catalunya (Government of Catalonia) and the University of Barcelona, IRB Barcelona is a Severo Ochoa Centre of Excellence—a seal that was awarded in 2011.

The institute is devoted to conducting research of excellence in biomedicine and to transferring results to clinical practice, thus improving people's quality of life, while simultaneously promoting the training of outstanding researchers, technology transfer, and public communication of science. Its 25 laboratories and seven core facilities address basic questions in biology and are orientated to diseases such as cancer, metastasis, Alzheimer's, diabetes, and rare conditions.

IRB Barcelona is an international centre that hosts 400 members and 30 nationalities. It is located in the Barcelona Science Park. IRB Barcelona forms part of the Barcelona Institute of Science and Technology (BIST) and the "Xarxa de Centres de Recerca de Catalunya" (CERCA).

IRB Barcelona is seeking a talented and highly motivated **Postdoctoral Researcher** to join the **Structural Bioinformatics and Network Biology group** (<https://sbnb.irbbarcelona.org>), led by **Dr. Patrick Aloy**, to work on **Generative Models** to create **Precision Drugs**. The candidate will work on the project "Valorización de EGA para la Industria y la Sociedad" (VEIS) funded by the Secretariat of Universities and Research of the Ministry of Business and Knowledge (Government of Catalonia) and by the European Regional Development Fund (FEDER) with reference number 001-P-001647.

Biological data is accumulating at an unprecedented rate, escalating the role of data-driven methods in computational drug discovery. The urge to couple biological data to cutting-edge machine learning has spurred developments in data integration and knowledge representation, especially in the form of heterogeneous, multiplex and semantically-rich biological networks. Today, thanks to the propitious rise in knowledge embedding techniques, these large and complex biological networks can be converted to a vector format that suits the majority of machine learning implementations. Indeed, we have generated biological embeddings (i.e. bioactivity signatures) that capture complex relationships between small molecules and other biological entities such as targets or diseases (Duran-Frigola *et al.* 2020 *Nat Biotechnol in press*, available at bioRxiv). However, only a tiny fraction of the possible chemical space has been so far explored, meaning that most compounds able to modulate biological activities (i.e. drugs) are yet to be discovered. Accordingly, the main objective of this project is to couple our bioactivity signatures to inverse design algorithms to generate new chemical entities with a desired functionality. In particular, we aim at generating new chemical entities (NCEs) to modulate the activity of a specific set of targets, selected from a combination of perturbagen profiles, to revert the pathological state induced by Alzheimer's disease (AD) and other complex disorders. All in all, the incorporation of machine learning methods to the drug discovery process will trigger the development of thousands of novel compounds, finally enabling precision medicine.

#### DUTIES

The successful candidate shall be responsible for the implementation of ML-based Generative Models (i.e. cVAEs or GANs) to create new small molecules that fulfill the required polypharmacological properties to revert AD pathological signatures.



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.

On 9th December, 2014, IRB Barcelona was awarded the "HR Excellence in Research" logo. This recognition reflects the commitment of the Institute to the continuous improvement of its human resources policies in line with the *Charter & Code*. The Institute works to ensure fair and transparent recruitment and appraisal procedures.

## EXPERIENCE, KNOWLEDGE, SKILLS & SELECTION CRITERIA

### Must Have - Required

- **Education:** Bachelor in Biosciences, Chemistry, Pharmacy or Engineering degree in Computer Sciences. PhD in Bioinformatics, machine learning or related areas.
- **Experience:** previous experience on the use of machine learning and data science techniques. Strong publications record according to his/her career stage.
- **Skills:**
  - o Excellent programming and scripting skills, with deep knowledge of Python.
  - o Excellent knowledge of machine learning techniques (TensorFlow/AdaNet).
  - o Competent in the use of HPC queue systems, virtual machines (OpenNebula) and Grid Containers (Docker, Singularity).
  - o Excellent interpersonal and communication skills. Highly motivated. Fluency in English.

### Desirable

- **Experience:** Previous experience working with biological data and in an international environment.
- **Skills:**
  - o Knowledge of ML-based generative models (e.g. cVAEs, GANs, etc)

## WORKING CONDITIONS & ENTITLEMENTS

- **Working conditions:** 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.
- **Training and Career:** Postdoctoral researchers joining IRB Barcelona gain access to the Institute's advanced research training and career development opportunities, all within in a competitive international environment. Courses and workshops on themes of particular interest to postdocs are offered regularly by the Institute.
- **International environment:** Nearly 90 Postdoctoral researchers (more than a half non-Spanish nationals) are currently working at IRB Barcelona.

## HOW TO APPLY & SELECTION PROCESS

Applications for the above opening should include a CV and a letter of interest and should be sent by e-mail to: [irbjobs@irbbarcelona.org](mailto:irbjobs@irbbarcelona.org) with the Reference: **PD/20/07**

- **Deadline for applications:** 31/03/2020  
If no suitable candidate is found, the deadline will be extended.
- **Number of positions available:** 1



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- Selection process
  - **Pre-selection:** Will be based on CV, motivation letter and experience.
  - **Interviews:** Short-listed candidates will be interviewed.
  - **Job offer:** Will be sent to the successful candidate after the interview.

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For more information please visit our website at: [www.irbbarcelona.org](http://www.irbbarcelona.org)

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

*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: [irbreruitment.suggestions@irbbarcelona.org](mailto:irbreruitment.suggestions@irbbarcelona.org) You will receive a response within a month.*