Universitat Pompeu Fabra Barcelona

Master in Bioinformatics for Health Sciences

Master project 2021-2022

Personal Information

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Project

Structural bioinformatics

Project Title:

Development and validation of a ligand docking workflow for PELE

Keywords:

Computational Chemistry, Molecular Modeling, Docking,

Summary:

PELE is our Monte Carlo algorithm to explore the potential energy surface of biomolecular systems. Since its origin, 15 years ago, it has proved to be an outstanding tool to simulate migration pathways of ligands, predict binding modes and their affinities, or engineer enzymes. Recently, we have developed a platform to automate different workflows for drug design and enzyme engineering applications. However, we currently do not have a method to generate the initial structure with the ligand already inside the protein cavity that we want to study. As a consequence, we are forced to either predict the whole entrance of the ligand to the desired cavity, resulting in a very expensive calculation, or to dock it with external tools. The solution is to develop a method to generate this initial structure by trying to fit a 3D conformer of a small molecule into a specific protein cavity. Then, we could use some of the algorithms of PELE to sample and rank the different ligand binding modes. The goal of this project is to develop and validate a package to dock a ligand and rank its binding modes in a predefined protein cavity with PELE.

Expected skills::

Biochemistry with programming skills or knowledge

Possibility of funding::

Yes

Possible continuity with PhD: :

To be discussed

Comments:

Initial duration: 6-8 months