Master « Sciences, Technologie, Santé »
Mention « In Silico Drug Design »
Second Year

OFFER AN INTERNSHIP
Academic Year 2014 – 2015

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Speciality training : Research

a few key words to describe the subject of training : computational chemistry - molecular modeling - molecular dynamics - protein flexibility - G protein-coupled receptor - opioid receptor

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Title of internship:

Supramolecular organization of opioid receptors and their biological partners

this subject is a first step towards a thesis: Yes

Short text describing your project

The G protein-coupled receptors (GPCRs) family are one of the largest family of transmembrane proteins in vertebrates. They are crucial in pharmaceutical research area as representing the molecular targets for nearly half of the therapeutic drugs that are prescribed. Despite the fact that several new crystallographic structures of GPCRs appeared in the literature during the past five years, crystallographic techniques present intrinsically major limitations as they are not able to capture the dynamics of these receptors. GPCRs are indeed very flexible proteins that are able to exhibit a large spectrum of conformations depending on the type of ligand, the oligomerization state, etc. We therefore propose various Master internship projects related to the influence of partners of opioid receptors as GPCRs on their dynamical properties. More specifically, we will use classical Molecular Dynamics (MD) simulation techniques, to decipher the molecular interactions that occur between GPCRs and one of their partners, *i.e.*, the agonist/antagonist as ligands, the presence of other receptors in oligomerized states, the consideration of their corresponding G-protein, but also the influence of the membrane composition on intrinsic dynamical aspects of opioid receptors. A practical problem encountered in all-atom (AA) MD techniques is the computing resources, as related GPCR mechanisms like many other protein mechanisms occur at the microsecond or even millisecond time scale. To take into account these issues, coarse grain (CG) models have rather recently been developed by merging atoms into a limited number of particles. According to the Master thesis projet considered, diverse CG techniques could then be taken onto account.