The Conformation of C-Galactosyl and C-Aminogalactosyl Inositols.

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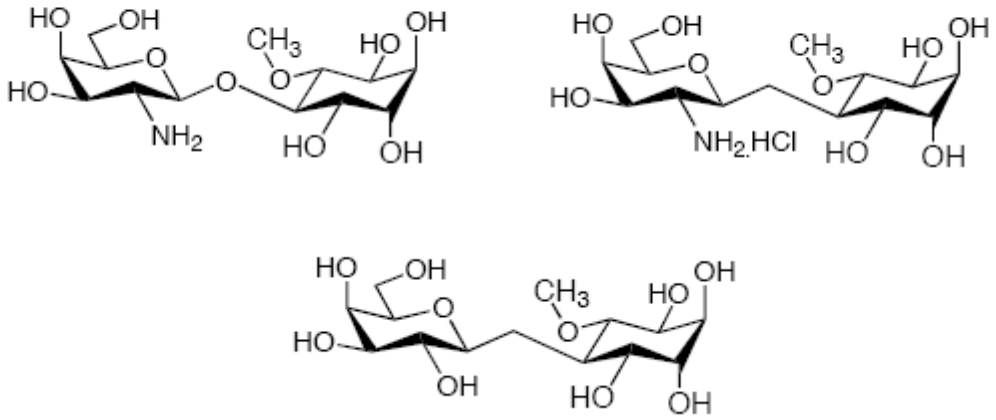
The conformational behaviour of C-glycosyl compounds in comparison to that of their natural glycosides has been a matter of debate for years[1].

The conformation of C-glycosyl inositols has not been yet evaluated. In this work, we have studied the behaviour in water solution of a variety of C-galactosyl inositols, using a combination of NMR methods and molecular mechanics calculations. Modern NMR methods including 1D and 2D NOE-based experiments have been quantitatively explained through dynamic models employing the geometries deduced from the application of different force fields with different protocols.



[1] Tony K. A., Denton R. W., Dilhas A., Jimenez-Barbero J., Mootoo D. R., *Organic Lett.*, 2007, *9*, 1441-1444; Pérez-Castells J., Hernández-Gay J. J., Denton R. W., Tony K. A., Mootoo D. R., Jiménez-Barbero J., *Org. Biomol. Chem.*, 2007, *5*, 1087-1092, and references therein.