

Master Thesis proposal 2023

Master Thesis title:

Development of a web-based toolkit for the visualization of molecular data in PlayMolecule.com

Supervisors: [Gianni De Fabritiis](#) + [Mariona Torrens](#)

Company: Acellera Labs (www.acellera.com)

ABOUT THE PROJECT:

PlayMolecule (www.playmolecule.com), the first online platform of cutting-edge tools for computer-aided drug discovery launched by Acellera in 2017. The platform provides scientists and medicinal chemists all over the world with easy access to cutting-edge applications for drug discovery problems. PlayMolecule's appeal and impact in the popularization of computer-aided drug discovery is proven by its over 4.500 users and 145k jobs submitted.

This master thesis will focus on the development of an interactive viewer for the study of molecular data. This includes the visualization of 3D structures, protein sequences, small molecule libraries and interactive plots. The goal of the project is to obtain a data visualization toolkit that facilitates the computational study of this data to researchers with any background, causing a direct impact on drug discovery. The outcome of this project is expected to be publishable in a scientific journal.

The candidate will work in close collaboration with Acellera's software developers. Moreover, Acellera's internal medicinal chemist team will help the candidate to identify and describe the most common and useful molecular visualization tools for drug discovery.

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, Python
- And maybe also have some knowledge of: React, SQL databases, Mol*
- You have very good communication skills in English

Funding: YES

Continuity with PhD: to be discussed

About Acellera

Our mission is to accelerate the transition to rational, computerized drug discovery via simulations and machine learning. In order to fulfill it, we work with our customers by becoming key technology partners, boosting their discovery workflow with the most innovative solutions. Science, research, development and innovation are the founding pillars of our company.

Acellera is devoted to bringing state-of-the-art technologies to drug discovery. Founded in 2006, we were one of the first companies worldwide to leverage the use of novel accelerator processor technology (GPU) for molecular dynamics. We developed the first online platform for drug design based on deep learning and are now leading the introduction of machine learning techniques into the drug discovery pipeline. Our Culture is Innovation First. Our purpose is to change the way things are done by constantly increasing the rate of innovation. Our mission is to transform drug

discovery into a computable task, by developing the algorithms to run it. Our impact is on the real world and not inside a screen, therefore molecules must be made and assays performed as a delivery path of our innovation.

WHAT WE OFFER:

- Real in-company work experience.
- Possibility to participate in the development of a commercial software product
- The possibility to join Acellera after finalising the MSc.