

Additional file 10: Table S6. Molecular dynamics-derived stability metrics and MM-PBSA binding energetics of Car_Chit-(GlcNAc)4 complexes (production window: 10-100 ns).

Gene	Family	Backbone RMSD (Å)	Ligand RMSD (Å)	Rg (Å)	RMSF (Å)	RMSF Max (Å)	H-bonds (mean)	COM Distance (Å)	ΔG_{bind} (kcal/mol)
Car_Chit-4	GH19	1.95 $\pm$ 0.26	1.29 $\pm$ 0.22	17.92 $\pm$ 0.41	1.23 $\pm$ 0.84	4.53	7.30 $\pm$ 2.45	10.24 $\pm$ 1.92	-6.89 $\pm$ 14.67
Car_Chit-11	GH19	2.18 $\pm$ 0.20	2.17 $\pm$ 0.14	17.58 $\pm$ 0.11	1.17 $\pm$ 1.06	9.40	1.46 $\pm$ 1.08	30.89 $\pm$ 4.63	-11.65 $\pm$ 8.55
Car_Chit-20	GH19	1.51 $\pm$ 0.16	0.85 $\pm$ 0.15	17.93 $\pm$ 0.18	1.10 $\pm$ 0.66	4.90	4.05 $\pm$ 1.92	12.76 $\pm$ 1.75	-8.25 $\pm$ 9.59
Car_Chit-14	GH18	1.92 $\pm$ 0.26	0.85 $\pm$ 0.15	20.12 $\pm$ 0.08	1.16 $\pm$ 0.58	4.90	4.43 $\pm$ 2.10	16.01 $\pm$ 1.63	-13.93 $\pm$ 6.43
Car_Chit-17	GH18	2.57 $\pm$ 0.21	2.84 $\pm$ 0.40	21.19 $\pm$ 0.14	0.86 $\pm$ 0.57	3.52	3.10 $\pm$ 1.85	11.43 $\pm$ 1.28	-18.51 $\pm$ 6.75
Car_Chit-19	GH18	1.24 $\pm$ 0.11	2.01 $\pm$ 0.54	20.12 $\pm$ 0.08	0.77 $\pm$ 0.36	3.03	3.60 $\pm$ 1.78	14.06 $\pm$ 1.56	-11.24 $\pm$ 13.68
Car_Chit-27	GH18	2.11 $\pm$ 0.38	0.72 $\pm$ 0.14	18.05 $\pm$ 0.21	1.29 $\pm$ 0.73	4.23	4.62 $\pm$ 2.05	14.83 $\pm$ 1.68	-10.16 $\pm$ 8.61