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

OFFER AN INTERNSHIP
Academic Year 2012 – 2013
Send to Mrs Pr Camproux :
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Name of the head of laboratory or company: Prof. T. Hackeng

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Specialty training : Research ☒ Professional ☐

a few key words to describe the subject of training : structural bioinformatics – virtual screening - hit identification - lead optimization - direct binding analysis

Title of internship: Targetting of NETosis through structure-based virtual ligand screening.

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

Short texte describing your project

Neutrophils respond to infection with formation of neutrophil extracellular traps (NETs) in a process that was discovered relatively recently and is named nettosis. Several proteins are involved in nettosis, and currently we are prioritizing these proteins via cell based assay systems. The aim of our studies is to discover molecules that can prevent nettosis and thereby dampen the inflammatory response of neutrophils. This way we envision that we may be able to describe a new generation of anti-inflammatory drugs. Inflammatory disease remains to be a major threat to public health in Western countries, but more so in third world countries.

In this project we will use a combination of data mining and structural bioinformatics, including virtual screening, molecular docking, MD simulation and binding free energy calculation to select most suitable targets and discover and optimize drug-like molecules that may serve as starting points for drug development. Functional testing of molecules will be performed in-house in specific assay systems as well as through direct binding studies using Biacore and/or nanoITC technologies. Depending on skills and interests, the potential candidate will be involved in the wet lab screening, as well as in the *in silico* part of this study.