Master « In Silico Drug Design »
Second Year

OFFER AN INTERNSHIP
Academic Year 2015/2016
Send to Mrs Pr Camproux
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iS·DD in Silico Drug Design — new insight to disease & therapy

Name of the head of laboratory or company: Sylviane Boucharens (Bioascent)

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Specialty training :   Research   ☐   Professional   X

a few key words to describe the subject of training : cheminformatics, data analysis, polypharmacology, ADMET

Title of internship: Polypharmacology and ADMET prediction of an internal chemical library

this subject is a first step towards a thesis: Yes

Short texte describing your project

BioAscent is a compound provider located in Scotland (http://www.bioascent.com/) and has recently released a 4480 compound library aimed for phenotypic screening. This library combines a set of chemically diverse compounds together with reference compounds with known MOA. A special care and attention has been brought to the quality of the annotations. Classically, many chemicals related properties are associated to hit compounds - guiding the compound selection process, but only sparse and variable biological information is available. However, this type of information is of critical importance in drug discovery.

The aim of this project is to investigate the potential pharmacological profile of this library using an ensemble of cheminformatics and in silico drug design tools. Based on the chemical structure of each compound of the library, the student will have to assess potential interactions with proteins (using for example ChemProt) and further potential pathways and diseases associated to compound.

Toxicity alerts (mutagenicity, carcinogenicity…), off-target prediction and ADME properties will be also investigated based on the development of machine learning prediction tools.

The final objective is to integrate all the biological information into a database that could be linked to the internal compound library database.

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