



Universitat  
Pompeu Fabra  
Barcelona

Departament  
de Ciències Experimentals  
i de la Salut



**Date of publication of the job offer – May 30th**

**Job Offer** Machine Learning position available at the Computational Science Group

**Job Description**

Success in the fields of machine learning and artificial intelligence has led to dramatic improvements in applications towards other areas. One of such is drug discovery, which entails a multi-objective optimization problem spanning several length scales, from solubility (angstroms) to in vivo toxicity (meters). A main focus of Acellera is to develop tools that provide understanding and guidance in several structural biology and chemoinformatics tasks.

The candidate is expected to advance the current state of the art in machine learning applications related to drug discovery and develop those for the free drug discovery platform [www.playmolecule.org](http://www.playmolecule.org). Examples include:

- Protein-ligand binding affinity [1]
- De novo compound generation [2]
- Protein-protein interface prediction [3]
- Forward and retrosynthesis prediction [4]
- ADMET modeling [5]

**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.

**Methods:** Modern deep learning approaches such as convolutional, recurrent neural networks, as well as generative models such as variational autoencoders and generative adversarial networks are some examples of the models we currently use.

**Candidate Profile:** The candidate will preferably have a profile in statistics,



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chemistry, medicinal chemistry or mathematics.

Requirements. Very good communication skills in English. Previous exposure to machine-learning pipelines, Python proficiency, familiarity with Linux and the ability to work with version control systems (e.g. git).

**Benefits of the Position:** One year contract, around 1200 euro/month gross, with the possibility of continuing with an industrial PhD.

**Facilities:** Acellera has access to GPU workstations and non-public datasets. Furthermore, it collaborates with several pharmaceutical companies worldwide.

**Location:** Acellera labs, C/ Dr Trueta 183, Barcelona, Website:

<http://www.acellera.com>; <http://www.playmolecule.org>

**Information on the application process:** Send CV and letter of interest, to [carina.oliver@upf.edu](mailto:carina.oliver@upf.edu)

**Deadline to submit applications** - June 14<sup>th</sup>, 2019