



Call for applicants to get a 3-year PhD grant from LabEx Arcane (Grenoble, France)
Deadline for application : 10 May 2015

Inclusion complexes of amylose: morphogenesis, crystal structure and chiral separation of bioactive molecules

Objective:

This work aims at determining the structure of amylose crystals prepared in the presence of selected complexing molecules. These compounds will serve as models to understand the entrapment and release properties of small active ligands in starchy products and evaluate the potential use of this crystallization method for chiral separation of enantiomers.

Abstract:

Amylose is a natural polymer with a significant industrial interest since starch, from which it is extracted, is a basic substance for the food industry. As a homopolymer of glucose, amylose can occur under different crystalline forms. So-called A and B types are found in native starch granules and are constituted of double helices. The V type is described by single helices that form by *in vitro* crystallization in the presence of small molecules (alcohols, lipids, etc.) and spontaneously self-assemble into crystals. The molecular organization of these V-amylose complexes is only partially known. This thesis will focus on unraveling the crystallization mechanisms of amylose in the presence of a selection of molecules. The ligands will be chosen depending of their potential interest for industrial applications (aromas, bioactive compounds, etc.). The experimental approach will be coupled to the molecular modeling of the structures, which will allow to study, among other aspects, the localization and the mobility of the complexing agent in the crystal lattice. The study will be divided into two parts: 1) set up of an instrumented reactor and optimization of the crystallization protocols using an experimental design method; 2) structural characterization of the complexes and evaluation of the chiral separation properties by complex formation.

Methods:

Set up of a crystallization reactor, optimization of the crystallization protocols using an experimental design approach, morphological characterization using scanning and transmission electron microscopy, structural analysis by X-ray and electron diffraction, solid-state NMR, infrared spectroscopy, optical rotation, molecular modeling.

Profile of the applicant:

Preferably with a background in polymer sciences, the applicant must be interested in fundamental research, instrumentation and structural analysis. He/she will need to follow crystallization protocols and bring some fresh ideas to optimize them and control the size and morphology of the crystals. Several structural characterization techniques are available in-house so this work offers a unique opportunity to get a basic training on various imaging, diffraction and spectroscopy equipments. Depending on the candidate affinity for computer work, a basic training in molecular modeling can also be considered. As the number of grants offered by LabEx Arcane is very small, the selection will be based on the applicant excellence, with very good grades during his/her master degree.

- **Research laboratory:** Centre de Recherches sur les Macromolécules Végétales (Grenoble, France), "Structure and Properties of Glycomaterials" group (<http://www.cermav.cnrs.fr/>)
- **Associated laboratory:** Département de Pharmacochimie Moléculaire (Grenoble, France), "New Tools for Drug Delivery and Analysis" group (<http://dpm.ujf-grenoble.fr/>)
- **Doctoral school :** Chimie et Sciences du Vivant, Univ. de Grenoble (<http://edcsv.ujf-grenoble.fr/>)
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Send your résumé, grades and a motivation letter, indicating clearly which aspects of your curriculum and training are relevant for the proposed subject.