

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

> OFFER AN INTERNSHIP Academic Year 2012 – 2013 Send to Mrs Pr Camproux : anne-claude.camproux@univ-paris-diderot.fr



Name of the head of laboratory or company: Dipartimento di Chimica e Tecnologia del Farmaco, Faculty of

Pharmacy, University of Perugia.

Adress : via del Liceo 1, 06123, Perugia, Italy

E-mail: antonio@chimfarm.unipg.it

## Name of training supervisor: Antonio Macchiarulo

Phone number : +39 075 5855160 Fax : +39 075 5855161 E-mail : antonio@chimfarm.unipg.it

Specialty training :	Research		Professional

## **Title of internship:**

Application of molecular dynamic simulations (MD) and replica exchange molecular dynamics (REMD) to study the cross-talk of PARP-1 domains in presence and absence of small molecule inhibitor.

this subject is a first step towards a thesis: No

## Short texte describing your project

Exploring and defining the conformational space of target proteins is pivotal to improve structure-based drug discovery approaches. Poly(ADP-ribose) polymerase-1 (PARP-1) is a multi-domain enzyme that couples DNA damage detection to poly(ADP-ribosyl)ation activity through a hitherto elusive mechanism. Using the recent disclosed crystal structure of PARP-1 domains (Langelier MF Science 2012), the applicant will apply molecular dynamic simulations (MD) and replica exchange molecular dynamics (REMD) to study the cross-talk of PARP-1 domains in presence and absence of small molecule inhibitors.

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