

Master « Sciences, 1 ecnnologie, Sante » Mention « In Silico Drug Design » Second Year

> OFFER AN INTERNSHIP Academic Year 2014 – 2015 Send to Mrs Pr Camproux : anne-claude.camproux@univ-paris-diderot.fr



Name of the head of laboratory or company: Pr. Matthieu Schapira

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Specialty training :	Research	Х	

Professional

a few key words to describe the subject of training :

computational chemistry, structure-based drug design, structural bioinformatics, virtual screening

**<u>Title of internship</u>**: Structural chemistry of the RNA methylation pathway: binding site analysis and drug design.

this subject is a first step towards a thesis: No

Short texte describing your project

Epigenetic mechanisms are central to the etiology of cancer and other diseases. Proteins involved in epigenetic mechanisms are emerging as promising targets in drug discovery, and novel chemical inhibitors targeting these proteins are currently in Phase I and II clinical trials. Epigenetic modifications of RNA molecules represent the next frontier in this area of biology, with unique translational opportunities. This project will first focus on the structural analysis of binding pockets found on proteins involved in the RNA methylation pathway (evaluation of druggability, identification of interaction hot-spots, and structural diversity). Lessons learned from this analysis will then serve as a foundation for a second step, consisting in screening virtually chemical libraries, and designing inhibitor candidates that will be purchased. The compounds will be screened in vitro and hits co-crystallized by another research group at the Structural Genomics Consortium with strong experimental expertise on the biochemistry of the RNA methylation pathway.