Synthesis of new functional cages based on trigonal peptidic building blocks by dynamic covalent chemistry

Molecular capsules are single molecules or systems of molecules that possess cavities that are large enough to accommodate other molecules. This feature allows for their use as transporters, sensors or nanoreactors or for storage and controlled release of other substances (reactive intermediated or drug molecules). However, their design and synthesis remains very challenging, because conventional methods of organic synthesis are inefficient for such complex and often hindered molecules. This project includes synthesis of molecular capsules composed of many components (up to 14) connected dynamically with each other. For this purpose, I will employ dynamic covalent chemistry, which takes advantages of reversible reactions. This approach introduces the possibility of controlling the reaction progress and obtaining "non-random" thermodynamically stable products. The project assumes formation of molecular capsules from the combination of two types of building blocks, trigonal and tetragonal blocks, which will be connected by imine or hydrazone bonds. Potential products will reveal an octahedral symmetry, large cavity and will be partially permeable (Fig. 1).



Fig. 1. Model of designed octahedral capsule.

The research tasks of the project include:

- synthesis of model building blocks;
- optimization of the reaction conditions for obtaining molecular capsules;
- incorporation of a series of functional amino acids for construction of building blocks and in the subsequent steps in capsules' formation;
- encapsulation experiments in the interior of the derived capsules.

Implementation of these research goals will result in obtaining a series of molecular capsules with unique properties, expanded interiors, chirality, dynamic character and numerous functional groups. Owing to these properties, target multi-component molecular capsules may exhibit applications as transporters and magazines for other molecules or as nanoreactors. It will also be a significant contribution to the basic knowledge, especially concerning the synthesis of complex materials composed of many components and the advantages of dynamic systems.