



Master project 2024-2025

Personal Information

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Project

Web development & bioinformatic tools

Project Title:

Development of machine learning methods applied to drug discovery

Keywords:

machine learning, reinforcement learning, drug discovery, software development

Summary:

This master thesis project aims to develop machine learning methods applied to molecular systems and chemistry. The aim is to go substantially beyond the state-of-the-art in machine learning and GPU computing, exploring supervised, unsupervised, and reinforcement learning approaches. Along the project, the candidate will closely work with Acellera scientists and software developers to develop new learning approaches and applications derived from deep learning applied to medicinal chemistry for drug discovery. 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. This is a strong computational project, so we encourage applications from students who love algorithms, computing, and programming.

References:

<https://www.acellera.com/science/>

Expected skills:

Good programming skills and a background in either chemistry, biology, computer science, or similar. Prior knowledge of neural networks and deep learning frameworks (PyTorch) is desirable. Specific knowledge of any of these areas is less critical, however, than strong research skills, and a history of innovation and accomplishment.

Possibility of funding:

Yes

Possible continuity with PhD:

Yes

Comments:

About Acellera Developing The Algorithms To Automate Drug Discovery Our mission is to accelerate the transition to rational, computerized drug discovery via simulations and machine learning. To fulfill our vision, we work with our customers by becoming key technology partners, boosting their discovery workflow with the most innovative solutions. Science, research, innovation, and

development are the founding pillars of our company. Our Background Acellera is devoted to bringing state-of-the-art technologies to drug discovery. 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 office is located in Poble Nou and we have a flexible working schedule.