

**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](mailto:anne-claude.camproux@univ-paris-diderot.fr)

Name of the head of laboratory or company: Prof. G. Wolber

Adress : Köngin-Luise-Str. 2+4, 14195 Berlin

E-mail : gerhard.wolber@fu-berlin.de

---

**Name of training supervisor: Alexandra Naß**

Phone number :

Fax :

E-mail : alexandra.nass@fu-berlin.de

Specialty training :    Research    ☒                      Professional    ☐

a few key words to describe the subject of training : computational drug design, structure and ligand based methods

---

**Title of internship:** Selective small molecule inhibitors of LMW-PTP

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

---

**Short texte describing your project**

LMW-PTP has been found to be related to different types of tumors and diabetes mellitus. Small molecule inhibitors could be a first step towards drugs. In order to find novel selective inhibitors with physicochemical properties appropriate for lead compounds structure and ligand based methods will be used : based on the available 3D protein structure in the PDB and known structure activity relationships 3D pharmacophore models can be created and used to screen different vendor databases. Protein-ligand docking can then be employed to select the hits and give hints for further refinement.