Universitat Pompeu Fabra Barcelona | Master in Bioinformatics for Health Sciences

Master project 2020-2021

Personal Information

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Project

Web development & bioinformatic tools

Project Title:

Machine learning in computational structural biology and drug discovery

Keywords:

machine learning; GPU computing; medicnal chemistry for drug discovery; PlayMolecule

Summary:

This project aims to develop machine learning methods applied to structural biology, drug discovery and computational chemistry. The aim is to go substantially beyond the state-of-the-art in the use of machine learning and GPU computing, exploring supervised, unsupervised and reinforcement learning approaches. We expect the candidate to participate in the development of new learning approaches and applications derived from deep learning applied to medicinal chemistry for drug discovery. By working in this project, the researcher will have access to state of the art computational resources. This project is expected to lead to discoveries that will be publishable in the highest impact scientific journals. Some examples of applications can be seen in PlayMolecule.org, a drug discovery platform used by thousands of scientists worldwide and pharmas and biotech companies. The platform is based on two main pillars, physical-based molecular simulations on GPUs and machine learning/AI, thus contributing to the company mission of accelerating the transition towards computerized drug discovery process. The platform was born in 2017 and serves as a repository of web applications for molecular modelling tools such as ProteinPrepare [Martínez-Rosell2017; doi:10.1021/acs.jcim.7b00190] and pioneering deep learning applications such as Kdeep [Jiménez2018; doi:10.1021/acs.jcim.7b00650] WHO WE ARE: Founded in 2006, Acellera was one of the first companies worldwide to leverage the use of novel accelerator processor technology (GPU) for molecular simulations. Among our clients, we count 10 of the top 50 pharmaceutical companies. We were selected as one of the Top30 AI Drug Discovery companies in 2019. Our software includes PlayMolecule, ACEMD, HTMD, KDEEP, etc. and it's used by hundreds of users both in academia and the private sector. In particular, PlayMolecule.com is the first platform to democratize the use of molecular dynamics and machine learning applications for drug discovery.

Expected skills::

You have VERY good programming skills and a background in either chemistry, biology, computer science or similar Prior knowledge in neural information processing, deep learning frameworks (pyTorch, Tensorflow) is desirable Very good knowledge of Python and good coding practices This is a strongly computational position, so we encourage application of people that love algorithms, computing, programming and likes to apply it

Possibility of funding::

Yes

Possible continuity with PhD: :

To be discussed

Comments:

What we offer: - Real in-company work experience. - Possibility to participate in the development of a real software product - After graduation, it is possible to stay in the company