Supplementary Material

Computational Study on the Encapsulation of Glucosamine Anomers by Cucurbit[6]uril and Cucurbit[8]uril in Aqueous Solution

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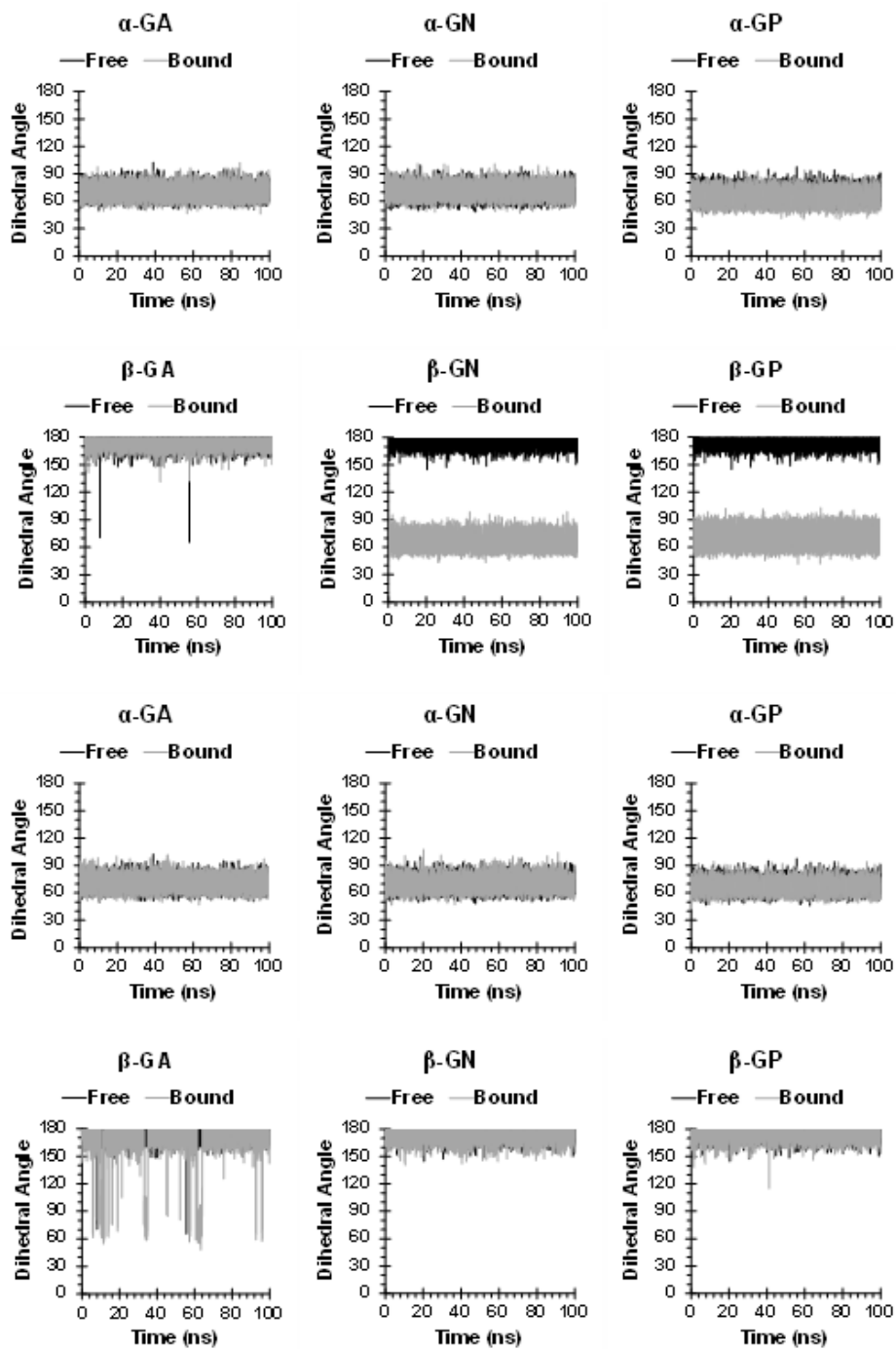
Figure S1. The dihedral angle O_1-C_1-O_5-C_5 versus time for the free and bound glucosamines with CB6 (first and second rows) and CB8 (third and fourth rows).
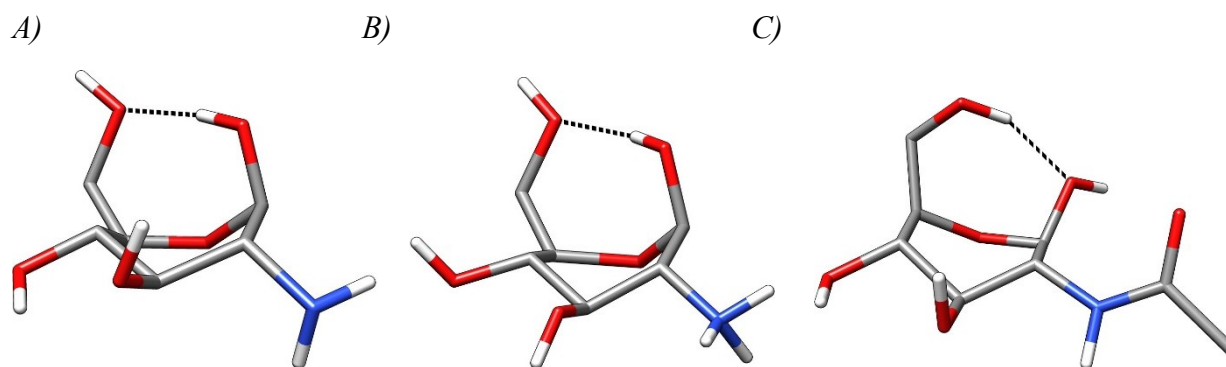
Figure S2. Sampled snapshots depicting ring distortion of β-GN in CB6 complex (A), β-GP in CB6 complex (B), and β-GA in CB8 complex (C) (CB removed for clarity).

Table S1. The computed relative binding free energies for CB6 complexes using TI in kcal/mol.

Mutations	$\Delta\Delta G_1$	$\Delta\Delta G_2$	$\Delta\Delta G_3$	$\Delta\Delta G_{ELE}$	$\Delta\Delta G$
α-GA→β-GA	-1.77	5.15	-6.08	-7.85	-2.69
α-GN→β-GN	-1.40	4.05	-3.17	-4.57	0.52
α-GP→β-GP	3.81	0.13	-1.49	2.32	2.64
α-GP→α-GN	-3.71	0.25	-1.33	-5.04	-4.79
β-GP→β-GN	0.68	0.65	1.60	2.28	2.93

Table S2. The computed relative binding free energies for CB8 complexes using TI in kcal/mol.

Mutations	$\Delta\Delta G_1$	$\Delta\Delta G_2$	$\Delta\Delta G_3$	$\Delta\Delta G_{ELE}$	$\Delta\Delta G$
α-GA→β-GA	-0.77	0.93	0.51	-0.26	0.69
α-GN→β-GN	1.10	2.01	0.70	1.80	1.61
α-GP→β-GP	-0.58	0.42	0.05	-0.53	-0.11
α-GP→α-GN	0.39	1.02	0.92	1.31	1.89
β-GP→β-GN	0.73	0.82	1.27	2.09	2.83

$\Delta\Delta\Delta G_{vdW} = \Delta\Delta G_2,\ \Delta G_{ELE} = \Delta\Delta G_1 + \Delta\Delta G_3;\ \Delta\Delta G = \Delta\Delta G_1 + \Delta\Delta G_2 + \Delta\Delta G_3$