OFFER AN INTERNSHIP
Academic Year 2014 – 2015
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Specialty training :   Research   ☒   Professional   ☐

A few key words to describe the subject of training :

Protein-ligand interactions, electronic effects, scoring functions, Monte Carlo

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Title of internship:

Study protein-ligand interactions at an atomic and electronic and atomic energy level. Improving PELE's score functions.

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

Short texte describing your project

The main goal will center on improving existing scoring functions, to better describe protein-ligand recognition at an energy level, by adding corrections obtained from quantum mechanics (QM) to existing molecular mechanics (MM) force fields. A second alternative will be based on solely using QM techniques on MM snapshots. The overall project will be implemented in the frame of the PELE software, which combines a Monte Carlo algorithm with protein structure prediction techniques.

We will use fragment molecular orbital theories (FMO) to compute at a 'full' QM level the non-bonding interaction energy of a ligand with the protein. This energy will be used to approximate the enthalpy of bonding and compared with several experimental measures. The correlation will be compared with simpler MM methods.

These improvements will then be implemented into PELE's force fields, adding correction terms and doing single point reevaluation of binding enthalpies on the fly along the MM exploration. We could also explore adding entropic corrections to the binding energies (enthalpies), providing a free energy scoring function on the fly (along the MM sampling).

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