

Facial Selectivity between Carbohydrates and Aromatic Amino Acids Explained by a Combination of NCI, NBO and EDA Techniques with NMR Spectroscopy

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Chemical shift perturbation

Glc-Trp

Table S1. ¹H chemical shift perturbation of Glc (2 mmol L⁻¹) with different concentrations of Trp in D₂O

Anomer	Hydrogen	¹ H chemical shift perturbation / Hz			
		2 mmol L ⁻¹	8 mmol L ⁻¹	16 mmol L ⁻¹	32 mmol L ⁻¹
α	H1	-0.36	-1.24	-2.68	-4.88
	H2	-0.35	-1.42	-2.99	-5.37
	H3	-0.20	-1.00	-1.84	-3.45
	H4	-0.22	-1.29	-2.72	-5.06
	H5	-0.34	-1.28	-2.65	-4.83
	H6a	-0.24	-1.29	-2.67	-4.99
	H6b	-0.35	-1.40	-3.01	-5.55
β	H1	-0.42	-1.60	-3.49	-6.46
	H2	-0.28	-1.12	-2.28	-4.17
	H3	-0.38	-1.41	-2.90	-5.34
	H4	-0.37	-1.35	-2.77	-5.07
	H5	-0.46	-1.87	-4.06	-7.45
	H6a	-0.37	-1.47	-3.10	-5.69
	H6b	-0.39	-1.45	-3.00	-5.57

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Glc-Phe

Table S2. ^1H chemical shift perturbation of Glc (2 mmol L $^{-1}$) with different concentrations of Phe D $_2$ O

Anomer	Hydrogen	^1H chemical shift perturbation / Hz			
		2 mmol L $^{-1}$	8 mmol L $^{-1}$	16 mmol L $^{-1}$	32 mmol L $^{-1}$
α	H1	−0.45	−1.30	−1.45	−3.07
	H2	−0.44	−1.29	−1.49	−3.30
	H3	−0.43	−0.71	−1.04	−2.62
	H4	−0.39	−0.58	−1.29	−2.88
	H5	−0.40	−1.30	−1.46	−3.42
	H6a	−0.49	−1.39	−1.54	−3.52
	H6b	−0.47	−1.38	−1.55	−3.38
β	H1	−0.45	−1.33	−1.55	−3.62
	H2	−0.42	−1.17	−1.26	−2.59
	H3	−0.42	−1.20	−1.61	−3.22
	H4	−0.43	−1.26	−1.56	−3.31
	H5	−0.43	−1.76	−1.76	−3.89
	H6a	−0.44	−1.35	−1.56	−3.46
	H6b	−0.39	−1.13	−1.61	−3.54

Glc-His

Table S3. ^1H chemical shift perturbation of Glc (2 mmol L $^{-1}$) with different concentrations of His D $_2$ O

Anomer	Hydrogen	^1H chemical shift perturbation / Hz			
		2 mmol L $^{-1}$	8 mmol L $^{-1}$	16 mmol L $^{-1}$	32 mmol L $^{-1}$
α	H1	−0.10	−0.30	−0.50	−1.40
	H2	0.10	−0.10	−0.40	−1.35
	H3	0.00	−0.15	−0.30	−1.20
	H4	0.20	−0.05	−0.30	−1.25
	H5	−0.15	−0.30	−0.50	−1.20
	H6a	−0.10	−0.35	−0.07	−1.60
	H6b	−0.05	−0.40	−0.50	−1.55
β	H1	−0.20	−0.30	−0.75	−1.40
	H2	0.00	−0.05	−0.55	−1.05
	H3	0.05	−0.10	−0.55	−1.15
	H4	0.00	−0.20	−0.65	−1.30
	H5	−0.35	−0.55	−1.60	−1.85
	H6a	−0.10	−0.25	−0.85	−1.55
	H6b	−0.10	−0.25	−0.75	−1.50

Glc-Gly

Table S4. ^1H chemical shift perturbation of Glc (2 mmol L $^{-1}$) with different concentrations of L-glycine D $_2$ O

Anomer	Hydrogen	^1H chemical shift perturbation / Hz			
		2 mmol L $^{-1}$	8 mmol L $^{-1}$	16 mmol L $^{-1}$	32 mmol L $^{-1}$
α	H1	−0.01	−0.11	−0.24	−0.52
	H2	0.08	−0.01	0.00	−0.49
	H3	0.05	−0.14	−0.20	−0.58
	H4	0.22	0.08	−0.04	−0.39
	H5	0.03	−0.10	−0.15	−0.66
	H6a	0.07	−0.02	−0.16	−0.65
	H6b	0.06	−0.01	−0.11	−0.52
β	H1	0.01	−0.11	−0.26	−0.51
	H2	0.03	−0.10	−0.24	−0.53
	H3	0.02	−0.13	−0.24	−0.50
	H4	0.02	−0.11	−0.26	−0.53
	H5	0.07	−0.11	−0.25	−0.53
	H6a	0.01	−0.15	−0.30	−0.63
	H6b	−0.01	−0.14	−0.28	−0.58

Gal-Trp

Table S5. ^1H chemical shift perturbation of Gal (2 mmol L $^{-1}$) with different concentrations of Trp D $_2$ O

Anomer	Hydrogen	^1H chemical shift perturbation / Hz			
		2 mmol L $^{-1}$	8 mmol L $^{-1}$	16 mmol L $^{-1}$	32 mmol L $^{-1}$
α	H1	−0.20	−1.10	−2.25	−5.20
	H2	−0.45	−1.30	−2.40	−5.60
	H3	−0.45	−1.75	−3.50	−8.10
	H4	−0.60	−2.40	−4.75	−10.85
	H5	−0.80	−2.10	−4.15	−9.00
	H6	−0.55	−1.70	−3.25	−7.45
β	H1	−0.45	−2.20	−4.25	−9.60
	H2	−0.25	−1.30	−2.50	−5.50
	H3	−0.55	−2.80	−5.50	−12.30
	H4	−0.30	−2.65	−5.25	−11.85
	H5	−0.55	−3.10	−6.20	−14.15
	H6	−0.30	−1.75	−3.45	−7.45

Gal-Phe

Table S6. ^1H chemical shift perturbation of Gal (2 mmol L^{-1}) with different concentrations of Phe D_2O

Anomer	Hydrogen	^1H chemical shift perturbation / Hz			
		2 mmol L^{-1}	8 mmol L^{-1}	16 mmol L^{-1}	32 mmol L^{-1}
α	H1	-0.24	-0.43	-1.01	-1.58
	H2	-0.29	-0.43	-1.02	-1.57
	H3	-0.32	-0.57	-1.25	-2.04
	H4	-0.29	-0.72	-1.41	-2.53
	H5	-0.37	-0.74	-1.35	-2.75
	H6a	-0.16	-0.48	-1.12	-1.91
	H6b	-0.08	-0.66	-1.17	-1.91
β	H1	-0.33	-0.57	-1.31	-2.22
	H2	-0.29	-0.43	-0.95	-1.31
	H3	-0.36	-0.68	-1.50	-2.59
	H4	-0.33	-0.63	-1.52	-2.55
	H5	-0.36	-0.81	-1.77	-3.07
	H6a	-0.33	-0.52	-1.27	-2.12
	H6b	-0.42	-0.65	-1.38	-2.16

Gal-His

Table S7. ^1H chemical shift perturbation of Gal (2 mmol L^{-1}) with different concentrations of His D_2O

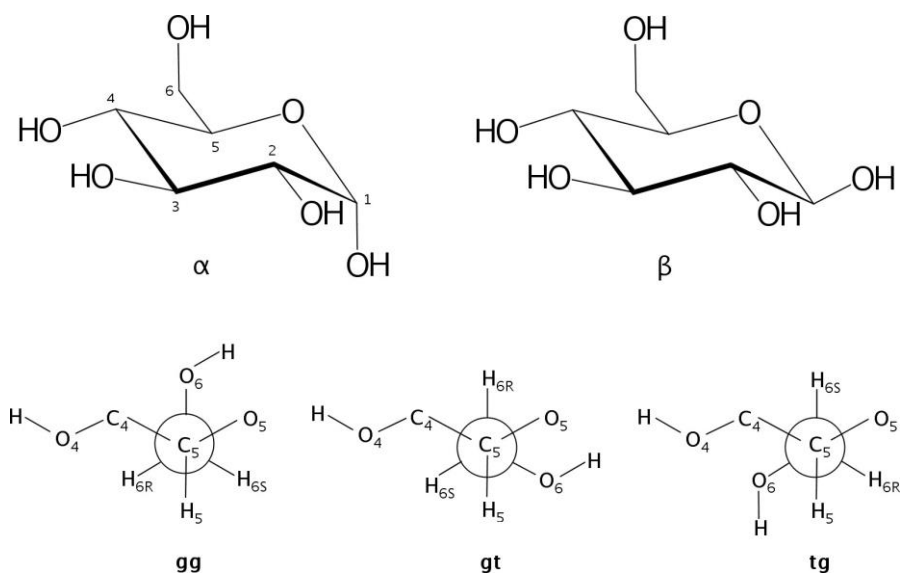
Anomer	Hydrogen	^1H chemical shift perturbation / Hz			
		2 mmol L^{-1}	8 mmol L^{-1}	16 mmol L^{-1}	32 mmol L^{-1}
α	H1	-0.30	-0.46	-1.02	-1.37
	H2	-0.24	-0.30	-0.84	-1.13
	H3	-0.26	-0.37	-1.00	-1.36
	H4	-0.61	-0.70	-1.26	-1.91
	H5	-0.27	-0.50	-1.15	-1.78
	H6a	-0.42	-0.59	-1.08	-1.64
	H6b	-0.58	-0.80	-1.19	-1.90
β	H1	-0.26	-0.39	-1.01	-1.35
	H2	-0.22	-0.31	-0.78	-1.04
	H3	-0.28	-0.42	-1.08	-1.49
	H4	-0.55	-0.72	-1.38	-1.77
	H5	-0.20	-0.47	-1.16	-2.38
	H6a	-0.30	-0.53	-1.11	-1.81
	H6b	-0.24	-0.41	-1.00	-1.77

Table S8. ^1H chemical shift perturbation of Gal (2 mmol L^{-1}) with different concentrations of L-glycine D_2O

Anomer	Hydrogen	^1H chemical shift perturbation / Hz			
		2 mmol L^{-1}	8 mmol L^{-1}	16 mmol L^{-1}	32 mmol L^{-1}
α	H1	-0.13	-0.26	-0.35	-0.62
	H2	-0.13	-0.31	-0.38	-0.69
	H3	-0.15	-0.31	-0.39	-0.70
	H4	-0.06	-0.24	-0.33	-0.62
	H5	-0.13	0.01	-0.39	-0.55
	H6a	-0.27	-0.33	-0.49	-0.74
	H6b	-0.17	-0.30	-0.32	-0.68
β	H1	-0.08	-0.21	-0.31	-0.53
	H2	-0.08	-0.24	-0.41	-0.66
	H3	-0.08	-0.22	-0.34	-0.56
	H4	-0.07	-0.27	-0.32	-0.56
	H5	-0.06	-0.24	-0.37	-0.63
	H6a	-0.11	-0.26	-0.44	-0.69
	H6b	0.17	-0.17	-0.26	-0.69

Carbohydrate Conformational Search

The anomers α and β with the different conformations (*gauche-gauche*, *gauche-trans* and *trans-gauche*) of the carbohydrate Glc and Gal are shown in Figures S1 and S2, respectively.

**Figure S1.** Conformations of Glc.

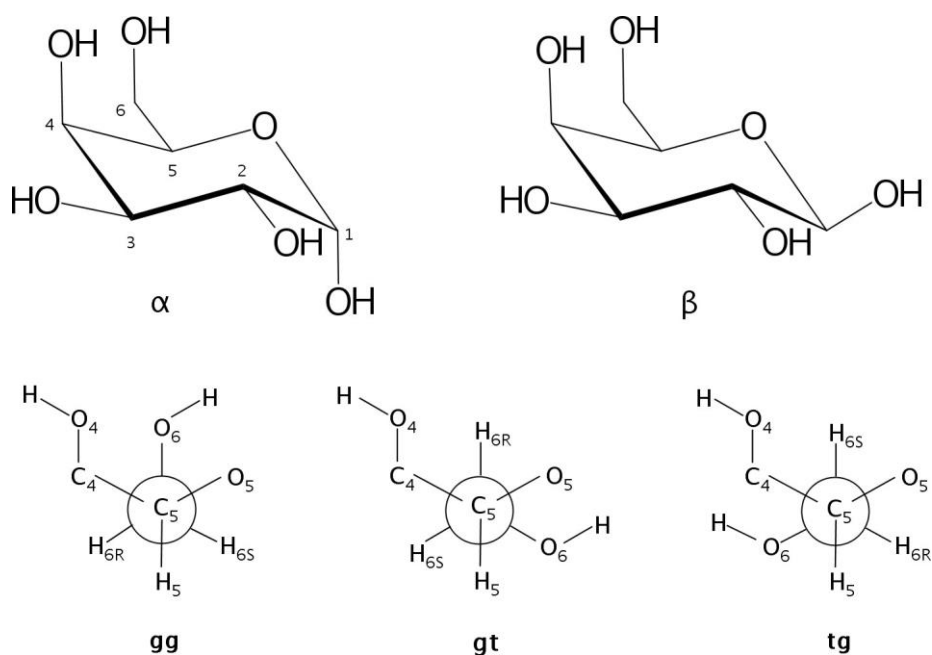


Figure S2. Conformations of Gal.

2D potential energy surface involving the dihedrals $O_5-C_5-C_6-O_6$ and $C_5-C_6-O_6-H$ were calculated at M06-2X/6-31G level in vacuum and water (IEF-PCM/Bondi) with 24 steps of 15 degrees for both anomers of Glc and Gal (Figures S3 and S4, respectively).

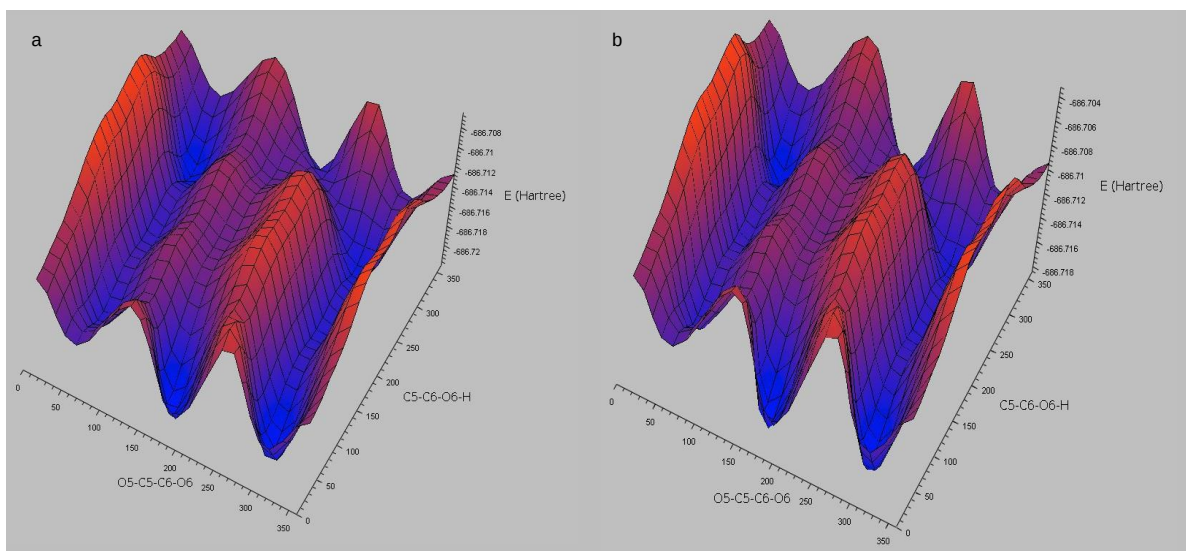


Figure S3. Potential energy surface of Glc calculated at M06-2X/6-31G level in water (IEF-PCM/Bondi). (a) α -D-Glc; (b) β -D-Glc.

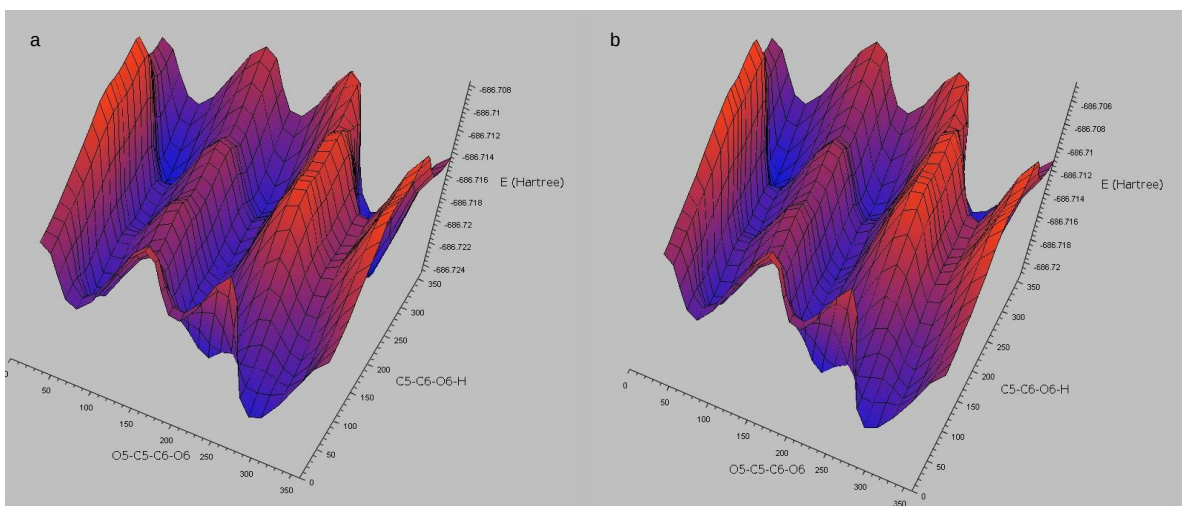


Figure S4. Potential energy surface of Gal calculated at M06-2X/6-31G level in water (IEF-PCM/Bondi). (a) α -D-Gal; b) β -D-Gal.

Each minimum was posteriorly optimized at the M06-2X/6-31++G(d,p) level both in vacuum and in water (IEF-PCM/Bondi) and at the MP2/6-31++G(d,p) level in water (IEF-PCM/Bondi). The results are shown in Tables S9 and S10 for Glc and Gal, respectively.

Table S9. Relative energy of the conformations of Glc (with ZPE correction) at the M06-2X/6-31++G(d,p) level in vacuum and water (IEF-PCM/Bondi) and at the MP2/6-31++G(d,p) level in water (IEF-PCM/Bondi)

entry	Conformation	M06-2X		MP2
		$\Delta E_{\text{vac}} / (\text{kcal mol}^{-1})$	$\Delta E_{\text{water}} / (\text{kcal mol}^{-1})$	$\Delta E_{\text{water}} / (\text{kcal mol}^{-1})$
1	α -gg ⁻	1.86	0.78	0.76
2	α -gg ⁺	0.00	0.00	0.00
3	α -gg	2.43	0.69	0.78
4	α -gt ⁻	0.13	0.05	0.07
5	α -gt ⁺	2.59	0.99	1.05
6	α -gt	2.30	1.00	1.07
7	α -tg ⁻	^a	2.84	3.15
8	α -tg ⁺	0.12	0.78	1.19
9	α -tg	^a	3.10	3.39
10	β -gg ⁻	3.03	1.08	1.06
11	β -gg ⁺	0.90	0.28	0.27
12	β -gg	3.62	1.14	1.08
13	β -gt ⁻	1.10	0.24	0.19
14	β -gt ⁺	3.60	0.93	0.97
15	β -gt	3.34	1.02	1.08
16	β -tg ⁻	^b	3.17	3.31
17	β -tg ⁺	1.20	1.18	1.44
18	β -tg	^b	3.38	3.49

19	α -gg ^{+cw}	0.59	1.57	1.84
20	α -gt ^{-cw}	2.18	1.85	2.08
21	α -tg ^{-cw}	0.93	2.45	3.10
22	β -gg ^{+cw}	3.27	2.07	2.40
23	β -gt ^{-cw}	4.60	2.51	2.58
24	β -tg ^{+cw}	3.51	3.01	3.76

^aConverted to α -tg⁺; ^bconverted to β -tg⁺.

Table S10. Relative energy of the conformations of Gal (with ZPE correction) at the M06-2X/6-31++G(d,p) level in vacuum and water (IEF-PCM/Bondi) and at the MP2/6-31++G(d,p) level in water (IEF-PCM/Bondi)

entry	Conformation	M06-2X		MP2
		$\Delta E_{\text{vac}} / (\text{kcal mol}^{-1})$	$\Delta E_{\text{water}} / (\text{kcal mol}^{-1})$	$\Delta E_{\text{water}} / (\text{kcal mol}^{-1})$
1	α -gg ⁻	0.60	0.00	0.37
2	α -gg ⁺	^a	1.99	2.35
3	α -gg	7.77	3.04	3.25
4	α -gt ⁻	0.00	0.03	0.07
5	α -gt ⁺	2.99	0.68	0.70
6	α -gt	2.01	0.69	0.73
7	α -tg ⁻	2.39	0.95	1.14
8	α -tg ⁺	0.41	0.98	1.34
9	α -tg	1.40	1.15	1.36
10	β -gg ⁻	2.04	0.39	0.58
11	β -gg ⁺	^b	2.21	2.48
12	β -gg	9.31	3.37	3.49
13	β -gt ⁻	1.37	0.09	0.00
14	β -gt ⁺	4.33	0.88	0.78
15	β -gt	3.37	0.81	0.67
16	β -tg ⁻	3.79	1.10	1.15
17	β -tg ⁺	1.56	1.23	1.30
18	β -tg	2.61	1.16	1.37

^aConverted to α -gg⁻; ^bconverted to β -gg⁻.

The most stable structure for each conformation of both anomer of *Glc* and *Gal* are presented in Figures S5 and S6, respectively, and were employed in the study of the interaction with the different amino acids.

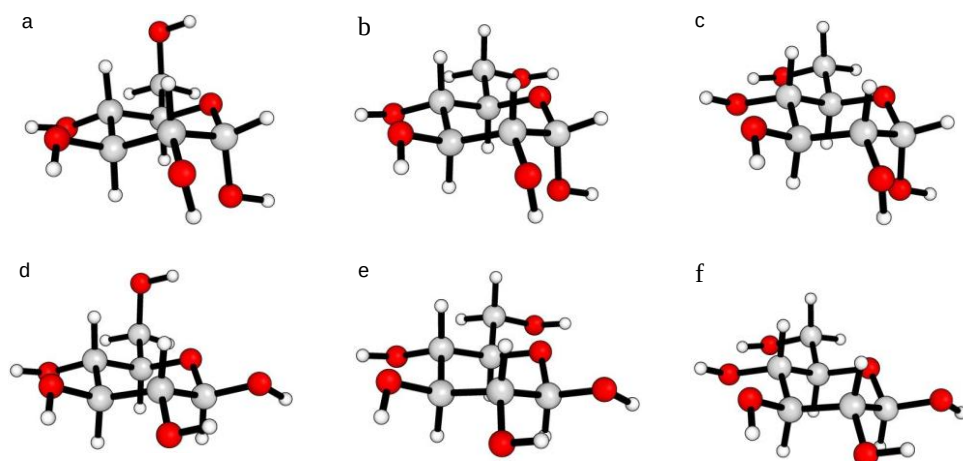


Figure S5. Optimized conformations of Glc at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi). (a) α -Glc-gg⁺; (b) α -Glc-gt⁻; (c) α -Glc-tg⁺; (d) β -Glc-gg⁺; (e) β -Glc-gt⁻; (f) β -Glc-tg⁺.

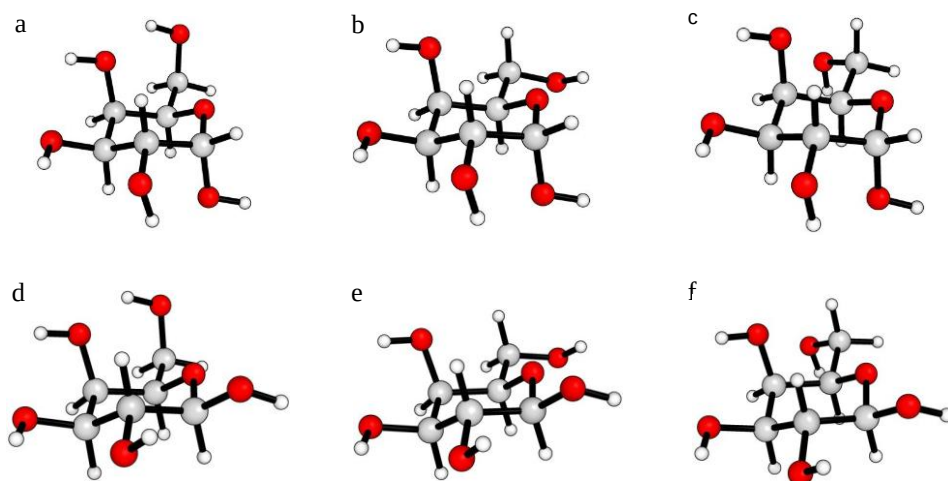


Figure S6. Optimized conformations of Gal at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi). (a) α -Gal-gg⁻; (b) α -Gal-gt⁻; (c) α -Gal-tg⁻; (d) β -Gal-gg⁻; (e) β -Gal-gt⁻; (f) β -Gal-tg⁻.

Theoretical Calculations Data of the Complexes

Glc-Trp

Table S11. Energy, ZPE and BSSE corrections and relative energy for the complexes between Glc and Trp at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

entry	Complex	Energy / Hartree	ZPE / Hartree	BSSE / Hartree	$\Delta E /$ (kcal mol ⁻¹)
1	α -Glc-gg_Trp_bottom	-1373.1706123	0.4227064	0.0031256251	0.60
2	α -Glc-gg_Trp_upper	-1373.1713087	0.4231601	0.0030594645	0.41
3	α -Glc-gt_Trp_bottom	-1373.1706414	0.4223524	0.0030792623	0.33
4	α -Glc-gt_Trp_upper	-1373.1715207	0.4231132	0.0026683030	0.00
5	α -Glc-tg_Trp_bottom	-1373.1694223	0.4235752	0.0031062657	1.88
6	α -Glc-tg_Trp_upper	-1373.1696536	0.4234618	0.0028119314	1.48
7	β -Glc-gg_Trp_bottom	-1373.1708421	0.4225045	0.0029053293	0.19
8	β -Glc-gg_Trp_upper	-1373.1704734	0.4226153	0.0032472485	0.71
9	β -Glc-gt_Trp_bottom	-1373.1711114	0.4222743	0.0033840289	0.18
10	β -Glc-gt_Trp_upper	-1373.1704102	0.4223406	0.0032364388	0.57
11	β -Glc-tg_Trp_bottom	-1373.1700650	0.4225603	0.0032579203	0.94
12	β -Glc-tg_Trp_upper	-1373.1689330	0.4226480	0.0030368492	1.56

ZPE: zero point energy correction; BSSE: basis set superposition error.

Table S12. Relative energy (in water), sum of NBO interactions and distance between Glc and Trp calculated at the M06-2X/6-31++G(d,p) level

entry	Complex	$\Delta E /$ (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å	
			1	1 $\rightarrow$ 2	2 $\rightarrow$ 1	2	Total	1	1 $\rightarrow$ 2	2	Total		
1	α -Glc-gg_Trp_bottom	0.60	267.34	0.74	3.17	852.40	1123.65	406.70	10.94	493.21	910.85	2.5384	2.5081
2	α -Glc-gg_Trp_upper	0.41	256.72	3.73	3.87	1214.79	1479.11	404.22	13.84	492.52	910.58	2.5115	2.3900
3	α -Glc-gt_Trp_bottom	0.33	266.45	0.69	3.05	852.98	1123.17	407.73	10.67	493.88	912.28	2.5687	2.5065
4	α -Glc-gt_Trp_upper	0.00	268.04	0.19	4.84	849.80	1122.87	404.80	11.53	495.06	911.39	2.3693	2.4495
5	α -Glc-tg_Trp_bottom	1.88	270.57	0.32	4.15	855.59	1130.63	407.91	10.47	494.53	912.91	2.3462	3.1717
6	α -Glc-tg_Trp_upper	1.48	271.71	0.16	4.78	856.14	1132.79	406.17	12.07	492.75	910.99	2.3953	2.3819
7	β -Glc-gg_Trp_bottom	0.19	260.27	0.91	5.76	1219.56	1486.50	404.71	16.39	492.68	913.78	2.5056	2.3349
8	β -Glc-gg_Trp_upper	0.71	258.29	2.74	4.23	1213.56	1478.82	403.49	13.19	492.70	909.38	2.5279	2.3856
9	β -Glc-gt_Trp_bottom	0.18	259.15	0.87	5.43	1212.15	1477.60	405.51	14.84	493.44	913.79	2.5598	2.3177
10	β -Glc-gt_Trp_upper	0.57	258.34	0.84	3.82	1205.54	1468.54	404.26	11.38	494.36	910.00	3.2290	2.3498
11	β -Glc-tg_Trp_bottom	0.94	261.99	0.39	5.30	860.51	1128.19	406.22	13.88	494.19	914.29	2.4608	2.3568
12	β -Glc-tg_Trp_upper	1.56	264.16	0.20	5.37	856.79	1126.52	405.36	12.11	492.94	910.41	2.4161	2.3726

1: carbohydrate; 2: amino acid; Distance: distance between the nearest hydrogen to the center of the two aromatic rings.

