1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title:

Studying the molecular mechanisms of starch processing using computational biophysics tools.

1.1. Project goals

- To build realistic theoretical models of starch
- To use molecular modelling techniques like all-atom and coarse-grained molecular dynamics methods
- To find best computational protocols for simulations of starch processing
- To find better techniques of starch processing

1.2. Outline

Efficient and inexpensive food processing is of high importance these days. Technological companies are able to pay big money to develop a faster and more efficient process to produce large quantities of food cheaply in a given time. In the human diet, the main source of carbohydrates is starch, which acts as an energy store in plants. Starch is an organic chemical compound, a plant polysaccharide, consisting solely of glucose mers linked by α-glycosidic bonds. It is a semicrystalline substance, insoluble in cold water, in fact consisting of two fractions: unbranched amylose made of glucose residues linked to each other by oxygen atoms through α-1,4-glycosidic bonds, and branched amylopectin, in which there are additional α-1,6-glycosidic bonds. Starch is deposited in plant cells in the form of grains, the size and shape of which are characteristic of individual plant species. Sources of starch include cereals (rice, wheat, corn), potatoes or manioc.

The Ph.D. project involves conducting research using computational molecular physics methods (e.g., molecular dynamics) of thermal processing of starch, learning about the physico-chemical factors occurring during this process, and then selecting processing parameters so that the most optimal starch processing process can be proposed to food technologists, taking into account, among other things, pressure, temperature, pH, the presence of salts and other chemical compounds. Starch retrogradation will be studied. One of the problems to be solved is the construction of a correct model of starch derived from rice and wheat, so that it will be as simple as possible and at the same time well reproduce the real system. It is assumed that all-atom simulations as well as coarse-grained methods will be carried out.

The research will be carried out in close cooperation with Ningbo University, Ningbo, China, (Dr. Shangyuan Sang), which will provide preliminary data on the physical-chemical conditions on the basis of initial experimental data, and will be able to check the tractability of the predictions of the simulation methods once the simulations have been carried out and better parameters selected.

1.3. Work plan

I. Mastering molecular dynamics and coarse-grained molecular dynamics techniques

II. Find realistic starch models.

III. To propose proper calculation protocols used in starch processing

IV. To propose better starch processing technique

1.4. Literature (max. 10 listed, as a suggestion for a PhD candidate)

[1] V. Krishnan, et al., Starch-lipid interaction alters the molecular structure and ultimate starch bioavailability: A comprehensive review, Int J Biol Macromol 182 (2021) 626.

[2] F. Cui, et al., A study of starch-urea-water mixtures with a combination of molecular dynamics simulation and traditional characterization methods, Int J Biol Macromol 148 (2020) 121.

[3] J.R. Perilla, et al., Molecular dynamics simulations of large macromolecular complexes, Curr Opin Struct Biol 31 (2015) 64.

[4] A. Hospital, et al., Molecular dynamics simulations: advances and applications, Adv Appl Bioinform Chem 8 (2015) 37.

[5] T. Hansson, et al., Molecular dynamics simulations, Curr Opin Struct Biol 12(2) (2002) 190.

[6] C.G. Biliaderis, The structure and interactions of starch with food constituents, Can J Physiol Pharmacol 69(1) (1991) 60.

[7] M. Zubair, et al., Emerging trends and challenges in polysaccharide derived materials for wound care applications: A review, Int J Biol Macromol (2024) 132048.

[8] N. Mahmood, et al., Influences of emerging drying technologies on rice quality, Food Res Int 184 (2024) 114264.

1.5. Required initial knowledge and skills of the PhD candidate

- Ability to work in Linux system
- Basic knowledge of programming in bash, C, Python
- Understanding of molecular biology and physics
- Basic knowledge about chemistry, biology and food technology.
- Analytical thinking
- Eager to learn

1.6. Expected development of the PhD candidate's knowledge and skills

- Better understanding of advanced modeling methods used in computer physics and computational biophysics
- Practical knowledge of designing starch models
- Programming and Linux skills (bash, C, Python)
- "Fluency" in work in collaboration with international scientific groups