Functionalized Chiral Bambusurils: Synthesis and Host-Guest Interactions with Chiral Carboxylates

Jan Sokolov, Adam Štefek, Vladimír Šindelář*

Department of Chemistry and RECETOX, Faculty of Science, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic. E-mail: sindelar@chemi.muni.cz

Bambusurils are a group of macrocyclic compounds that features notable anion recognition properties.¹ Bambusurils can bind inorganic anions as well as carboxylates, sulfonates or organic phosphates.²⁻⁴ Recently we started investigating enantioselective binding of chiral carboxylates by chiral bambusuril derivatives.⁵ Hereby we report synthesis and supramolecular behavior of two new representatives of chiral bambusuril macrocycles bearing ester groups (Figure 1) that are suitable for further modifications.⁶ Supramolecular properties of the new macrocycles were studied by means of NMR. New bambusurils exhibit enantioselective binding of chiral carboxylate anions. Comparison of the new macrocycle with a previously reported one shows that introduction of the substituents has significant impact on the enantioselectivity. The results also indicate that selectivity towards structurally different carboxylates is governed by bulkiness of the substituents that surround bambusuril portals. Lastly, we would like to show the application of the previously reported chiral bambusuril as chiral solvating agent.



Figure 1. Structures of new chiral bambusuril macrocycles.

References

- ¹T. Lizal, and V. Sindelar, *Isr. J. Chem.* **2018**, 58 (3-4), 326–333.
- ²V. Havel and V. Sindelar, *ChemPlusChem* **2015**, *80* (11), 1601–1606.
- ³V. Havel, V. Sindelar, M. Necas, and A. E. Kaifer, *Chem Commun* **2014**, *50* (11), 1372–1374.
- ⁴ T. Fiala and V. Sindelar, *Supramol. Chem.* **2016**, *28* (9-10), 810–816.
- ⁵ J. Sokolov, and V. Šindelář, *Chem. Eur. J.* **2018**, *24* (58), 15482–15485.
- ⁶ J. Sokolov, A. Štefek and V. Šindelář, *ChemPlusChem* **2020**, 85 (6), 1307–1314.