CYCLOFRUCTINS: GEOMETRIES, ELECTROSTATIC AND LIPOPHILICITY PATTERNS, AND INCLUSION COMPLEXES

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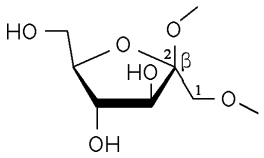
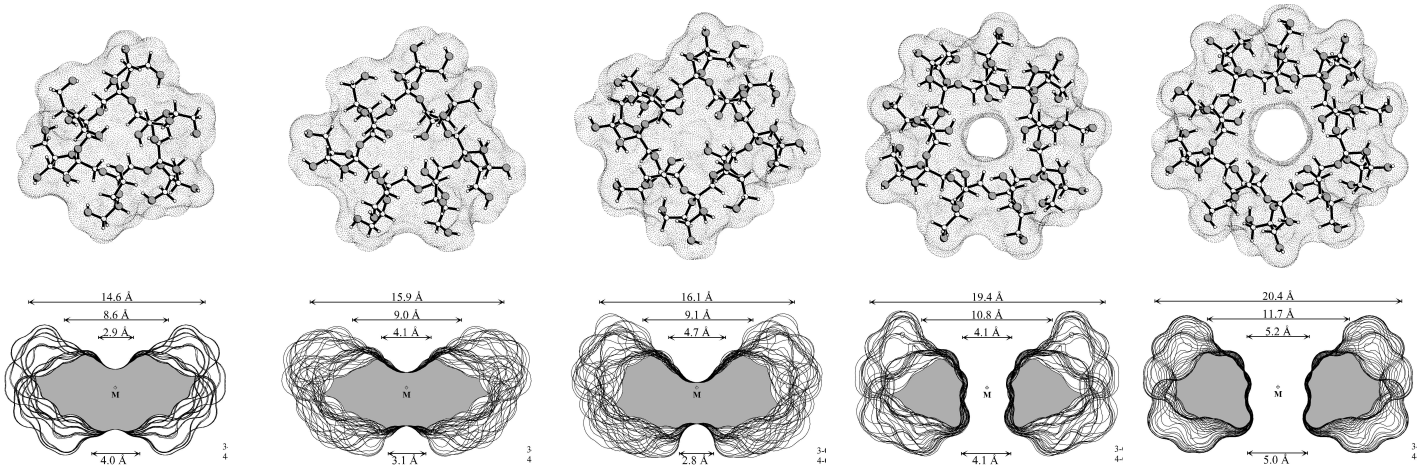
Cyclofructins composed of six (α-CF, **1**) to ten (ε-CF, **5**) β(1→2)-linked fructofuranose units (i.e. *cyclo*[D-Fru*f*β(1→2)]$_n$ with n = 6 - 10) were subjected to conformational analysis using "Monte-Carlo" simulations based on the PIMM91[1] force field[2,3]. Far-reaching similarities and identical over-all conformations of the solid-state geometry[4] of α-cyclofructin (**1**) and its computer-generated form provide information about the reliability of the computational analysis.



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

Calculation of the molecular surfaces for the energy-minimum structures establishes a disk-type shape of the cyclofructins with six to eight residues, ring enlargement to nine and ten residues leads to torus-shaped molecules with central cavities that conceivably allow for the formation of inclusion complexes. The color-coded projection of molecular lipophilicity patterns (MLPs)[5] and electrostatic potential profiles (MEPs) onto these surfaces displays the crown ether-like properties of the disk-shaped cyclofructins. The central cavities of **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)]$_{10}$

Fig. 1. Geometries with the dotted contact surfaces and cross section plots of the global energy-minimum structures (PIMM91) of the cyclofructins **1 - 5** composed of six to ten β(1→2)-linked fructose units.

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[3] S. Immel, F. W. Lichtenthaler, to be submitted.

[4] M. Sawada, T. Tanaka, Y. Takai, T. Hanafusa, T. Taniguchi, M. Kawamura, T. Uchiyama, *Carbohydr. Res.* **1991**, *217*, 7-17.

[5] M. Waldherr-Teschner, T. Goetze, W. Heiden, M. Knoblauch, H. Vollhardt, J. Brickmann, in: *Advances in Scientific Visualization* (Eds.: F. H. Post, A. J. S. Hin), Springer Verlag, Heidelberg, **1992**, pp. 58-67.