

Supplementary Material

The individual conformational Φ , Ψ samplings resulting from 1-ns simulations within $30 \times 30 \times 30 \text{ \AA}^3$ solvent boxes are presented in the supplementary online material for the ABH histo-blood group tri- and tetrasaccharides. The reader can thus examine the behavior at each glycosidic linkage in the tri- and tetrasaccharides.

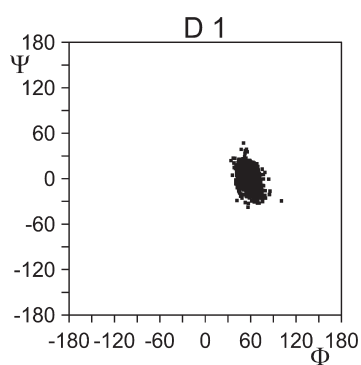
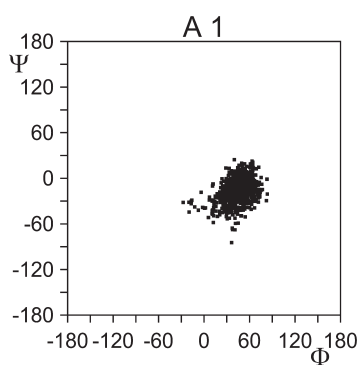
Supplementary conformational maps:

Trisaccharides

Tetrasaccharides

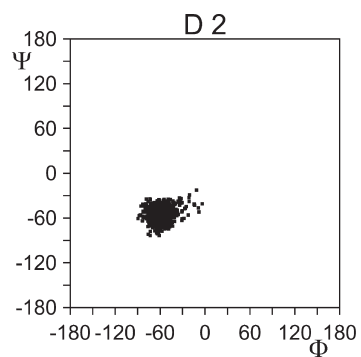
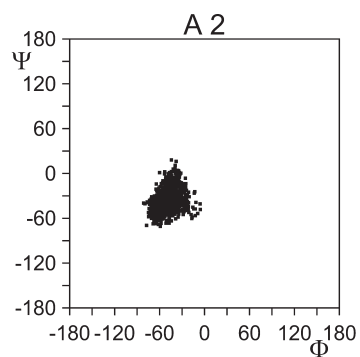
A-1 Galp- β 1,3GlcNAcp

D-1 Galp- β 1,3GlcNAcp



A-2 Galp- α 1,3Galp

D-2 Galp- α 1,3Galp

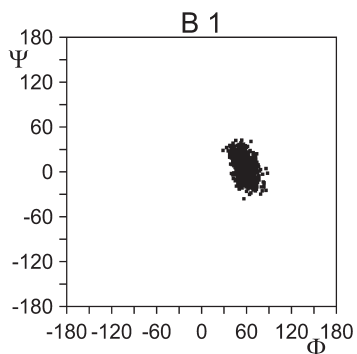


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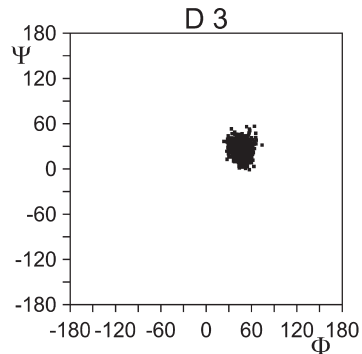
Trisaccharides

Tetrasaccharides

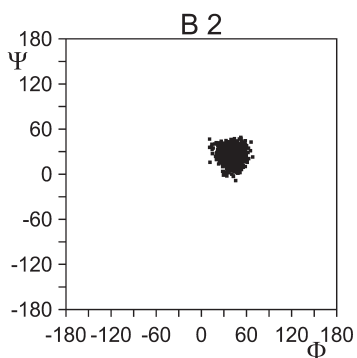
B-1 Galp- β 1,3GlcNAc



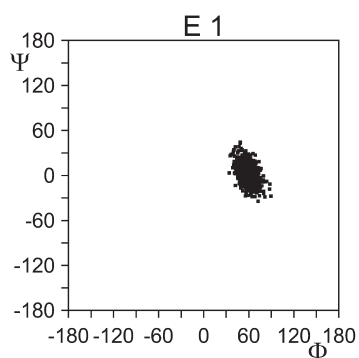
D-3 Fucp- α 1,2Galp



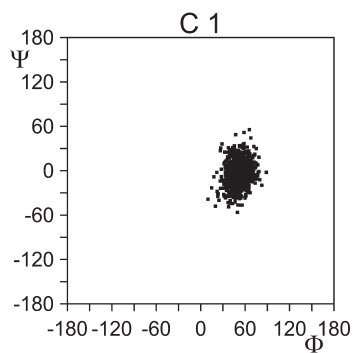
B-2 Fucp- α 1,2Galp



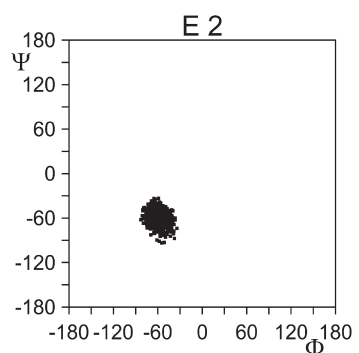
E-1 Galp- β 1,3GlcNAcp



C-1 Galp β 1,3GlcNAcp



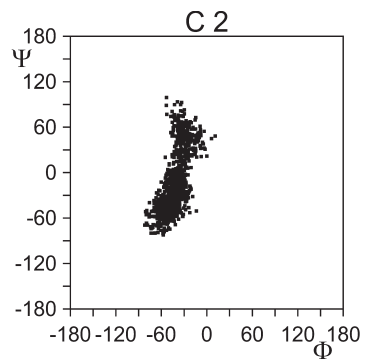
E-2 GalNAcp- α 1,3Galp



continued

Trisaccharides

C-2 GalNAc β -1,3Gal β



Tetrasaccharides

E-3 Fuc β -1,2Gal β