Table S13. C–H NBO bond dipole moment (D) for complexes between Glc and Trp calculated at M06-2X/6-31++G(d,p)

entry	Complex	C1-H	C2-H	C3-H	C4-H	C5-H	C6-Ha	C6-Hb
1	α -Glc-gg	1.861	1.796	1.885	1.808	1.843	1.898	1.737
2	α -Glc-gt	1.860	1.796	1.871	1.878	1.801	1.735	1.900
3	α -Glc-tg	1.856	1.797	1.865	1.873	1.801	1.908	1.790
4	β -Glc-gg	1.950	1.826	1.891	1.789	1.922	1.895	1.738
5	β -Glc-gt	1.939	1.826	1.875	1.860	1.881	1.735	1.887
6	β -Glc-tg	1.945	1.826	1.867	1.855	1.882	1.895	1.785
7	α -Glc-gg_Trp_bottom	1.862	1.788	1.902	1.821	1.840	1.910	1.747
8	α -Glc-gg_Trp_upper	1.863	1.754	1.889	1.821	1.833	1.877	1.717
9	α -Glc-gt_Trp_bottom	1.860	1.790	1.882	1.877	1.807	1.746	1.884
10	α -Glc-gt_Trp_upper	1.904	1.787	1.881	1.834	1.809	1.727	1.898
11	α -Glc-tg_Trp_bottom	1.856	1.787	1.860	1.873	1.807	1.897	1.798
12	α -Glc-tg_Trp_upper	1.874	1.757	1.876	1.855	1.797	1.976	1.796
13	β -Glc-gg_Trp_bottom	1.910	1.830	1.920	1.785	1.940	1.900	1.760
14	β -Glc-gg_Trp_upper	1.950	1.785	1.897	1.811	1.904	1.875	1.720
15	β -Glc-gt_Trp_bottom	1.881	1.834	1.881	1.859	1.893	1.721	1.879
16	β -Glc-gt_Trp_upper	1.937	1.794	1.882	1.876	1.884	1.703	1.904
17	β -Glc-tg_Trp_bottom	1.948	1.835	1.826	1.859	1.872	1.882	1.780
18	β -Glc-tg_Trp_upper	1.945	1.794	1.875	1.848	1.874	1.971	1.786

Table S14. NBO atomic charge for hydrogens of C-H bonds for complexes between Glc and Trp
calculated at M06- 2X/6-31++G(d,p)

entry	Complex	H1	H2	H3	H4	H5	H6a	H6b
1	α -Glc-gg	0.21985	0.24813	0.22333	0.23430	0.23841	0.20483	0.24247
2	α -Glc-gt	0.22016	0.24804	0.22650	0.21991	0.24373	0.24258	0.20117
3	α -Glc-tg	0.22135	0.24800	0.22735	0.22249	0.24199	0.19841	0.22822
4	β -Glc-gg	0.19026	0.23492	0.22185	0.23866	0.22327	0.20552	0.24186
5	β -Glc-gt	0.19266	0.23492	0.22541	0.22404	0.22812	0.24219	0.20432
6	β -Glc-tg	0.19170	0.23485	0.22672	0.22655	0.22635	0.20109	0.22899
7	α -Glc-gg_Trp_bottom	0.21869	0.25009	0.21885	0.23233	0.23932	0.20277	0.24074
8	α -Glc-gg_Trp_upper	0.21890	0.25631	0.22378	0.22916	0.24133	0.20864	0.24562
9	α -Glc-gt_Trp_bottom	0.21910	0.24958	0.22404	0.22039	0.24418	0.24004	0.20459
10	α -Glc-gt_Trp_upper	0.20998	0.24565	0.22579	0.23029	0.24316	0.24283	0.20033
11	α -Glc-tg_Trp_bottom	0.22091	0.25030	0.22663	0.22287	0.24167	0.20132	0.22651
12	α -Glc-tg_Trp_upper	0.21786	0.25349	0.22721	0.22343	0.24367	0.18120	0.22771
13	β -Glc-gg_Trp_bottom	0.19691	0.23433	0.21552	0.23996	0.21711	0.20298	0.23655
14	β -Glc-gg_Trp_upper	0.19108	0.24326	0.22152	0.23259	0.22773	0.20874	0.24465
15	β -Glc-gt_Trp_bottom	0.20399	0.23434	0.22345	0.22536	0.22461	0.24468	0.20644
16	β -Glc-gt_Trp_upper	0.19342	0.24069	0.22515	0.22188	0.22898	0.24676	0.19789
17	β -Glc-tg_Trp_bottom	0.19170	0.23420	0.23606	0.22700	0.22669	0.20476	0.22967
18	β -Glc-tg_Trp_upper	0.19222	0.24074	0.22610	0.22664	0.22887	0.18362	0.22850

Table S15. Energy, ZPE and BSSE corrections and relative energy for the complexes between Glc and D-phenylalanine at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

entry	Complex	Energy / Hartree	ZPE / Hartree	BSSE / Hartree	$\Delta E /$ (kcal mol ⁻¹)
1	α -Glc-gg_Phe_H1	-1241.6272032	0.3932709	0.0020739934	0.70
2	α -Glc-gg_Phe_H2	-1241.6285549	0.3934054	0.0022915527	0.07
3	α -Glc-gg_Phe_H3	-1241.6288845	0.3933954	0.0025175540	0.00
4	α -Glc-gg_Phe_H4	-1241.6270297	0.3930715	0.0024164532	0.90
5	α -Glc-gg_Phe_H5	-1241.6281769	0.3933706	0.0023636874	0.33
6	α -Glc-gg_Phe_H6	-1241.6267441	0.3930209	0.0021947019	0.91
7	α -Glc-gt_Phe_H1	-1241.6263829	0.3929509	0.0019202445	0.92
8	α -Glc-gt_Phe_H2	-1241.6279686	0.3931970	0.0023188824	0.33
9	α -Glc-gt_Phe_H3	-1241.6286916	0.3932052	0.0025360913	0.01
10	α -Glc-gt_Phe_H4	-1241.6277836	0.3928945	0.0023248882	0.26
11	α -Glc-gt_Phe_H5	-1241.6265183	0.3931960	0.0025421589	1.38
12	α -Glc-gt_Phe_H6	-1241.6248461	0.3932003	0.0014703140	1.75
13	α -Glc-tg_Phe_H1	-1241.6255793	0.3934119	0.0019389675	1.72
14	α -Glc-tg_Phe_H2	-1241.6270778	0.3935588	0.0023229316	1.11
15	α -Glc-tg_Phe_H3	-1241.6283631	0.3939175	0.0026622507	0.75
16	α -Glc-tg_Phe_H4	-1241.6269306	0.3930205	0.0022522322	0.82
17	α -Glc-tg_Phe_H5	-1241.6248165	0.3934810	0.0018123806	2.16
18	α -Glc-tg_Phe_H6	-1241.6259172	0.3931813	0.0020588513	1.44
19	β -Glc-gg_Phe_H1	-1241.6279281	0.3931105	0.0024416148	0.37
20	β -Glc-gg_Phe_H2	-1241.6273707	0.3925139	0.0025278091	0.40
21	β -Glc-gg_Phe_H3	-1241.6277712	0.3930865	0.0025024406	0.50
22	β -Glc-gg_Phe_H4	-1241.6265145	0.3927871	0.0025195185	1.11
23	β -Glc-gg_Phe_H5	-1241.6277444	0.3925033	0.0025084970	0.15
24	β -Glc-gg_Phe_H6	-1241.6254142	0.3923710	0.0021944721	1.33
25	β -Glc-gt_Phe_H1	-1241.6279368	0.3924296	0.0025697318	0.02
26	β -Glc-gt_Phe_H2	-1241.6273057	0.3928202	0.0025942233	0.68
27	β -Glc-gt_Phe_H3	-1241.6280019	0.3931237	0.0025780685	0.42
28	β -Glc-gt_Phe_H4	-1241.6273883	0.3927913	0.0025400934	0.57
29	β -Glc-gt_Phe_H5	-1241.6270997	0.3923513	0.0022393413	0.29
30	β -Glc-gt_Phe_H6	-1241.6269772	0.3927311	0.0025033975	0.77
31	β -Glc-tg_Phe_H1	-1241.6269086	0.3930151	0.0026001615	1.05
32	β -Glc-tg_Phe_H2	-1241.6262422	0.3926459	0.0025062398	1.18
33	β -Glc-tg_Phe_H3	-1241.6268202	0.3933070	0.0026428427	1.32
34	β -Glc-tg_Phe_H4	-1241.6267274	0.3930463	0.0025356666	1.15
35	β -Glc-tg_Phe_H5	-1241.6261901	0.3927435	0.0020956893	1.02
36	β -Glc-tg_Phe_H6	-1241.6253141	0.3931307	0.0023365917	1.96

ZPE: zero point energy correction; BSSE: basis set superposition error.

Table S16. Relative energy (in water), sum of NBO interactions and distance between Glc and Phe calculated at the M06-2X/6-31++G(d,p) level

entry	Complex	$\Delta E /$ (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å
			1	1→2	2→1	2	Total	1	1→2	2	Total	
1	α -Glc-gg_Phe_H1	0.70	266.49	0.82	3.43	636.12	906.86	406.07	9.86	356.93	772.86	2.5001
2	α -Glc-gg_Phe_H2	0.07	266.30	0.70	2.53	636.99	906.52	405.75	10.26	356.82	772.83	2.3471
3	α -Glc-gg_Phe_H3	0.00	267.23	0.61	3.54	637.73	909.11	405.29	11.07	356.26	772.62	2.3811
4	α -Glc-gg_Phe_H4	0.90	268.17	0.67	1.91	635.73	906.48	404.77	6.98	356.74	768.49	2.6400
5	α -Glc-gg_Phe_H5	0.33	268.73	0.76	2.45	634.03	905.97	406.95	9.93	357.08	773.96	2.4370
6	α -Glc-gg_Phe_H6	0.91	270.03	1.18	1.51	636.04	908.76	406.59	9.10	357.25	772.94	2.7490
7	α -Glc-gt_Phe_H1	0.92	267.99	0.36	2.19	636.81	907.35	405.90	8.97	357.28	772.15	2.4069
8	α -Glc-gt_Phe_H2	0.33	268.06	0.37	2.73	637.30	908.46	405.02	9.26	355.79	770.07	2.3611
9	α -Glc-gt_Phe_H3	0.01	267.68	0.73	3.78	637.19	909.38	405.75	11.39	355.64	772.78	2.3811
10	α -Glc-gt_Phe_H4	0.26	266.60	0.32	4.58	637.19	908.69	405.35	8.84	357.44	771.63	2.5033
11	α -Glc-gt_Phe_H5	1.38	268.14	0.79	2.64	635.96	907.53	406.90	7.80	354.35	769.05	3.1324
12	α -Glc-gt_Phe_H6	1.75	267.73	0.25	2.18	634.89	905.05	406.17	6.50	356.32	768.99	2.6157
13	α -Glc-tg_Phe_H1	1.72	270.66	0.92	2.19	637.04	910.81	408.00	9.95	357.11	775.06	2.4030
14	α -Glc-tg_Phe_H2	1.11	271.70	0.40	2.71	637.80	912.61	406.71	9.43	355.66	771.8	2.3544
15	α -Glc-tg_Phe_H3	0.75	270.24	0.66	3.95	635.14	909.99	407.57	11.23	356.65	775.45	2.3496
16	α -Glc-tg_Phe_H4	0.82	270.86	0.35	4.37	636.37	911.95	406.39	8.82	356.34	771.55	2.4560
17	α -Glc-tg_Phe_H5	2.16	267.90	0.77	1.70	635.60	905.97	408.29	5.99	354.15	768.43	3.5349
18	α -Glc-tg_Phe_H6	1.44	271.55	0.69	2.83	635.88	910.95	406.92	7.78	357.89	772.59	2.5387
19	β -Glc-gg_Phe_H1	0.37	259.60	0.61	3.70	638.26	902.17	403.98	12.71	356.80	773.49	2.3754
20	β -Glc-gg_Phe_H2	0.40	259.31	0.20	3.46	636.51	899.48	404.24	8.88	355.41	768.53	2.3445
21	β -Glc-gg_Phe_H3	0.50	259.05	0.49	3.85	636.92	900.31	404.50	10.03	356.99	771.52	2.3500
22	β -Glc-gg_Phe_H4	1.11	259.19	0.69	2.10	634.97	896.95	403.94	7.32	356.73	767.99	2.6585
23	β -Glc-gg_Phe_H5	0.15	259.89	0.45	3.56	635.40	899.30	404.97	11.14	357.19	773.30	2.3512
24	β -Glc-gg_Phe_H6	1.33	260.69	1.42	1.82	634.38	898.31	404.99	8.98	357.03	771.00	2.7206

Table S16. Relative energy (in water), sum of NBO interactions and distance between Glc and Phe calculated at the M06-2X/6-31++G(d,p) level (cont.)

entry	Complex	ΔE / (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å
			1	1→2	2→1	2	Total	1	1→2	2	Total	
25	β -Glc-gt_Phe_H1	0.02	256.42	0.29	5.03	637.59	899.33	405.31	10.77	357.25	773.33	2.3161
26	β -Glc-gt_Phe_H2	0.68	258.10	0.17	3.69	637.03	898.99	404.28	8.82	356.45	769.55	2.3556
27	β -Glc-gt_Phe_H3	0.42	257.77	0.42	3.90	636.24	898.33	405.82	10.02	356.73	772.57	2.3570
28	β -Glc-gt_Phe_H4	0.57	256.44	0.60	2.93	636.87	896.84	404.38	9.42	357.07	770.87	2.4108
29	β -Glc-gt_Phe_H5	0.29	257.19	0.56	3.51	637.35	898.61	406.44	10.82	354.95	772.21	2.7390
30	β -Glc-gt_Phe_H6	0.77	255.80	1.58	2.76	634.80	894.94	404.35	9.68	357.5	771.53	2.4353
31	β -Glc-tg_Phe_H1	1.05	259.20	0.38	4.64	637.36	901.58	407.35	10.72	356.96	775.03	2.3623
32	β -Glc-tg_Phe_H2	1.18	262.61	0.47	3.17	635.76	902.01	405.81	9.07	355.93	770.81	2.3903
33	β -Glc-tg_Phe_H3	1.32	262.85	0.46	4.04	637.63	904.98	406.34	10.31	357.17	773.82	2.3688
34	β -Glc-tg_Phe_H4	1.15	261.30	0.68	3.06	635.98	901.02	405.31	9.66	357.30	772.27	2.4158
35	β -Glc-tg_Phe_H5	1.02	260.14	0.65	3.63	636.35	900.77	406.70	11.82	354.36	772.88	2.5029
36	β -Glc-tg_Phe_H6	1.96	260.14	0.70	2.70	635.59	899.13	405.68	8.57	357.57	771.82	2.4549

1: carbohydrate; 2: amino acid; Distance: distance between the nearest hydrogen to the center of the aromatic ring.

Table S17. Energy decomposition analyse for the complex between Glc and Phe through SAPT0/6-31++G(d,p)

entry	Complex	Energy / (kcal mol ⁻¹)				
		Electrostatic	Exchange	Induction	Dispersion	Total
1	α -Glc-gg_Phe_H1	-7.18792326	10.09852267	-2.35339270	-8.17791931	-7.62071260
2	α -Glc-gg_Phe_H2	-3.89069534	10.35298215	-1.57721195	-9.73559655	-4.85052170
3	α -Glc-gg_Phe_H3	-5.04634560	11.94281389	-1.92761430	-9.84421280	-4.87535882
4	α -Glc-gg_Phe_H4	-1.76370411	8.93666232	-1.38214576	-8.78543269	-2.99462023
5	α -Glc-gg_Phe_H5	-3.38049345	10.16549241	-1.44203157	-9.45457189	-4.11160450
6	α -Glc-gg_Phe_H6	-3.83814041	9.09980208	-1.50083198	-8.26084068	-4.50001100
7	α -Glc-gt_Phe_H1	-5.30366369	8.49065158	-1.46837782	-7.73268002	-6.01406995
8	α -Glc-gt_Phe_H2	-4.91213568	10.03638884	-1.42121307	-9.43792522	-5.73488513
9	α -Glc-gt_Phe_H3	-5.86859552	12.26909511	-2.07219409	-9.88217188	-5.55386638
10	α -Glc-gt_Phe_H4	-5.25434802	10.96961203	-1.50033555	-9.81206604	-5.59713757
11	α -Glc-gt_Phe_H5	-1.04480783	8.92636566	-1.51384727	-8.55353231	-2.18582176
12	α -Glc-gt_Phe_H6	-3.06182411	7.18237326	-0.87841743	-6.30137385	-3.05924213
13	α -Glc-tg_Phe_H1	-5.99214160	8.94458085	-1.63006679	-7.82865911	-6.50628665
14	α -Glc-tg_Phe_H2	-4.40750704	10.08022057	-1.45158092	-9.43756280	-5.21643019
15	α -Glc-tg_Phe_H3	-9.23022177	12.05342742	-2.20905436	-10.40897586	-9.79482457
16	α -Glc-tg_Phe_H4	-5.85374143	10.81362087	-1.54783658	-9.70009877	-6.28805591
17	α -Glc-tg_Phe_H5	-4.82056681	7.83174979	-1.21175638	-7.52885200	-5.72942540
18	α -Glc-tg_Phe_H6	-2.50966052	9.27367422	-1.38857811	-8.73124386	-3.35580827
19	β -Glc-gg_Phe_H1	-7.15600645	12.42013477	-2.31234813	-9.77826527	-6.82648507
20	β -Glc-gg_Phe_H2	-6.68303768	9.66076060	-1.56941357	-9.24114083	-7.83283149
21	β -Glc-gg_Phe_H3	-5.73525368	10.93490971	-1.69555791	-9.73203368	-6.22793555
22	β -Glc-gg_Phe_H4	-3.59927956	9.34332411	-1.39161097	-9.14352352	-4.79108994
23	β -Glc-gg_Phe_H5	-5.73110258	11.22114973	-1.83506121	-9.88699364	-6.23200770
24	β -Glc-gg_Phe_H6	-3.63104481	8.89740242	-1.56421515	-7.95241497	-4.25027250
25	β -Glc-gt_Phe_H1	-7.90940983	11.22388946	-2.06987126	-9.75510128	-8.51049291
26	β -Glc-gt_Phe_H2	-4.68885247	9.99598870	-1.55670772	-9.55332120	-5.80289269
27	β -Glc-gt_Phe_H3	-7.33306970	10.79659811	-1.70598068	-9.77553579	-8.01798806
28	β -Glc-gt_Phe_H4	-5.83487288	11.06754370	-1.62217488	-10.06977148	-6.45927554
29	β -Glc-gt_Phe_H5	-7.28518953	10.71871336	-1.93218780	-9.56962138	-8.06828535
30	β -Glc-gt_Phe_H6	-5.48151487	11.02962934	-1.85810528	-9.64919566	-5.95918647
31	β -Glc-tg_Phe_H1	-8.08309221	11.33745924	-2.07138636	-9.91901421	-8.73603353
32	β -Glc-tg_Phe_H2	-3.86355250	10.08205669	-1.48918862	-9.60651622	-4.87720064
33	β -Glc-tg_Phe_H3	-4.26290410	10.98569096	-1.72469366	-9.96920396	-4.97111075
34	β -Glc-tg_Phe_H4	-6.66294897	11.24449159	-1.76555302	-10.23066697	-7.41467737
35	β -Glc-tg_Phe_H5	-6.41742201	11.00500784	-2.01943087	-9.50591454	-6.93775959
36	β -Glc-tg_Phe_H6	-4.33265969	9.73396014	-1.71560083	-8.99052685	-5.30482723

Table S18. Energy, ZPE and BSSE corrections and relative energy for the complexes between Glc and D-Histidine at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

entry	Complex	Energy / Hartree	ZPE / Hartree	BSSE / Hartree	$\Delta E /$ (kcal mol ⁻¹)
1	α -Glc-gg_His_H1	-1235.6232898	0.3644632	0.0016819889	5.06
2	α -Glc-gg_His_H2	-1235.6276981	0.3654229	0.0027449108	3.57
3	α -Glc-gg_His_H3	-1235.6290496	0.3651065	0.0026063386	2.43
4	α -Glc-gg_His_H4	-1235.6266150	0.3647330	0.0024369412	3.62
5	α -Glc-gg_His_H5	-1235.6262145	0.3640428	0.0021761730	3.27
6	α -Glc-gg_His_H6	-1235.6261932	0.3642129	0.0022996638	3.47
7	α -Glc-gt_His_H1	-1235.6214966	0.3647328	0.0015374996	6.27
8	α -Glc-gt_His_H2	-1235.6247185	0.3641846	0.0022932874	4.37
9	α -Glc-gt_His_H3	-1235.6273032	0.3656392	0.0025938232	3.85
10	α -Glc-gt_His_H4	-1235.6242002	0.3644056	0.0024026991	4.91
11	α -Glc-gt_His_H5	-1235.6251346	0.3650851	0.0024899751	4.80
12	α -Glc-gt_His_H6	-1235.6297514	0.3648079	0.0021658306	1.53
13	α -Glc-tg_His_H1	-1235.6219014	0.3649309	0.0015873380	6.17
14	α -Glc-tg_His_H2	-1235.6249700	0.3646482	0.0021684179	4.43
15	α -Glc-tg_His_H3	-1235.6281007	0.3657911	0.0025611183	3.43
16	α -Glc-tg_His_H4	-1235.6245118	0.3653139	0.0022044359	5.16
17	α -Glc-tg_His_H5	-1235.6302324	0.3656027	0.0031274143	2.33
18	α -Glc-tg_His_H6	-1235.6222591	0.3641624	0.0013940734	5.34
19	β -Glc-gg_His_H1	-1235.6247389	0.3639584	0.0023572618	4.26
20	β -Glc-gg_His_H2	-1235.6273537	0.3645725	0.0029554949	3.38
21	β -Glc-gg_His_H3	-1235.6331597	0.3648377	0.0031103318	0.00
22	β -Glc-gg_His_H4	-1235.6291725	0.3646080	0.0028101695	2.17
23	β -Glc-gg_His_H5	-1235.6247854	0.3640338	0.0022354801	4.20
24	β -Glc-gg_His_H6	-1235.6222295	0.3638675	0.0015334319	5.26
25	β -Glc-gt_His_H1	-1235.6236479	0.3643936	0.0024616896	5.28
26	β -Glc-gt_His_H2	-1235.6244228	0.3642671	0.0025076045	4.75
27	β -Glc-gt_His_H3	-1235.6318408	0.3644775	0.0031322975	0.62
28	β -Glc-gt_His_H4	-1235.6242739	0.3642598	0.0023630303	4.74
29	β -Glc-gt_His_H5	-1235.6244473	0.3649667	0.0025130600	5.17
30	β -Glc-gt_His_H6	-1235.6297007	0.3649596	0.0020414210	1.58
31	β -Glc-tg_His_H1	-1235.6238332	0.3645971	0.0023496673	5.22
32	β -Glc-tg_His_H2	-1235.6291788	0.3647520	0.0029874778	2.37
33	β -Glc-tg_His_H3	-1235.6322335	0.3657752	0.0031214795	1.18
34	β -Glc-tg_His_H4	-1235.6281771	0.3645033	0.0027628199	2.70
35	β -Glc-tg_His_H5	-1235.6241787	0.3645529	0.0022853372	4.94
36	β -Glc-tg_His_H6	-1235.6207438	0.3640923	0.0013641665	6.23

ZPE: zero point energy correction; BSSE: basis set superposition error.

Table S19. Relative energy (in water), sum of NBO interactions and distance between Glc and His calculated at the M06-2X/6-31++G(d,p) level

entry	Complex	ΔE / (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å
			1	1→2	2→1	2	Total	1	1→2	2	Total	
1	α -Glc-gg_His_H1	5.06	266.43	0.09	1.85	597.90	866.27	405.29	5.43	403.58	814.30	2.4120
2	α -Glc-gg_His_H2	3.57	263.68	13.10	3.10	604.50	884.38	403.12	15.87	403.56	822.55	2.4402
3	α -Glc-gg_His_H3	2.43	267.30	0.92	9.65	598.52	876.39	403.59	13.02	402.64	819.25	2.4759
4	α -Glc-gg_His_H4	3.62	271.16	1.06	11.20	594.41	877.83	403.48	10.79	401.73	816.00	2.6943
5	α -Glc-gg_His_H5	3.27	269.11	1.14	2.43	596.89	869.57	406.16	9.54	403.30	819.00	2.4061
6	α -Glc-gg_His_H6	3.47	267.59	1.59	2.65	592.71	864.54	406.17	9.43	408.51	824.11	2.6667
7	α -Glc-gt_His_H1	6.27	264.54	0.23	2.22	594.10	861.09	403.29	5.48	402.31	811.08	2.3678
8	α -Glc-gt_His_H2	4.37	266.73	2.11	2.98	595.87	867.69	402.98	8.89	402.91	814.78	2.4438
9	α -Glc-gt_His_H3	3.85	266.60	1.03	10.12	597.75	875.50	401.68	12.91	402.09	816.68	2.4794
10	α -Glc-gt_His_H4	4.91	267.04	1.30	3.05	596.06	867.45	403.48	8.35	403.11	814.94	2.3591
11	α -Glc-gt_His_H5	4.80	266.23	1.55	3.02	592.02	862.82	405.10	9.40	403.47	817.97	2.4875
12	α -Glc-gt_His_H6	1.53	270.43	2.03	31.24	601.17	904.87	402.64	21.41	405.50	829.55	2.7176
13	α -Glc-tg_His_H1	6.17	270.51	0.15	1.96	596.36	868.98	406.88	5.54	402.35	814.77	2.3848
14	α -Glc-tg_His_H2	4.43	270.84	1.58	2.94	599.40	874.76	406.71	8.55	403.07	818.33	2.4557
15	α -Glc-tg_His_H3	3.43	270.86	0.88	10.36	600.04	882.14	405.34	13.03	402.78	821.15	2.4907
16	α -Glc-tg_His_H4	5.16	270.82	0.25	3.22	595.69	869.98	406.59	6.86	401.98	815.43	2.3840
17	α -Glc-tg_His_H5	2.33	275.02	3.07	26.98	589.04	894.11	411.04	21.78	403.75	836.57	2.7254
18	α -Glc-tg_His_H6	5.34	271.12	0.83	1.15	596.31	869.41	407.43	7.43	404.23	819.09	2.6682
19	β -Glc-gg_His_H1	4.26	258.25	0.47	3.84	599.44	862.00	404.88	8.16	403.25	816.29	2.3124
20	β -Glc-gg_His_H2	3.38	254.67	11.89	2.90	602.32	871.78	402.49	14.55	401.62	818.66	2.4957
21	β -Glc-gg_His_H3	0.00	263.95	2.32	40.48	594.80	901.55	406.35	26.75	403.84	836.94	2.5682
22	β -Glc-gg_His_H4	2.17	260.61	2.70	21.76	602.60	887.67	405.34	19.04	404.46	828.84	2.6798
23	β -Glc-gg_His_H5	4.20	261.78	0.81	2.97	597.30	862.86	403.62	9.51	401.96	815.09	2.3969
24	β -Glc-gg_His_H6	5.26	257.65	0.62	1.91	597.18	857.36	404.62	5.55	402.72	812.89	2.5265
25	β -Glc-gt_His_H1	5.28	257.02	0.81	3.36	598.89	860.08	402.91	8.35	403.14	814.40	2.3428
26	β -Glc-gt_His_H2	4.75	258.56	2.04	2.78	595.36	858.74	402.36	7.81	402.59	812.76	2.4616

Table S19. Relative energy (in water), sum of NBO interactions and distance between Glc and His calculated at the M06-2X/6-31++G(d,p) level (cont.)

entry	Complex	ΔE / (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å
			1	1→2	2→1	2	Total	1	1→2	2	Total	
27	β -Glc-gt_His_H3	0.62	263.30	2.24	39.41	596.38	901.33	404.99	25.89	404.17	835.05	2.5685
28	β -Glc-gt_His_H4	4.74	259.32	1.18	3.75	599.42	863.67	402.76	8.25	402.56	813.57	2.4227
29	β -Glc-gt_His_H5	5.17	260.66	1.33	4.35	600.10	866.44	402.10	9.10	402.49	813.69	2.6238
30	β -Glc-gt_His_H6	1.58	258.36	1.46	37.86	596.53	894.21	401.24	23.92	404.53	829.69	2.6979
31	β -Glc-tg_His_H1	5.22	259.71	0.60	3.31	599.38	863.00	406.54	7.94	403.67	818.15	2.3447
32	β -Glc-tg_His_H2	2.37	262.25	4.65	36.38	590.69	893.97	406.72	25.09	403.14	834.95	2.6303
33	β -Glc-tg_His_H3	1.18	267.59	2.23	41.11	594.25	905.18	408.64	26.38	403.90	838.92	2.5931
34	β -Glc-tg_His_H4	2.70	264.64	2.89	22.32	604.61	894.46	406.69	20.07	404.28	831.04	2.4460
35	β -Glc-tg_His_H5	4.94	262.18	2.05	2.75	594.30	861.28	405.63	9.63	402.92	818.18	2.5009
36	β -Glc-tg_His_H6	6.23	259.53	0.33	1.45	596.56	857.87	406.01	4.88	403.08	813.97	2.5998

1: carbohydrate 2: amino acid; Distance: distance between the nearest hydrogen to the center of the aromatic ring.

