

Summary of the Ph.D Thesis:

Monosaccharides functionalized receptors in chiral anions recognition

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The main aim of this Ph.D Thesis was to investigate chiral recognition of anions by neutral receptors containing monosaccharides. To accomplish this goal, a hybrid anion receptor has been synthesized. It contained diindolylmethane as a binding pocket and D-glucuronic acid as enantio-differentiating part. The chiral recognition ability of this receptor was carried out by ^1H NMR titrations in demanding solvents. This receptor was able to recognize anions obtained from chiral α -hydroxyacids and *N*-Boc-protected α -amino acids. Structures of the supramolecular complexes were investigated using 2D ROESY NMR technique which showed that anions are located differently inside anion binding pocket (*Org. Lett.* **2013**, 15, 4730-4733).

Chiral anion binding by the above-mentioned receptors is accompanied by unusual anion-binding-induced chemical shift changes, particularly those of protons of acetyl groups and protons of glucopyranose ring. On that basis, the changes have been associated with chirality of anionic guests. Principal Component Analysis (PCA) of chemical shift changes for 26 anionic guests showed discrimination for most of anions based on their configuration. On the other hand, application of artificial neural network (ANN) allowed for guest chirality classification, based on anion-binding-induced chemical shift changes (*Chem. Eur. J.* **2014**, 20, 12368-12372).

Conclusions obtained from diindolylmethane receptor studies allowed for designing and synthesizing an anion receptor containing a new bispyrrolylbenzene anion binding motif. Investigation of binding properties showed that this anion receptor can undergo conformational changes, induced by fluoride, chloride, and dihydrogenphosphate anion binding. Additionally process of fluoride anion binding modifies the barrier of rotation of pyrrole with respect to the benzene ring (as a slow equilibrium on the NMR time scale). The above-mentioned results were the starting point to consider this anion receptor as a molecular logic gate. Anion receptor acted as INHIBIT and NAND logic gate, using a fluoride and dihydrogenphosphate anions as inputs and UV/VIS and fluorescence readout, respectively (*Chem. Eur. J.* **2014**, 20, 12790-12795).