Universitat Pompeu Fabra Barcelona | Master in Bioinformatics for Health Sciences

Master project 2020-2021

Personal Information

Supervisor	Gianni De Fabritiis
Email	g.defabritiis@acellera.com
Institution	Acellera Labs SL
Website	www.acellera.com
Group	-

Project

Web development & bioinformatic tools

Project Title:

Development of frontend capabilities and graphic user interface (GUI) for PlayMolecule.org

Keywords:

frontend; GUI, in silico drug discovery; HTML, Phyton

Summary:

This master thesis will focus on the development and release of a new graphic user interface (GUI) for PlayMolecule, a popular platform for biomolecular-related applications with hundreds of unique users every month available at https://www.playmolecule.org. PlayMolecule is 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]. The position is based within the informatic and innovation hub of Barcelona (Spain). Acellera values excellence, merits and scientific innovation above anything else. WHAT YOU WILL BE WORKING ON: 1. You will closely work with Acellera developers to develop and improve the GUI capabilities for PlayMolecule. 2. You will mostly work in front-end tasks such as: - Collaborate with medicinal chemists to improve the capabilities and usability of PlayMolecule web interface - Development of 3D novel graphical interface to better access molecular structural information and dynamic plots ready to interface with the PlayMolecule back-end. 3. You may additionally work in back-end tasks such as: - Development of functionalities necessary to make custom GUI molecular selections 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::

THIS PROJECT IS FOR YOU IF: You have good programming skills and a background in either chemistry or computer science You are proficient in: HTML, CSS/CSS3, Javascript, AngularJS, Python And maybe also have some knowledge of: Flask, SQL databases,

Plotly.js, NGL.js You have very good communication skills in English

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, possibility to stay in the company.