Table S20. Energy decomposition analyse for the complex between Glc and His through SAPT0/6-31++G(d,p)

entry	Complex	Energy / (kcal mol ⁻¹)				
		Electrostatic	Exchange	Induction	Dispersion	Total
1	α -Glc-gg_His_H1	-0.76492743	5.70935931	-1.01086757	-5.55749607	-1.62393175
2	α -Glc-gg_His_H2	-14.79106547	16.64548857	-4.01872399	-11.24066990	-13.40497079
3	α -Glc-gg_His_H3	-9.20127824	15.26192426	-3.31770184	-9.55625469	-6.81331051
4	α -Glc-gg_His_H4	-10.23133054	14.23551860	-3.12578060	-8.60299715	-7.72458969
5	α -Glc-gg_His_H5	-4.30966857	9.71010947	-1.53535828	-8.85262330	-4.98754068
6	α -Glc-gg_His_H6	-4.14789458	9.59152616	-1.71438324	-8.77619275	-5.04694441
7	α -Glc-gt_His_H1	-2.25310418	5.43084526	-0.87447941	-5.24454388	-2.94128222
8	α -Glc-gt_His_H2	-5.55261395	9.91572071	-1.86385122	-9.16652955	-6.66727402
9	α -Glc-gt_His_H3	-9.63795923	15.20282935	-3.42525612	-9.33109107	-7.19147707
10	α -Glc-gt_His_H4	-6.07802824	8.95718458	-1.30080521	-8.18943219	-6.61108107
11	α -Glc-gt_His_H5	-4.15303298	10.69035929	-1.83232522	-9.52517764	-4.82017655
12	α -Glc-gt_His_H6	-16.66468752	22.97654029	-7.45254150	-9.95917663	-11.09986536
13	α -Glc-tg_His_H1	-0.83502457	5.69506970	-0.94249292	-5.40403628	-1.48648407
14	α -Glc-tg_His_H2	-5.43743424	9.46634173	-1.62685694	-8.81097955	-6.40892900
15	α -Glc-tg_His_H3	-10.26925474	15.40811853	-3.59073884	-9.47505399	-7.92692904
16	α -Glc-tg_His_H4	-4.04170094	7.86436031	-1.15892869	-7.80430390	-5.14057322
17	α -Glc-tg_His_H5	-20.23674475	24.66778018	-7.08421346	-12.50692195	-15.16009999
18	α -Glc-tg_His_H6	-3.95655801	6.15989192	-0.98550627	-5.59062215	-4.37279452
19	β -Glc-gg_His_H1	-4.56174343	9.03352472	-1.48198042	-7.82935403	-4.83955316
20	β -Glc-gg_His_H2	-16.41504492	16.33340531	-3.93043895	-11.33620954	-15.34828809
21	β -Glc-gg_His_H3	-23.62826270	28.85873983	-9.88082705	-12.44440292	-17.09475284
22	β -Glc-gg_His_H4	-15.70114638	21.85180876	-5.90479723	-11.60647067	-11.36060552
23	β -Glc-gg_His_H5	-2.14290337	8.81524350	-1.26042406	-8.24675614	-2.83484006
24	β -Glc-gg_His_H6	-0.77132919	6.41428033	-0.89932622	-5.84631379	-1.10268887
25	β -Glc-gt_His_H1	-4.55435676	9.10253070	-1.43207322	-7.89902989	-4.78292916
26	β -Glc-gt_His_H2	-7.33381109	9.84666745	-1.95970343	-9.23542089	-8.68226796
27	β -Glc-gt_His_H3	-22.39776071	28.08073709	-9.51979868	-12.30695788	-16.14378017
28	β -Glc-gt_His_H4	-7.05029966	9.47786967	-1.47736656	-8.92714196	-7.97693851
29	β -Glc-gt_His_H5	-1.11245566	9.93077109	-2.11886927	-8.64991469	-1.95046852
30	β -Glc-gt_His_H6	-19.73813149	25.23155059	-8.77859136	-9.67497814	-12.96015041
31	β -Glc-tg_His_H1	-3.64739592	8.66644531	-1.45695903	-7.72738310	-4.16529275
32	β -Glc-tg_His_H2	-26.77287049	29.20433405	-9.50252186	-12.59275797	-19.66381627
33	β -Glc-tg_His_H3	-23.69958334	28.43499396	-9.86666422	-12.30153313	-17.43278672
34	β -Glc-tg_His_H4	-18.16234633	22.58485675	-5.95708794	-11.91007639	-13.44465390
35	β -Glc-tg_His_H5	-0.95865668	9.33878549	-1.57577215	-8.81922936	-2.01487270
36	β -Glc-tg_His_H6	-3.05155989	5.10747300	-0.75528277	-5.12556547	-3.82493513

Gal-Trp

Table S21. Energy, ZPE and BSSE corrections and relative energy for the complexes between *Gal* and *Trp* at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

entry	Complex	Energy / Hartree	ZPE / Hartree	BSSE / Hartree	ΔE / (kcal mol ⁻¹)
1	α -Gal-gg_Trp_bottom	-1373.1715012	0.4235385	0.0026794018	0.36
2	α -Gal-gg_Trp_upper	-1373.1698584	0.4237930	0.0026109260	1.50
3	α -Gal-gt_Trp_bottom	-1373.1712727	0.4227011	0.0027199662	0.00
4	α -Gal-gt_Trp_upper	-1373.1693046	0.4233954	0.0025509387	1.56
5	α -Gal-tg_Trp_bottom	-1373.1700469	0.4231957	0.0030203869	1.27
6	α -Gal-tg_Trp_upper	-1373.1677713	0.4234427	0.0025809160	2.58
7	β -Gal-gg_Trp_bottom	-1373.1706582	0.4227393	0.0029716792	0.57
8	β -Gal-gg_Trp_upper	-1373.1686966	0.4232148	0.0029873335	2.11
9	β -Gal-gt_Trp_bottom	-1373.1708584	0.4223645	0.0030337424	0.25
10	β -Gal-gt_Trp_upper	-1373.1681896	0.4226876	0.0028508909	2.01
11	β -Gal-tg_Trp_bottom	-1373.1694747	0.4226382	0.0031802100	1.38
12	β -Gal-tg_Trp_upper	-1373.1665996	0.4230462	0.0028375581	3.22

ZPE: zero point energy correction; BSSE: basis set superposition error.

Table S22. Relative energy (in water), sum of NBO interactions and distance between Gal and Trp calculated at the M06-2X/6-31++G(d,p) level

entry	Complex	$\Delta E /$ (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å	
			1	1→2	2→1	2	Total	1	1→2	2	Total		
1	α -Gal-gg_Trp_bottom	0.36	279.54	0.39	3.93	857.08	1140.94	411	13.7	494.94	919.64	2.3904	2.5128
2	α -Gal-gg_Trp_upper	1.50	278.09	0.43	2.21	859.85	1140.58	411.09	11.13	495.31	917.53	3.3331	2.3618
3	α -Gal-gt_Trp_bottom	0.00	270.35	0.43	4.00	855.33	1130.11	408.32	13.89	494.78	916.99	2.3966	2.5014
4	α -Gal-gt_Trp_upper	1.56	268.82	0.20	2.53	886.30	1157.85	408.4	11.09	494.12	913.61	3.3634	2.3528
5	α -Gal-tg_Trp_bottom	1.27	270.05	0.36	3.81	856.75	1130.97	406.49	13.42	494.58	914.49	2.3447	2.6467
6	α -Gal-tg_Trp_upper	2.58	267.78	0.46	2.23	859.25	1129.72	406.6	11.16	494.96	912.72	3.3331	2.3571
7	β -Gal-gg_Trp_bottom	0.57	269.88	0.24	4.20	858.49	1132.81	408.69	14.12	494.61	917.42	2.3604	2.3945
8	β -Gal-gg_Trp_upper	2.11	269.38	0.52	3.09	854.89	1127.88	410.7	9.35	493.18	913.23	2.3728	3.1607
9	β -Gal-gt_Trp_bottom	0.25	262.00	0.30	4.40	857.57	1124.27	407.09	14.1	494.58	915.77	2.3895	2.3738
10	β -Gal-gt_Trp_upper	2.01	259.91	0.39	3.05	856.00	1119.35	407.36	8.6	493.99	909.95	2.3922	3.1481
11	β -Gal-tg_Trp_bottom	1.38	258.01	0.23	4.58	856.12	1118.94	404.96	14.3	495.58	914.84	2.4110	2.3446
12	β -Gal-tg_Trp_upper	3.22	260.57	0.45	2.75	855.51	1119.28	405.55	8.13	493.38	907.06	2.3971	3.1676

1: carbohydrate; 2: amino acid; Distance: distance between the nearest hydrogen to the center of the two aromatic rings.

Table S23. C–H NBO bond dipole moment (D) for complexes between Gal and Trp calculated at M06-2X/6-31++G(d,p)

entry	Complex	C1–H	C2–H	C3–H	C4–H	C5–H	C6–Ha	C6–Hb
1	α -Gal-gg	1.848	1.752	1.886	1.882	1.880	1.801	1.931
2	α -Gal-gt	1.857	1.756	1.890	1.885	1.846	1.832	1.782
3	α -Gal-tg	1.857	1.753	1.905	1.839	1.933	1.689	1.898
4	β -Gal-gg	1.978	1.782	1.892	1.884	1.959	1.798	1.931
5	β -Gal-gt	1.956	1.787	1.894	1.887	1.927	1.831	1.768
6	β -Gal-tg	1.974	1.784	1.909	1.843	2.012	1.676	1.895
7	α -Gal-gg_Trp_bottom	1.844	1.751	1.885	1.843	1.924	1.818	1.931
8	α -Gal-gg_Trp_upper	1.860	1.736	1.878	1.882	1.876	1.792	1.925
9	α -Gal-gt_Trp_bottom	1.853	1.753	1.892	1.846	1.894	1.831	1.772
10	α -Gal-gt_Trp_upper	1.868	1.738	1.886	1.887	1.841	1.829	1.800
11	α -Gal-tg_Trp_bottom	1.852	1.751	1.901	1.830	1.966	1.685	1.909
12	α -Gal-tg_Trp_upper	1.867	1.736	1.900	1.842	1.928	1.707	1.887
13	β -Gal-gg_Trp_bottom	1.985	1.796	1.849	1.928	1.920	1.811	1.983
14	β -Gal-gg_Trp_upper	1.972	1.788	1.877	1.882	1.950	1.797	1.925
15	β -Gal-gt_Trp_bottom	1.959	1.801	1.845	1.929	1.903	1.877	1.758
16	β -Gal-gt_Trp_upper	1.949	1.794	1.879	1.887	1.921	1.831	1.777
17	β -Gal-tg_Trp_bottom	1.984	1.796	1.866	1.886	1.967	1.674	1.889
18	β -Gal-tg_Trp_upper	1.969	1.792	1.894	1.844	2.005	1.687	1.888

Table S24. NBO atomic charge for hydrogens of C–H bonds for complexes between Gal and Trp calculated at M06- 2X/6-31++G(d,p)

entry	Complex	H1	H2	H3	H4	H5	H6a	H6b
1	α -Gal-gg	0.22306	0.25733	0.22537	0.22816	0.23465	0.22666	0.19866
2	α -Gal-gt	0.22059	0.25637	0.22483	0.22651	0.23961	0.22260	0.22586
3	α -Gal-tg	0.22102	0.25700	0.22194	0.23665	0.21988	0.24511	0.20377
4	β -Gal-gg	0.18360	0.24461	0.22384	0.22754	0.21935	0.22715	0.19811
5	β -Gal-gt	0.18840	0.24370	0.22357	0.22577	0.22380	0.22226	0.22918
6	β -Gal-tg	0.18476	0.24423	0.22070	0.23544	0.20424	0.24818	0.20424
7	α -Gal-gg_Trp_bottom	0.22379	0.25844	0.22280	0.23538	0.22448	0.22269	0.19745
8	α -Gal-gg_Trp_upper	0.21909	0.25968	0.22758	0.22792	0.23571	0.22823	0.19980
9	α -Gal-gt_Trp_bottom	0.22130	0.25772	0.22164	0.23397	0.22967	0.22139	0.22736
10	α -Gal-gt_Trp_upper	0.21689	0.25878	0.22631	0.22594	0.24083	0.22283	0.22207
11	α -Gal-tg_Trp_bottom	0.22182	0.25820	0.21912	0.23858	0.21271	0.24613	0.20087
12	α -Gal-tg_Trp_upper	0.21733	0.25926	0.22348	0.23582	0.22105	0.24131	0.20596
13	β -Gal-gg_Trp_bottom	0.18257	0.24310	0.23202	0.21870	0.22191	0.22449	0.18770
14	β -Gal-gg_Trp_upper	0.18488	0.24040	0.22731	0.22714	0.22128	0.22698	0.19909
15	β -Gal-gt_Trp_bottom	0.18847	0.24204	0.23278	0.21718	0.22482	0.21275	0.23115
16	β -Gal-gt_Trp_upper	0.18983	0.23931	0.22696	0.22512	0.22522	0.22205	0.22694
17	β -Gal-tg_Trp_bottom	0.18333	0.24305	0.22790	0.22664	0.21008	0.24872	0.20528
18	β -Gal-tg_Trp_upper	0.18601	0.23973	0.22407	0.23464	0.20584	0.24537	0.20557

Gal-Phe

Table S25. Energy, ZPE and BSSE corrections and relative energy for the complexes between Gal and D-phenylalanine at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

entry	Complex	Energy / Hartree	ZPE / Hartree	BSSE / Hartree	$\Delta E /$ (kcal mol ⁻¹)
1	α -Gal-gg_Phe_H1	-1241.6272696	0.3935528	0.0020328427	1.09
2	α -Gal-gg_Phe_H2	-1241.6289284	0.3942662	0.0022993614	0.67
3	α -Gal-gg_Phe_H3	-1241.6294548	0.3938958	0.0023286959	0.12
4	α -Gal-gg_Phe_H4	-1241.6275071	0.3940978	0.0017839342	1.13
5	α -Gal-gg_Phe_H5	-1241.6289923	0.3936664	0.0020004167	0.06
6	α -Gal-gg_Phe_H6	-1241.6268503	0.3939559	0.0020528915	1.62
7	α -Gal-gt_Phe_H1	-1241.6269885	0.3931441	0.0020091356	1.00
8	α -Gal-gt_Phe_H2	-1241.6280082	0.3934321	0.0022175656	0.67
9	α -Gal-gt_Phe_H3	-1241.6289741	0.3930903	0.0024558843	0.00
10	α -Gal-gt_Phe_H4	-1241.6289293	0.3940198	0.0020521008	0.36
11	α -Gal-gt_Phe_H5	-1241.6293227	0.3938133	0.0022938758	0.13
12	α -Gal-gt_Phe_H6	-1241.6278148	0.3936324	0.0020897052	0.84
13	α -Gal-tg_Phe_H1	-1241.6245056	0.3933221	0.0017460806	2.50
14	α -Gal-tg_Phe_H2	-1241.6264794	0.3936980	0.0022621626	1.83
15	α -Gal-tg_Phe_H3	-1241.6262559	0.3933981	0.0022192151	1.75
16	α -Gal-tg_Phe_H4	-1241.6271281	0.3939877	0.0024688112	1.73
17	α -Gal-tg_Phe_H5	-1241.6285049	0.3936805	0.0025311930	0.71
18	α -Gal-tg_Phe_H6	-1241.6234491	0.3935222	0.0015696715	3.18
19	β -Gal-gg_Phe_H1	-1241.6277129	0.3935837	0.0024735990	1.11
20	β -Gal-gg_Phe_H2	-1241.6274182	0.3936014	0.0023355928	1.22
21	β -Gal-gg_Phe_H3	-1241.6275410	0.3932786	0.0024080320	0.99
22	β -Gal-gg_Phe_H4	-1241.6274929	0.3936724	0.0019810085	1.00
23	β -Gal-gg_Phe_H5	-1241.6282367	0.3935208	0.0023736962	0.68
24	β -Gal-gg_Phe_H6	-1241.6257694	0.3937053	0.0020742959	2.16
25	β -Gal-gt_Phe_H1	-1241.6277968	0.3926855	0.0025301122	0.53
26	β -Gal-gt_Phe_H2	-1241.6277806	0.3933285	0.0024402863	0.89
27	β -Gal-gt_Phe_H3	-1241.6273468	0.3925612	0.0023732978	0.64
28	β -Gal-gt_Phe_H4	-1241.6275597	0.3928445	0.0021615545	0.55
29	β -Gal-gt_Phe_H5	-1241.6281539	0.3934719	0.0023144522	0.67
30	β -Gal-gt_Phe_H6	-1241.6247452	0.3926386	0.0015879680	1.83
31	β -Gal-tg_Phe_H1	-1241.6262745	0.3937002	0.0024808984	2.09
32	β -Gal-tg_Phe_H2	-1241.6258937	0.3931113	0.0022964605	1.85
33	β -Gal-tg_Phe_H3	-1241.6257863	0.3927741	0.0021268464	1.60
34	β -Gal-tg_Phe_H4	-1241.6256707	0.3931341	0.0021593125	1.91
35	β -Gal-tg_Phe_H5	-1241.6265625	0.3932971	0.0022898123	1.54
36	β -Gal-tg_Phe_H6	-1241.6250366	0.3931627	0.0021718925	2.34

ZPE: zero point energy correction; BSSE: basis set superposition error.

Table S26. Relative energy (in water), sum of NBO interactions and distance between Gal and Phe calculated at the M06-2X/6-31++G(d,p) level

entry	Complex	$\Delta E /$ (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å
			1	1→2	2→1	2	Total	1	1→2	2	Total	
1	α -Gal-gg_Phe_H1	1.09	277.66	0.50	2.52	635.32	916.00	410.97	9.60	357.44	778.01	2.4620
2	α -Gal-gg_Phe_H2	0.67	278.31	0.43	2.53	635.94	917.21	411.42	9.70	357.17	778.29	2.4319
3	α -Gal-gg_Phe_H3	0.12	279.77	0.68	2.73	637.99	921.17	410.44	11.18	357.57	779.19	2.3932
4	α -Gal-gg_Phe_H4	1.13	279.04	0.46	2.51	636.36	918.37	411.20	8.97	356.78	776.95	2.4887
5	α -Gal-gg_Phe_H5	0.06	279.11	0.42	2.85	636.48	918.86	411.23	11.12	356.12	778.47	2.4088
6	α -Gal-gg_Phe_H6	0.89	280.49	1.71	1.61	636.40	920.21	410.48	9.21	357.07	776.76	2.5113
7	α -Gal-gt_Phe_H1	1.00	268.01	0.50	2.59	635.81	906.91	408.75	9.85	357.81	776.41	2.4418
8	α -Gal-gt_Phe_H2	0.67	269.81	0.32	2.46	636.21	908.80	408.64	9.58	356.45	774.67	2.4075
9	α -Gal-gt_Phe_H3	0.00	267.75	0.74	2.51	636.01	907.01	409.03	11.02	357.07	777.12	2.3979
10	α -Gal-gt_Phe_H4	0.36	269.73	0.47	3.14	637.56	910.90	409.03	11.03	358.05	778.11	2.4608
11	α -Gal-gt_Phe_H5	0.13	270.96	0.61	2.84	637.67	912.08	409.56	10.94	357.12	777.62	2.4392
12	α -Gal-gt_Phe_H6	0.84	270.21	0.40	2.20	637.59	910.40	409.25	9.66	357.10	776.01	2.5896
13	α -Gal-tg_Phe_H1	2.50	266.79	0.26	2.67	635.94	905.66	406.08	7.96	356.34	770.38	2.3776
14	α -Gal-tg_Phe_H2	1.83	268.06	0.81	2.12	635.57	906.56	406.33	9.62	356.87	772.82	2.4134
15	α -Gal-tg_Phe_H3	1.75	268.24	0.35	5.59	638.37	912.55	406.56	9.91	355.94	772.41	3.1232
16	α -Gal-tg_Phe_H4	1.73	270.20	0.57	3.11	637.32	911.20	407.16	9.98	357.10	774.24	2.6106
17	α -Gal-tg_Phe_H5	0.71	269.24	1.03	3.95	637.58	911.80	407.17	11.95	357.53	776.65	2.5992
18	α -Gal-tg_Phe_H6	3.18	267.71	0.16	1.19	633.20	902.26	406.74	5.36	356.09	768.19	2.5033
19	β -Gal-gg_Phe_H1	1.11	269.73	0.40	4.08	639.00	913.21	409.22	10.45	356.97	776.64	2.3509
20	β -Gal-gg_Phe_H2	1.22	270.90	0.53	3.43	635.45	910.31	410.11	9.91	355.71	775.73	2.4010
21	β -Gal-gg_Phe_H3	0.99	270.69	0.47	3.27	636.40	910.83	409.41	10.28	357.09	776.78	2.3370
22	β -Gal-gg_Phe_H4	1.00	270.20	0.47	2.65	637.81	911.13	409.28	10.43	357.64	777.35	2.4570
23	β -Gal-gg_Phe_H5	0.68	269.26	0.39	3.58	637.31	910.54	409.94	11.54	357.53	779.01	2.3424
24	β -Gal-gg_Phe_H6	2.16	273.07	0.37	2.53	636.45	912.42	408.24	9.05	357.27	774.56	2.4213
25	β -Gal-gt_Phe_H1	0.53	260.40	0.25	4.79	638.03	903.47	407.01	10.78	356.96	774.75	2.3165

Table S26. Relative energy (in water), sum of NBO interactions and distance between Gal and Phe calculated at the M06-2X/6-31++G(d,p) level (cont.)

entry	Complex	ΔE / (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å
			1	1→2	2→1	2	Total	1	1→2	2	Total	
26	β-Gal-gt_Phe_H2	0.89	260.74	0.47	2.99	637.75	901.95	406.72	10.08	356.03	772.83	2.4149
27	β-Gal-gt_Phe_H3	0.64	259.71	0.46	3.19	637.71	901.07	407.87	9.80	355.58	773.25	2.3525
28	β-Gal-gt_Phe_H4	0.55	262.07	0.51	3.26	637.77	903.61	407.49	10.66	357.55	775.70	2.4860
29	β-Gal-gt_Phe_H5	0.67	260.28	0.50	3.76	636.89	901.43	408.41	11.30	356.99	776.70	2.3683
30	β-Gal-gt_Phe_H6	1.83	261.58	0.32	1.99	635.54	899.43	406.88	7.28	355.28	769.44	2.4984
31	β-Gal-tg_Phe_H1	2.09	257.93	0.38	4.24	638.21	900.76	405.96	10.52	356.61	773.09	2.3481
32	β-Gal-tg_Phe_H2	1.85	259.55	0.41	2.71	638.03	900.70	405.99	9.79	356.88	772.66	2.3820
33	β-Gal-tg_Phe_H3	1.60	259.38	0.41	2.98	775.98	1038.75	406.05	9.98	356.54	772.57	2.3609
34	β-Gal-tg_Phe_H4	1.91	259.80	1.19	2.10	635.97	899.06	406.07	9.99	357.14	773.20	2.4839
35	β-Gal-tg_Phe_H5	1.54	259.22	0.53	2.97	636.57	899.29	408.34	11.27	357.92	777.53	2.4277
36	β-Gal-tg_Phe_H6	2.34	261.40	0.80	1.92	636.46	900.58	405.27	9.77	357.35	772.39	2.5349

1: carbohydrate; 2: amino acid; Distance: distance between the nearest hydrogen to the center of the aromatic ring.

Table S27. Energy decomposition analyse for the complex between Gal and Phe through SAPT0/6-31++G(d,p)

entry	Complex	Energy / (kcal mol ⁻¹)				
		Electrostatic	Exchange	Induction	Dispersion	Total
1	α -Gal-gg_Phe_H1	-4.71450808	8.87942607	-1.62562020	-8.27751311	-5.73821532
2	α -Gal-gg_Phe_H2	-7.34304199	9.99836062	-1.90628690	-9.67198593	-8.92295419
3	α -Gal-gg_Phe_H3	-4.31035931	11.14976462	-1.65677682	-9.98385172	-4.80122323
4	α -Gal-gg_Phe_H4	-5.44249896	9.88124729	-1.37920103	-8.40313459	-5.34358730
5	α -Gal-gg_Phe_H5	-6.22622362	11.51735454	-1.44928045	-9.56042425	-5.71857378
6	α -Gal-gg_Phe_H6	-3.59119730	8.80674231	-1.30370218	-7.95809132	-4.04624850
7	α -Gal-gt_Phe_H1	-5.14257341	9.01103469	-1.55177345	-8.22263332	-5.90594550
8	α -Gal-gt_Phe_H2	-3.88735381	9.64951375	-1.51089702	-9.21548675	-4.96422383
9	α -Gal-gt_Phe_H3	-4.98164217	11.03713809	-1.55218141	-9.97703462	-5.47372010
10	α -Gal-gt_Phe_H4	-6.99393620	10.82417987	-1.69279829	-9.56200471	-7.42455933
11	α -Gal-gt_Phe_H5	-4.21188199	11.37955176	-1.63621122	-10.16882126	-4.63736272
12	α -Gal-gt_Phe_H6	-3.00536575	9.36778174	-1.57642445	-8.71158068	-3.92558914
13	α -Gal-tg_Phe_H1	-6.08726948	8.05829162	-1.64168629	-6.59792025	-6.26858440
14	α -Gal-tg_Phe_H2	-4.37818837	9.72937169	-1.55512411	-9.19296124	-5.39690203
15	α -Gal-tg_Phe_H3	-5.41410954	12.22093646	-2.60783352	-9.09276398	-4.89377058
16	α -Gal-tg_Phe_H4	-3.60536010	11.07994705	-1.78308352	-9.69671092	-4.00520749
17	α -Gal-tg_Phe_H5	-8.19032020	12.95588308	-2.52951209	-10.63651418	-8.40046339
18	α -Gal-tg_Phe_H6	-0.63302195	5.85462445	-0.83887319	-6.08549397	-1.70276467
19	β -Gal-gg_Phe_H1	-4.81269445	11.28159756	-1.90621727	-9.60882336	-5.04613752
20	β -Gal-gg_Phe_H2	-7.21739979	10.73859349	-1.91889383	-9.06448319	-7.46218332
21	β -Gal-gg_Phe_H3	-4.18714677	10.75788246	-1.68525436	-9.45575767	-4.57027635
22	β -Gal-gg_Phe_H4	-4.76690818	10.73508270	-1.61872065	-9.14733263	-4.79787876
23	β -Gal-gg_Phe_H5	-6.81811655	11.86195749	-1.94581434	-10.01681116	-6.91878455
24	β -Gal-gg_Phe_H6	-0.70526613	8.38787794	-1.45709423	-7.77314177	-1.54762419
25	β -Gal-gt_Phe_H1	-5.95567371	11.29197723	-1.99492456	-9.64516307	-6.30378411
26	β -Gal-gt_Phe_H2	-4.23229386	10.63814628	-1.70090189	-9.16094403	-4.45599351
27	β -Gal-gt_Phe_H3	-4.77610933	10.58396188	-1.68431341	-9.35170806	-5.22816891
28	β -Gal-gt_Phe_H4	-4.26391981	11.03511880	-1.66357597	-9.48677459	-4.37915157
29	β -Gal-gt_Phe_H5	-6.09582097	11.72710719	-1.98918564	-10.11234429	-6.47024371
30	β -Gal-gt_Phe_H6	-2.70734193	7.27580894	-1.11240004	-6.59468761	-3.13862063
31	β -Gal-tg_Phe_H1	-6.50804881	11.24215054	-1.91737687	-9.64456268	-6.82783781
32	β -Gal-tg_Phe_H2	-5.13006762	10.53072956	-1.71491445	-9.03813854	-5.35239105
33	β -Gal-tg_Phe_H3	-5.75782431	10.22805994	-1.53621378	-9.01469580	-6.08067395
34	β -Gal-tg_Phe_H4	-4.99019083	10.20377258	-1.53060394	-9.06537397	-5.38239616
35	β -Gal-tg_Phe_H5	-6.16355207	11.14601224	-1.91961875	-9.96832288	-6.90548147
36	β -Gal-tg_Phe_H6	-2.87914623	9.41027805	-1.40752501	-8.62417936	-3.50057255

Table S28. Energy, ZPE and BSSE corrections and relative energy for the complexes between Gal and D-Histidine at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

entry	Complex	Energy / Hartree	ZPE / Hartree	BSSE / Hartree	$\Delta E /$ (kcal mol ⁻¹)
1	α -Gal-gg_His_H1	-1235.6257430	0.3653442	0.0021355632	3.77
2	α -Gal-gg_His_H2	-1235.6272433	0.3654630	0.0024423660	3.10
3	α -Gal-gg_His_H3	-1235.6266178	0.3656858	0.0021927608	3.47
4	α -Gal-gg_His_H4	-1235.6252407	0.3653226	0.0017637206	3.84
5	α -Gal-gg_His_H5	-1235.6271076	0.3655259	0.0024125117	3.20
6	α -Gal-gg_His_H6	-1235.6256340	0.3653638	0.0019168443	3.71
7	α -Gal-gt_His_H1	-1235.6317111	0.3654182	0.0026060089	0.37
8	α -Gal-gt_His_H2	-1235.6328617	0.3656778	0.0029113818	0.00
9	α -Gal-gt_His_H3	-1235.6260225	0.3647418	0.0021615479	3.23
10	α -Gal-gt_His_H4	-1235.6249693	0.3648726	0.0020600241	3.91
11	α -Gal-gt_His_H5	-1235.6265184	0.3651487	0.0021340703	3.16
12	α -Gal-gt_His_H6	-1235.6314759	0.3654979	0.0023138079	0.38
13	α -Gal-tg_His_H1	-1235.6236263	0.3648449	0.0019439542	4.67
14	α -Gal-tg_His_H2	-1235.6249122	0.3651213	0.0023740551	4.30
15	α -Gal-tg_His_H3	-1235.6248757	0.3659582	0.0021473571	4.71
16	α -Gal-tg_His_H4	-1235.6241079	0.3650887	0.0023374269	4.76
17	α -Gal-tg_His_H5	-1235.6261206	0.3654018	0.0023975944	3.73
18	α -Gal-tg_His_H6	-1235.6210469	0.3646152	0.0013744881	5.78
19	β -Gal-gg_His_H1	-1235.6255706	0.3654623	0.0025012716	4.18
20	β -Gal-gg_His_H2	-1235.6267365	0.3656107	0.0029033803	3.80
21	β -Gal-gg_His_H3	-1235.6247804	0.3648586	0.0021165868	4.06
22	β -Gal-gg_His_H4	-1235.6239143	0.3642500	0.0017337504	3.98
23	β -Gal-gg_His_H5	-1235.6245529	0.3649475	0.0020707154	4.23
24	β -Gal-gg_His_H6	-1235.6226131	0.3644441	0.0014109324	4.72
25	β -Gal-gt_His_H1	-1235.6252924	0.3641248	0.0023077079	3.40
26	β -Gal-gt_His_H2	-1235.6251847	0.3647390	0.0024703702	3.95
27	β -Gal-gt_His_H3	-1235.6250026	0.3644757	0.0023042787	3.80
28	β -Gal-gt_His_H4	-1235.6239666	0.3642916	0.0017884983	4.01
29	β -Gal-gt_His_H5	-1235.6258578	0.3648716	0.0021503286	3.41
30	β -Gal-gt_His_H6	-1235.6220208	0.3641650	0.0013509100	4.87
31	β -Gal-tg_His_H1	-1235.6244189	0.3644458	0.0025650557	4.31
32	β -Gal-tg_His_H2	-1235.6244208	0.3639138	0.0026896788	4.05
33	β -Gal-tg_His_H3	-1235.6316706	0.3654192	0.0029867998	0.63
34	β -Gal-tg_His_H4	-1235.6235494	0.3646352	0.0019475442	4.58
35	β -Gal-tg_His_H5	-1235.6247037	0.3645652	0.0025574701	4.20
36	β -Gal-tg_His_H6	-1235.6205547	0.3640431	0.0013608666	5.72

ZPE: zero point energy correction; BSSE: basis set superposition error.

