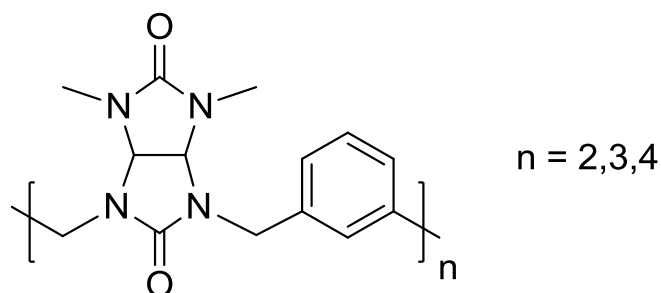


# Bambusuril analogs based on alternating glycoluril and xylylene units

Tomáš Lízal, Vladimír Šindelář

Glycoluril is a urea-based heterocyclic molecule, which is a suitable building block for macrocyclic receptors. These host molecules can interact with cationic, anionic or neutral guests. Bambusurils<sup>1</sup> are potent anion receptors that were used to detect and quantify anions in a complex mixture by NMR<sup>2</sup>. In order to allow anion sensing by UV-VIS spectroscopy, we designed a new bambusuril derivative incorporating aromatic groups in its structure.

Here we present synthesis of the new hybrid macrocycles consisting of glycoluril and aromatic units. Inspired by work of prof. Shimizu<sup>3</sup>, we employed basic synthetic conditions which afforded us with mixture of macrocyclic of various sizes. The macrocyclic homologues were separated by reverse-phase flash chromatography and characterized by the means of NMR spectroscopy and X-ray crystallography. The conformational behavior of separated isomers was investigated using DFT models and variable-temperature NMR.



**Figure 1.** Xylylene-glycoluril macrocycle.

## References

- [1] J. Švec, M. Nečas, V. Šindelář, *Angew. Chemie Int. Ed.* **2010**, *49*, 2378;
- [2] V. Havel, M. A. Yawer, V. Šindelář, *Chem. comm.* **2015**, *51*, 4666;
- [3] K. Roy, C. Wang, P. J. Pellechia, L. S. Shimizu, *J. Org. Chem.* **2010**, *75*, 5453.