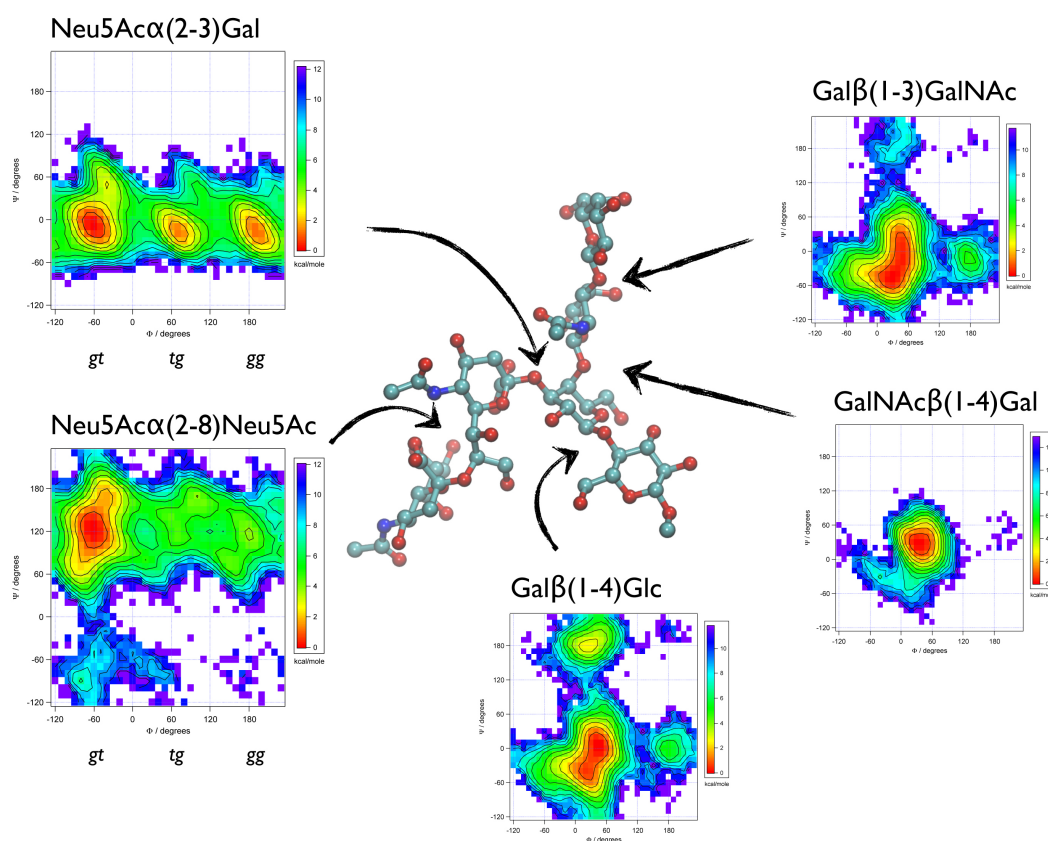


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Supplemental Figure S1.

Conformational energy maps for the GD1b oligosaccharide showing the accessible conformational space of the glycosidic linkages. The maps are calculated based on 200000 snapshots sampled from a 100ns MD simulation at 700 K using TINKER/MM3 as described in (Frank et al., 2007). Three local energy minima are predicted for the internal Neu5Aca(2-3)Gal linkage.



Reference:

Frank, M., Lutteke, T., and von der Lieth, C.W. (2007). GlycoMapsDB: a database of the accessible conformational space of glycosidic linkages. *Nucl Acid Res* 35, 287-290.