Table S29. Relative energy (in water), sum of NBO interactions and distance between Gal and His calculated at the M06-2X/6-31++G(d,p) level

entry	Complex	$\Delta E /$ (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å
			1	1→2	2→1	2	Total	1	1→2	2	Total	
1	α -Gal-gg_His_H1	3.77	278.93	1.66	1.93	599.12	881.64	412.26	8.91	402.78	823.95	2.4878
2	α -Gal-gg_His_H2	3.10	276.95	1.85	2.90	598.28	879.98	411.26	9.21	403.34	823.81	2.4731
3	α -Gal-gg_His_H3	3.47	278.16	0.58	3.19	599.47	881.40	409.63	8.02	402.62	820.27	2.4588
4	α -Gal-gg_His_H4	3.84	279.80	0.14	2.70	595.23	877.87	410.19	6.95	404.05	821.19	2.4325
5	α -Gal-gg_His_H5	3.20	280.61	0.52	3.36	597.25	881.74	410.31	9.18	408.94	828.43	2.4257
6	α -Gal-gg_His_H6	3.71	279.54	0.38	2.11	597.02	879.05	409.95	7.30	402.70	819.95	2.5696
7	α -Gal-gt_His_H1	0.37	270.28	2.73	32.31	603.93	909.25	408.75	23.77	406.99	839.51	2.4297
8	α -Gal-gt_His_H2	0.00	272.29	2.93	21.58	610.35	907.15	408.14	20.16	407.08	835.38	2.4056
9	α -Gal-gt_His_H3	3.23	269.66	0.21	2.77	598.43	871.07	408.07	8.49	402.06	818.62	2.3825
10	α -Gal-gt_His_H4	3.91	269.17	1.41	2.16	595.94	868.68	408.41	8.80	403.75	820.96	2.3740
11	α -Gal-gt_His_H5	3.16	269.51	0.49	3.08	599.95	873.03	408.87	9.24	401.02	819.13	2.4616
12	α -Gal-gt_His_H6	0.38	271.04	2.63	30.95	602.18	906.80	406.35	21.45	404.77	832.57	2.5185
13	α -Gal-tg_His_H1	4.67	268.74	1.60	1.86	598.95	871.15	407.49	8.06	403.95	819.50	2.5082
14	α -Gal-tg_His_H2	4.30	267.08	1.82	2.77	598.40	870.07	407.58	8.92	403.24	819.74	2.4638
15	α -Gal-tg_His_H3	4.71	267.25	0.73	3.01	599.25	870.24	405.90	8.13	402.75	816.78	2.4519
16	α -Gal-tg_His_H4	4.76	267.21	1.61	1.65	594.32	864.79	407.05	8.22	403.34	818.61	2.4468
17	α -Gal-tg_His_H5	3.73	269.21	0.56	2.83	594.11	866.71	408.10	9.69	403.45	821.24	2.4924
18	α -Gal-tg_His_H6	5.78	266.82	0.66	1.43	594.71	863.62	406.84	6.59	403.21	816.64	2.5149
19	β -Gal-gg_His_H1	4.18	269.84	0.80	7.01	596.51	874.16	408.89	10.52	408.83	828.24	2.3950
20	β -Gal-gg_His_H2	3.80	275.87	0.84	20.18	597.13	894.02	404.08	15.95	400.42	820.45	2.3974
21	β -Gal-gg_His_H3	4.06	271.85	0.45	2.78	596.84	871.92	408.43	8.50	404.73	821.66	2.3898
22	β -Gal-gg_His_H4	3.98	270.88	0.14	2.75	595.36	869.13	408.34	7.05	404.49	819.88	2.4177
23	β -Gal-gg_His_H5	4.23	271.46	0.08	2.86	597.88	872.28	408.56	8.89	405.02	822.47	2.3386
24	β -Gal-gg_His_H6	4.72	268.33	0.18	2.23	597.10	867.84	408.99	5.80	402.70	817.49	2.5151
25	β -Gal-gt_His_H1	3.40	261.42	0.90	3.72	600.27	866.31	407.07	8.49	401.83	817.39	2.3763

Table S29. Relative energy (in water), sum of NBO interactions and distance between Gal and His calculated at the M06-2X/6-31++G(d,p) level

entry	Complex	ΔE / (kcal mol ⁻¹)	NBO / (kcal mol ⁻¹)					Steric / (kcal mol ⁻¹)				Distance / Å
			1	1→2	2→1	2	Total	1	1→2	2	Total	
26	β -Gal-gt_His_H2	3.95	259.86	1.78	3.00	598.36	863.00	407.01	8.61	401.95	817.57	2.3873
27	β -Gal-gt_His_H3	3.80	260.41	0.88	2.87	596.51	860.67	407.51	8.23	403.19	818.93	2.3615
28	β -Gal-gt_His_H4	4.01	260.35	0.08	2.68	595.18	858.29	406.54	6.95	401.97	815.46	2.4395
29	β -Gal-gt_His_H5	3.41	260.27	2.53	2.85	595.09	860.74	408.13	10.96	404.20	823.29	2.4754
30	β -Gal-gt_His_H6	4.87	260.73	0.33	1.50	593.22	855.78	406.86	5.62	402.74	815.22	2.4891
31	β -Gal-tg_His_H1	4.31	258.46	0.66	7.36	599.87	866.35	405.24	11.33	411.29	827.86	2.3631
32	β -Gal-tg_His_H2	4.05	259.22	1.41	2.92	595.49	859.04	406.06	10.32	404.21	820.59	2.3466
33	β -Gal-tg_His_H3	0.63	262.25	2.14	40.38	596.07	900.84	408.58	26.17	404.13	838.88	2.5867
34	β -Gal-tg_His_H4	4.58	255.16	13.10	1.10	599.55	868.91	404.25	10.86	399.33	814.44	3.0901
35	β -Gal-tg_His_H5	4.20	258.11	1.22	3.50	602.08	864.91	405.87	9.36	409.94	825.17	2.4439
36	β -Gal-tg_His_H6	5.72	257.85	0.15	1.47	594.55	854.02	405.27	5.68	404.13	815.08	2.5565

1: carbohydrate; 2: amino acid; Distance: distance between the nearest hydrogen to the center of the aromatic ring.

Table S30. Energy decomposition analyse for the complex between Gal and His through SAPT0/6-31++G(d,p)

entry	Complex	Energy / (kcal mol ⁻¹)				
		Electrostatic	Exchange	Induction	Dispersion	Total
1	α -Gal-gg_His_H1	-7.77227214	9.02718339	-2.36336803	-8.34399038	-9.45244717
2	α -Gal-gg_His_H2	-8.39411850	9.52136985	-2.05060909	-9.26570940	-10.18906714
3	α -Gal-gg_His_H3	-0.85754487	8.65571064	-1.29019934	-8.10661003	-1.59864361
4	α -Gal-gg_His_H4	-0.89121513	7.87738347	-1.15746033	-7.17718025	-1.34847223
5	α -Gal-gg_His_H5	-2.27929815	10.04534478	-1.52459394	-9.56422950	-3.32277682
6	α -Gal-gg_His_H6	-2.58894716	8.10449003	-1.13334715	-7.53821770	-3.15602198
7	α -Gal-gt_His_H1	-23.63907706	25.47724539	-8.27373851	-11.60030223	-18.03587241
8	α -Gal-gt_His_H2	-17.20464182	22.02775073	-6.49558240	-12.80056646	-14.47303996
9	α -Gal-gt_His_H3	-2.60719446	8.44575776	-1.17361958	-8.08680617	-3.42186246
10	α -Gal-gt_His_H4	-5.76347355	9.04042784	-1.27430761	-7.82833908	-5.82569240
11	α -Gal-gt_His_H5	-4.24947364	9.09719290	-1.29948100	-8.68231462	-5.13407635
12	α -Gal-gt_His_H6	-17.09645315	22.63075252	-7.39900824	-10.04929525	-11.91400411
13	α -Gal-tg_His_H1	-6.18146410	8.48427324	-1.69544228	-7.85029240	-7.24292554
14	α -Gal-tg_His_H2	-7.38960662	9.33605252	-1.72298716	-8.98166510	-8.75820637
15	α -Gal-tg_His_H3	-1.03562526	8.72015418	-1.28326098	-8.08449557	-1.68322763
16	α -Gal-tg_His_H4	-5.02118996	9.08521177	-1.24227656	-8.20246865	-5.38072340
17	α -Gal-tg_His_H5	-5.76499248	9.80226830	-1.72373564	-9.71483166	-7.40129149
18	α -Gal-tg_His_H6	-4.14312044	5.50679019	-0.91638488	-4.84631576	-4.39903090
19	β -Gal-gg_His_H1	-1.56484507	11.71279065	-2.23224080	-9.44416971	-1.52846493
20	β -Gal-gg_His_H2	-15.98215180	18.79284805	-5.59438918	-9.55000767	-12.33370059
21	β -Gal-gg_His_H3	-1.23598972	8.56625377	-1.29220754	-7.97115819	-1.93310169
22	β -Gal-gg_His_H4	-0.47573661	7.98489060	-1.20323869	-7.14127625	-0.83536095
23	β -Gal-gg_His_H5	-0.96423347	8.93298384	-1.26404428	-7.94235072	-1.23764463
24	β -Gal-gg_His_H6	-3.56710495	6.84066980	-0.94150869	-5.80605962	-3.47400348
25	β -Gal-gt_His_H1	-4.90632391	9.61030894	-1.55465170	-8.52804390	-5.37871058
26	β -Gal-gt_His_H2	-7.12824866	8.85573824	-1.54026155	-7.98747699	-7.80024896
27	β -Gal-gt_His_H3	-5.72484226	8.70565122	-1.28725008	-8.15560792	-6.46204904
28	β -Gal-gt_His_H4	-2.32162129	7.58061133	-1.17080283	-7.02640290	-2.93821570
29	β -Gal-gt_His_H5	-4.58674616	10.55115874	-1.92780460	-9.01939784	-4.98278985
30	β -Gal-gt_His_H6	-0.82376727	5.74535447	-0.79814210	-5.29506378	-1.17161869
31	β -Gal-tg_His_H1	-2.62903715	12.31182191	-2.32193945	-9.97240269	-2.61155738
32	β -Gal-tg_His_H2	-9.37867073	10.70809470	-2.00687834	-9.37374020	-10.05119458
33	β -Gal-tg_His_H3	-23.99552369	28.32559369	-9.67003029	-12.10331389	-17.44327418
34	β -Gal-tg_His_H4	-10.28601166	11.85493635	-3.38177369	-6.61817532	-8.43102431
35	β -Gal-tg_His_H5	-7.51089936	10.41647662	-1.84769795	-9.71555282	-8.65767352
36	β -Gal-tg_His_H6	-3.67989236	5.32003470	-0.69216091	-5.12002623	-4.17204479

Complementary figures

RGD Glc-Trp

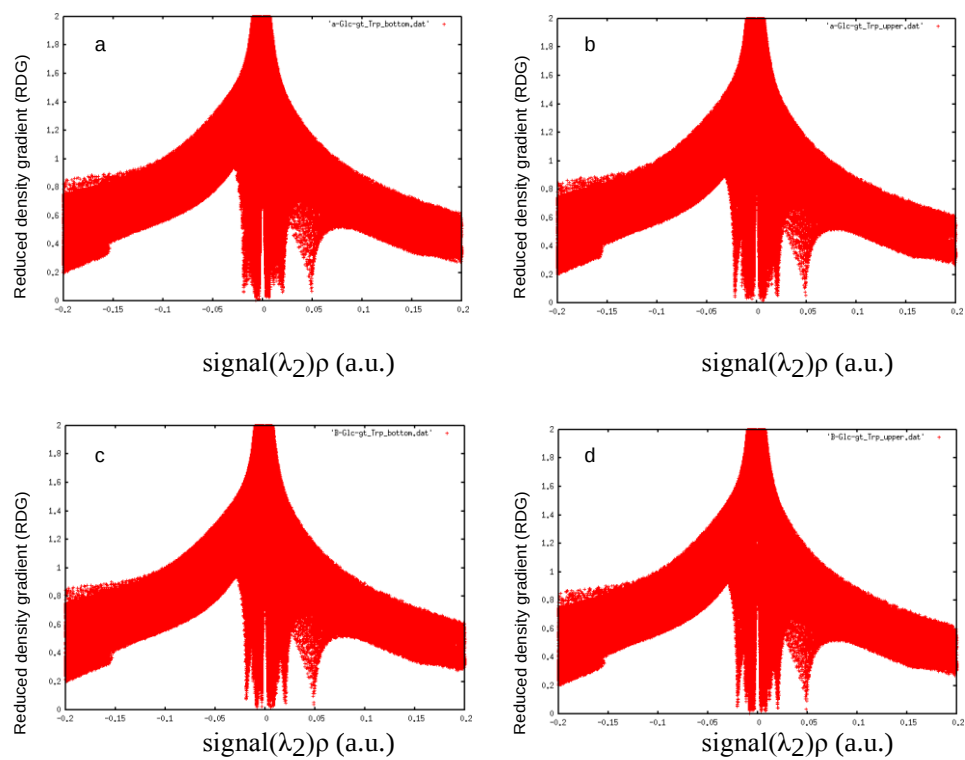


Figure S7. Plot of the reduced density gradient versus the electron density multiplied by the sign of $(\lambda_2)\rho$ for complexes (a) α -Glc-gt_Trp_bottom; (b) α -Glc-gt_Trp_upper; (c) β -Glc-gt_Trp_bottom and (d) β -Glc-gt_Trp_upper.

Glc-Phe

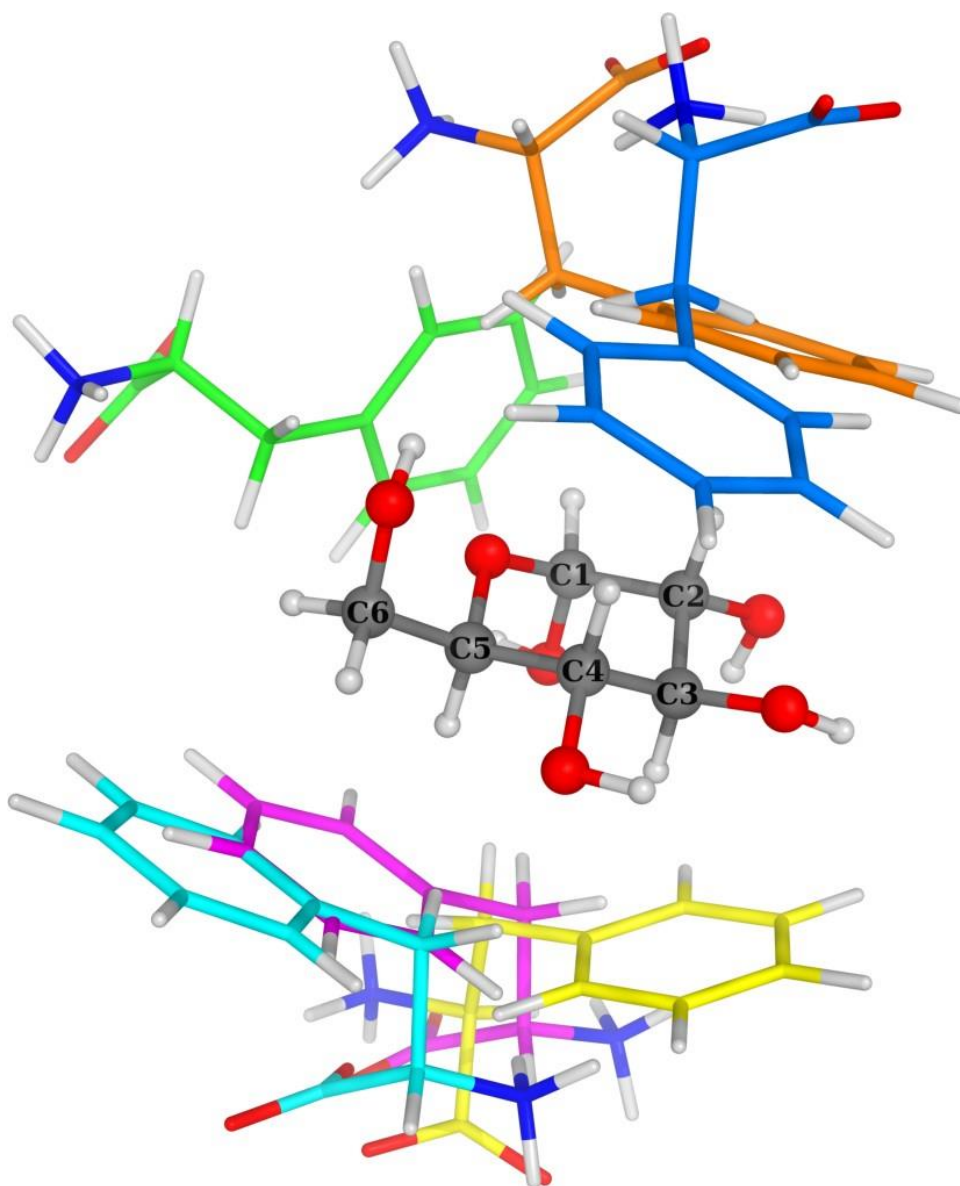


Figure S8. Superposition of all complexes of α -Glc *gauche-gauche* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

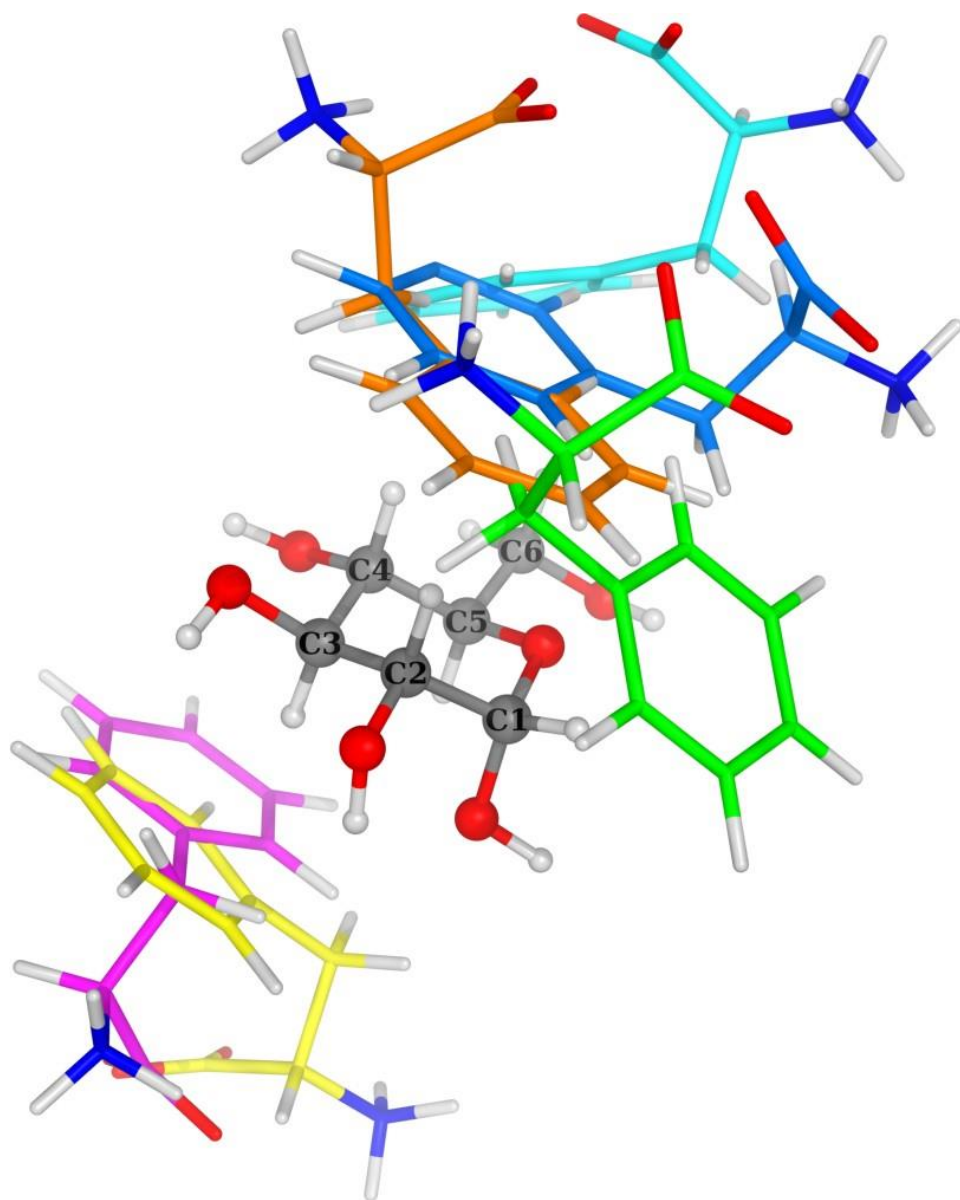


Figure S9. Superposition of all complexes of α -Glc *gauche-trans* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

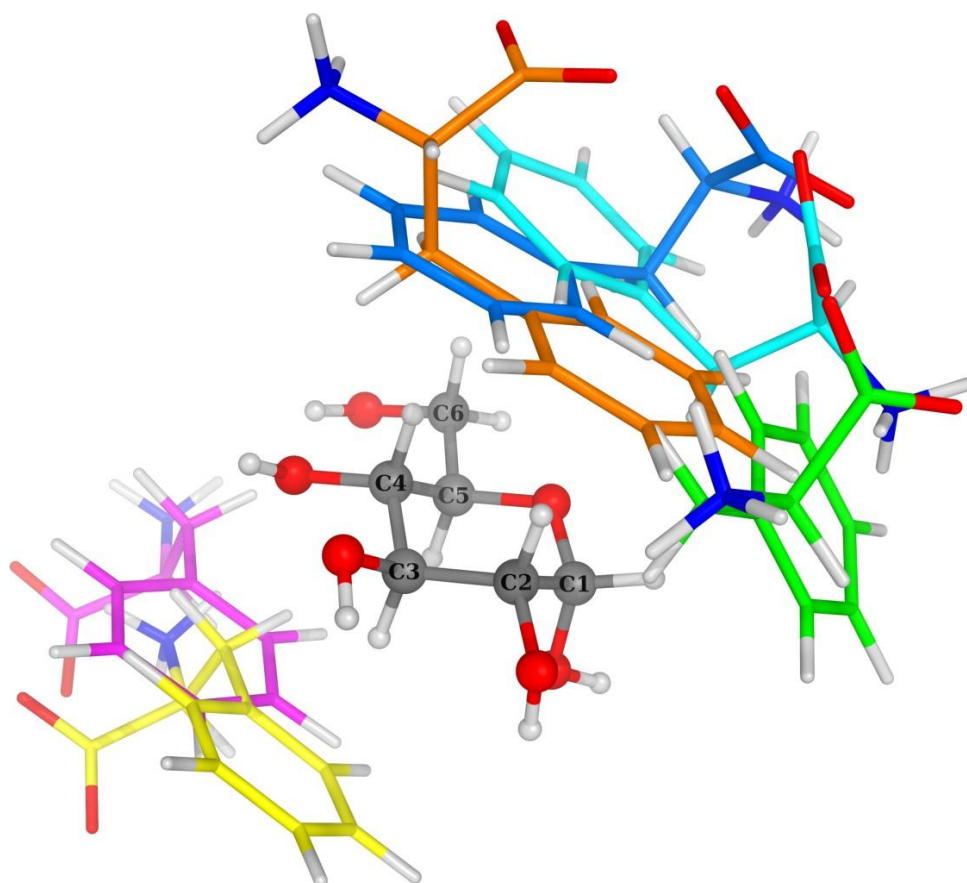


Figure S10. Superposition of all complexes of α -Glc *trans-gauche* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

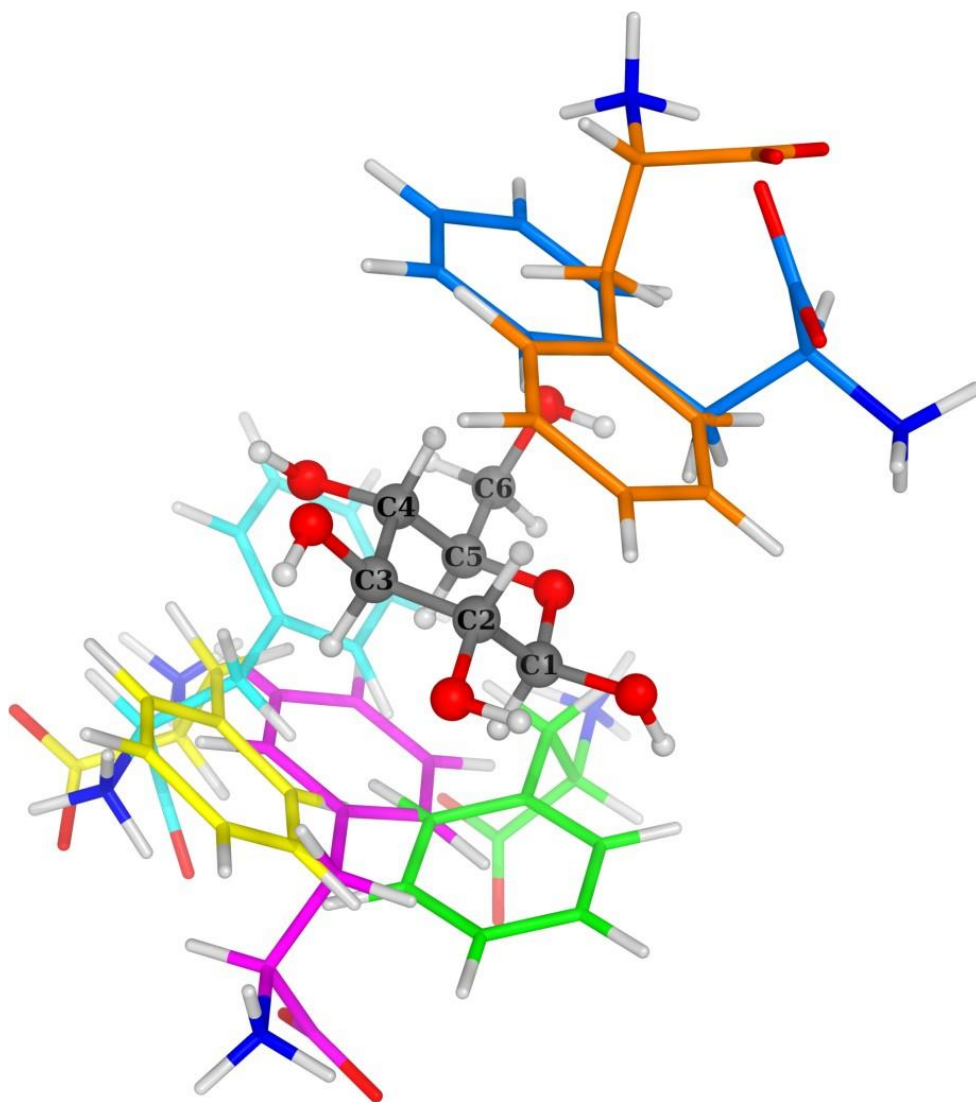
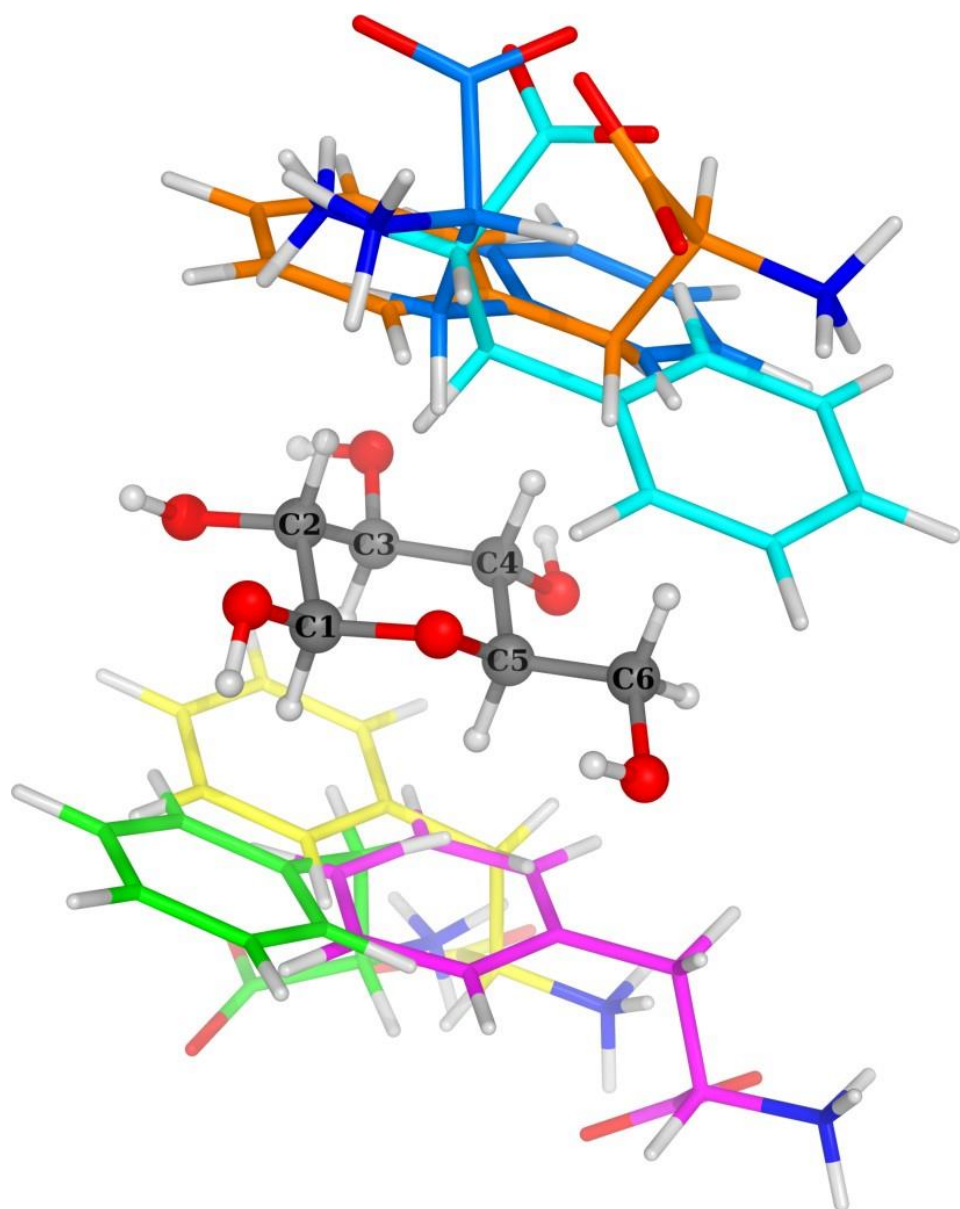
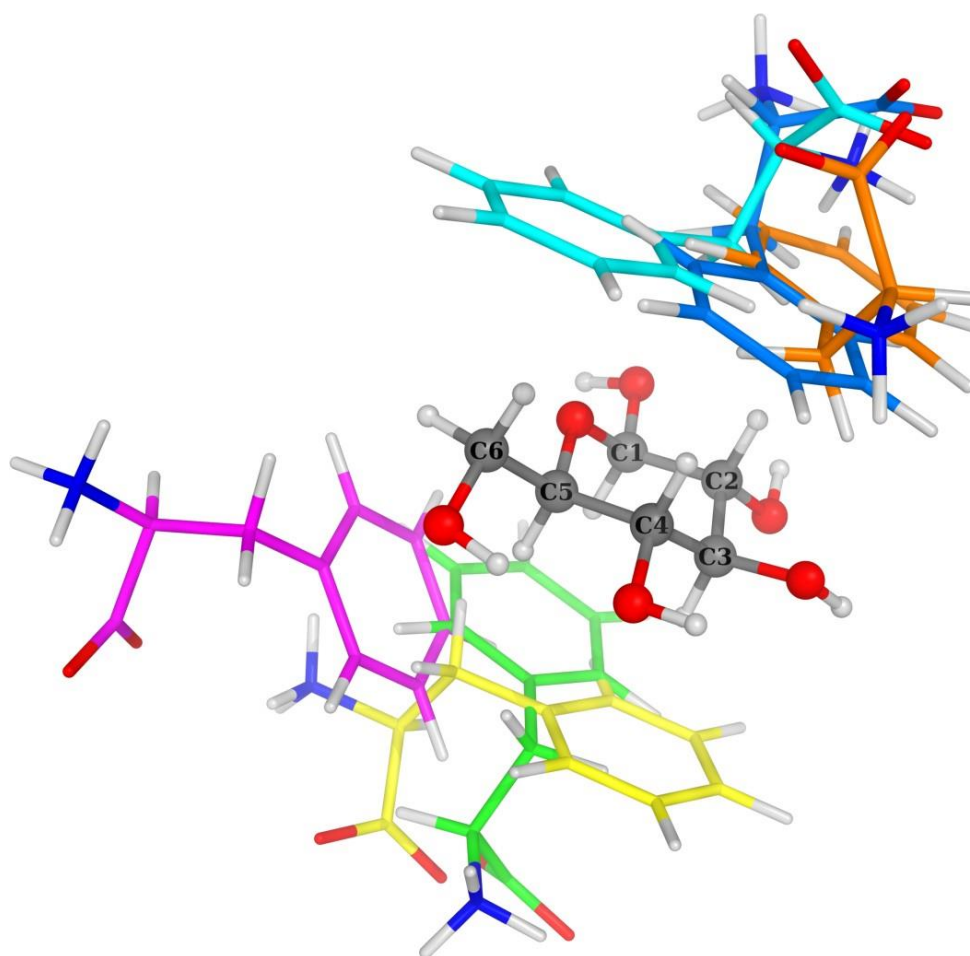


Figure S11. Superposition of all complexes of β -Glc *gauche-gauche* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).



