

# CHIRAL HEMICUCURBIT[*n*]URILS, THEIR SYNTHESIS, POST FUNCTIONALIZATION AND APPLICATION

Kamini A. Mishra, Riina Aav

Department of Chemistry and Biotechnology, Tallinn University of Technology,  
Akadeemia tee 15, 12618 Tallinn, Estonia  
e-mail: [kamini.mishra@taltech.ee](mailto:kamini.mishra@taltech.ee)

Supramolecular chemistry involving encapsulation of guest molecules by macrocyclic hosts, has become a challenging interdisciplinary field with a wide range of applications and a strong impact in analytical sciences. Hemicucurbiturils (HCs)<sup>[1]</sup> are neutral macrocyclic host molecules which is a subclass of cucurbiturils (CBs), well known pumpkin shaped host molecules synthesized in template controlled single step oligomerization reaction.<sup>[2]</sup> In the CB family, there aren't many examples of chiral hosts, which is a significant disadvantage. In this work we address various methods for inducing chirality in CB-type hosts,<sup>[3]</sup> and discuss the synthesis of cycHC[12] which is the largest substituted HC homolog to date.<sup>[4]</sup> An efficient mechanochemical protocol is developed to assist in tuning of macrocyclic structure as well as for synthesis of peptides and amides.<sup>[5]</sup> We also show that cycHCs can bind neutral heterocycles and that sulfur-containing heterocycles can be efficiently isolated from water using solid-phase extraction.<sup>[6]</sup>

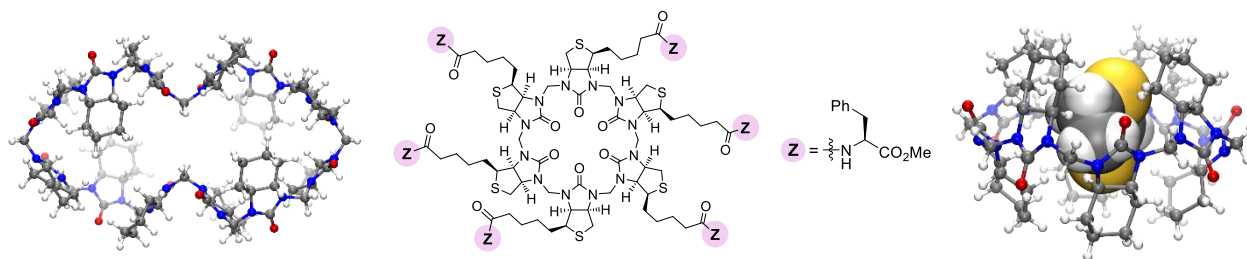


Figure 1. From left to right: cycHC[12]; hexa-amide-biotin[6]uril; and 1,3-dithiolane@cycHC[8]

## References

- [1] N. N. Andersen, M. Lisbjerg, K. Eriksen, M. Pittelkow, 2018, *Isr. J. Chem.*, 58, 435–448.
- [2] S. Kaabel, R. Aav, 2018, *Isr. J. Chem.*, 58, 296–313.
- [3] R. Aav, K. A. Mishra, 2018, *Symmetry*, 10, 98.
- [4] K. A. Mishra, J. Adamson, M. Öeren, S. Kaabel, M. Fomitšenko, R. Aav, 2020, *Chem. Commun.*, 56, 14645–14648.
- [5] T. Dalidovich, K. A. Mishra, T. Shalima, M. Kudrjašova, D. G. Kananovich, R. Aav, 2020, *ACS Sustainable Chem. Eng.*, 8, 15703–15715.
- [6] T. Shalima, K. A. Mishra, S. Kaabel, L. Ustrnul, S. Bartkova, K. Tõnsuaadu, I. Heinmaa, R. Aav, 2021, DOI 10.26434/chemrxiv.14458854.v1.

