



Universitat  
Pompeu Fabra  
Barcelona

Departament  
de Ciències Experimentals  
i de la Salut



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**Date of publication of the job offer : Jan 16 2020**

**Job Offer - Position at the Computational Science Group**

### Job Description

This project aims to develop machine learning models in physics and chemistry applied to drug discovery. We expect the candidate to help to develop methods and models for PlayMolecule.org, validate them with several industrial partners together with our spin-off [Acellera](#) and participate in challenges. This project is expected to lead next generation methods that are transformative in the field and publishable in the highest impact scientific journals. There will be ample opportunities to present his/her work at international meetings and conferences and to collaborate with other research groups in USA and Europe.

The candidate will be able to use <http://www.playmolecule.org>, a new platform for computational drug discovery. The laboratory is very well equipped with access to a local GPU and CPU cluster, hundreds of TB of storage and experimental facilities.

Universitat Pompeu Fabra and Prof. Gianni De Fabritiis, Icrea research professor <https://es.linkedin.com/in/gdefabritiis>, are looking to recruit a scientist on computational medicinal chemistry.

The laboratory is part of the Barcelona Biomedical Research Park which, with a privileged location on the shoreline of the Mediterranean sea, constitutes one of the most exciting interdisciplinary research centres in Southern Europe with more than 1000 scientists in the building alone. Lab website: <http://www.compscience.org/>

Relevant References: [https://scholar.google.es/citations?hl=en&user=-\\_kX4kMAAAAJ&view\\_op=list\\_works&sortby=pubdate](https://scholar.google.es/citations?hl=en&user=-_kX4kMAAAAJ&view_op=list_works&sortby=pubdate)

### Project and Institution that finance the contract

The work is supported by grant: AEI-BIO2017-82628-P (FEDER/UE) DE FABRITIIS from the Spanish Ministry of Economy (MINECO), FEDER and Agencia Estatal de Investigación sources and Acellera ([www.acellera.com](http://www.acellera.com)).

**Official number reference:** PR07118 - AEI-BIO2017-82628-P (FEDER/UE) FABRITIIS

### Skills and Experience

- The candidate will preferably have a profile in pharmacy, medicinal chemistry,



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organic chemistry or similar discipline.

- We seek exceptional candidates with a passion for using computation to solve real life problems in drug discovery. Experience in previous drug discovery projects and tools either from a method development perspective or from an application perspective is required.
- The capability to think out of the box, the ambition to work in very innovative projects and very good communication skills in English.
- Experience in statistics/machine learning and good knowledge of Python.

#### **Benefits of the opening**

Salary: We offer a competitive salary (gross around 30k eur) and 11 month contract with possibility of extension.

#### **Information on the application process:**

Please send an email to [carina.oliver@upf.edu](mailto:carina.oliver@upf.edu) with subject “GdF\_PN” with a CV and a cover letter.