Master « Sciences, Technologie, Santé »
Mention « In Silico Drug Design »
2ème année

PROPOSITION DE STAGE
Année Universitaire 2012 – 2013

A envoyer à Mme Pr Camproux :
anne-claude.camproux@univ-paris-diderot.fr
colette.geneix@univ-paris-diderot.fr

Nom du Responsable du Laboratoire ou de l'Entreprise:

Affiliation administrative (CNRS, INSERM,…) et Numéro d'affiliation de l'unité :

Centre for Drug Research, Faculty of Pharmacy

Adresse précise du Laboratoire :

PO BOX 56, FI-00014 University of Helsinki, Helsinki, Finland

Nom du Responsable de l'équipe d'accueil (EA) : Professor Arto Urtti

Equipes d'accueil

Dr Henri Xhaard
http://www.helsinki.fi/cdr/research/group_xhaard.htm
Equipe : 1 investigateur principal (PI), 2 postdocs, 7 doctorants, 2 doctorants invités

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Nom du Responsable du stage :

Dr Henri Xhaard

E-mail : henri.xhaard@helsinki.fi

Titre du stage :

Optimizing the hydrogen-bond network in GPCR models.

Description du sujet (quelques lignes):

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 write a software that will run an optimization protocol, optimizing the hydrogen bond network for the side-chains that face the binding pocket (not the side-chains of the loop domain) in GPCRs. 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 Schrödinger, Modeller 9v2, Swissmodeller, Tripos/Sybyl, Accelrys/Discovery studio) based on retrospective reconstruction of known Xray structures. Data already available: rotamer library for literature, code for parsing PDB files and most of the geometry calculations, starting model coordinates.