FigureS12. Superposition of all complexes of β -Glc *gauche-trans* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).



FigureS13. Superposition of all complexes of β -Glc *trans-gauche* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

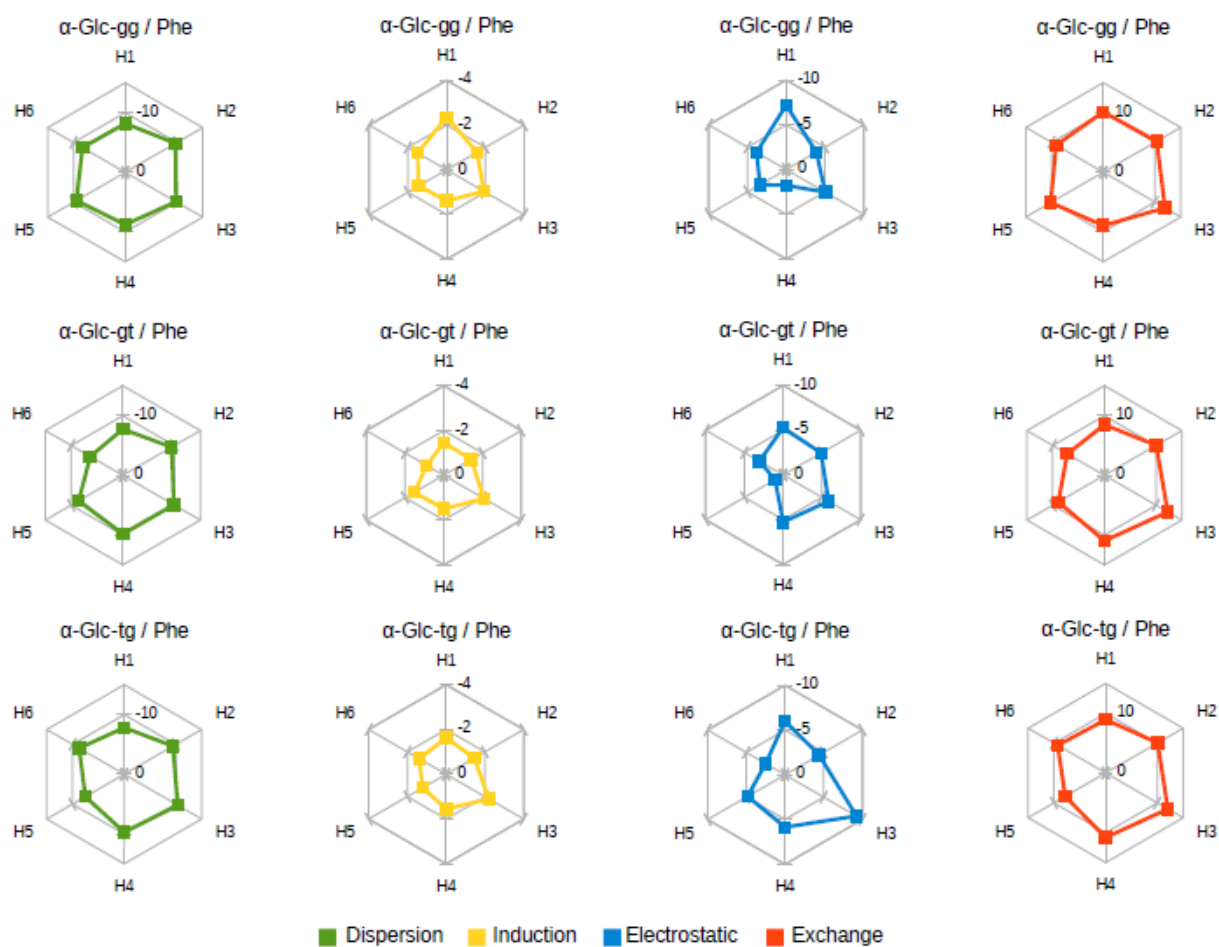


Figure S14. Energy decomposition analysis (kcal mol⁻¹) for the complexes between α -Glc and Phe through SAPT0/6-31++G(d,p) calculation.

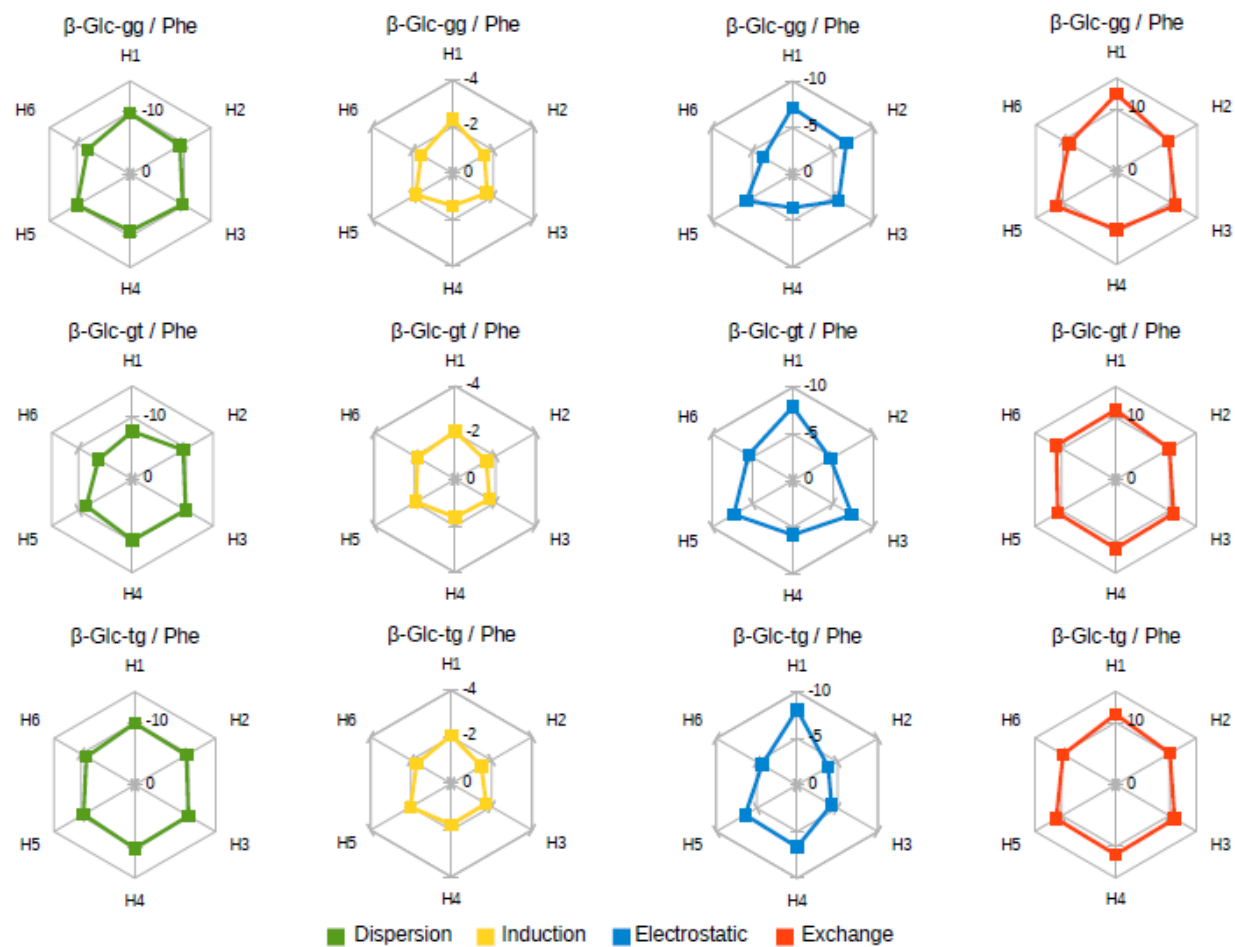


Figure S15. Energy decomposition analysis (kcal mol⁻¹) for the complexes between β -Glc and Phe through SAPT0/6-31++G(d,p) calculation.

Glc-His

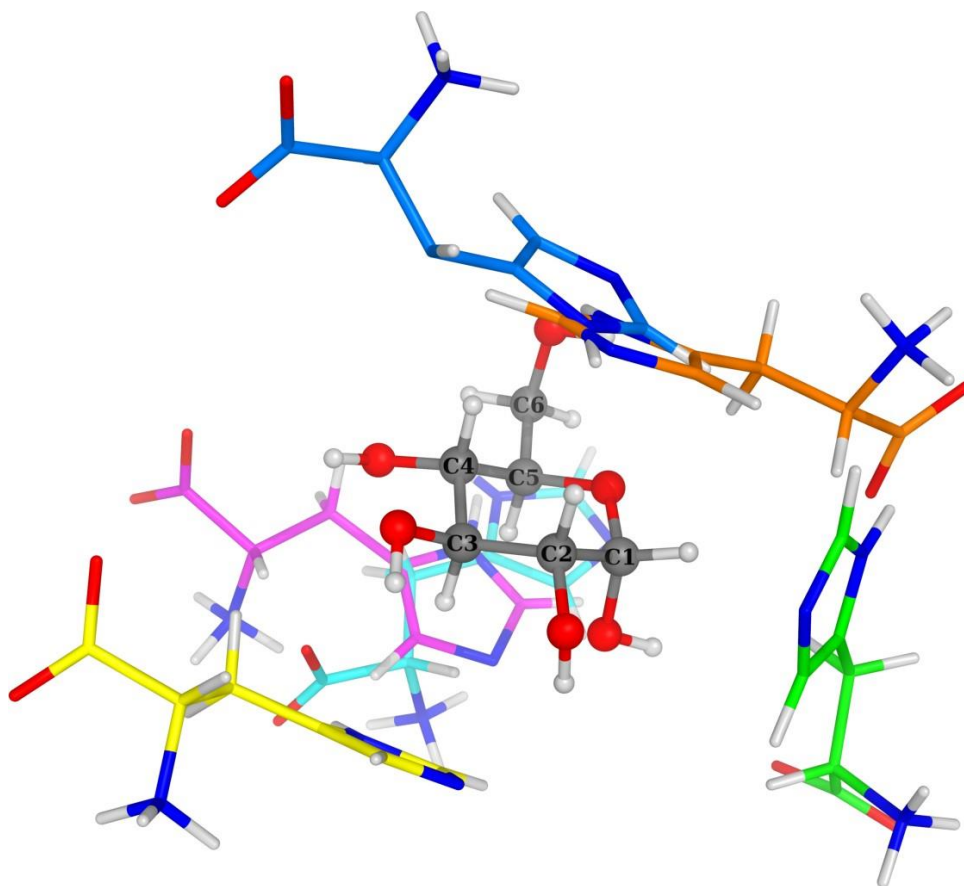


Figure S16. Superposition of all complexes of α -Glc *gauche-gauche* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

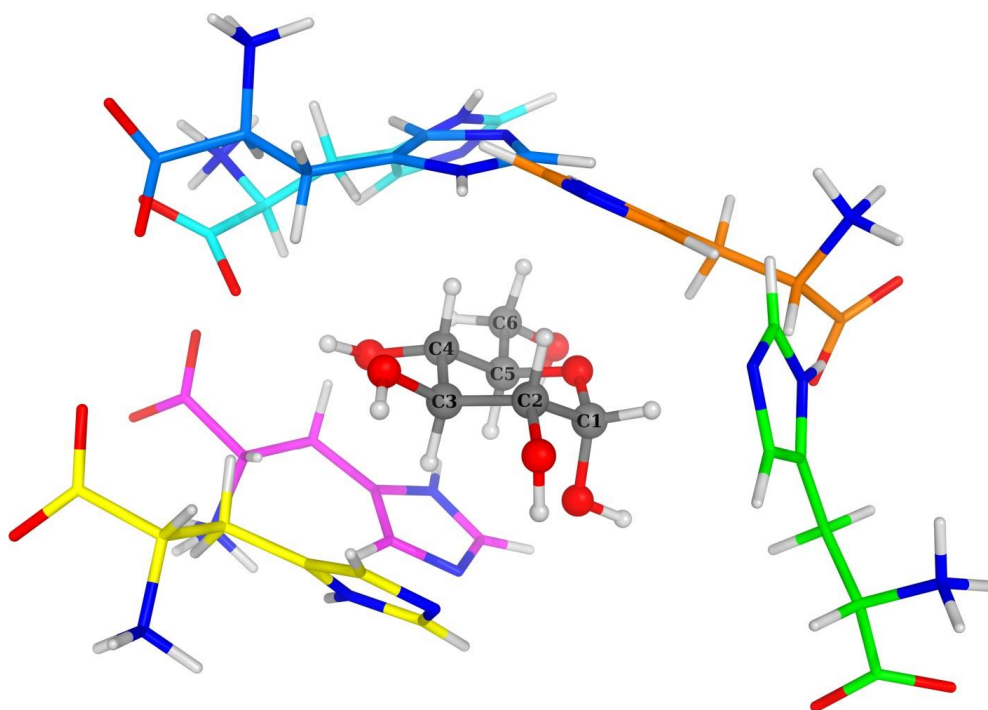


Figure S17. Superposition of all complexes of α -Glc *gauche-trans* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

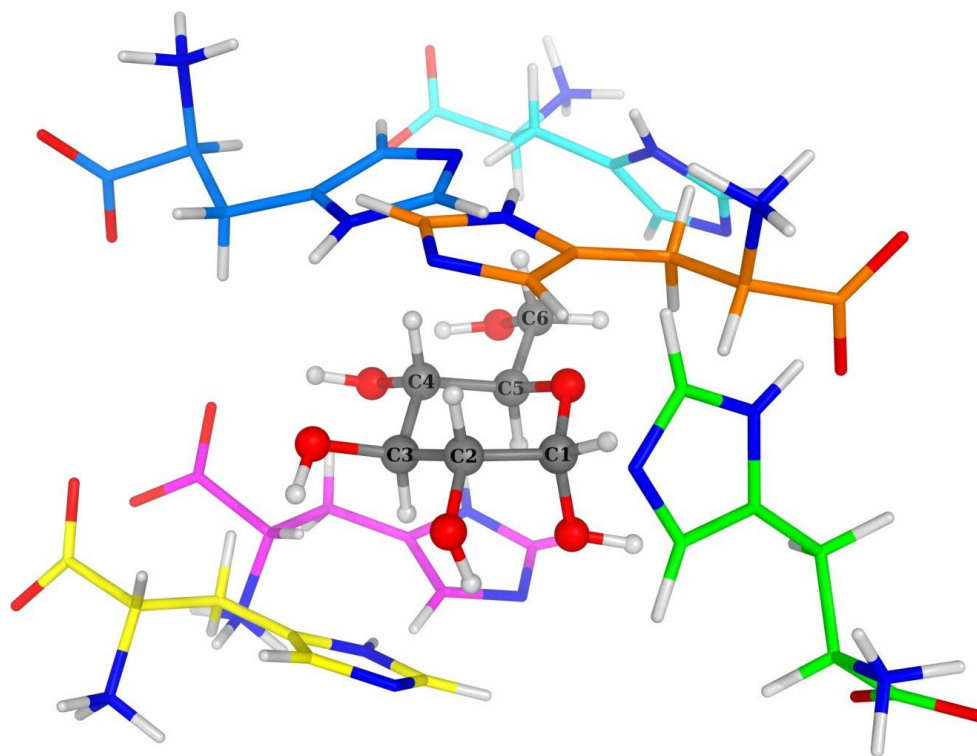


Figure S18. Superposition of all complexes of α -Glc *trans-gauche* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

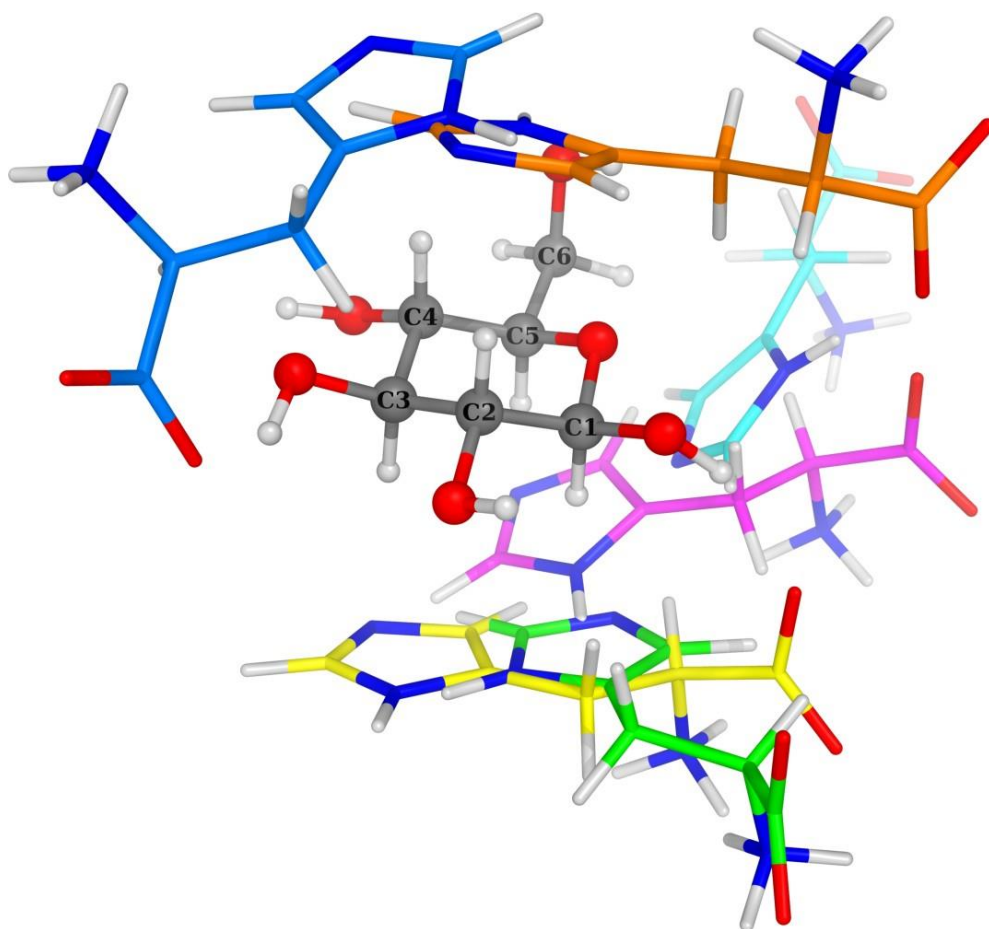
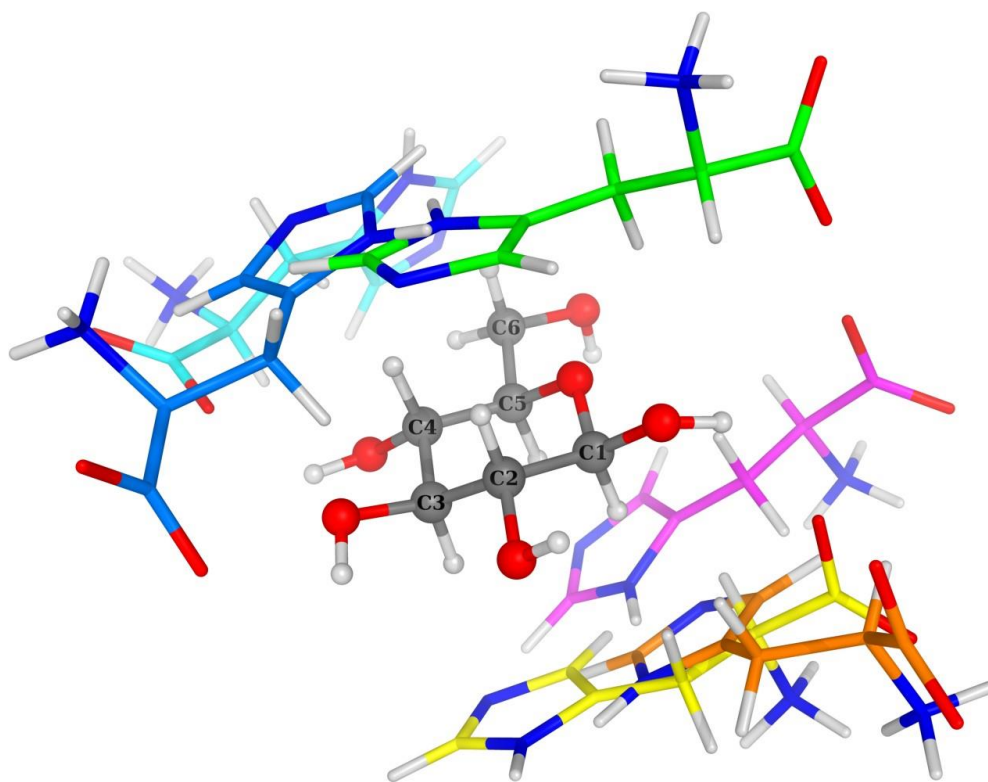
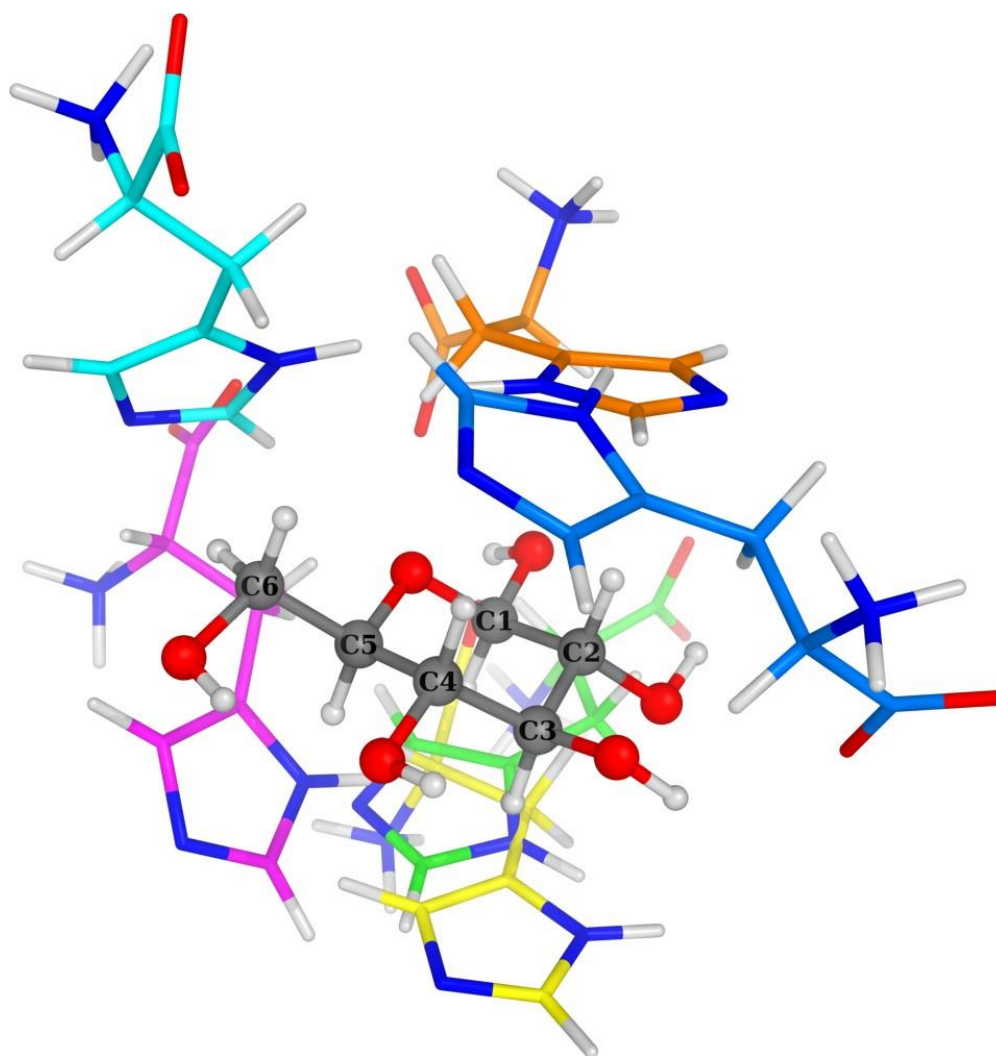


Figure S19. Superposition of all complexes of β -Glc *gauche-gauche* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).



FigureS20. Superposition of all complexes of β -Glc *gauche-trans* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).



FigureS21. Superposition of all complexes of β -Glc *trans-gauche* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

RGD Gal-Trp

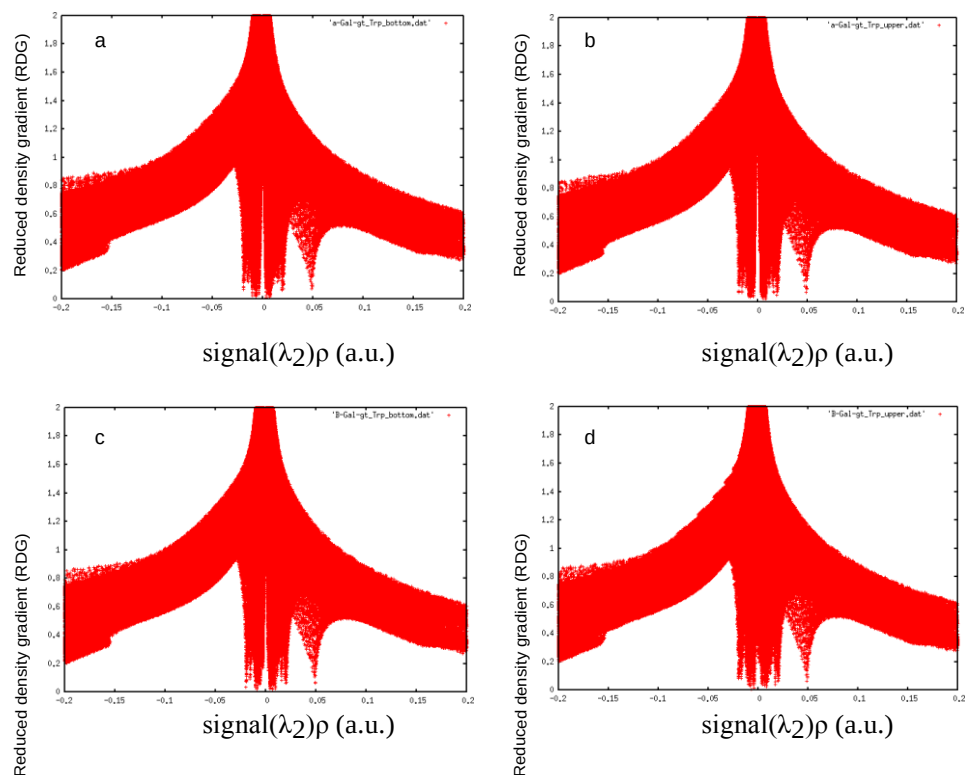


Figure S22. Plot of the reduced density gradient *versus* the electron density multiplied by the sign of $(\lambda_2)\rho$ for complexes (a) α -Gal-gt_Trp_bottom; (b) α -Gal-gt_Trp_upper; (c) β -Gal-gt_Trp_bottom and (d) β -Gal-gt_Trp_upper.

