

Carbohydrates are one of the key groups of compounds that determine the structure and functioning of all living organisms. Contrary to the studies focused on other types of biomolecules, e.g. proteins, lipids or nucleic acids, analogous studies on the structure, conformation and the role of carbohydrates in biological systems are much less advanced.

The main goal of the project is to create a series of computational tools designed to effectively study the behavior of carbohydrates and carbohydrate-containing systems by means of the molecular dynamics simulations technique. These tools will have a character of the so-called force fields, i.e. sets of parameters approximating the interactions that are present in real systems. In contrary to many existing force fields, we want to focus on the so-called coarse-grained models, which are based on a simplified representation of molecules, introducing pseudoatoms that simulate the behavior of whole groups of the real atoms. This allows for a significant increase in the efficiency of simulations and, as a result, consideration of large-scale systems and processes occurring within broader timescales.

We intend to create a coherent set of parameters covering a number of natural carbohydrates that exhibit various functionalizations, different types of glycosidic linkages, possible branching of the chain, etc. The developed parameters will be compatible with those already existing and dedicated to other types of biomolecules (proteins, lipids, nucleic acids ...). In the further perspective, such combination will allow to perform research concerning a wide range of natural systems of diverse composition in which carbohydrates are in contact with biomolecules of other types.

In addition, as a part of the project, the created parameters will be applied to study selected systems and processes that involve natural polysaccharides.