Master « Sciences, Technologie, Santé » Mention « In Silico Drug Design »

Second Year

OFFER AN INTERNSHIP Academic Year 2012 – 2013

Send to Mrs Pr Camproux:

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Name of the head of laboratory or company: Mateo VALERO CORTÉS

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Name of	training	supervisor: Jua	n FERNA	ÁNDEZ	-RECIO
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Specialty training:	Research	\boxtimes	Professional					
a few key words to describe the subject of training:								
Protein-protein docking, structural bioinformatics, flexible refinement.								
Title of internship:								
Optimization of pyDock for inhibitor prediction and flexible docking.								
this subject is a first step towards a thesis: Yes (Depending on funding)								

Short texte describing your project

The proposed project will focus on the optimization and benchmarking of a state-of-the-art protein-protein docking tool, in order to include cofactors, modified residues and ions, which can perform flexible refinement with standard forcefields and improve the predictions in many cases of biomedical interest. This will extend the knowledge acquired by the student during the first year of the Master. The proposed research project will facilitate the modeling of small-molecule ligands and inhibitors that modify protein-protein interactions of biomedical interest, a subject of large interest for drug discovery.

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