

**OFFER AN INTERNSHIP
Academic Year 2015/2016**

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Name of the head of laboratory or company:

Adress :
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Specialty training : Research ☐ Professional ☐

a few key words to describe the subject of training :

Title of internship:

Optimizing the position of water molecules at protein-ligand interface

this subject is a first step towards a thesis: Yes - No

Short texte describing your project

The goal of this internship is, from a previous work, to optimizing water molecules positioned in protein-ligand interfaces. This work is divided in two step, (i) develop and test a algorithm to keep the longest water sequence and propose a score of interaction based on the number of contact points and (ii) using MODELLER improve the water network. The long-term perceptive of this work is to proposing a new method, faster and less dependent of the molecular dynamic softwares, able to computed the energy of the solvent molecule in the protein-ligand interaction, largely missing in drug discovery studies but influencing the entropic and also the enthalpic of the protein-ligand system.

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