

PhD Project

Structure of carbohydrates investigated by NMR spectroscopy and molecular modeling

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Carbohydrates are the most abundant biomolecules with enormous structural diversity. They are present in the Nature in the form of mono-, di-, oligo- or polysaccharides but also as a part of glycoconjugates such as glycoproteins, peptidoglycans or glycolipids. Consequently, this structural variety makes carbohydrates the least exploited among biomolecules. In addition to the structural diversity originating from multi-linkage and branching of a monosaccharide, carbohydrates are usually flexible molecules that can exist in various conformations. All this makes structural studies of carbohydrates difficult and challenging.

NMR spectroscopy is among other experimental techniques the most exploited method in determination of carbohydrate structure. The advantage of NMR is the possibility to study molecules of interest in both solution and solid state and at the same time correlate multiple parameters (chemical shift, coupling constants, NOE, relaxation times) with the structure. On the other hand, NMR spectra of carbohydrates are complex due to significant signal overlap and averaging of NMR parameters in solution experiments. Many NMR parameters respond sensitively to changes in structure, however, the structure is not directly deducible from NMR spectra. Therefore, a combination of experimental NMR with molecular modeling techniques is frequently used in carbohydrate structure determination.

The aim of the PhD project is studying of carbohydrate structure by NMR spectroscopy and explore various NMR techniques in combination with molecular modelling that can be used in order to fulfill this task. Particular emphasis will be given to the sensitivity of NMR parameters to conformational changes and to the influence of the environment on carbohydrate structure. The studied compounds will be synthesized in collaborating laboratory of Dr. Kamil Parkan at UCT Prague.