New, non-macrocyclic amide and urea receptors in processes of anion recognition

Agnieszka Cholewiak

Promotor: prof. dr hab. Janusz Jurczak

The aim of this Ph.D. thesis was the synthesis and investigation of anion binding properties of new linear receptors of anions. These receptors are based on the new building block: 8-propyldithieno[3,2-*b*:2',3'-*e*]pyridine-3,5-diamine (DITIPIRAM) and are equipped with urea or amide hydrogen bond donors. The DITIPIRAM skeleton was chosen, among other due to the three-ring structure (advantageous in the anion binding process). In addition the number and the distribution of amine groups (easily convertible into amide or urea groups) were taken into consideration as well as the presence of the pyridine ring in the platform's structure (the interaction of nitrogen atom with urea or amide arms provides their arrangement in the favorable *syn-syn* conformation). This attractive building block has not been used yet in the supramolecular chemistry of anions.

This research was aimed at designing effective nonmacrocyclic anion receptors using the potential of DITIPIRAM, developing useful methods for their synthesis, and the detailed evaluation of their binding properties toward selected anions. The binding properties studies were carried out in solution (^{1}H NMR controlled titrations) and solid state (RAS).

The designed receptors have a favourable geometry of the binding site, which results in high stability constants toward model anions. The outcome of these studies, owing to the description of the full geometry of the binding pocket of the receptors confirmed the hypothesis that DITIPRAM is very useful as a platform for nonmacrocyclic anion receptors. These results were obtained by correlating the binding properties studies conducted in solution and in the solid state. In addition, the results may provide useful tips for designing both new building blocks (platforms) and efficient anion receptors.