





Date of publication of the job offer: March 1st 2021

Job Offer: Postdoctoral Position in Machine Learning at the Computational Science Laboratory

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 <u>Acellera</u> 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 http://www.upf.edu/ and Prof. Gianni De Fabritiis, ICREA research professor https://es.linkedin.com/in/gdefabritiis, are looking to recruit a postdoctoral scientist on computational medicinal chemistry.

Location: Barcelona, Spain, Barcelona Biomedical Research park. 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

Project and Institution that finance the contract:

The work is supported with H2020 European Commission Funds, by grant H2020-CompBioMed2-Gianni de Fabritiis

Official number reference: PREUR00419 - H2020-CompBioMed2-Gianni de Fabritiis

Skills and Experience:

The candidate will preferably have a profile in pharmacy, medicinal chemistry, 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.
- Very good publication record

Benefits of the opening: We offer a nine months contract, 32,5hrs/week, yearly gross salary around 30-35k Eur depending on experience.

Information on the application process: Send CV to carina.oliver@upf.edu (Ref. C2)

Deadline to submit applications March 25th, 2021