



Master project 2024-2025

Personal Information

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Project

Structural bioinformatics

Project Title:

Studying brain signaling and neurolipids using molecular dynamics simulations

Keywords:

Brain, lipids, molecular simulations, membrane proteins, neurotransmission

Summary:

GPCRs are the largest family of membrane proteins in the human genome. They respond to a broad range of stimuli, which trigger a series of conformational changes that result in the activation of intracellular heterotrimeric G proteins, the main transducers for GPCRs. While GPCRs are key signaling proteins, there are several aspects of their activation mechanism, such as their modulation by membrane lipids, that call for a deeper understanding of their conformational dynamics. Molecular dynamics (MD) simulations have become a very powerful technique to study relevant biomolecular processes at the atomic level, including membrane complexity and its influence in GPCR function. In this project, the student will use MD simulations to study the role of specific brain lipids on neuronal function, including the effect of membrane composition in neurotransmission and its interplay with key GPCRs in the brain.

References:

https://scholar.google.com/citations?user=eQ3yh_AAAAAJ&hl=en

Expected skills:

Molecular dynamics simulations, basic structural bioinformatics knowledge, good programming skills

Possibility of funding:

To be discussed

Possible continuity with PhD:

To be discussed