



Master project 2024-2025

Personal Information

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Project

Structural bioinformatics

Project Title:

Application of MD and machine learning to GPCR drug discovery

Keywords:

G protein coupled receptors, computer-assisted drug design, machine learning

Summary:

G protein-coupled receptors (GPCRs) represent the most prevalent class of receptors within the human body, found in nearly every cell type and regulating a myriad of physiological processes, including cognition, inflammation, and cardiovascular function. Their ubiquitous presence makes them targets for over 30% of existing drugs, with new GPCRs continually emerging as potential pharmacological targets for various diseases. Molecular dynamics (MD) stands out as a sophisticated technique capable of simulating protein behavior within a physiological context, offering valuable insights into GPCR function and dynamics. In this project, the Master student will apply MD in combination with machine learning to predict the functional outcome of drug candidates at an unprecedented temporal and spatial resolution. We expect that the results of this 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, molecular dynamics engines (GROMACS, NAMD, etc.), analysis tools/packages (VMD, Chimera, MDtraj...) and high level of English, oral and written.

Possibility of funding:

Yes

Possible continuity with PhD:

Yes