

**OFFER AN INTERNSHIP
year 2017/2018**

send to Pr Camproux
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Name of the head of laboratory or company: David van der Spoel

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Name of training supervisor: Jens Carlsson

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Specialty training : Research

a few key words to describe the subject of training : Molecular dynamics simulations, protein-ligand complexes, free energy calculations, scripting/programming, thermodynamics

Title of internship:

Understanding of the thermodynamic signatures of ligand binding using molecular dynamics free energy calculations and molecular dynamics simulations.

this subject is a first step towards a thesis: Yes/No (not sure)

Short texte describing your project

This project will involve running molecular dynamics simulations of proteins in complex with ligands. We will use high resolution crystal structures of ligands that have been thoroughly characterized by measuring free energy, enthalpy, and entropy. These energy terms will be calculated computationally using molecular dynamics free energy simulations to assess if force fields can reproduce these quantities accurately, which would be useful in drug design.

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