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:

Detection of novel druggable binding sites at G protein-coupled receptors

Keywords:

G protein-coupled receptors, molecular dynamics, data analysis, drug design

Summary:

G protein-coupled receptors (GPCRs) are the most abundant class of receptors in the human organism. They are present in almost every type of cell, and govern almost every process in the human body (i.e. cognitive and inflammatory processes or control of the cardiovascular system). Owing to their ubiquity, they are targets of more than 30% of current drugs, and every day new GPCRs are revealed to be pharmacological targets for existing diseases. Molecular dynamics (MD) is a sophisticated technique that enables to simulate protein behaviour in a physiological environment. In this project the Master student will develop a simulation-based pipeline that allows detecting druggable binding sites including cryptic pockets ("transient binding pockets"). This pipeline involves (i) the setup of simulation systems including small chemical fragments to probe the entire protein surface for druggable binding sites, (ii) running production runs, (iii) automated detection of binding sites and (iii) intuitive visualization. The pipeline will be implemented into our GPCRmd server and detected sites will be exploited for the discovery of new molecular GPCR modulators. We expect that the results of the analysis will be published in a high impact journal, and the expertise acquired by the student will make her/him a valuable asset for pharma companies in future. We are looking for a highly motivated and skilled student with exceptional academic records that allows pursuing a PhD afterwards.

References:

Rodríguez-Espigares & Torrens-Fontanals et al. GPCRmd uncovers the dynamics of the 3D-GPCRome, Nature Methods 2020, DOI: 10.1038/s41592-020-0884-y

Expected skills::

Experience in structural biology, programming in python/bash, molecular dynamics engines (GROMACS, NAMD, etc.), analysis tools/packages (VMD, Chimera, MDtraj…) and high level of English, oral and written.

Possibility of funding::

To be discussed

Possible continuity with PhD: :

Yes