HOST-GUEST COMPLEXES WITH A CHIRAL HEMICUCURBIT[8]URIL

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Molecular recognition, as the foundation of most biological systems, has inspired the development of synthetic receptors for e.g. sensors, pharmaceuticals, separation systems and catalysis. [1] Our group has focused on chiral macrocyclic receptor molecules – cyclohexanohemicucurbit[*n*]urils (cycHC[*n*]), notable for their size- and shape-selective encapsulation of anions. [2][3][4]

More recently, we have set our aim to establish the scope of neutral guests that form host-guest complexes with the barrel shaped (*all-R*)-cycHC[8] (Figure, left). Inspired by the potential application of cycHC[8] as a chiral catalyst, a number of small heterocyclic compounds were chosen for the study, resulting in several 1:1 host-guest complexes which have been characterized by single crystal X-ray diffraction in solid state (Figure, right) and NMR spectroscopic methods in solution.

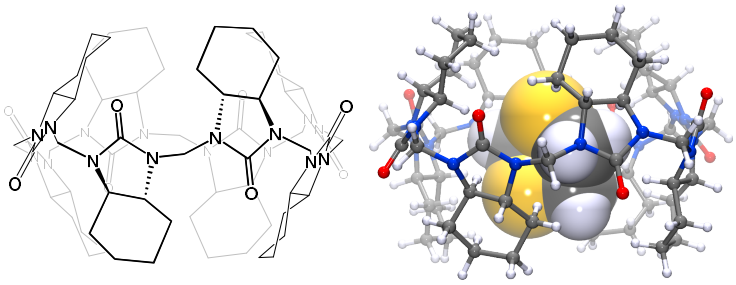

Fig.1 The molecular structure of (all-R)-cycHC[8] (left) and the crystal structure of its host-guest complex with 1,3-dithiolane (right)

References

1. E. M. Peck, B. D. Smith, in *Synthetic Receptors for Biomolecules: Design Principles and Applications*; ed B. D. Smith, Royal Society of Chemistry, Cambridge, 2015; ch. 1, pp 1–38.
2. R. Aav, E. Shmatova, I. Reile, M. Borissova, F. Topić, K. Rissanen, 2013, *Org. Lett.* 15, 3786.
3. E. Prigorchenko, M.Öeren, S. Kaabel, M. Fomitšenko, I. Reile, I. Järving, T. Tamm, F. Topić, K. Rissanen, R. Aav, 2015, *Chem. Commun.* 51, 10921.
4. S. Kaabel, J.Adamson, F. Topić, A. Kiesilä, E. Kalenius, M. Öeren, M. Reimund, E. Prigorchenko, A. Lõokene, H. J. Reich, K. Rissanen and R. Aav, 2017, *Chem. Sci*, 10.1039/C6SC05058A.

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