Novel chiral nanospaces for molecular confinement

Description of the POMOST Project

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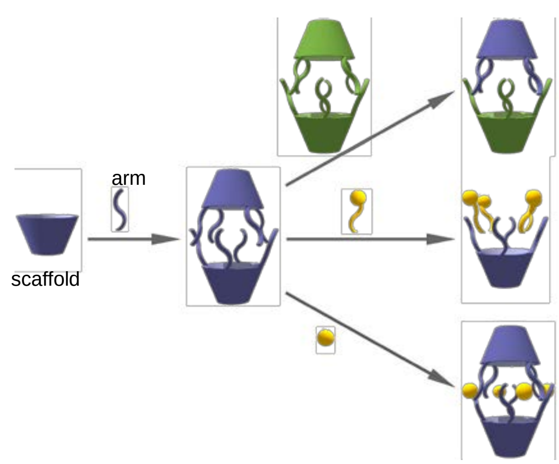
Living cells are able to perform hundreds of chemical reactions at the same time with unusual selectivity and effectiveness. This is possible owing to spatial separation of the processes using various cellular containers. Synthesis of artificial containers is a step towards mimicking functionality and complexity of natural systems. Synthetic molecular containers can be used to mimic enzyme's functions, they can also serve as selective sensors, gas storage media, reaction vessels or as hollow parts of advanced nanomaterials.

It is the goal of this project to design and synthesize new chiral capsules and cavitands having polar and functional interiors with the aim of using them as molecular reactors. Currently most of the known synthetic container molecules (capsules and cavitands) have walls composed of aromatic rings. Therefore, they have smooth and hydrophobic interiors incapable of directional interactions with guests, recognition of polar guests, distinguishing of enantiomers, performing in asymmetric reactions or generation of unidirectional motion. Their nonpolar interiors are disadvantageous for catalytic purposes since the only possible catalytic mechanism involves bringing the reactants together, whereas electrostatic effects were identified to have main catalytic contribution for natural systems. Synthetic container molecules with chiral and polar walls capable of directional interactions with guests can potentially overcome these drawbacks and therefore are of great interest. We have recently succeeded, for the first time, in synthesis of well-ordered capsular dimer with hydrophobic outer surface and polar and chiral interior. In the current project the methodology will be extended to produce new container molecules and applications of the resulting functional nanospaces as reaction vessels will be tested.

Tasks in the project

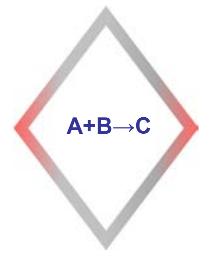


1. ***Synthesis of new polar capsules and cavitands*** based on amino acids and peptides. The synthesis will include a combination of classical organic synthesis and non-covalent assembly. The design includes capsules having various cavity sizes (in order to accommodate various/multiple guests), chiral cavitand molecules (in order to tune kinetics of guest uptake/release) and metal-

organic capsules (in order to modulate properties of capsule's walls.

2. ***Structural characterization of the assemblies*** involving molecular modeling, advanced NMR (2D techniques including DOSY), CD and X-ray techniques.

3. ***Investigation of the resulting assemblies as reaction nanovessels.*** The great advantage of a nanovessel as a reaction medium is separation of reacting species from the hostile environment and bringing reactants into a close proximity. It results in a considerable catalytic effect. However, for enzymes, electrostatic effects give, by far, the largest contribution to catalysis. The currently known molecular vessels with hydrophobic cavities have limited possibility of utilizing electrostatic interaction. The advantage of the currently designed containers is their internal polarity and chirality. Therefore, we expect their better performance in reactions proceeding through polar transition states (majority of the organic reactions) and possible application in asymmetric reactions.



References:

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