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Supporting Information

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Supporting Information

for

Assessing Carbohydrate–Carbohydrate Interactions by NMR Spectroscopy: The Trisaccharide Epitope from the Marine Sponge *Microciona prolifera*

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A) F_1 vs. Y_1 B) F_1 vs. Y_1

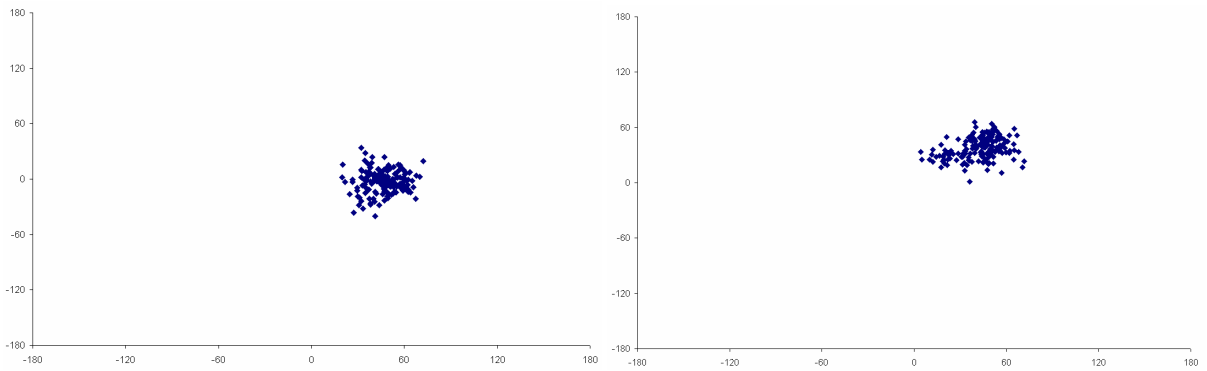
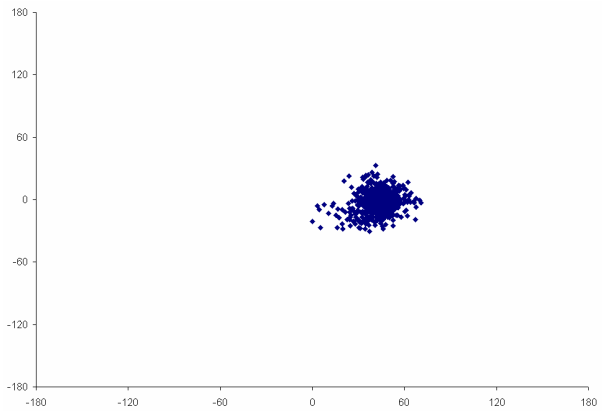
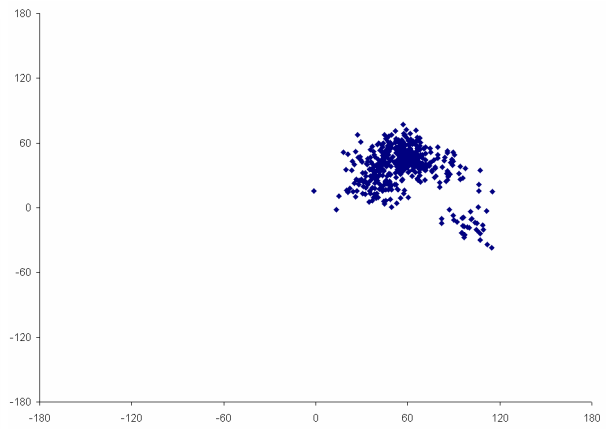


Figure S1. The trajectories of **1-All**, represented as F/Y scattered plots, according to 2 ns MD simulations in explicit water.

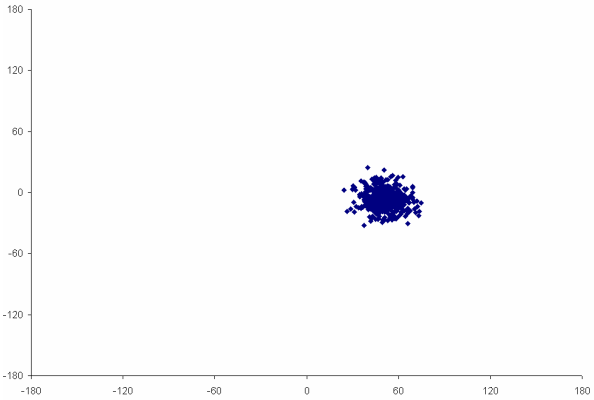
A) F_1 vs. Y_1 (residue 1)



B) F_2 vs. Y_2 (residue 1)



C) F_1 vs. Y_1 (residue 2)



D) F_2 vs. Y_2 (residue 2)

