Universitat Pompeu Fabra Barcelona | Master in Bioinformatics for Health Sciences

Master project 2024-2025

Personal Information

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Group	Molecular Neurobiology

Project

Pharmacoinformatics & systems pharmacology

Project Title:

Exploring neurodegeneration: In silico drug screening and assessment of GPCRs interactome

Keywords:

Drug screening, neurology, chemistry, molecular dynamics.

Summary:

The study aims to elucidate the underlying structural mechanisms governing the functionality of G protein-coupled receptors (GPCRs) by utilizing molecular docking and molecular dynamics techniques. The main focus is on examining receptors associated with neurodegenerative disorders such as adenosine and cannabinoid receptors. Furthermore, in silico drug screening will be utilized to pinpoint potential binding sites on GPCRs that have yet to be thoroughly characterized. Very relevant: The candidate will gain proficiency in utilizing various tools within a state-of-the-art professional software (Maestro-Schrödinger) suite for tasks such as molecular dynamics, drug screening, and molecular docking, among other functionalities.

Expected skills:

Valued: Programming (Python and/or R), basic chemistry knowledge

Possibility of funding:

No

Possible continuity with PhD:

To be discussed

Comments:

Remote/hybrid work is possible. Physical location of the lab is: Fac og Biology (UB) Diagonal 643. Edifici Prevosti