Gal-Phe

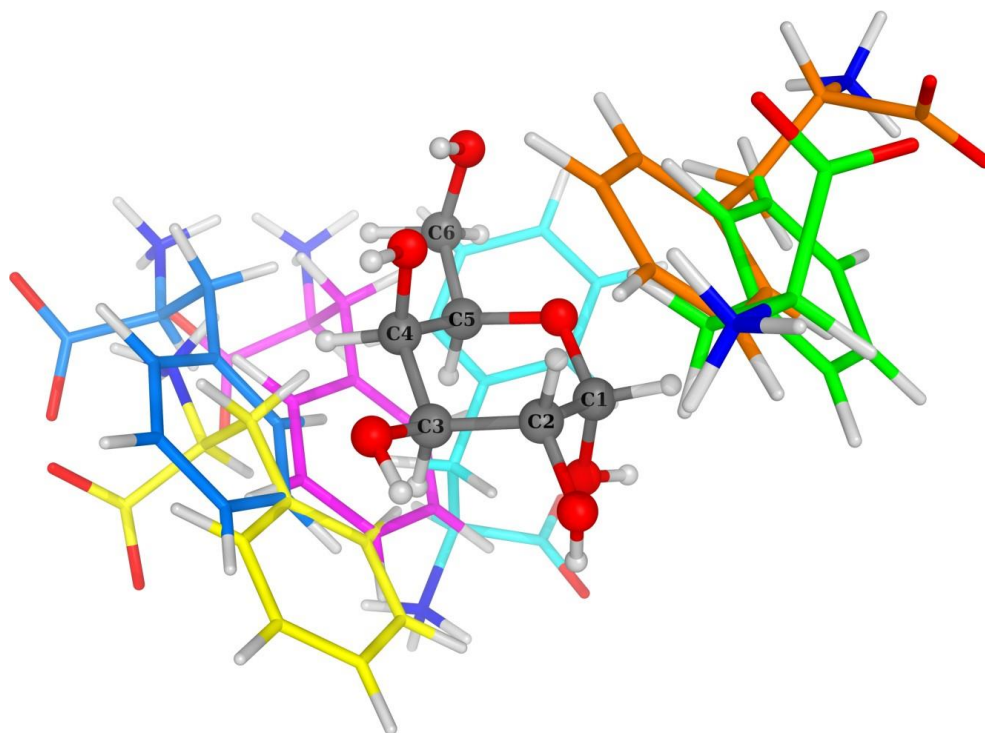


Figure S23. Superposition of all complexes of α -Gal *gauche-gauche* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

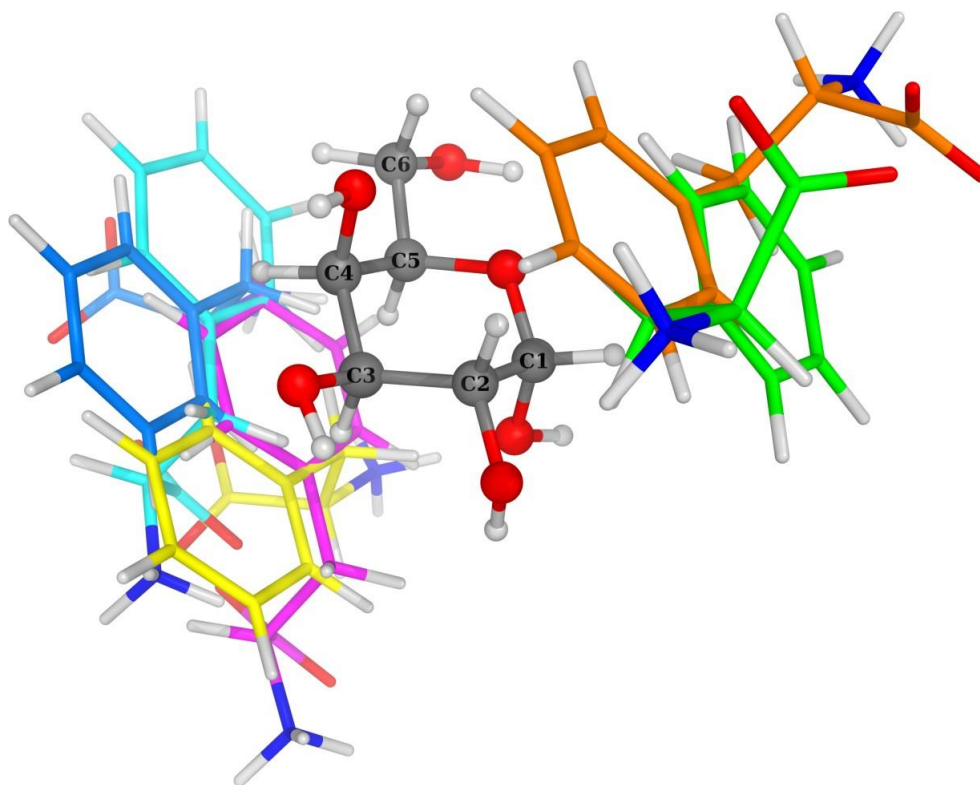


Figure S24. Superposition of all complexes of α -Gal *gauche-trans* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

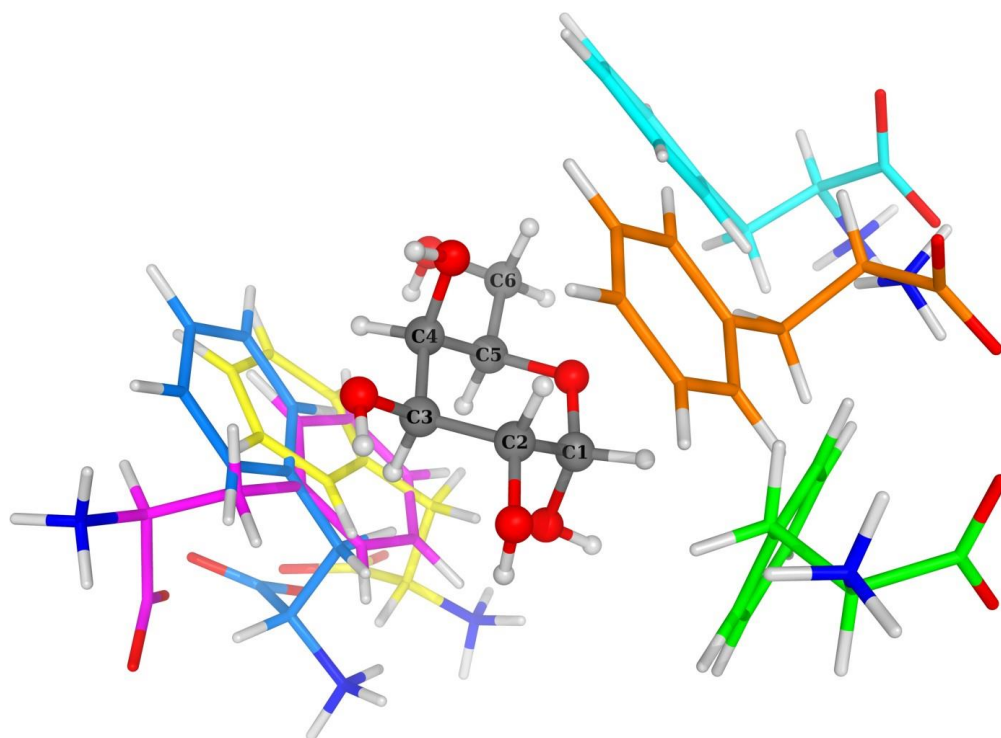


Figure S25. Superposition of all complexes of α -Gal *trans-gauche* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

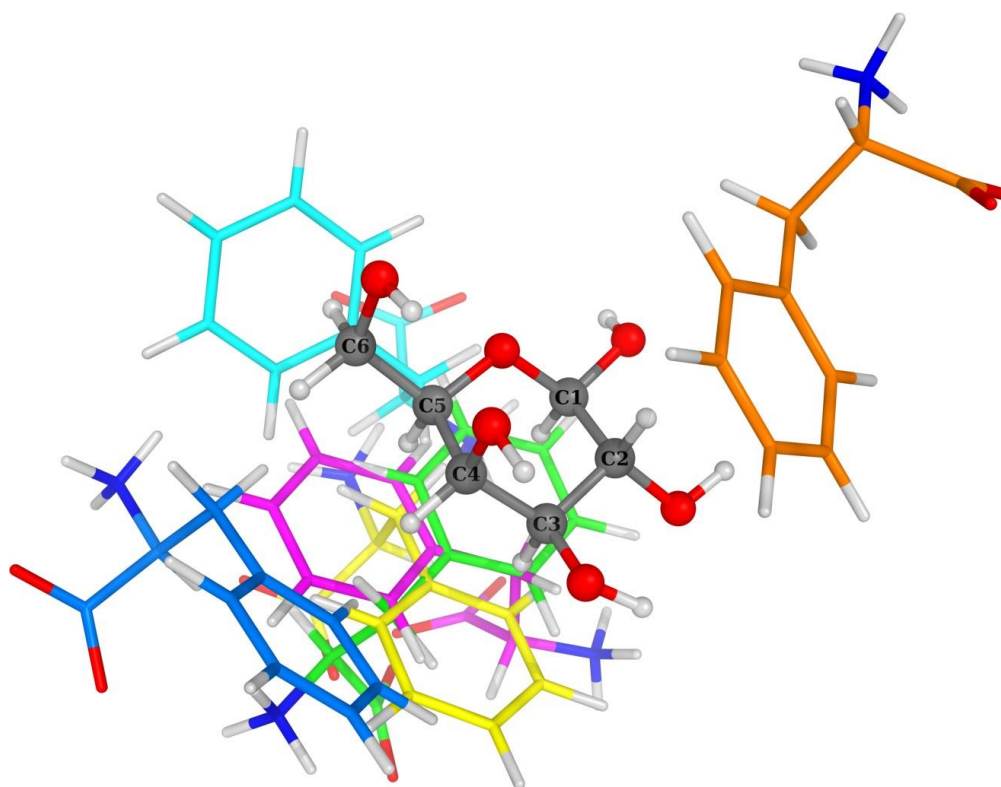


Figure S26. Superposition of all complexes of β -Gal *gauche-gauche* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

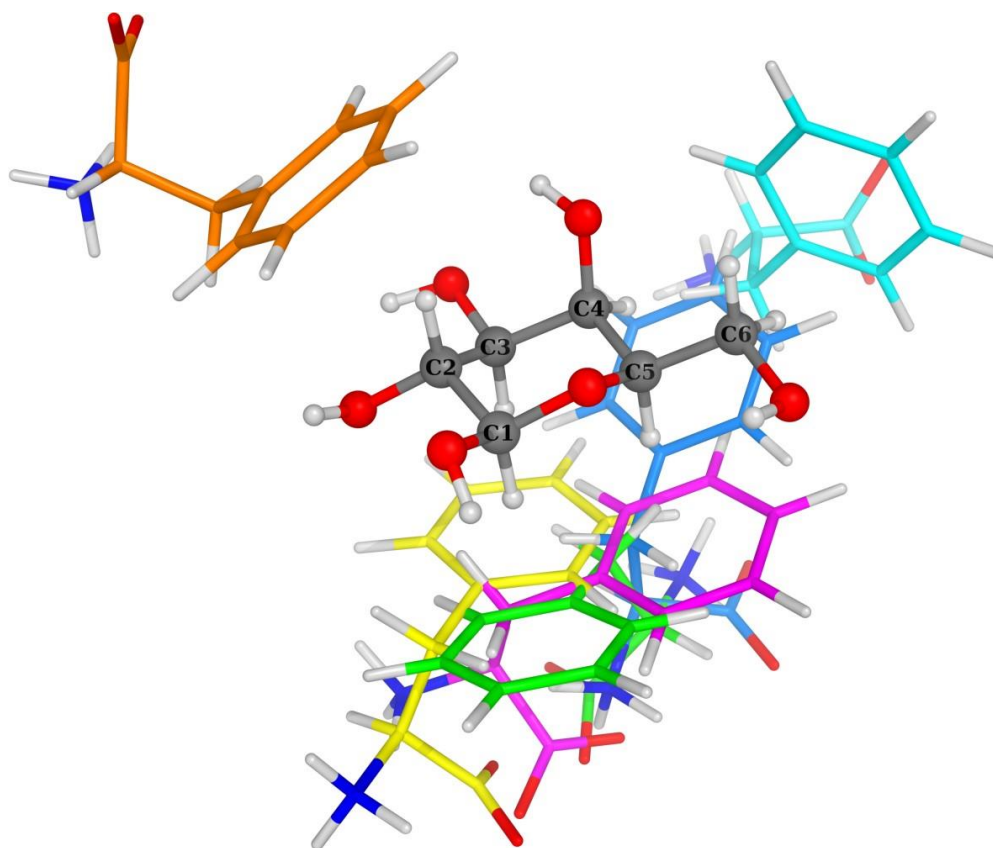


Figure S27. Superposition of all complexes of β -Gal *gauche-trans* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

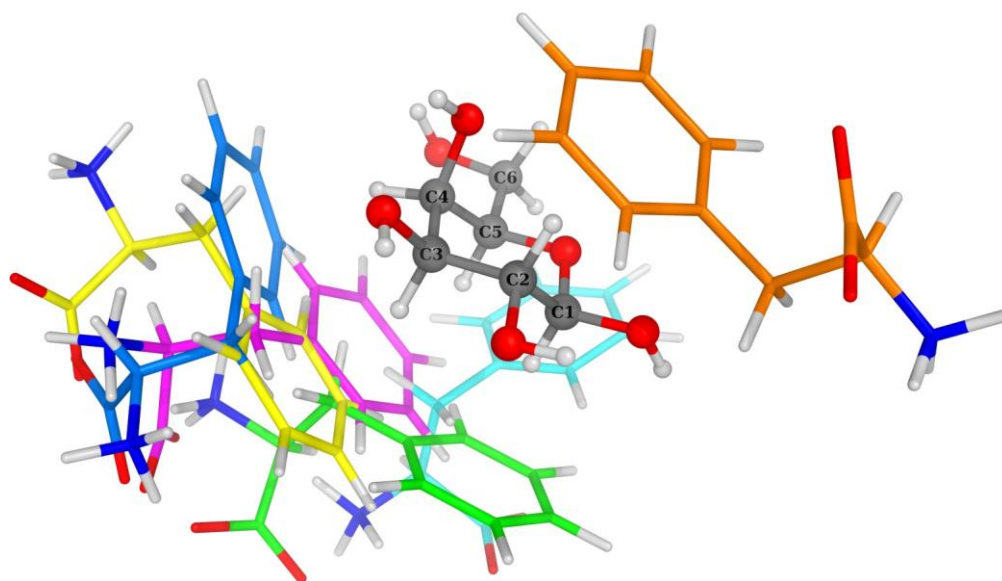


Figure S28. Superposition of all complexes of β -Gal *trans-gauche* (gray structure) with Phe (green for Phe_H1, orange for Phe_H2, yellow for Phe_H3, marine for Phe_H4, magenta for Phe_H5 and cyan for Phe_H6).

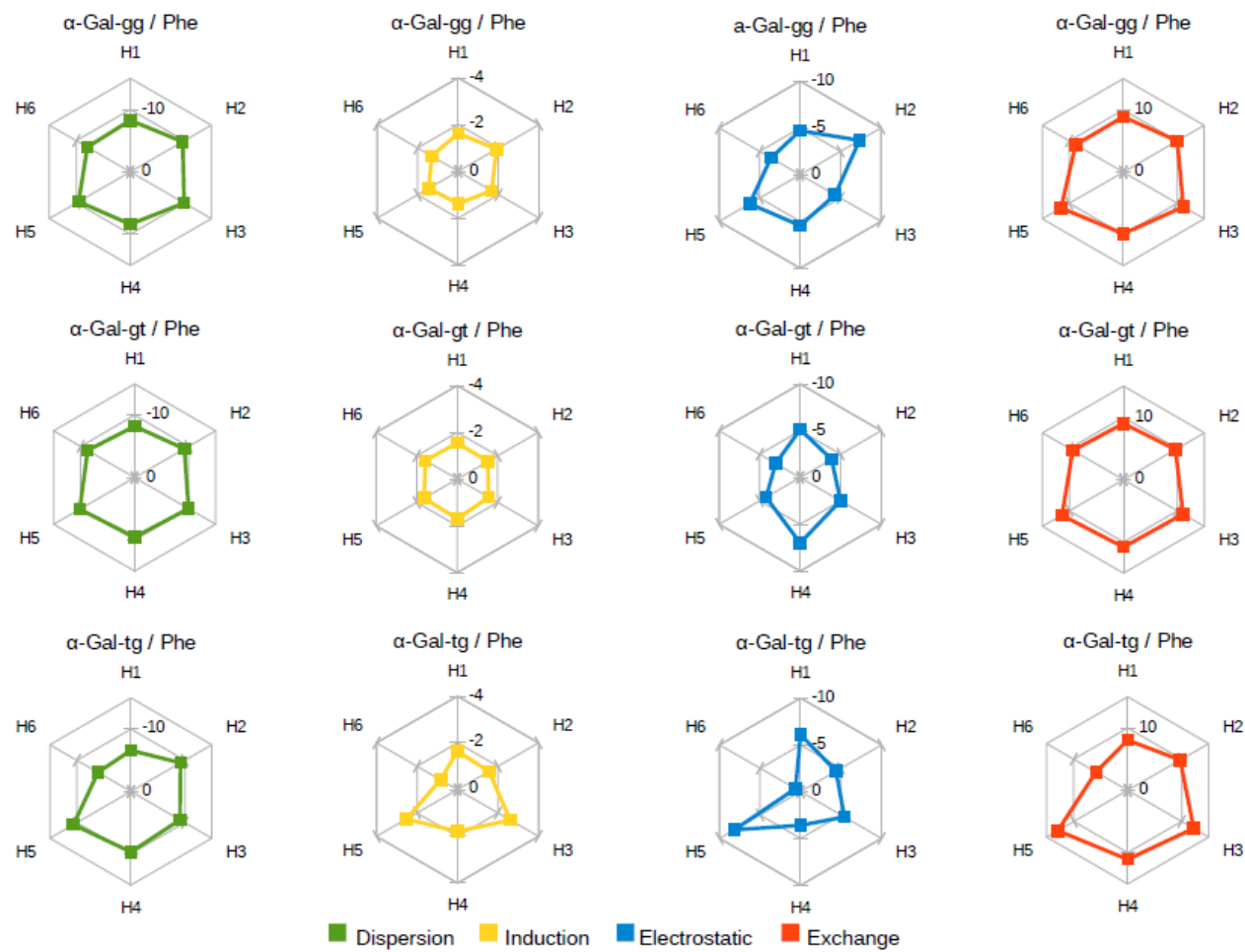


Figure S29. Energy decomposition analysis (kcal mol⁻¹) for the complexes between α -Gal and Phe through SAPT0/6-31++G(d,p) calculation.

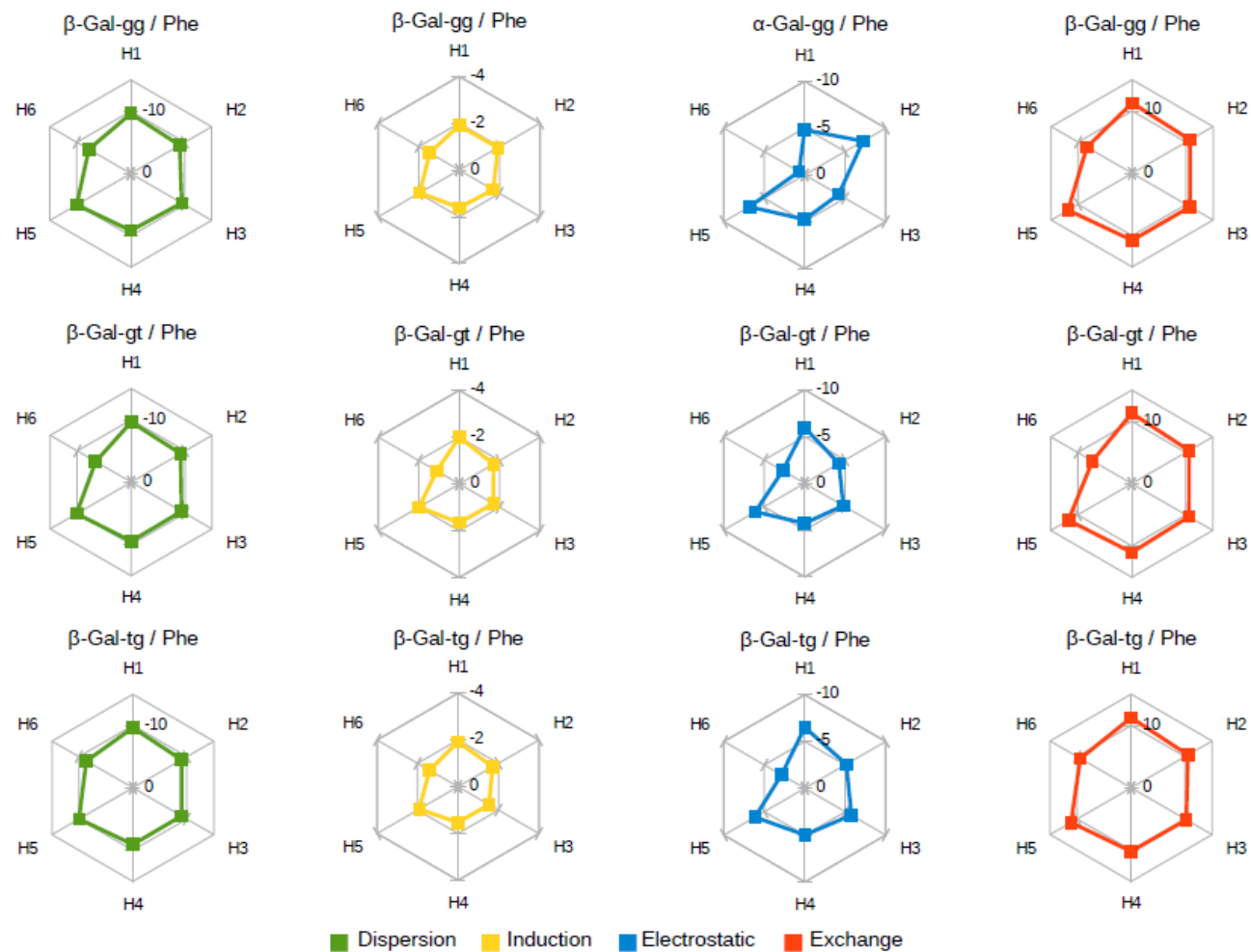


Figure S30. Energy decomposition analysis (kcal mol⁻¹) for the complexes between β -Gal and Phe through SAPT0/6-31++G(d,p) calculation.

Gal-His

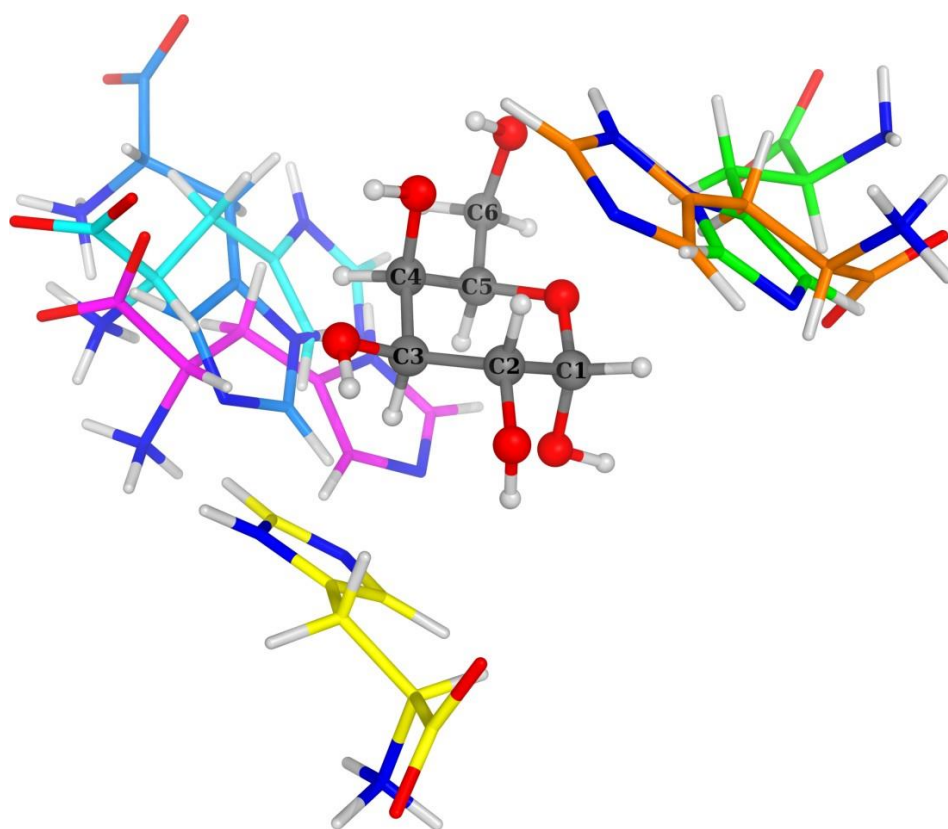


Figure S31. Superposition of all complexes of α -Gal *gauche-gauche* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

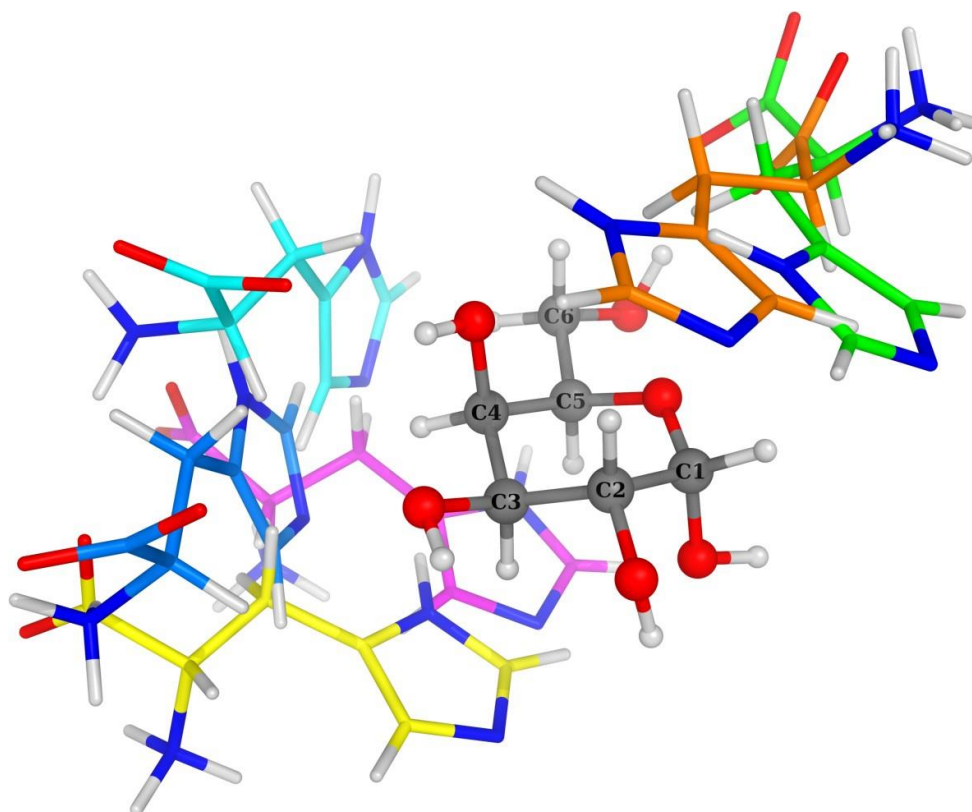


Figure S32. Superposition of all complexes of α -Gal *gauche-trans* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

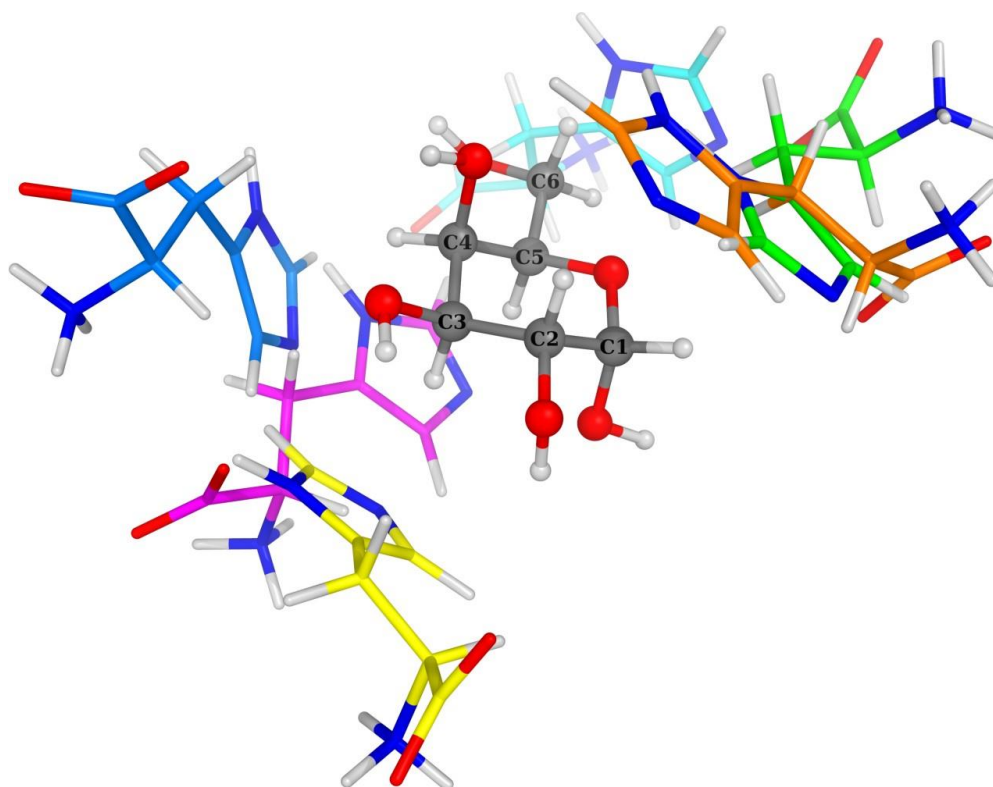


Figure S33. Superposition of all complexes of α -Gal *trans-gauche* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

