CYCLOFRUCTINS: CONFORMATIONS, MOLECULAR ELECTROSTATIC AND LIPOPHILICITY PATTERNS, AND INCLUSION COMPLEXES

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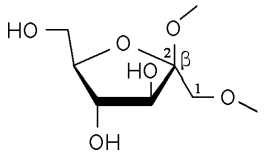
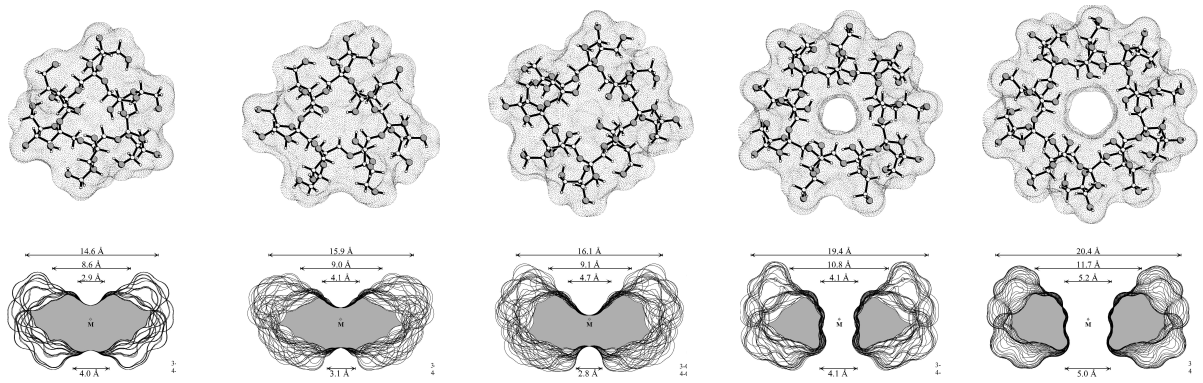
Conformational analysis of cyclofructins[1] composed of six (α-CF, **1**) to ten (ε-CF, **5**) β(1→2)-linked fructofuranose units (i.e. *cyclo*[D-Fru*f* β(1→2)]$_n$ with n = 6 - 10) was carried out in vacuum and aqueous solution using molecular mechanics (Monte Carlo) and dynamics simulation techniques.

Calculation of molecular surfaces and cross section cuts (cf. below) for the energy-minimum geometries reveals a disk-type shape of **1 - 3** without a "through-going" cavity. The larger ring homologs with nine (**4**) and ten (**5**) fructose units feature torus-like structures with central cavities of 4.1 or 5.2 Å diameter, respectively.



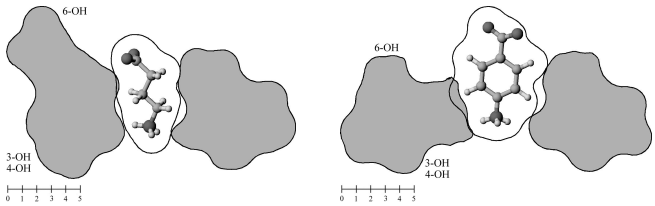
cyclo[D-Fru*f*β(1→2)]$_n$ with n = 6-10
1 - 5

Evaluation of the molecular electrostatic and lipophilicity patterns displays the crown-ether like properties of the cyclofructins **1 - 5**. The pronouncedly hydrophobic cavities for **4** and **5** should be amenable to the formation of inclusion complexes similar to those formed by cyclodextrins.



cyclo[D-Fru*f*β(1→2)]$_6$ *cyclo*[D-Fru*f*β(1→2)]$_7$ *cyclo*[D-Fru*f*β(1→2)]$_8$ *cyclo*[D-Fru*f*β(1→2)]$_9$ *cyclo*[D-Fru*f*β(1→2)]$_{10}$

Cross-section contours through the surfaces of the most stable structures computed for the inclusion complexes of **4** with β-alanin (left) and **5** with *p*-amino benzoic acid (right).



[1] S. Immel, F. W. Lichtenthaler, *Liebigs Ann. Chem.* **1996**, 39-44.