**Master « Sciences, Technologie, Santé »**
**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: **Prof. Antonio Macchiarulo**

Adress : **Via del Liceo 1, 06123, Perugia (ITALY).**

E-mail : antonio.macchiarulo@unipg.it

**Name of training supervisor: Prof. Antonio Macchiarulo**

Phone number : ++ 39 075 585 5160
Fax : ++ 39 075 585 5161
E-mail : antonio.macchiarulo@unipg.it


Specialty training : Research ☑ Professional ☐

a few key words to describe the subject of training : molecular docking; steered molecular dynamics; enzyme; inhibitor; kinetic constants; unbinding.

**Title of internship: Study of the Interaction Mode of IDO Inhibitors by Steered Molecular Dynamics.**

this subject is a first step towards a thesis: **No**

**Short texte describing your project**


Indoleamine 2,3-dioxygenase (IDO) is a master regulator of immune tolerance in pregnancy, cancer disease and host-pathogen interactions. As a consequence, IDO is attracting a great deal of attention as drug target to developing new therapeutic opportunities for cancer and autoimmune diseases.
Starting from the available crystal structure of the enzyme, this project aims to study the interaction mode of selected inhibitors to IDO. Specifically, molecular docking and steered molecular dynamics will be used to study the binding/unbinding process of the two isomers of 1-methyltryptophan. From data in literature, 1-Me-D-Trp has shown superior *in vivo* anticancer activity compared with 1-Me-L-Trp. Nevertheless, 1-Me-L-Trp proved to be endowed with higher specificity and inhibition potency to IDO than the other isomer. The results of this study are expected to shed lights on key residues involved in the stereo-specificity of ligand recognition in IDO and suggest routes of lead compound optimization to designing more potent and selective inhibitors of the enzyme.


Send by e-mail: laurence.muller-wurtz@univ-paris-diderot.fr
anne-claude.camproux@univ-paris-diderot.fr