DESCRIPTION FOR THE GENERAL PUBLIC

Supramolecular chemistry concentrates on the complex structures and, unlike organic chemistry, studies intermolecular interactions such as Van der Waals forces, hydrogen bonds, π-π and electrostatic interactions that are responsible for the shape of protein molecules, transport of ions and small molecules across different types of membranes or their aggregation into larger systems. Analyzing these interactions is essential for the understanding of all processes occurring in living organisms. The supramolecular chemistry assumptions are based on the phenomenon of molecular recognition and self-organization of molecules. A host molecule with a cavity or pockets on its surface recognizes and binds the guest molecule. As a result of such self-organization, which requires the chemical and geometrical compatibility of the interacting molecules, a host-guest complex is formed. The most commonly used hosts in such supramolecular systems are macrocyclic compounds.

The aim of the project is designing, obtaining and analyzing supramolecular complexes between carboxylatopillar[*n*]arenes (*n* = 5, 6) (CPA5 and CPA6) and guanidine and amidine derivatives, taking into account the influence of conditions such as pH, stoichiometry or solvent type on their formation and structure. The essence of my project is to combine the studies on the complexation of selected organic cations of guanidine and amidine derivatives by CPA5 and CPA6 in the solution by techniques such as NMR spectroscopy and calorimetric titration ITC with solid state studies using single crystal X-ray diffraction method. This project aims to precisely characterize the obtained supramolecular systems, analyze intermolecular interactions responsible for the formation of host-guest complexes, and supramolecular architectures in the solid state. Additionally, the thermal stabilities of CPA5 and CPA6 complexes with guanidine and amidine derivatives by determining their melting point.

Carboxylatopillar[*n*]arenes (*n* = 5, 6) are in the center of interest in the studies of their ability of complexation different biologically important molecules. However, almost all studies on the host-guest complexes of CPA5 and CPA6 performed so far have been carried out in solution. Moreover, there is only one report on the complexation abilities of CPA5 in the solid state. Despite of many studies on host-guest complexes between CPA5 and CPA6 and biorelevant molecules, there were no investigation on the complexation process of such important bioactive compounds as guanidine and amidine derivatives by carboxylatopillar[*n*]arenes (*n* = 5, 6). The formation of host-guest complexes between CPA5 and CPA6 and guanidine and amidine pharmaceutics may increase their solubility in aqueous solution, prevent side effects and enable the obtaining of new transport and drug release systems under different conditions, e.g. pH.

The combination of solution and solid state studies will provide new information on the formation of the host-guest complexes of CPA5 and CPA6 with guanidine and amidine derivatives, the interactions responsible for their formation, the aggregation of molecules in the crystal lattice and the influence of solvent and pH on their structure. In a broader perspective, my project will be a basis for the understanding of the complexation process of guanidine and amidine derivatives by the CPA5 and CPA6, which may have potential applications in drug delivery systems and new supramolecular formulations of active pharmaceutical ingredients (APIs).