Master « In Silico Drug Design »
2ème année

PROPOSITION DE STAGE
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Spécialité du stage : Recherche

Indiquez par quelques mots clés, l'orientation scientifique du sujet : protein-protein interaction networks – protein-protein docking – pathogenicity prediction of mutations

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Titre du stage :

Application of protein-protein docking to help caracterizing disease-related mutations for personalized medicine

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

Description du sujet (quelques lignes):

The general goal of this proposal is to computationally characterize protein-protein interactions involving proteins with mutations associated to diseases detected in newborn screening, so that this knowledge can be applied to increase the accuracy of pathogenicity predictions of new mutations. This will be done in close collaboration with Prof. Xavier de la Cruz (Vall d'Hebron Institut de Reserca; VHIR), in the context of an Interreg-POCTEFA European project.

The main activities for this 6-month project will be:

1) Build a list of proteins with mutations associated to diseases included in the newborn screening in North Spain and South France (POCTEFA region), using databases such as OMIM/ClinVar, UniProt, Exac, HGMD, and 1000Genomes.
2) Build protein interaction networks for the above list of proteins, using available resources such as Interactome3D, PRISM.
3) Characterize proteins and interaction networks involving disease-related SNPs, using structural data, and biophysical properties: number of protein-protein pairs, number of partners per protein, number of cases with available 3D structure, number of residues at interface, types of interface residues according to accessibility (core or rim), number of distinct interfaces per partner, mutation density per interface residue, etc.
4) Test pathogenicity predictors (PolyPhen-2, SIFT, PON-P2) on the above list of disease-related proteins and identify those proteins in which standard methods show low predictive success.