Master « In Silico Drug Design »
Second Year

OFFER AN INTERNSHIP
Academic Year 2015/2016
Send to Mrs Pr Camproux
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Name of the head of laboratory or company: **RIKEN Structural Bioinformatics Team** - Division of Structural and Synthetic Biology - Center for Life Science Technologies

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Specialty training : Research ☒ Professional ☐

a few key words to describe the subject of training :

Drug design, Virtual screening, Docking, Shape and electrostatic matching

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Title of internship:

In silico screening for inhibitors of DNMT3B

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

Short texte describing your project

DNMT3B is required for genome-wide de novo methylation and is essential for the establishment of DNA methylation patterns during development. It is implicated in several diseases including cancer. However, there are no small molecule inhibitors reported to date.

The goal of this project is to discover small molecule inhibitors of DNMT3B in collaboration with biologists and medicinal chemists. During his/her internship, the student will be trained on using various advanced computational tools to perform virtual screening for the identification of hit compounds. Initially, a large collection of commercially available compounds will be screened using the state-of-the-art docking program, Glide from Schrodinger Inc., to identify potential hits. These potential hits will be purchased and assayed by our collaborating biologists. The assay confirmed hits will be further optimized by searching for analogs using shape and electrostatics matching tools, ROCS and EON from OpenEye Inc. Finally, new compounds will be designed using the MOE suite from the Chemical Computing Group and synthesized by our collaborating medicinal chemists.

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