Universitat Pompeu Fabra Barcelona

Master in Bioinformatics for Health Sciences

Master project 2024-2025

Personal Information

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Institution	Pharmacelera
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Group	R&D

Project

Pharmacoinformatics & systems pharmacology

Project Title:

Use of novel 3D molecular descriptors for the representation and search of quantum molecular fields with application in rational drug design

Keywords:

Computational chemistry, Virtual screening, Drug discovery, Small molecule, Molecular fields

Summary:

Pharmacelera offers a position to evaluate the impact of a novel methodology for 3D molecule alignment and comparison. In the project you will evaluate a novel and efficient way of representing 3D molecular energy fields with simple vectors invariant to rotation and translation. Regarding the published literature, it would be the first time that these descriptors are used with small molecules of pharmaceutical interest and, therefore, the results of this project might lead to a scientific publication. The usage of these descriptors has potential applications in a wide range of computational chemistry methods (e.g. virtual screening of molecules with similar 3D molecular fields, docking) and in the generation of predictive models with artificial intelligence (including the prediction of quantum properties). The student will characterize multiple small molecule benchmarking datasets of different receptor families and evaluate the impact that these novel methods have in virtual screening performance in comparison with state-of-the-art techniques. Eventually, the student will be able to propose improvements to these methods after evaluating the results. The student will receive a small economic compensation for his work and, if agreed between both parties, there might be options to perform an industrial PhD after the completion of the Master. About Pharmacelera Pharmacelera is a Computer-Aided Drug Design software company based in Barcelona that improves the productivity of pharmaceutical R&D through the usage of Quantum-Mechanics algorithms, High Performance Computing and machine learning techniques. We help pharmaceutical companies find new drugs at the early stages of drug design reducing costs and time-to-market.

References:

Vazquez J., Deplano A., Herrero A., Gibert, E., Herrero E., Luque F. J., J. of Chem Inf and Mod, 60(9), May 2020 https://doi.org/10.1021/acs.jcim.9b01191

Expected skills:

Python programming, experience with small molecule drug discovery software tools is a plus

Possibility of funding:

Yes

Possible continuity with PhD:

To be discussed

Comments:

We are located at the Parc Científic de Barcelona and the position would enable a hybrid work model.