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

**PROPOSITION DE STAGE**
**Année Universitaire 2012 – 2013**
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**Nom du Responsable du Laboratoire ou de l'Entreprise:**

Affiliation administrative (CNRS, INSERM,…) et Numéro d'affiliation de l'unité :

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HDR : oui ou non

Ecole doctorale de rattachement :

Spécialité du stage : Recherche ☐ Professionnel ☐

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

**Titre du stage :** STRUCTURAL BIOINFORMATICS STUDY OF AMYLASES, CHITINASES AND CELLULASES

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

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**Description du sujet (quelques lignes):**

The most abundant organic compounds on earth are cellulose, starch, and chitin, all of them being renewable and important sources of energy, their digestion in glucose being the subject of large amount of research work. To valorize the carbohydrate-rich waste by extracting useful carbohydrates is still an open problem with high importance for environmental protection. Usually, there are two common ways to convert cellulose, starch and chitin to glucose: chemical and enzymatic. From enzymatic viewpoint, cellulose is degraded by cellulases, starch is degraded by amylases and chitin is degraded by chitinases. Alpha 1-4 linkages make starch fairly easily broken down by enzymes whereas beta 1-4 linkages result in linear microfibrils of cellulose which are difficult to break down. In case of chitin, the substitution of the hydroxyl group by an acetyl amine one increases the hydrogen bonding between adjacent polymers and chitin is also difficult to break down. There are major differences regarding the efficiency of these three classes of enzymes. Comparison of the kinetic parameters reveal that chitinases and cellulases are less efficient than amylases. The aim of this study is to perform a bioinformatics analysis in order to identify sequence and structure similarities/dissimilarities between amylases, cellulases and chitinases with direct

consequences on their catalytic activity and to identify possible actions to enhance catalytic activity of cellulases and chitinases.

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