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:

Why is water essential for GPCR functionality?

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. As for the whole life, water is critical for GPCR functionality at a nanoscopic scale. It forms important intermolecular networks that mediate the signaling response of the receptor. Our group owns an extraordinary dataset with unprecedented information about the implication of water molecules in GPCR structural dynamics and the binding of small drug-like molecules. We believe that stabilized or disrupted intermolecular water signatures drive the functional consequences of a drug-like molecule. In this project, the Master student will seek for the underlying molecular mechanism of the water-mediated functional responses. For this, she/he will (i) develop an analysis pipeline to extract relevant information from our unique dataset and (ii) setup control simulations to validate obtained conclusions. 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