RECOGNITION OF RING EXPANDED CARBOHYDRATES BY CONCANAVALIN A: EFFECT OF ANOMERIC CONFIGURATION ON BINDING

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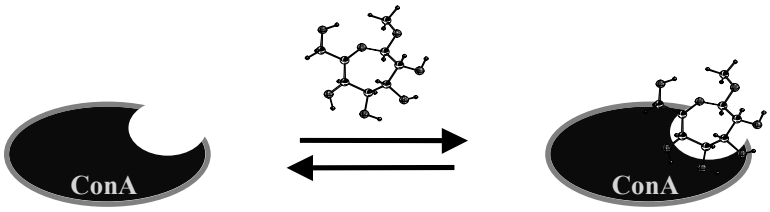

A major research theme of the the group is the design and preparation of new carbohydrate compounds and the analysis of their interactions with proteins. Our investigation of protein-carbohydrate molecular recognition events is from the perspective of bioorganic chemistry. That is, we use a full complement of assay techniques and spectroscopies to investigate how incremental changes in carbohydrate structure can effect binding to target proteins. The synthesis and conformational analysis of unnatural carbohydrate structures is considered the foundation of our current and future research investigations.

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We have recently reported on the synthesis[1, 2] and conformational analysis[3] of a family of ring expanded carbohydrates characterized by having seven (septanose) rather than five (furanose) or six (pyranose) atoms in their ring. The ability of the jack bean lectin Concanavalin A (ConA) to bind septanose monosaccharides has been investigated by Isothermal Titration Calorimetry (ITC) and Saturation Transfer Difference (STD) NMR spectroscopy. The data reveal a selectivity by ConA for septanosides of the beta rather than alpha anomeric configuration. This is opposite to the preference observed in anomeric configuration observed for pyranosides, the natural ligands of ConA. A model for the observed selectivity was developed based on known crystal structures of ConA-pyranoside complexes.

[1] (a) Peczuh, M. W.; Synder, N. L. *Tetrahedron Lett*. **2003**, *44*, 4057-4061. (b) Castro, S.; Peczuh, M. W. *J. Org. Chem.* **2005**, *70*, ASAP.
[2] (a) Fyvie, W. S.; Morton, M.; Peczuh, M. W. *Carbohydr. Res.* **2004**, *339*, 2363-2370. (b) Peczuh, M. W.; Snyder, N. L.; Fyvie, W. S. *Carbohydr. Res*. **2004**, *339*, 113-1171.
[3] DeMatteo, M.; Snyder, N. L..; Morton, M.; Baldisseri, D. M.; Hadad, C. M.; Peczuh, M. W. *J. Org. Chem.* **2005**, *70*, 24-38.