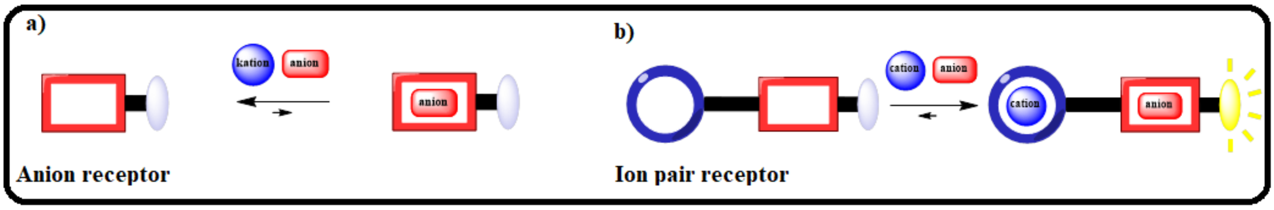
Studying the abilities of molecular receptors to form complexes with ions is one of the main trends of research in contemporary supramolecular chemistry. Taking advantage of noncovalent interactions, this line of work strives to achieve strong and selective binding between receptors and ions. However, while the study of cation complexation is quite well established, the design of receptors capable effectively complexing anions still poses a serious problem. Anions are characterized by varied geometry and more diffused charge than cations, making receptors capable of complexing them is much more difficult to design. When we further consider the optical properties (chirality) of anions, their enantioselective complexation becomes even more difficult. To resolve these problems, many research efforts strive to design monotopic receptors capable of interacting with cations or anions in particular ways. Such laboratory studies make use of the respective salts containing charge diffuse counterions, which are treated as having negligible influence on the binding of ions by the receptor (tetrabutylammonium or hexafluorophosphate salts). In nature, such salts do not occur, and cations and anions are generally strongly bound with their counterions; monotopic receptors dedicated to binding cations or anions are therefore generally ineffective for such ion pairs, having to compete with the counterion. This problem may be resolved through the design of ditopic receptors, capable of binding cations and anions simultaneously.



Binding of ion pair by a) mono- and b) ditopic receptor

Unfortunately, the simple combination of effective cation and anions receptors does not always yield effective ion pair receptors. In designing such receptors, it is very important to ensure the proper positioning of the binding domains. If they are properly attached to the receptor platform, the binding of one of the ions by the receptor may facilitate the binding of the corresponding counterion (e.g. by changing the conformation). In particular, this property may be utilized in the case of complexing weakly interacting ions (Br^-, NO_3^-, ClO_4^-). The receptor's binding of ion pairs may proceed in several ways. One way is for the ion pair to be bound to the receptor while its constituent ions are not in direct contact with one another. The most desired property for such receptors, however, is the ability to bind a salt in the form of a contact ion pair. In such situations, there is a very strong electrostatic interaction between the cation and anion, which additionally stabilizes the complex of the receptor and salt. Receptors with such properties are frequently macrocyclic compounds obtained by combining domains capable of binding both cations and anions. However, obtaining such compounds is very difficult because macrocyclic reactions are characterized by low efficiency. Macrocyclic receptors are usually structures not equipped with functional groups that might be utilized for further modification. An alternative to such receptors is offered by acyclic ion pair receptors. The proper spatial arrangement of binding domains on properly chosen molecular platforms may lead to effective salt receptors. Such receptors are easier to synthesize and more amenable to further modification with the aim of introducing new binding domains, adding additional functional groups (facilitating complexation studies, such as chromophores, fluorophores or electroactive units), or incorporating receptors into polymer networks.

The purpose of this project is to synthesize family of new, squaramide based and modular ion pairs receptors. Based on proposed idea the synthesis of the receptors library seems straightforward to achieve by combining of properly designed modules containing binding domains or reporters. I intend to investigate how the individual components of the proposed receptors (appropriate modules) affect the ability to bind cations, anions and ion pairs. Modular structure of the receptors allows to modify selected liquid and solid supports and thereby obtain functional material containing the receptor units. Both, the ion pair receptors and materials functionalized with them, will be used in extraction of harmful salts from water or in salt transport across membranes.