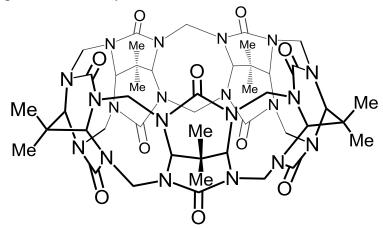
## Pressocucurbit[5]urils: synthesis and supramolecular properties

Lukáš Ustrnul, Vladimír Šindelář

Cucurbit[*n*]urils (CB[*n*]) are macrocyclic compounds known for ability to bind organic and inorganic guests in water with high affinity.<sup>1</sup> The smallest derivative of this family of compounds - CB[5] consist of five glycoluril monomer units and it is able to include only small solvent molecules and gases in its cavity.<sup>2</sup> CB[*n*] chemistry was explored almost exclusively in water and acidic media due to limited solubility in organic solvents.

Synthesis and properties of novel macrocycles constructed from propanediurea  $(Me_{10}prCB[5])^{3,4}$  and glycoluril  $(GU_1-Me_8prCB[5])^5$  unit will be presented. In comparison to other cucurbiturils this compound differs in a shorter carbonyl portals distance and has better solubility in water and organic solvents.

GU<sub>1</sub>-Me<sub>8</sub>prCB[5] is well soluble in methanol. It allowed us to look deeply into supramolecular chemistry of CB[*n*]s in this organic polar solvent. We described exceptionally strong binding of cations which is even higher than interaction between potassium and crown ethers. The same pressoCB[5] derivative exhibits cation-modulated self-assembly into tetrameric aggregate. The tetramer is stabilized by the addition of up to one equivalent of a cation but is fully disassembled in the presence of 2 equivalents of the cation. Cations can thus be used to tune the aggregation of macrocycle in solution.



(1) J. Lagona, P. Mukhopadhyay, S. Chakrabati, L. Isaacs, Angew. Chem. Int. Ed. 2005, 44, 4844

- (2) Y. Miyahara, K. Abe, T. Inazu, Angew. Chem. Int. Ed. 2002, 41, 3020-3023
- (3) X. Jiang, X. Yao, X. Huang, Q. Wang, H. Tian, Chem. Commun. 2015, 51, 2890
- (4) L. Ustrnul, P. Kulhanek, T. Lizal, V. Sindelar, Org. Lett. 2015, 17, 1022
- (5) L. Ustrnul, M. Babiak, P. Kulhanek, V. Sindelar, in process of publication