MASTER « *In Silico* Drug Design »

2ème année

PROPOSITION DE STAGE
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Ecole doctorale de rattachement : Compléxité du Vivant

Spécialité du stage : Recherche ☒ Professionnel ☐

Indiquez par quelques mots clés, l'orientation scientifique du sujet :

Pocket, protein-protein interactions, 3D structure, clustering, high dimensionality space, distances, classification

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Titre du stage : Determination of similarities within the Protein-Protein Interaction pocketome.

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

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Description du sujet (quelques lignes):

The development of small molecules as drugs requires first to identify, within the chosen therapeutic target, a so-called druggable pocket that can accommodate a small molecule and consequently allow their modulation. This concept of pockets being a central dogma in drug design for small molecules, it imposes itself to all the chosen therapeutic targets, but constitutes a real challenge on families of complicated targets such as protein-protein interactions (PPIs). It is therefore essential to understand which PPIs can be drugged on the basis of a characterization of the pockets within them.

As part of a multidisciplinary project involving our group, the C3BI of the Institut Pasteur and the rest of the structural bioinformatics unit of Pr Nilges, we aim to characterize the pockets present at the core of the protein-protein interfaces. Using an already published approach, we have fully mapped the complete set heterodimeric

complexes in the PDBe and have detected, within them, pockets in the form of negative images of cavities constituted of interacting probes.

The aim of this internship is to establish, within this PPI pocketome, similarities between pockets for purposes of classification and determination of proximities within the pocket space. Several methods will be tested to establish a robust protocol for selecting relevant neighbors within this space. The objective is to validate this protocol on known examples to eventually proceed to the selection of target candidates on the basis of their proximity to already liganded systems.

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