Master « In Silico Drug Design »
Second Year

OFFER AN INTERNSHIP
Academic Year 2016/2017
Send to Mrs Pr Camproux
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Name of the head of laboratory or company: Ole Thastrup, Professor, PhD

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Specialty training : Research X ☐ Professional ☐

a few key words to describe the subject of training : The project is part of an intensive computational chemistry based approach to study the structure-activity relationships of cytochromes P450 and other drug metabolising enzymes at the Biostructural Research group (http://www.farma.ku.dk/br) at University of Copenhagen.

Title of internship:

From SMARTCyp towards a Virtual Liver

This subject is a first step towards a thesis: Yes

The project is a research project and the candidate will be able to base his/her Master thesis on it.

Short text describing your project

In the Biostructural Research group at University of Copenhagen, we have developed the SMARTCyp program to predict cytochrome P450 mediated site-of-metabolism. The program is widely used by the pharmaceutical industry all over the world and is available via a Web-server (http://www.farma.ku.dk/smartcyp/) or as an open-source JAVA-based program to be installed locally or being embedded in other software packages (e.g. in the Schrödinger and MOE software). The SMARTCyp program is based on density functional theory (DFT) calculations on model compound leading to a library of reactivities of fragments representative for most drug compounds.

At present, we are working on several extensions and improvements of the original SMARTCyp program:

1) extending the SMARTCyp concept to other drug metabolising enzymes (aldehyde oxidase, sulfotransferase etc.),

2) predicting not only site-of-metabolism, but also predicting and ranking the possible metabolites,

3) developing annotated output, i.e. with references to the computational model and similarity to model,

4) designing and developing a graphically user-friendly intereface (GUI),

5) porting the present developing version from Python to Java.

We expect a student who wants to take responsibility and be an active partner in the project. We expect the project will result in a scientific publication.

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