



Master « In Silico Drug Design » Second Year



OFFER AN INTERNSHIP

Academic Year 2016/2017

Send to Mrs Pr Camproux

anne-claude.camproux@univ-paris-diderot.fr



Name of the head of laboratory or company: Pr Johannes Kirchmair

Address : University of Hambourg, Center for Bioinformatics, Bundesstrasse 43, 20146 Hambourg, Germany

E-mail : kirchmair@zbh.uni-hamburg.de

Name of training supervisors : Pr Johannes Kirchmair

Phone number : +49 (0)40 42838 7303 Fax : +49 (0)40 42838 7352

E-mail : kirchmair@zbh.uni-hamburg.de

Specialty training : Research Professional

A few key words to describe the subject of training :

« conformer prediction », « protein-bound ligand conformation », « conformer ensemble generation »

Title of internship :

Statistical analysis of the known conformational space of protein-bound ligands

This subject is a first step towards a PhD :

Short text describing your project

The research group of Pr Kirchmair has devised a cheminformatics pipeline for the fully automated extraction of a comprehensive set of high-quality ligand conformations from the Protein Data Bank (PDB). This integrated approach includes the scoring of the electron density support of atoms based on the 2fo-fc electron density difference map.

The aim of this internship is to study in detail the known conformational space of protein bound ligands: (a) How diverse are the experimentally observed protein-bound ligand conformations of individual ligands? (b) How do these conformations differ from low energy conformations observed in the gas phase? (c) How well and to which extent can protein-bound ligand conformations be represented by conformer ensembles computed with some of the best available algorithms? The student will deepen her knowledge in Python, R, C++ and statistics. She will use conformer ensemble generators and possibly also explore molecular dynamics simulation techniques.

Send by e-mail : anne-claude.camproux@univ-paris-diderot.fr