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Carbohydrates are one of the most essential chemical compounds that occur in nature. They are structural components of living organisms (e.g. constituents of DNA and RNA), energy source for them and play a crucial role in numerous, natural biochemical processes. One of the basic distinctions that can be applied to carbohydrates is based on the type of their monomer residues: pyranoses contain six-membered rings whereas furanoses are five-membered ring sugars.

As an alternative to the commonly used experimental methods which can be used to study the structure and role of carbohydrate molecules, one can also use the tools provided by computational chemists, such as methods of computer simulations. Contrary to pyranoses, furanoses are relatively rarely studied in that way. One of the reasons for that is the lack of appropriate tools and methods which can be applied to effectively and accurately investigate the molecular features of furanoses by means of the molecular dynamics-based methods of computational chemistry.

Our project aims at development of such tools. In particular, we want to create the set of parameters (called the biomolecular force field) which can subsequently be used to perform simulations of furanose-containing biomolecular systems. The developed force field will be validated against the available experimental and quantum-mechanical data and extensively tested for the most chemically/biochemically significant furanose-containing systems. The final version of the force field (distributed free of charge) will be possible to apply in simulations of various biomolecular systems containing furanoses.

The subsequent stage of our research will include the extensive theoretical study (with the use of the newly-developed force field) on the conformational features exhibited by the molecules of furanose-containing saccharides. Additionally, we plan to investigate the molecular details of interactions between furanoses and the biomolecular systems of other types (e.g. lipid membranes or proteins).