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

PROPOSITION DE STAGE
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HDR : oui

Ecole doctorale de rattachement : ED 393 – Santé publique

Spécialité du stage : Recherche X Professionnel ☐

Indiquez par quelques mots clés, l'orientation scientifique du sujet : polypharmacology, network biology, SAR index development.

Titre du stage : Development of a SARI approach based on pharmacophore fingerprint and assessment with side effects clinical outcomes

Ce sujet constitue-t-il un premier pas vers un travail de thèse : Potentiellement

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Description du sujet (quelques lignes):

The old drug design paradigm, i.e., drugs interact selectively with one or two targets (proteins), resulting in treatment and prevention of diseases, is now challenged by several studies showing that most of the drugs interact with multiple targets ("polypharmacology"). Acquiring knowledge of the full pharmacology profile has inspired new strategies to predict and to characterize drug-target associations in order to improve the success rates of current drug discovery paradigms, i.e. increase the efficacy and reduce toxicity and adverse effects.
To facilitate the analysis of such massive amount of data, network-like graphs illustration have started to be implemented to explore the chemical effect across multiple layers of complexity, from chemical space

In this project, we would like to develop the Structure-Activity Relationship Indices (SARI) approaches based on large chemogenomics databases (1). A structural similarity approach based on diverse fingerprint will be developed based on the study of Waver et al. and matched to side effect information. Then, network biology will be implemented to help the visualisation of the results. Such analysis would be useful to understand potential mechanisms of action related to side effects.

For the project, we look for a motivated and autonomous student would like to do network biology, data mining and who is not afraid to develop some small scripts.
You are welcome to contact me (olivier.taboureau@univ-paris-diderot.fr) if you have some questions.

References:
Waver, M., Peltason, L., Weskamp, N., Teckentrup, A., Bajorath, J. (2008) Structure-activity relationship anatomy by network-like similarity graphs and local structure-activity relationship indices. *J. Med. Chem*., **51**, 6075-6084.