Master « In Silico Drug Design »

Second Year

INTERNSHIP OFFER

Academic Year 2016/2017

Send to Mrs Pr Camproux
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Name of the head of laboratory or company: Rousu Juho

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Specialty training : Research ☒ Professional ☐

A few key words to describe the subject of training : molecular dynamics, machine learning, protein-ligand interactions

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Title of internship : building hybrid models combining molecular dynamics and machine learning for predicting protein-ligand interactions

This subject is a first step towards a PhD : Yes

Short text describing your project

The internship is related to research projects in Prof. Juho Rousu's group in Aalto University, concerned on building new predictive models for protein ligand interaction using machine learning and molecular dynamics models. The task of the intern include the following:

(1) Together with instructors, identifying a set of proteins and candidate ligands of interest, as well as appropriate molecular dynamics simulation tools

(2) Running molecular dynamics simulations for selected proteins and ligands

(3) Preparing datasets for machine learning models composed of descriptors of proteins and ligands and their affinities

(4) Training machine learning models for the prediction of previously unseen protein-ligand paris

(5) Reporting on the research regularly in group meetings

(6) Writing a final report on the internship

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