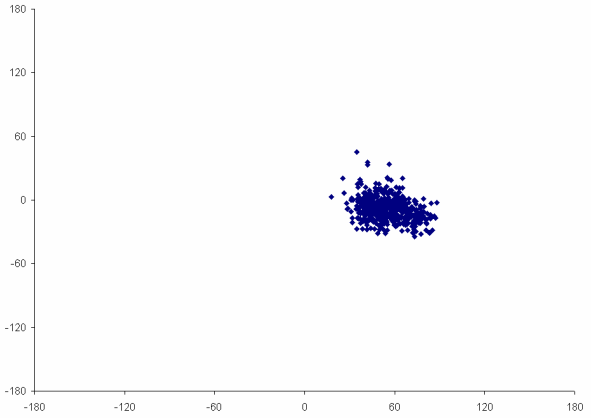


Figure S2. The trajectories of the dimeric model of **1-AII**, when Ca^{2+} is coordinated with atoms belonging to set 2, represented as F/Y scattered plots, according to 1 ns MD simulations in explicit water.

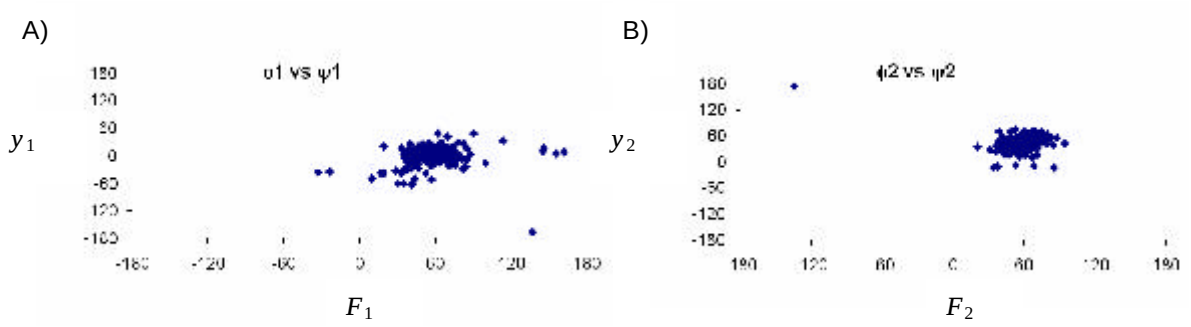


Figure S3. The trajectories of **1-All,** represented as F/Y scattered plots, according to 5 ns MD simulations. A well defined conformational behavior with fluctuations around the global minimum was found. A) The Gal*p*4,6(*R*)Pyr(β1-4)Glc*p*NAc linkage. B) The Glc*p*NAc(β1-3)Fuc*p*- linkage. C) The Fuc*p*(α1-OAll linkage. F_1 is defined as H1 Gal-C1 Gal-O-C4 GlcNAc. Y_1 is C1 Gal-O-C4 GlcNAc-H4 GlcNAc. F_2 is defined as H1 GlcNAc-C1 GlcNAc-O-C3 Fuc. Y_2 is C1 GlcNAc-O-C3 Fuc–H3 Fuc. In all cases, the major conformation takes values around F/Y 60:0.

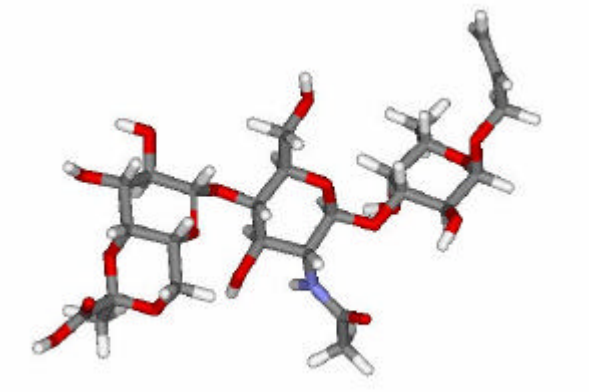


Figure S4. The global minimum of **1-All** according to MM3* calculations.

Table S1. Average distances between the five Ca^{2+} cations coordinated with the corresponding five sets of atoms shown in Figure 6.

	Distance (Å) with the corresponding Ca^{2+} atom
Set 1 (carboxilate group)	Ca-O 2.485 Ca-O 2.525
Set 2 (O2-Gal and O6-GlcNAc)	Ca-O2(Gal) 2.571 Ca-O6(GlcNAc) 2.529
Set 3 (O1-Fuc, O2-Fuc, and allyl group)	Ca-O1 2.718 Ca-O2 3.016 Ca-ethylene carbons (average) 2.892
Set 4 (O4-Fuc and endocyclic O-Fuc)	Ca-O4 2.528 Ca-O (endocyclic) 3.442
Set 5 (O3-GlcNAc, carboxamide oxygen, and O6-Gal)	Ca-O3(ClcNAc) 2.589 Ca-carboxamide oxygen 2.759 Ca-O6(Gal) 2.680