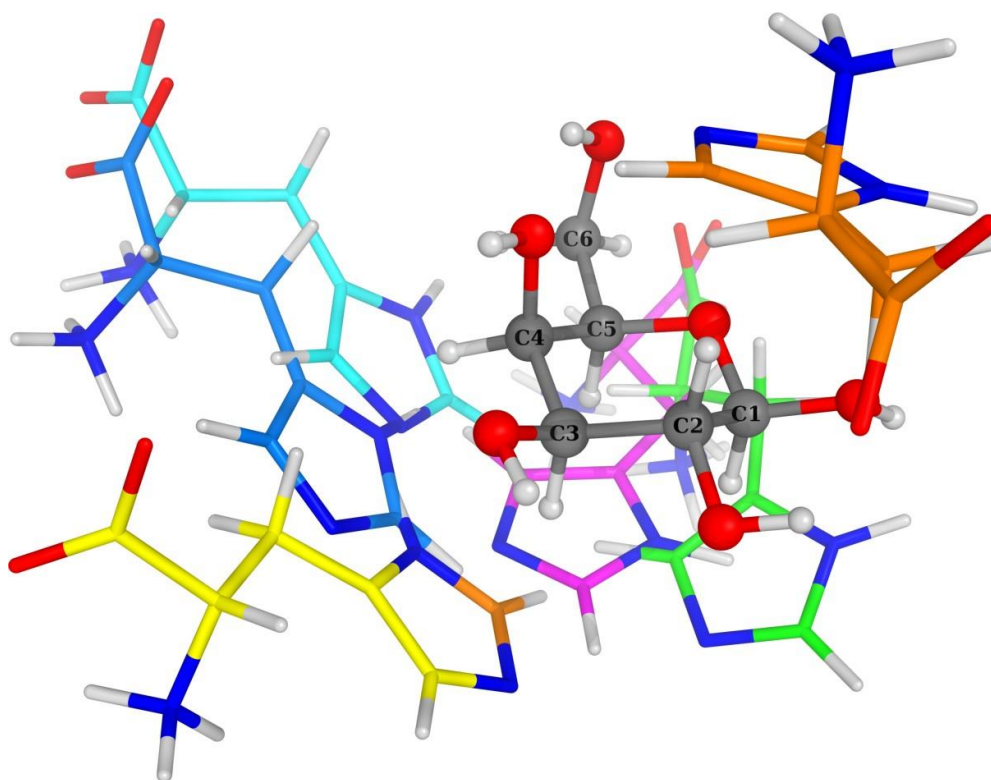


Figure S34. Superposition of all complexes of β -Gal *gauche-gauche* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

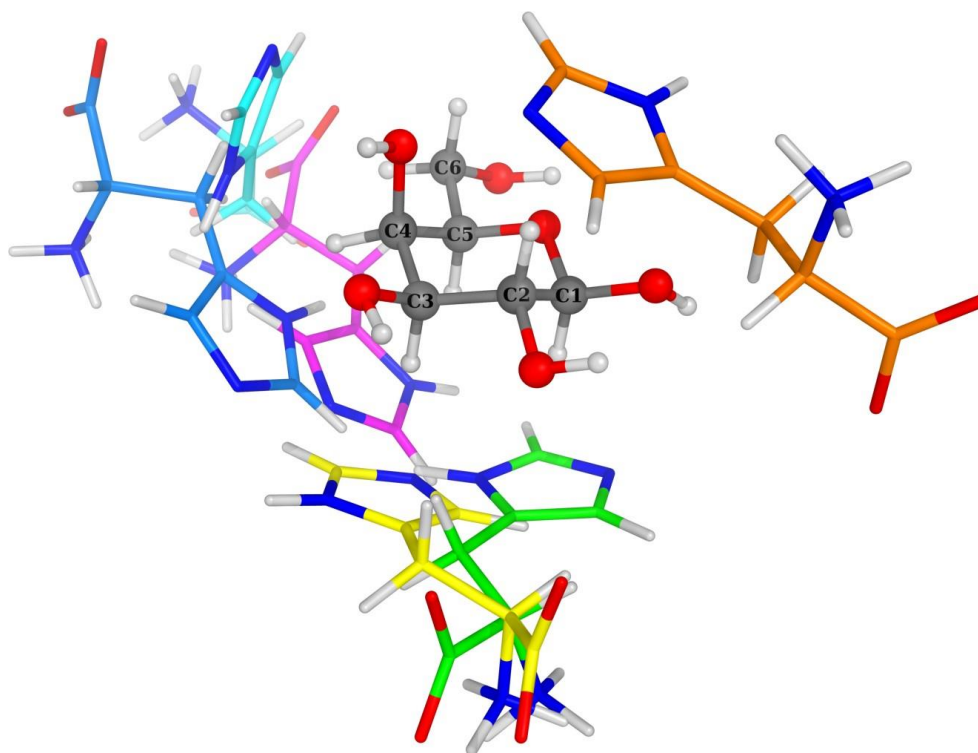


Figure S35. Superposition of all complexes of β -Gal *gauche-trans* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

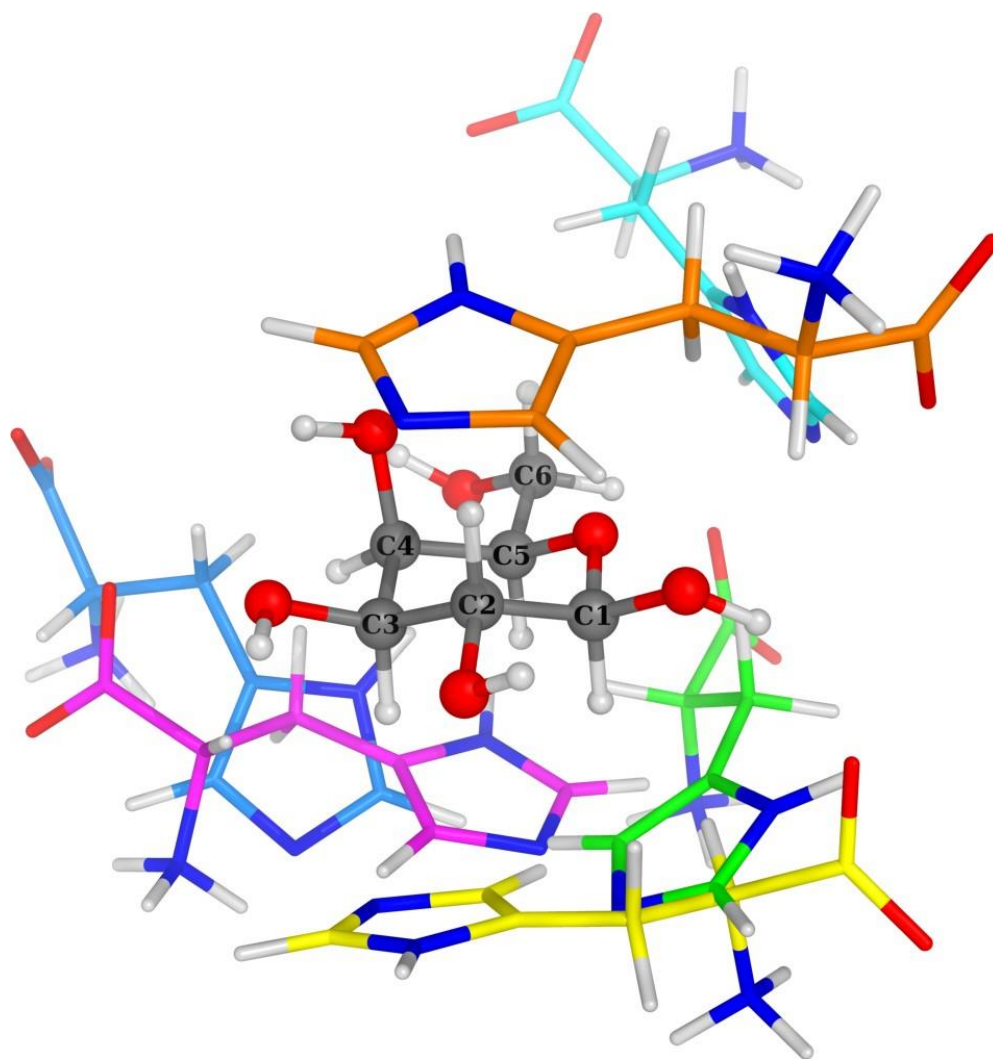


Figure S36. Superposition of all complexes of β -Gal *trans-gauche* (gray structure) with His (green for His_H1, orange for His_H2, yellow for His_H3, marine for His_H4, magenta for His_H5 and cyan for His_H6).

Effect of the intermolecular distance between carbohydrate and amino acid on the EDA

In order to obtain more insight at the recognition process involving the aromatic ring of amino acids and monosaccharides, EDA analysis of the complexes with different distances between the carbohydrates Glc and Gal and the amino acid Trp were performed. From the minimum energy structure (structure 0) of each complex the intermolecular distance was increased in five steps of 0.5 Å (structures 1-5) and decreased in two steps of 0.5 Å (structures -1 and -2). All the structures of these complexes can be seen at the supplementary material in video format that also shows the NCI surfaces for each step. Figure S37 presents the decomposition analyses for the complex α -Glc-gt_Trp_bottom and Table S31 presents the energy values for all complexes.

As the distance between the molecules decreased, the exchange component presented the greatest energy variations. This component has a destabilizing character and increases exponentially with the decrease in the intermolecular distance. With the exception of the structure in which the two molecules are closer (structure -2), the dispersion component was the one with the highest stabilizing energy, followed by the electrostatic component. The energy values of the induction component were the smallest ones. The electrostatic component overcomes the dispersion component only at structures in step -2. At larger distances in the complexes with Glc, the electrostatic component presented a positive energy, that is, an energy of destabilizing character.

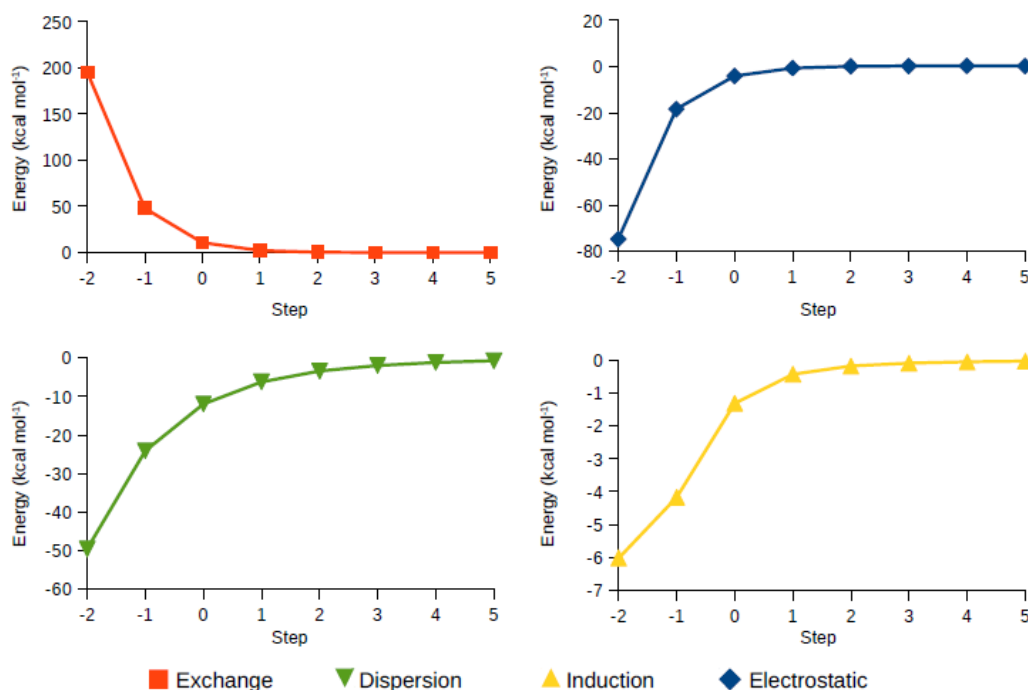


Figure S37. Energy decomposition analyses for the complex α -Glc-gt_Trp_bottom through SAPT0/6-31++G(d,p) with variation of the intermolecular distance.

In general, it was observed that the energy of the dispersion component is greater than that of the electrostatic one, being the main responsible for counterbalancing the exchange component from greater distance to the point of less energy. In the structure with the smallest intermolecular distance analyzed, the electrostatic component exceeds the dispersion component.

Table S31. Energy decomposition analyse for the complexes between Glc and Gal with Trp through SAPT0/6-31++G(d,p) with variation of the intermolecular distance

Complex	Component	Energy / (kcal mol ⁻¹)							
		Step							
		-2	-1	0	1	2	3	4	5
α -Glc-gt_Trp_bottom	electrostatic	-74.7302	-18.3628	-4.0351	-0.6155	0.1421	0.2953	0.3118	0.2968
	exchange	195.4384	48.0126	10.9146	2.3321	0.4673	0.0887	0.0170	0.0035
	induction	-6.0124	-4.1660	-1.3174	-0.4392	-0.1903	-0.1049	-0.0647	-0.0439
	dispersion	-49.6123	-24.1173	-11.9626	-6.2054	-3.3843	-1.9411	-1.1680	-0.7338
	total	65.0836	1.3665	-6.4005	-4.9279	-2.9652	-1.6619	-0.9039	-0.4774
β -Glc-gt_Trp_bottom	electrostatic	-86.0996	-23.3258	-6.1634	-1.5460	-0.2424	0.1905	0.3638	0.4408
	exchange	228.0513	59.3107	14.0640	3.1135	0.6490	0.1276	0.0239	0.0043
	induction	-2.2460	-5.3640	-2.0028	-0.6794	-0.2737	-0.1357	-0.0756	-0.0471
	dispersion	-53.9185	-26.5525	-13.1554	-6.7939	-3.6824	-2.0969	-1.2528	-0.7818
	total	85.7872	4.0683	-7.2576	-5.9059	-3.5495	-1.9146	-0.9407	-0.3839
α -Glc-gt_Trp_upper	electrostatic	-77.8299	-20.7731	-5.6124	-1.6625	-0.5766	-0.2153	-0.0626	0.0144
	exchange	206.6371	52.2490	12.0150	2.5910	0.5298	0.1032	0.0195	0.0036
	induction	-0.8276	-4.3656	-1.4545	-0.4284	-0.1539	-0.0720	-0.0396	-0.0252
	dispersion	-48.8516	-23.8730	-11.7420	-6.0496	-3.2785	-1.8701	-1.1202	-0.7011
	total	79.1280	3.2373	-6.7939	-5.5496	-3.4791	-2.0541	-1.2030	-0.7084
β -Glc-gt_Trp_upper	electrostatic	-75.6584	-19.3203	-4.6108	-1.0078	-0.1680	0.0398	0.1024	0.1287
	exchange	202.5947	52.4893	12.4037	2.7219	0.5606	0.1100	0.0211	0.0038
	induction	-3.9211	-4.4029	-1.4732	-0.4360	-0.1499	-0.0673	-0.0355	-0.0227
	dispersion	-51.9173	-25.4594	-12.6387	-6.5538	-3.5662	-2.0386	-1.2223	-0.7651
	total	71.0979	3.3067	-6.3190	-5.2756	-3.3235	-1.9561	-1.1343	-0.6553

Table S31. Energy decomposition analyse for the complexes between Glc and Gal with Trp through SAPT0/6-31++G(d,p) with variation of the intermolecular distance (cont.)

Complex	Component	Energy / (kcal mol ⁻¹)							
		Step							
		-2	-1	0	1	2	3	4	5
α -Gal-gt_Trp_bottom	electrostatic	-80.0398	-21.6854	-6.1895	-2.0736	-0.9010	-0.4963	-0.3141	-0.2120
	exchange	209.6462	53.3993	12.7482	2.9076	0.6357	0.1330	0.0269	0.0054
	induction	-1.5593	-4.4043	-1.5388	-0.4862	-0.1775	-0.0802	-0.0436	-0.0276
	dispersion	-47.6415	-23.8469	-12.0906	-6.3709	-3.5116	-2.0290	-1.2265	-0.7725
	total	80.4056	3.4627	-7.0708	-6.0231	-3.9545	-2.4724	-1.5572	-1.0067
β -Gal-gt_Trp_bottom	electrostatic	-84.7100	-23.3982	-6.9142	-2.5904	-1.3774	-0.9374	-0.7108	-0.5600
	exchange	222.6078	57.0300	13.2474	2.8770	0.5897	0.1138	0.0208	0.0037
	induction	-0.0542	-5.1347	-1.8799	-0.6179	-0.2424	-0.1170	-0.0632	-0.0383
	dispersion	-51.5442	-25.3671	-12.5422	-6.4685	-3.5004	-1.9912	-1.1890	-0.7419
	total	86.2993	3.1300	-8.0889	-6.7997	-4.5305	-2.9318	-1.9421	-1.3365
α -Gal-gt_Trp_upper	electrostatic	-65.6237	-15.8937	-4.2410	-1.5032	-0.8382	-0.6363	-0.5404	-0.4724
	exchange	178.8431	42.6178	9.7541	2.1588	0.4629	0.0972	0.0204	0.0043
	induction	-3.5427	-3.6671	-1.2137	-0.3758	-0.1304	-0.0551	-0.0277	-0.0164
	dispersion	-42.3022	-20.4733	-10.1876	-5.3060	-2.9018	-1.6663	-1.0029	-0.6299
	total	67.3745	2.5838	-5.8882	-5.0262	-3.4075	-2.2604	-1.5505	-1.1144
β -Gal-gt_Trp_upper	electrostatic	-60.0721	-14.0140	-2.9189	-0.4594	-0.0229	-0.0189	-0.0832	-0.1402
	exchange	169.3727	40.4592	9.2775	2.0854	0.4603	0.1003	0.0219	0.0048
	induction	-9.2293	-4.5990	-1.5528	-0.5857	-0.2669	-0.1416	-0.0829	-0.0532
	dispersion	-39.0797	-19.2682	-9.8683	-5.2897	-2.9779	-1.7595	-1.0862	-0.6969
	total	60.9916	2.5780	-5.0625	-4.2495	-2.8074	-1.8197	-1.2304	-0.8855

Methodology used for the generation of the initial structures of the complexes

Different orientations of the aromatic ring of Trp over each face of Glc (upper and bottom faces) were optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM) for the three different conformations of the carbohydrate (*gauche-gauche*, *gauche-trans* and *trans-gauche*), but always seeking an interaction of the amino acid aromatic group with the C–H bonds of the carbohydrate. That is, complexes orientations with only hydrogen bonds between the amino or carboxylic group of the amino acid with the hydroxyl groups of the carbohydrate were not investigated. The most stable complexes with the amino acid at each of the faces were then used for the NBO, NCI and EDA calculations.

The intermolecular distance was investigated for the complexes with Trp and the results were presented in “Effect of the intermolecular distance between carbohydrate and amino acid on the EDA” sub-section of this Supplementary Material. It was also performed calculations modifying the position of the amino acid in a perpendicular plane (if the distance variation were the z axis of a Cartesian space, this variation were at the plane xy). These calculations confirmed that the most stable orientations are indeed the ones with the C–H bond pointed to the center of the aromatic ring.

With these results, initial structures for the complexes with Phe and His were prepared in order to obtain each C–H bond of the carbohydrate oriented at the center of the aromatic ring for the three different conformation of the carbohydrate. The amino acid and the carbohydrate were positioned a little closer in the input than in the optimized structure with Trp. The most stable complexes with the aromatic ring centered at each C–H bond for each conformation were then studied.

Cartesian coordinates

Glc

Table S32. Cartesian coordinates of α -Glc-gg optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9928739			
ZPE / Hartree = 0.1989039			
C	0.8402010000	-1.5028870000	-0.1945850000
C	1.5094790000	-0.1999890000	-0.6359880000
C	0.9450440000	0.9779960000	0.1528820000
C	-0.5695610000	1.0035480000	0.0300810000
C	-1.1436460000	-0.3349330000	0.4890410000
C	-2.6444250000	-0.4448270000	0.2872860000
O	-0.5643050000	-1.3940230000	-0.2794060000
O	1.2722050000	-1.7608850000	1.1158100000
O	2.9162930000	-0.2808140000	-0.5115890000
O	1.4303130000	2.2142690000	-0.3474100000
O	-1.1328390000	2.0168910000	0.8449660000
O	-3.0122040000	-0.2922750000	-1.0752880000
H	1.1088300000	-2.3247310000	-0.8632190000
H	1.2974250000	-0.0465710000	-1.6990090000
H	1.2131820000	0.8730260000	1.2149290000
H	-0.8358930000	1.1675120000	-1.0243630000
H	-0.9200090000	-0.4759120000	1.5553020000
H	-2.9801630000	-1.4145440000	0.6736880000
H	-3.1452780000	0.3482110000	0.8458630000
H	1.1273520000	-2.6934850000	1.3262580000
H	3.1163110000	-0.5869690000	0.3865000000
H	2.3839410000	2.2570630000	-0.1915890000
H	-0.7080020000	2.8544410000	0.6112280000
H	-2.5559540000	-0.9768040000	-1.5845550000

Table S33. Cartesian coordinates of α -Glc-gt optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9926431			
ZPE / Hartree = 0.1987525			
C	0.4959800000	-1.5664160000	-0.2645730000
C	1.5468040000	-0.4920850000	-0.5531430000
C	1.1991450000	0.8002080000	0.1809610000
C	-0.2170490000	1.2316890000	-0.1651310000
C	-1.1844280000	0.0949060000	0.1507730000
C	-2.6035060000	0.3996250000	-0.2902060000
O	-0.7959430000	-1.0821920000	-0.5633100000
O	0.6338390000	-1.9207460000	1.0861720000
O	2.8445370000	-0.9437170000	-0.2176030000
O	2.0657120000	1.8580560000	-0.1965850000
O	-0.6075210000	2.3623790000	0.5940690000
O	-3.4849060000	-0.6619270000	0.0417760000
H	0.6380190000	-2.4346300000	-0.9131070000
H	1.5513790000	-0.2952970000	-1.6299470000
H	1.2608200000	0.6349320000	1.2669390000
H	-0.2644730000	1.4575630000	-1.2420300000
H	-1.1704000000	-0.1071690000	1.2306060000
H	-2.9637610000	1.2902890000	0.2274700000
H	-2.6116790000	0.5892090000	-1.3720230000
H	0.2160050000	-2.7788530000	1.2406280000
H	2.8110550000	-1.2930230000	0.6864110000
H	2.9571190000	1.6509840000	0.1162260000
H	0.0675970000	3.0457110000	0.4741660000
H	-3.1591020000	-1.4621010000	-0.3935690000

Table S34. Cartesian coordinates of α -Glc-tg optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9917886			
ZPE / Hartree = 0.1990655			
C	1.1220720000	-1.4354560000	-0.2739260000
C	1.7022170000	-0.0382280000	-0.5047650000
C	0.8473170000	1.0191960000	0.1895320000
C	-0.5999070000	0.8674260000	-0.2452970000
C	-1.0799390000	-0.5545150000	0.0422560000
C	-2.4983050000	-0.8097550000	-0.4569880000
O	-0.2396410000	-1.4795800000	-0.6469670000
O	1.3085820000	-1.7358580000	1.0838880000
O	3.0505090000	0.0308500000	-0.0825670000
O	1.2651850000	2.3283110000	-0.1607140000
O	-1.4505100000	1.7638430000	0.4557740000
O	-3.4695870000	-0.1576120000	0.3454590000
H	1.6192380000	-2.1725560000	-0.9094540000
H	1.7002330000	0.1613720000	-1.5811120000
H	0.9061130000	0.8848590000	1.2798560000
H	-0.6691860000	1.0511980000	-1.3283030000
H	-1.0415240000	-0.7407800000	1.1244960000
H	-2.5776340000	-0.4967110000	-1.5069970000
H	-2.7014410000	-1.8817310000	-0.3983210000
H	1.2303660000	-2.6904560000	1.2181040000
H	3.0941970000	-0.3151360000	0.8223400000
H	2.1652180000	2.4599940000	0.1685640000
H	-1.1783000000	2.6691650000	0.2490390000
H	-3.2243230000	0.7791400000	0.3979280000

Table S35. Cartesian coordinates of β -Glc-gg optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9918835			
ZPE / Hartree = 0.1983654			
C	-0.9872670000	-1.2733800000	-0.3822580000
C	-1.5535330000	-0.0337950000	0.3025050000
C	-0.7886610000	1.1941050000	-0.1656320000
C	0.7046970000	1.0023230000	0.0526890000
C	1.1663630000	-0.2963110000	-0.6090070000
C	2.6232520000	-0.6228490000	-0.3319270000
O	0.3989700000	-1.3829590000	-0.0952670000
O	-1.6323010000	-2.3864610000	0.1410660000
O	-2.9148610000	0.1589680000	-0.0300550000
O	-1.1716650000	2.3581740000	0.5478590000
O	1.4408780000	2.0672630000	-0.5219440000
O	2.8871680000	-0.7508920000	1.0567330000
H	-1.1262900000	-1.2069990000	-1.4723110000
H	-1.4277420000	-0.1547040000	1.3881930000
H	-0.9729480000	1.3362640000	-1.2417220000
H	0.8984510000	0.9403280000	1.1332310000
H	1.0244720000	-0.2152290000	-1.6983020000
H	2.8833880000	-1.5456640000	-0.8635130000
H	3.2528850000	0.1874030000	-0.7044490000
H	-1.5092050000	-3.1405080000	-0.4521080000
H	-3.4366080000	-0.5431020000	0.3824690000
H	-2.0786300000	2.5865730000	0.3027070000
H	1.0951070000	2.8953270000	-0.1592460000
H	2.3424970000	-1.4729870000	1.3996950000

Table S36. Cartesian coordinates of β -Glc-gt optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9918086			
ZPE / Hartree = 0.1982153			
C	-0.5860220000	-1.4233360000	-0.2659190000
C	-1.5754470000	-0.3731850000	0.2298080000
C	-1.1087430000	1.0072140000	-0.2069230000
C	0.3263220000	1.2547740000	0.2358040000
C	1.2198360000	0.1125310000	-0.2439850000
C	2.6379630000	0.2268590000	0.2824370000
O	0.7054180000	-1.1243300000	0.2439650000
O	-0.9806790000	-2.6578280000	0.2318760000
O	-2.8626120000	-0.5782150000	-0.3196080000
O	-1.9034590000	2.0362740000	0.3578670000
O	0.8234510000	2.4616410000	-0.3132240000
O	3.4505520000	-0.8346680000	-0.1916120000
H	-0.5482050000	-1.4286260000	-1.3660480000
H	-1.6050630000	-0.4227320000	1.3278820000
H	-1.1498440000	1.0612410000	-1.3056630000
H	0.3550040000	1.2924520000	1.3358330000
H	1.2341300000	0.0970920000	-1.3455590000
H	3.0848810000	1.1576540000	-0.0709970000
H	2.6128910000	0.2391680000	1.3803880000
H	-0.5580520000	-3.3626520000	-0.2781890000
H	-3.2394370000	-1.3806900000	0.0665700000
H	-2.7887040000	1.9908220000	-0.0283510000
H	0.2051710000	3.1694820000	-0.0813170000
H	3.0524070000	-1.6653400000	0.1040180000

Table S37. Cartesian coordinates of β -Glc-tg optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9907721			
ZPE / Hartree = 0.1986866			
C	-1.2176560000	-1.2090460000	-0.2800830000
C	-1.6651310000	0.1669310000	0.2046480000
C	-0.6385710000	1.2145910000	-0.1993520000
C	0.7428130000	0.7990410000	0.2805370000
C	1.0716940000	-0.6101360000	-0.2181720000
C	2.4050560000	-1.1250160000	0.3144140000
O	0.0687920000	-1.5056160000	0.2464470000
O	-2.1175420000	-2.1459640000	0.2094800000
O	-2.9009130000	0.5372650000	-0.3751530000
O	-0.9254730000	2.4784380000	0.3739720000
O	1.7431410000	1.6804290000	-0.2075600000
O	3.5081160000	-0.4769340000	-0.2979320000
H	-1.1708170000	-1.2336180000	-1.3797340000
H	-1.7411840000	0.1331230000	1.3011200000
H	-0.6230070000	1.2933160000	-1.2971920000
H	0.7500900000	0.7905610000	1.3808850000
H	1.1000920000	-0.6103490000	-1.3197670000
H	2.4306610000	-1.0046630000	1.4059650000
H	2.4873570000	-2.1889070000	0.0801640000
H	-2.0384630000	-2.9673230000	-0.2949450000
H	-3.5948000000	-0.0302670000	-0.0122780000
H	-1.7456210000	2.8138170000	-0.0134890000
H	1.5676960000	2.5661450000	0.1405110000
H	3.3797970000	0.4790210000	-0.1972290000

Gal

Table S38. Cartesian coordinates of α -Gal-gg optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9933157			
ZPE / Hartree = 0.1996877			
C	0.7695340000	-1.3973860000	-0.4855320000
C	1.4639040000	-0.0380960000	-0.5786340000
C	1.0050840000	0.8707730000	0.5570140000
C	-0.5161310000	0.9718020000	0.5686840000
C	-1.1231330000	-0.4284680000	0.6114930000
C	-2.6439900000	-0.4389040000	0.5341390000
O	-0.6306680000	-1.2405820000	-0.4574570000
O	1.2586540000	-2.0272770000	0.6716570000
O	2.8729620000	-0.1793710000	-0.5790530000
O	1.5184070000	2.1828400000	0.3936500000
O	-0.9790030000	1.6429560000	-0.5986150000
O	-3.1601300000	-0.0261500000	-0.7218320000
H	0.9783570000	-2.0000390000	-1.3733800000
H	1.1947180000	0.4208890000	-1.5340920000
H	1.3351110000	0.4486020000	1.5168060000
H	-0.8366550000	1.5173220000	1.4661540000
H	-0.8410750000	-0.8755760000	1.5742050000
H	-2.9987890000	-1.4597520000	0.6951740000
H	-3.0279590000	0.1921600000	1.3465070000
H	1.0757000000	-2.9756010000	0.6233460000
H	3.1135530000	-0.7383530000	0.1761030000
H	2.4689570000	2.1161000000	0.2220620000
H	-0.4999280000	2.4815810000	-0.6721050000
H	-2.7353770000	0.8150250000	-0.9505620000

