



Universitat
Pompeu Fabra
Barcelona

Departament
de Ciències Experimentals
i de la Salut



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Job Offer - Position to develop machine learning models in physics and chemistry applied to drug discovery 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 [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 <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: Combiomed project has received funding from the European Union's Horizon 2020 research and innovation programme, under grant agreement No 675451.

PR08416 – Combiomed – Gianni de Fabritiis



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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

Salary: Gross year salary 30.000 eur.

Duration: Initially 1 month contract with the possibility of extension.

Information on the application process:

Please send an email to CM carina.oliver@upf.edu with subject "CM" with a CV and a cover letter together with the names of up to three contacts for requesting recommendations.

Deadline to submit applications –22/07/2019