Synthesis and properties of cryptands with sucrose scaffold

DESCRIPTION FOR THE GENERAL PUBLIC (IN ENGLISH)

Supramolecular chemistry, an area rapidly developing for many years, deals with the non-covalent 'host-guest' interactions. A particularly interesting aspect of this research is the enantioselective complexation of chiral cations, *i.e.* their ability to distinguish two optical antipodes. The enantiomers, which are indistinguishable in achiral environment, may show a different affinity in biological systems. For example, one of the enantiomers may have therapeutic properties while its optical antypod can be toxic. Chiral receptors able to differentiate the enantiomers are therefore an object of study in many research groups.

One of the very interesting molecules are cryptands, compounds with strong complexing properties, much more expressed than in crown ethers and their aza-analogs. Cryptands form the complexes with the guest molecules which are located in the center of the crypt. Cryptands with sugar scaffold are known for quite a long time; the first synthesis of such molecule was realized in 1983. However, cryptands with a di-saccharide structure are rare.

In the current project, the synthesis and study of the properties of the new class of receptors: cryptands with sucrose scaffold is proposed. This type of derivatives is so far unknown. Sucrose is the most abundant disaccharide occuring in Nature; its yearly production exeeds 160 million tonnes, most of which is absorbed by the food market. However, there is a huge overproduction (a few percent = several million tonnes), which stimulates many research groups to use this 'redundant' sucrose also in other fields. The importance of this of these studies may be exemplified by the fact that they are referred to as *'sucrochemistry*' (by analogy to the '*petrochemistry*'). Synthesis of cryptands proposed in this project will be based mainly on penta-*O*-benzyl-sucrose in which all terminal positions are unprotected. This will allow to connect them with appropriate linkers.

Our earlier study on sucrose-based receptors displayed the interesting complexing properties of the analogs of aza-crown ethers. These receptors not only bind the ammonium cations, but also do it with high enantioselectivity. For example, α-phenylethyl ammonium cation with the *S*-configuration is complexed by several of our receptors while the *R*-enantiomer is completely not recognized by these hosts.

We reason that cryptands with sucrose scaffold, which we plan to obtain, will have even better complexing properties than 'sucrose-based' crown ether analogs. This assuption is supported by a literature data which clearly indicate that cryptands usually show much greater affinity to ammonium salts than the corresponding aza-crown ethers. In the proposed project we will prepare a wide range of cryptands with sucrose unit in the structure and will investigate their complexing properties. The first step will involve examination of the ability of such complexing agents to chiral α-phenylethylamine. The next task will be the investigatation of the complexation of amino acids.

The cryptands obtained in this project built on 'benzylated' sucrose, could be fully de-protected which should enable to obtain the molecules soluble in water. Thus, the complexing study in such demanding solvent could be carried out.

The structure of cryptands and/or their complexes (cryptates) will be assigned using the X-Ray methodology (which can be a big challenge) as well as *in silico*. The project should broaden our understanding of the nature of chiral cryptands and their complexing abilities.