Universitat Pompeu Fabra Barcelona | Master in Bioinformatics for Health Sciences

# Master project 2020-2021

## Personal Information


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## Project

# Web development & bioinformatic tools

**Project Title:**

Developing web-based analysis tools for the study of GPCRs


**Keywords:**

web-based tools, data-sharing, structural biology, G protein coupled receptors


**Summary:**


G protein–coupled receptors (GPCRs) are major targets for the pharmaceutical industry (more than 30% of all FDA-approved drugs act on a GPCR) and present an immense potential for future drug development. Although GPCRs have been extensively studied over the past decades, the underlying molecular and structural mechanisms responsible for many critical regulatory processes of this protein superfamily remain elusive. Understanding the dynamics of receptor functionality is currently a major challenge in molecular biophysics and a requirement for the rational design of drugs with improved therapeutic profile. For this reason, a promising approach to elucidate the molecular basis of GPCR functionality are molecular dynamics (MD) simulations, a potent computational technique capable of generating atomic-resolution simulations of the structural motions of a molecular system. Consequently, MD simulations are increasingly being applied to the study of GPCRs, as reflected by the rapid upsurge of publications concerning this topic. In view of the growing importance of MD simulations, the GPCRmd project was created with the purpose to build the GPCRmd database, a database of MD simulations of GPCRs capable to foster data from all-over the world (www.gpcrmd.org). This web-based platform provides visualization and analysis tools specifically designed for the evaluation of structural and dynamic data of GPCR family members. In this Master project, the student will be involved in the design and development of new interactive analysis tools for the study of GPCRs, which will be incorporated in the GPCRmd viewer webpage. Such analysis tools will be focused on the study of the complex signalling network of intra-protein interactions that ultimately determine the response of the GPCR to a given drug. This includes the automatized detection and classification of different types of relevant interactions, comparison of the interaction network of different receptors (phylogenetically related receptors, wild type vs. mutant, ...), comparison of the network at different stages of a given molecular process, etc. Moreover, the obtained analysis tools will be applied to a case-study with the final aim to better understand how the intra-protein interaction network of a receptor of interest is affected by different stimuli or alterations (binding of a given ligand, receptor mutations, ...). The student will learn about GPCR biology, protein dynamics and in silico drug design, as well as web development, biomedical data analysis and biological databases. The internship can be extended into a PhD thesis. We expect that the GPCRmd database will have high impact on GPCR research and the discovery for new drugs. This will be communicated in a relevant publication to which the Master student will contribute.

**References:**

https://www.biorxiv.org/content/biorxiv/early/2019/12/17/839597.full.pdf

**Expected skills::**

Experience in structural biology. Python, HTLM/CSS and web page design. Experience with molecular dynamics simulations and JavaScript is a plus. Good level of English (oral and written).

**Possibility of funding::**

To be discussed

**Possible continuity with PhD: :**

Yes