β(1→3)- AND β(1→6)-LINKED CYCLOGALACTOFURANOSIDES: CONFORMATIONS AND MOLECULAR SHAPES

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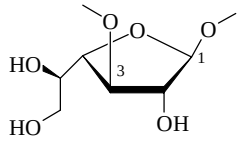
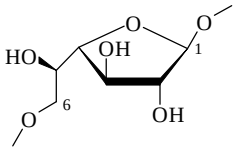
Various cyclooligosaccharides composed of β(1→3)-, β(1→5)-, and β(1→6)-linked galactofuranose units have been prepared by cycloglycosylation of tritylated 1,2-*O*-(1-cyano)ethylidene-derivatives of D-galactofuranose[1], yet information as to their molecular geometries and particularly to their inclusion complex behavior is essentially non-existent. To get a first assessment of the conformational features involved we have subjected the cyclogalactins **1** - **4** to PIMM91 Monte Carlo simulations:

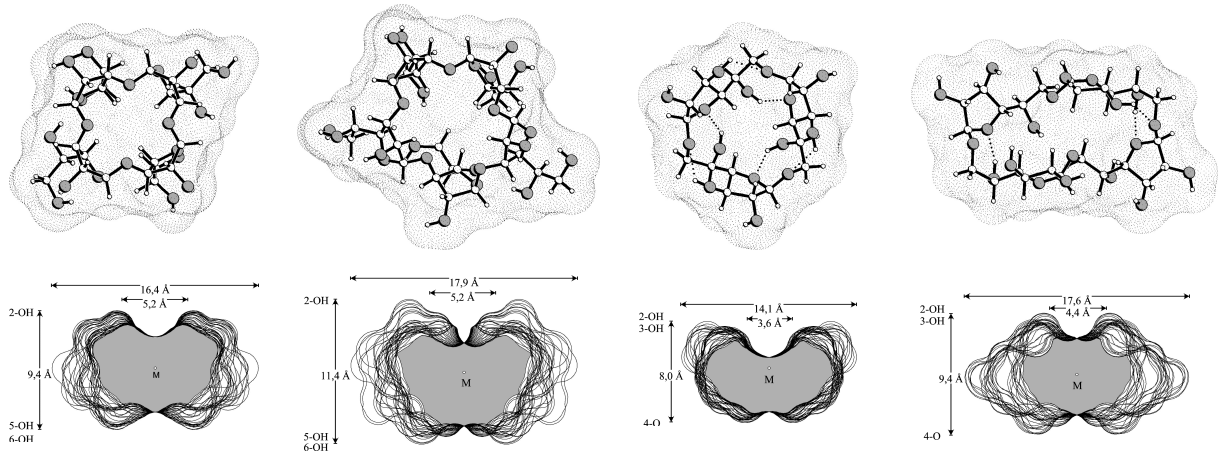


cyclo[D-Gal*f*β(1→3)]$_4$ **1**
cyclo[D-Gal*f*β(1→3)]$_5$ **2**



cyclo[D-Gal*f*β(1→6)]$_3$ **3**
cyclo[D-Gal*f*β(1→6)]$_4$ **4**

The results reveal a comparatively high flexibility of the cyclic furanosides, rendering the molecules with irregular, asymmetric overall shapes rather than symmetrical geometries. In contrast to cyclogalactins composed of pyranoid units[2], calculation of the corresponding molecular surfaces and the cross section cuts of **1** - **4** displays them to be disk-shaped and devoid of central cavities.



cyclo[D-Gal*f*β(1→3)]$_4$ **1**
cyclo[D-Gal*f*β(1→3)]$_5$ **2**
cyclo[D-Gal*f*β(1→6)]$_3$ **3**
cyclo[D-Gal*f*β(1→6)]$_4$ **4**

[1] N. K. Kochetkov; S. A. Nepogodiev, L. V. Backinowsky, *Carbohydr. Res.* **1989**, *185*, C1-C3; *Tetrahedron* **1990**, *46*, 139-150.

[2] F. W. Lichtenthaler, S. Immel, *Tetrahedron Asymmetry*, **1994**, *5*, 2045-2060.