

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



OFFER AN INTERNSHIP
Academic Year 2013 – 2014

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Specialty training : Research Professional

A few key words to describe the subject of training : A2A adenosine receptor, ligand optimization, molecular dynamics simulations, free energy estimations.

Title of internship: Prediction of receptor-ligand binding affinities using molecular dynamics simulations

This subject is a first step towards a thesis: Yes (depending on funding)

Short text describing your project :

The recent determination of the first crystal structures for G protein-coupled receptors have given the opportunity to use structure-based methods in design of ligands to this important class of drug targets. At the same time, the increased amount of computational power during the last years has made it possible to compute ligand binding energies with a precision that may enable ligand design. Computational methods that can be used to identify analogs of a lead compound are of particular interest because such approaches could improve the efficiency of the drug development process. The focus of the project is to test if molecular dynamics simulations in combination with rigorous free energy estimations can be used in optimization of GPCR ligands. We will mainly focus on identification of more potent ligands of the A2A Adenosine receptor, which is a target for development of drugs against Parkinson's disease. The goal of the project is to develop an automated protocol for ligand optimization based on molecular dynamics simulations.

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