Synthesis of Water-Soluble Amino-Functionalized Bambus[n]urils

Jacopo Torrisi,[1,2] Pia Jurček,[1,2] Vladimír Šindelář,[1,2]*
[1]Department of Chemistry and [2]RECETOX, Faculty of Science, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic,
jacopo.torrisi@mail.muni.cz

Anions are crucial for the existence of living organisms as many vital functions such as anion transmembrane transport are based on supramolecular recognition and interaction. Considering that most relevant biological interactions take place in water, supramolecular chemistry in water is a constantly growing area to research.[1]

Bambusurils (BUs) are a family of macrocyclic anion receptors formed by four or six glycolurils units presenting alternate conformations with two methine hydrogen atoms pointing toward the cavity and connected by methylene bridges. During the macrocyclization reaction, it is possible to form four- and six-membered rings, but only bambus[6]urils can bind anions inside their cavities due to their size.

Over the years, several functionalities have been attached to the BU portals to achieve higher binding constant, to form supramolecular gels, rotaxanes, and transmembrane transporters.[2] To date, water solubility of BUs has been achieved only by the insertion of PEG chains or carboxylic moieties on portals of the macrocycles.[3] Our aim is to explore the synthesis of BUs bearing amino groups (Fig. 1), other potentially water-soluble anion receptor. The synthesis of the amino-functionalized BU is challenging because the amino groups could react during the formation of the macrocycle and lead to side products. For this reason, different protective groups have been tested. Moreover, these new derivatives could be further functionalized to form corresponding ammonium salts, amides, and imines.

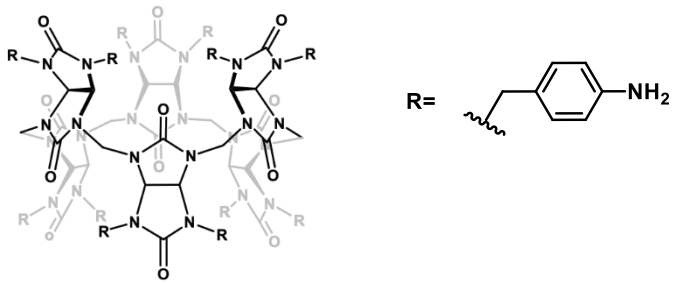

Fig. 1 Amino-functionalized bambus[6]uril.

1. Oshovsky, G., Reinhoudt, D. and Verboom, W., *Angew Chem. Int. Ed*. **2007**, 46: 2366-2393.
2. (a) Kokan, Z.; Dušková-Smrčková, M.; Šindelář, V., Chem, **2021**, 7, 2473-2490.(b) Kandrnálová, M.; Kokan, Z.; Havel, V.; Nečas, M.; Šindelář, V., *Angew Chem. Int. Ed.*, **2019**, 58, 18182-18185. (c) Valkenier, H.; Akrawi, O.; Jurček, P.; Sleziaková, K.; Lízal, T.; Bartik, K.; Šindelář, V., *Chem*, **2019**, 5, 429-444.
3. (a) Fiala ,T., Sleziakova, K., Marsalek, K., Salvadori, K., Šindelář, V., *J. Org. Chem.* **2018** *83* (4), 1903-1912. (b) Havel, V., Babiak, M., Šindelář, V., *Chem. Eur. J.* **2017**, *23*, 8963.