

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 :

Halogen Bond, Free energy, Molecular dynamics, Thermodynamic integration.

Title of internship:

Free energy calculations in halogen bonded systems of biological relevance

this subject is a first step towards a thesis: No

Short texte describing your project

Halogen bonding is gaining an increasing attention in drug design as a useful tool for increasing the affinity and the specificity of small drug like molecules for their target. Standard force fields allow a very poor description of halogen bond interactions, so different approaches have been devised to modify them as to obtain a satisfactory modeling of this important interaction. In our group we developed a model of halogen bonding based on extra point charges located the halogen atom. This simple model succeeded in reproducing the geometry of protein-ligand complexes of brominated and iodinated compounds. Now we aim at applying this model to the detailed calculation of the free energy of binding of such molecules to their target.

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