Master « In Silico Drug Design »
Second Year

OFFER AN INTERNSHIP
Academic Year 2015/2016

Send to Mrs Pr Camproux
anne-claude.camproux@univ-paris-diderot.fr

Name of the head of laboratory or company:

Adress :
CENTRE FOR DRUG RESEARCH
Faculty of pharmarcy
PO Box 56 (Viikinkaari 5 E)
FI-00014 University of Helsnki
E-mail :

Name of training supervisor: Dr Henri xhaard

Phone number :
Fax :
E-mail : xhaard@mappi.helsinki.fi

Specialty training : Research ☐ Professional ☐

a few key words to describe the subject of training :

Title of internship:

Optimizing the hydrogen-bond network in GPCR models

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

Short texte describing your project

To our experience, (1) molecular modeling softwares (even commercial) optimize very poorly - or simply do not optimize at all - the network of hydrogen bond formed by side-chains (and water molecules) when homology models are built and (2) virtual screening experiments perform less well in molecular models presenting a poor hydrogen bonding network. The aim of this training period is to continue developing the code generated by the previous ISDD internship to write a software that run an optimization protocol, optimizing the hydrogen bond network for the side-chains that face the binding pocket in GPCRs. There is a lot of room for new developments. The candidate will focus on a single algorithm among those that may be used (eg genetic, ant-colony, random forest, monte carlo). As much as possible the search space will be divided so that parallelized GRID computing can be used (collaboration with Finnish Center for Scientific computing). Performance will be compared to existing software (eg SchrÃ¶dinger, Modeller 9v2, Swissmodeller, Tripos/Sybyl, Accelrys/Discovery studio) based on retrospective reconstruction of known Xray structures. Data already available: object-oriented code that allow many geometrical definitions (helices, blocks of amino acids) and their transformations, code for parsing PDB files.

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