Table S39. Cartesian coordinates of *α -Gal-gt* optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9930331			
ZPE / Hartree = 0.1994516			
C	-0.4049200000	-1.4381900000	0.5016740000
C	-1.4945420000	-0.3648220000	0.5027970000
C	-1.2133780000	0.6860520000	-0.5680790000
C	0.1889160000	1.2613130000	-0.3906510000
C	1.1954400000	0.1179470000	-0.3681900000
C	2.6095040000	0.5754350000	-0.0638580000
O	0.8669750000	-0.8452020000	0.6404860000
O	-0.5326650000	-2.1530760000	-0.7003570000
O	-2.7797090000	-0.9334110000	0.3299920000
O	-2.1316600000	1.7626090000	-0.4662930000
O	0.2829100000	1.9870890000	0.8256360000
O	3.5309400000	-0.4997000000	-0.1762630000
H	-0.5142050000	-2.1022790000	1.3631930000
H	-1.4969410000	0.1186720000	1.4838040000
H	-1.2794740000	0.2210160000	-1.5620450000
H	0.4213070000	1.9150390000	-1.2429670000
H	1.1814310000	-0.3703020000	-1.3514790000
H	2.9094540000	1.3321300000	-0.7928510000
H	2.6472220000	1.0143780000	0.9393930000
H	-0.0643900000	-2.9958470000	-0.6257040000
H	-2.7499980000	-1.4981240000	-0.4577890000
H	-3.0241410000	1.3929780000	-0.3989260000
H	-0.4854590000	2.5753160000	0.8714210000
H	3.2747480000	-1.1758500000	0.4661790000

Table S40. Cartesian coordinates of α -Gal-tg optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9910743			
ZPE / Hartree = 0.199273			
C	-0.9675760000	-1.3877950000	0.4653370000
C	-1.6045140000	0.0021570000	0.4375790000
C	-0.8722750000	0.9035960000	-0.5520550000
C	0.6185000000	0.9374980000	-0.2322570000
C	1.1525590000	-0.4897630000	-0.1896930000
C	2.6041670000	-0.5696600000	0.2685870000
O	0.4137680000	-1.2938780000	0.7333600000
O	-1.2291780000	-1.9830570000	-0.7797280000
O	-2.9863450000	-0.0691900000	0.1360150000
O	-1.3585590000	2.2343930000	-0.4722500000
O	0.8475290000	1.5520200000	1.0264820000
O	3.4573990000	0.1925930000	-0.5693640000
H	-1.3822770000	-1.9887890000	1.2788710000
H	-1.5261350000	0.4349030000	1.4388000000
H	-1.0045350000	0.5107060000	-1.5701500000
H	1.1450840000	1.4857060000	-1.0245600000
H	1.0651740000	-0.9135030000	-1.1997450000
H	2.6915020000	-0.1519920000	1.2740350000
H	2.9096560000	-1.6212300000	0.2972300000
H	-1.1007520000	-2.9391210000	-0.7134400000
H	-3.0864660000	-0.5928010000	-0.6740920000
H	-2.3259190000	2.2034540000	-0.5012950000
H	0.3451380000	2.3799280000	1.0407160000
H	3.5274540000	-0.2464980000	-1.4274770000

Table S41. Cartesian coordinates of β -Gal-gg optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9922485			
ZPE / Hartree = 0.1992472			
C	-0.8396760000	1.3615830000	0.2450870000
C	-1.5065650000	0.0769580000	-0.2343940000
C	-0.9215690000	-1.1099090000	0.5155300000
C	0.5982180000	-1.1311250000	0.3908680000
C	1.1706600000	0.2313410000	0.7826730000
C	2.6793530000	0.3353340000	0.5995930000
O	0.5597350000	1.2755300000	0.0296150000
O	-1.3370260000	2.4117880000	-0.5168580000
O	-2.8986720000	0.0844960000	0.0242280000
O	-1.4071020000	-2.3359230000	-0.0044090000
O	0.9834260000	-1.4258630000	-0.9469270000
O	3.0963160000	0.3196820000	-0.7564860000
H	-1.0339700000	1.5195090000	1.3177100000
H	-1.3092610000	-0.0290080000	-1.3097790000
H	-1.1845080000	-1.0143310000	1.5794130000
H	1.0036830000	-1.8892260000	1.0736920000
H	0.9600880000	0.3761110000	1.8538370000
H	3.0203620000	1.2849480000	1.0187450000
H	3.1458720000	-0.4806990000	1.1668090000
H	-1.1483160000	3.2502330000	-0.0734420000
H	-3.3246950000	0.7051800000	-0.5823790000
H	-2.3716840000	-2.2791970000	-0.0639020000
H	0.5091990000	-2.2226470000	-1.2271200000
H	2.6772830000	-0.4436530000	-1.1830260000

Table S42. Cartesian coordinates of β -Gal-gt optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9921149			
ZPE / Hartree = 0.1986278			
C	0.4460870000	1.4262070000	-0.1677820000
C	1.5041100000	0.3742200000	0.1474870000
C	1.1552560000	-0.9318420000	-0.5517650000
C	-0.2615400000	-1.3760920000	-0.1971720000
C	-1.2295930000	-0.2243510000	-0.4518470000
C	-2.6458710000	-0.5288860000	-0.0007850000
O	-0.8227100000	0.9496830000	0.2516540000
O	0.7495460000	2.5707960000	0.5585800000
O	2.7820890000	0.7650150000	-0.3204300000
O	2.0372120000	-1.9705340000	-0.1608780000
O	-0.3429470000	-1.7528690000	1.1682040000
O	-3.5321280000	0.5238390000	-0.3511140000
H	0.4183470000	1.6355670000	-1.2487000000
H	1.5166940000	0.2206850000	1.2351610000
H	1.2108790000	-0.7718550000	-1.6385470000
H	-0.5425320000	-2.2194910000	-0.8427380000
H	-1.2352080000	-0.0141520000	-1.5324860000
H	-3.0001930000	-1.4296590000	-0.5075420000
H	-2.6580230000	-0.7020020000	1.0809760000
H	0.2864230000	3.3287900000	0.1762420000
H	3.1073830000	1.4896110000	0.2310670000
H	2.9449930000	-1.6445550000	-0.2446210000
H	0.4052550000	-2.3401300000	1.3518560000
H	-3.2332070000	1.3242140000	0.1023930000

Table S43. Cartesian coordinates of β -Gal-tg optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -686.9905628			
ZPE / Hartree = 0.1988957			
C	-1.0431070000	-1.2952700000	-0.2316500000
C	-1.5879360000	0.0844550000	0.1197950000
C	-0.7058850000	1.1548960000	-0.5052490000
C	0.7525270000	0.9602850000	-0.1000200000
C	1.1740130000	-0.4775900000	-0.3933020000
C	2.5693000000	-0.8068960000	0.1264020000
O	0.2926770000	-1.4048700000	0.2341030000
O	-1.8168080000	-2.2422400000	0.4275540000
O	-2.8950570000	0.2735790000	-0.3908090000
O	-1.0971360000	2.4501730000	-0.0801920000
O	0.9263180000	1.2128250000	1.2849590000
O	3.5459270000	0.0747350000	-0.4016060000
H	-1.0621550000	-1.4524670000	-1.3215650000
H	-1.5774100000	0.1864360000	1.2134240000
H	-0.7812610000	1.0733280000	-1.5996300000
H	1.3798540000	1.6389560000	-0.6923130000
H	1.1465760000	-0.6223130000	-1.4853150000
H	2.5875690000	-0.6872580000	1.2118550000
H	2.8003940000	-1.8496800000	-0.1163960000
H	-1.6751100000	-3.1107930000	0.0265980000
H	-3.5107710000	-0.2670380000	0.1222920000
H	-2.0554700000	2.5296790000	-0.1922660000
H	0.4785170000	2.0477740000	1.4856600000
H	3.6684400000	-0.1195160000	-1.3402660000

Table S44. Cartesian coordinates of α -Glc-gg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1706123			
ZPE / Hartree = 0.4227064			
BSSE / Hartree = 0.003125625123			
C	3.7079950000	-0.4999250000	-0.6689620000
C	2.9659630000	-1.8401480000	-0.7293450000
C	1.5625830000	-1.6987780000	-0.1461070000
C	1.6564290000	-1.1235270000	1.2566840000
C	2.3356410000	0.2403850000	1.1600340000
C	2.5034640000	0.9380130000	2.4954720000
O	3.6528030000	0.0572680000	0.6269520000
O	3.1073120000	0.3311230000	-1.6264020000
O	2.9264090000	-2.3380700000	-2.0533140000
O	0.9073430000	-2.9538190000	-0.0552230000
O	0.3768130000	-0.9572560000	1.8395690000
O	3.2615090000	0.1669320000	3.4155590000
H	4.7722770000	-0.6340820000	-0.8798950000
H	3.5217780000	-2.5728650000	-0.1354970000
H	0.9692370000	-1.0127760000	-0.7704250000
H	2.2724500000	-1.7900330000	1.8790530000
H	1.7474000000	0.8935230000	0.4983430000
H	2.9734480000	1.9146110000	2.3246570000
H	1.5197180000	1.0982030000	2.9427230000
H	3.6767330000	1.0934680000	-1.7986540000
H	2.6012420000	-1.6246340000	-2.6246530000
H	0.7344010000	-3.2761730000	-0.9506940000
H	-0.1285190000	-1.7674850000	1.6763800000
H	4.1358110000	0.0168470000	3.0296080000
H	-5.1848800000	1.4604210000	-0.6313860000
O	-5.5891710000	-0.2903480000	1.5341790000

Table S44. Cartesian coordinates of α -Glc-gg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

C	-5.0781950000	-1.0073480000	0.6384750000
O	-5.2298590000	-2.2373430000	0.4581430000
N	-4.2926170000	1.1672830000	-0.2263210000
H	-4.3118710000	1.4364820000	0.7632090000
H	-4.3364440000	-0.5853500000	-1.3655480000
C	-4.1051630000	-0.3103760000	-0.3349950000
H	-3.5450770000	1.6801310000	-0.7046830000
C	-2.6519860000	-0.6778420000	-0.0010990000
H	-2.5643060000	-1.7599890000	-0.1313650000
H	-2.4679840000	-0.4619400000	1.0589110000
C	-1.6411480000	0.0405840000	-0.8452190000
H	-1.5378820000	1.8406810000	1.5056520000
H	-1.4935300000	-1.1508480000	-2.7187590000
C	-1.2101130000	-0.3077900000	-2.1030140000
C	-0.9006440000	2.0628800000	0.6531360000
C	-0.9241180000	1.2401340000	-0.4914730000
N	-0.2712140000	0.5931900000	-2.5438490000
C	-0.0426420000	3.1508010000	0.6773590000
H	-0.0078680000	3.7895920000	1.5546330000
C	-0.0721290000	1.5517660000	-1.5808890000
H	0.2069840000	0.5482250000	-3.4327670000
C	0.7976600000	3.4436110000	-0.4231310000
C	0.7939700000	2.6544030000	-1.5628660000
H	1.4597570000	4.3024740000	-0.3716680000
H	1.4432560000	2.8692330000	-2.4060440000

Table S45. Cartesian coordinates of α -Glc-gg_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1713087			
ZPE / Hartree = 0.4231601			
BSSE / Hartree = 0.0030594645			
C	-3.4749270000	0.9842250000	-0.7122290000
C	-2.0931680000	0.8911720000	-1.3594800000
C	-1.7761350000	-0.5534280000	-1.7295970000
C	-1.9175290000	-1.4318970000	-0.4982410000
C	-3.3219170000	-1.2801510000	0.0826430000
C	-3.5186770000	-2.0278480000	1.3908340000
O	-3.5759650000	0.0962960000	0.3798440000
O	-4.4165620000	0.6987550000	-1.7135450000
O	-1.9929100000	1.7500870000	-2.4797040000
O	-0.4407780000	-0.6830620000	-2.1939370000
O	-1.7249000000	-2.8005910000	-0.8149680000
O	-2.6798450000	-1.5249680000	2.4222160000
H	-3.6396830000	1.9800230000	-0.2908420000
H	-1.3502070000	1.2369040000	-0.6341960000
H	-2.4766050000	-0.9030750000	-2.5031400000
H	-1.1816840000	-1.1064450000	0.2499220000
H	-4.0542230000	-1.6507450000	-0.6482890000
H	-4.5721180000	-1.9546810000	1.6850360000
H	-3.2644410000	-3.0802390000	1.2516410000
H	-5.2885680000	1.0105070000	-1.4355160000
H	-2.7485870000	1.5705380000	-3.0603910000
H	-0.3498730000	-0.1682520000	-3.0079690000
H	-0.8622320000	-2.8838530000	-1.2461220000
H	-2.9061200000	-0.5926470000	2.5510290000
H	5.1732330000	1.0576360000	1.4321580000
O	5.9518270000	0.3329450000	-1.2342160000
C	5.4024370000	-0.6902960000	-0.7552560000
O	5.6235920000	-1.8882110000	-1.0446300000
N	4.3903770000	0.9497790000	0.7829780000
H	4.5736810000	1.5759710000	-0.0093420000
H	4.4089190000	-1.1137880000	1.1379040000
C	4.2820220000	-0.4521200000	0.2794240000

H	3.5379130000	1.2491270000	1.2676810000
C	2.9020630000	-0.6699790000	-0.3598980000
H	2.8723150000	-1.7099410000	-0.6954220000
H	2.8225640000	-0.0351860000	-1.2516380000
C	1.7636060000	-0.3847680000	0.5737790000
H	1.8816220000	2.2845120000	-0.7080560000
H	1.4338730000	-2.2868640000	1.6777410000
C	1.2027800000	-1.2478030000	1.4843460000
C	1.1438430000	2.1147270000	0.0723940000
C	1.0581150000	0.8645590000	0.7173380000
N	0.2136940000	-0.6108730000	2.1940500000
C	0.2638320000	3.1204210000	0.4435190000
H	0.3132280000	4.0869830000	-0.0481670000
C	0.0833170000	0.6757630000	1.7317600000
H	-0.4644180000	-1.0807390000	2.7815280000
C	-0.7067090000	2.9070880000	1.4495470000
C	-0.8105370000	1.6890900000	2.1060990000
H	-1.3847450000	3.7130170000	1.7128250000
H	-1.5525150000	1.5263660000	2.8820810000

Table S46. Cartesian coordinates of α -Glc-gt_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1706414			
ZPE / Hartree = 0.4223524			
BSSE / Hartree = 0.0030792623			
C	-3.7068020000	-0.8330870000	0.3750470000
C	-2.9261000000	-2.1318250000	0.1431080000
C	-1.5166640000	-1.8253750000	-0.3593290000
C	-1.5994160000	-0.9416440000	-1.5934130000
C	-2.3285470000	0.3390060000	-1.2018690000
C	-2.4977150000	1.3093710000	-2.3530470000
O	-3.6496400000	-0.0000590000	-0.7636860000
O	-3.1442150000	-0.2250710000	1.5066100000
O	-2.8960010000	-2.9212850000	1.3168200000
O	-0.8239510000	-3.0076700000	-0.7252330000
O	-0.3138530000	-0.6100020000	-2.0842850000
O	-3.1670390000	2.4886220000	-1.9322590000
H	-4.7695500000	-1.0391010000	0.5281580000
H	-3.4497100000	-2.7197680000	-0.6175760000
H	-0.9541110000	-1.2875740000	0.4198970000
H	-2.1800330000	-1.4621790000	-2.3716460000
H	-1.7860930000	0.8363780000	-0.3850670000
H	-1.5140270000	1.6124040000	-2.7182530000
H	-3.0458240000	0.8189950000	-3.1691840000
H	-3.7276150000	0.4799680000	1.8196620000
H	-2.6139480000	-2.3496630000	2.0479450000
H	-0.6266380000	-3.5116330000	0.0761870000
H	0.2100570000	-1.4245210000	-2.1089380000
H	-4.0200200000	2.2253420000	-1.5589810000
H	5.0279030000	1.5933270000	0.8639660000
O	5.6260600000	0.1432240000	-1.4853860000
C	5.1642620000	-0.7139330000	-0.6919780000
O	5.4195630000	-1.9392250000	-0.6494440000
N	4.1793540000	1.2721690000	0.3922380000
H	4.2075370000	1.6492860000	-0.5612610000
H	4.3549940000	-0.5915040000	1.3268830000
C	4.1178770000	-0.2187630000	0.3288710000

H	3.3745920000	1.6655620000	0.8906390000
C	2.7075710000	-0.6642730000	-0.0841320000
H	2.7211100000	-1.7569550000	-0.1180640000
H	2.5115640000	-0.3074560000	-1.1033940000
C	1.6310640000	-0.1821580000	0.8421040000
H	1.5000080000	2.0643070000	-1.0852650000
H	1.4854110000	-1.7484330000	2.4152930000
C	1.1805970000	-0.8056740000	1.9810730000
C	0.8376320000	2.0814300000	-0.2229940000
C	0.8701440000	1.0369040000	0.7235830000
N	0.1923700000	-0.0543600000	2.5695980000
C	-0.0618040000	3.1199830000	-0.0433930000
H	-0.1049620000	3.9263390000	-0.7692590000
C	-0.0203740000	1.0800900000	1.8258300000
H	-0.3054900000	-0.3058870000	3.4122010000
C	-0.9356870000	3.1453750000	1.0693220000
C	-0.9276930000	2.1323340000	2.0152800000
H	-1.6305410000	3.9722810000	1.1793290000
H	-1.6041460000	2.1409810000	2.8644020000

Table S47. Cartesian coordinates of α -Glc-gt_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1715207			
ZPE / Hartree = 0.4231132			
BSSE / Hartree = 0.002668303			
C	-2.5814850000	-1.6436280000	-1.1622440000
C	-1.2859390000	-1.7431290000	-0.3576400000
C	-1.5458390000	-1.4713780000	1.1205270000
C	-2.2462550000	-0.1309570000	1.2734370000
C	-3.5283860000	-0.1356500000	0.4463770000
C	-4.2347910000	1.2066410000	0.4555080000
O	-3.2110310000	-0.4019020000	-0.9241770000
O	-3.3869170000	-2.7299010000	-0.7887590000
O	-0.6503770000	-2.9919700000	-0.5531370000
O	-0.3300270000	-1.4024180000	1.8497180000
O	-2.5925970000	0.1224930000	2.6245410000
O	-5.4314590000	1.1625260000	-0.3072320000
H	-2.3730290000	-1.6611560000	-2.2357110000
H	-0.5952590000	-0.9822010000	-0.7310310000
H	-2.1889750000	-2.2602820000	1.5393370000
H	-1.5801580000	0.6592390000	0.8950120000
H	-4.2091110000	-0.9116820000	0.8233910000
H	-4.5150250000	1.4660220000	1.4778890000
H	-3.5526180000	1.9752280000	0.0678680000
H	-4.0779710000	-2.8621020000	-1.4522220000
H	-1.3036610000	-3.6879060000	-0.3827300000
H	0.1182190000	-2.2569140000	1.7776910000
H	-1.7809400000	0.0790130000	3.1502720000
H	-5.1951930000	0.9036460000	-1.2089620000
H	5.2937350000	1.4866310000	-1.2431910000
O	6.2425560000	-1.0026430000	0.0788630000
C	5.3164360000	-0.5449370000	0.7943130000
O	5.1529810000	-0.6916120000	2.0265860000
N	4.7154430000	0.6445700000	-1.2813060000
H	5.3095790000	-0.1158210000	-1.6351380000
H	3.9861890000	1.1688930000	0.6153350000
C	4.2115380000	0.2521930000	0.0681650000

H	3.9475850000	0.8196590000	-1.9384640000
C	2.9475200000	-0.6081510000	-0.0900780000
H	2.6390940000	-0.9050880000	0.9176490000
H	3.2075080000	-1.5204650000	-0.6398010000
C	1.8372270000	0.1146010000	-0.7877410000
H	1.6758940000	1.5378240000	1.7980540000
H	1.7267450000	-0.8034860000	-2.8107620000
C	1.3925100000	-0.0863040000	-2.0728790000
C	0.9903660000	1.8266120000	1.0052660000
C	1.0315760000	1.1785940000	-0.2438410000
N	0.3583640000	0.7752770000	-2.3532760000
C	0.0583070000	2.8339680000	1.2051000000
H	0.0122510000	3.3437690000	2.1624560000
C	0.1150900000	1.5643980000	-1.2544870000
H	-0.1441370000	0.8158050000	-3.2288430000
C	-0.8419450000	3.2074630000	0.1806290000
C	-0.8309110000	2.5800670000	-1.0564950000
H	-1.5637510000	3.9962190000	0.3700250000
H	-1.5287600000	2.8572220000	-1.8407640000

Table S48. Cartesian coordinates of α -Glc-tg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1694223			
ZPE / Hartree = 0.4235752			
BSSE / Hartree = 0.0031062657			
C	-3.5258500000	-1.5330160000	0.5159810000
C	-2.3692350000	-2.2832150000	-0.1563200000
C	-1.3583090000	-1.2973590000	-0.7356270000
C	-2.0711620000	-0.3056360000	-1.6365590000
C	-3.1507400000	0.4078700000	-0.8279710000
C	-3.9473610000	1.4121720000	-1.6527940000
O	-4.0800870000	-0.5655930000	-0.3522680000
O	-3.0098600000	-0.9536770000	1.6855170000
O	-1.7566650000	-3.1792910000	0.7510870000
O	-0.3681360000	-1.9531770000	-1.5116170000
O	-1.1744860000	0.6717350000	-2.1415820000
O	-3.1972250000	2.5874610000	-1.9186330000
H	-4.3473790000	-2.2154240000	0.7484590000
H	-2.7783520000	-2.8904330000	-0.9700990000
H	-0.8828280000	-0.7402960000	0.0822170000
H	-2.5489690000	-0.8454150000	-2.4691550000
H	-2.6824980000	0.9327410000	0.0189160000
H	-4.2848060000	0.9389840000	-2.5851090000
H	-4.8266460000	1.7170580000	-1.0803670000
H	-3.7377860000	-0.7172210000	2.2768160000
H	-1.5243750000	-2.6746570000	1.5466870000
H	0.2829370000	-2.3441850000	-0.9123830000
H	-0.4231090000	0.2123070000	-2.5450130000
H	-2.3625980000	2.3173930000	-2.3314340000
H	5.1018710000	1.4277460000	1.0575160000
O	5.6465320000	0.4943210000	-1.5761530000
C	5.2300720000	-0.5127020000	-0.9512500000
O	5.5118660000	-1.7153460000	-1.1551590000
N	4.2540710000	1.1978100000	0.5337790000
H	4.2760060000	1.7530380000	-0.3295670000
H	4.4637450000	-0.8169280000	1.0681440000
C	4.2037870000	-0.2510230000	0.1722630000

H	3.4480330000	1.4801820000	1.1008580000
C	2.7904240000	-0.6227970000	-0.3029880000
H	2.8150870000	-1.6880530000	-0.5483370000
H	2.5777700000	-0.0781840000	-1.2320710000
C	1.7185500000	-0.3452260000	0.7088860000
H	1.6279570000	2.2837940000	-0.6570560000
H	1.5409260000	-2.2270590000	1.8827340000
C	1.2519420000	-1.2054450000	1.6746280000
C	0.9586300000	2.1118370000	0.1829600000
C	0.9748570000	0.8805110000	0.8689130000
N	0.2732580000	-0.5916130000	2.4181680000
C	0.0648490000	3.0912220000	0.5865520000
H	0.0367010000	4.0422640000	0.0638540000
C	0.0778770000	0.6843310000	1.9506230000
H	-0.2356860000	-1.0222010000	3.1776560000
C	-0.8193350000	2.8726300000	1.6686030000
C	-0.8265750000	1.6729900000	2.3634660000
H	-1.5086990000	3.6598570000	1.9578050000
H	-1.5086530000	1.4969860000	3.1895800000

Table S49. Cartesian coordinates of α -Glc-tg_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1696536			
ZPE / Hartree = 0.4234618			
BSSE / Hartree = 0.0028119314			
C	-3.5337210000	0.8782130000	-0.4105560000
C	-2.2294920000	1.0255680000	-1.1950950000
C	-1.7335890000	-0.3324950000	-1.6834860000
C	-1.6336760000	-1.2697950000	-0.4938750000
C	-2.9891190000	-1.3713350000	0.2021140000
C	-2.9346600000	-2.2353310000	1.4576990000
O	-3.3885030000	-0.0683560000	0.6285840000
O	-4.5273710000	0.5071530000	-1.3292360000
O	-2.3721250000	1.9421370000	-2.2635880000
O	-0.4417820000	-0.2255990000	-2.2604110000
O	-1.2347320000	-2.5779130000	-0.8814640000
O	-2.8394400000	-3.6167080000	1.1485810000
H	-3.7915270000	1.8161400000	0.0892870000
H	-1.4748840000	1.4456920000	-0.5236020000
H	-2.4396940000	-0.7511280000	-2.4165970000
H	-0.9085590000	-0.8546240000	0.2200560000
H	-3.7335040000	-1.7885030000	-0.4905030000
H	-2.0917420000	-1.9112150000	2.0839600000
H	-3.8604780000	-2.0951890000	2.0208580000
H	-5.3996530000	0.6735180000	-0.9465420000
H	-3.1477480000	1.6764760000	-2.7814710000
H	-0.4948400000	0.3802170000	-3.0132080000
H	-0.3281080000	-2.5326730000	-1.2174100000
H	-2.0792130000	-3.7294320000	0.5569180000
H	5.2371950000	1.1994690000	0.9542420000
O	5.7212920000	-0.0566520000	-1.4704520000
C	5.1519290000	-0.9403620000	-0.7835730000
O	5.2753940000	-2.1833760000	-0.8737320000
N	4.3423280000	1.0112700000	0.4959710000
H	4.3622720000	1.4983680000	-0.4063720000
H	4.3209640000	-0.9465700000	1.2293970000
C	4.1394610000	-0.4516690000	0.2737710000
H	3.5998840000	1.4119420000	1.0779150000

C	2.7004980000	-0.7127490000	-0.1950860000
H	2.6076130000	-1.7934690000	-0.3311390000
H	2.5617260000	-0.2465410000	-1.1787690000
C	1.6538820000	-0.2145900000	0.7572540000
H	1.8019390000	2.2172650000	-0.9312980000
H	1.3246320000	-1.8986660000	2.1736770000
C	1.1182880000	-0.8956830000	1.8247260000
C	1.1091720000	2.2086950000	-0.0931280000
C	1.0098590000	1.0754780000	0.7398080000
N	0.1839340000	-0.1154170000	2.4603770000
C	0.3079850000	3.3083570000	0.1728460000
H	0.3729310000	4.1870460000	-0.4612380000
C	0.0895120000	1.0952700000	1.8196650000
H	-0.3572700000	-0.3973020000	3.2659550000
C	-0.6052820000	3.3029810000	1.2532090000
C	-0.7295990000	2.2018880000	2.0871980000
H	-1.2237640000	4.1775030000	1.4298410000
H	-1.4325590000	2.1905720000	2.9144000000

Table S50. Cartesian coordinates of β -Glc-gg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1708421			
ZPE / Hartree = 0.4225045			
BSSE / Hartree = 0.0029053293			
C	-2.0092940000	0.5049880000	-1.2450860000
C	-3.5010080000	0.2895340000	-1.0190610000
C	-3.7021920000	-0.4247540000	0.3078240000
C	-2.8848540000	-1.7073230000	0.3454460000
C	-1.4205030000	-1.4006000000	0.0314020000
C	-0.5534870000	-2.6427200000	-0.0598490000
O	-1.3372130000	-0.7465830000	-1.2332500000
O	-1.8311770000	1.0905920000	-2.4917440000
O	-4.1853860000	1.5260580000	-0.9456600000
O	-5.0577980000	-0.7823260000	0.5194970000
O	-2.9362830000	-2.3019440000	1.6303310000
O	-1.0313520000	-3.5632230000	-1.0293920000
H	-1.5972090000	1.1399060000	-0.4481570000
H	-3.8951850000	-0.3298000000	-1.8379220000
H	-3.3568550000	0.2366960000	1.1187540000
H	-3.2768610000	-2.3989760000	-0.4139830000
H	-1.0150100000	-0.7464530000	0.8201410000
H	0.4726310000	-2.3328020000	-0.2906600000
H	-0.5558660000	-3.1592130000	0.9024020000
H	-0.9885120000	1.5689330000	-2.4941450000
H	-4.1390140000	1.9545420000	-1.8116810000
H	-5.5770750000	0.0253380000	0.6339680000
H	-3.8675990000	-2.4337810000	1.8584480000
H	-1.0136110000	-3.1264040000	-1.8923050000
N	4.3364510000	1.2402070000	0.0293060000
H	4.3512270000	1.3713580000	-0.9884990000
H	5.2102440000	1.6286300000	0.3918210000
H	3.5647660000	1.7807250000	0.4325100000
C	4.2183410000	-0.2170930000	0.3370690000
H	4.4768380000	-0.3435570000	1.3896770000
C	2.7809620000	-0.6981610000	0.0832700000
C	5.2104590000	-0.9900010000	-0.5582570000

H	2.5634780000	-0.6156180000	-0.9895610000
H	2.7644650000	-1.7611750000	0.3390000000
C	1.7470880000	0.0462180000	0.8753480000
O	5.6569500000	-0.3779890000	-1.5599300000
C	1.3149030000	-0.2468020000	2.1469640000
C	1.0336920000	1.2326670000	0.4727140000
H	1.5978850000	-1.0639200000	2.7968530000
N	0.3856820000	0.6783640000	2.5542590000
C	0.1931860000	1.6006080000	1.5562870000
C	1.0230610000	2.0196850000	-0.6977970000
H	-0.0871390000	0.6735710000	3.4473040000
C	-0.6434880000	2.7251500000	1.5080210000
C	0.1995730000	3.1351120000	-0.7476470000
H	1.6557120000	1.7586770000	-1.5432770000
H	-1.2787570000	2.9863420000	2.3485530000
C	-0.6267020000	3.4835780000	0.3469810000
H	0.1859670000	3.7545370000	-1.6396300000
H	-1.2618730000	4.3607430000	0.2738770000
O	5.4390070000	-2.1719350000	-0.2136270000

Table S51. Cartesian coordinates of β -Glc-gg_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1704734			
ZPE / Hartree = 0.4226153			
BSSE / Hartree = 0.0032472485			
C	3.5056900000	0.7449060000	0.9895950000
C	2.0722280000	0.7237470000	1.5086270000
C	1.6752000000	-0.7085120000	1.8236050000
C	1.8624490000	-1.5742710000	0.5876660000
C	3.3002070000	-1.4497670000	0.0803000000
C	3.5404500000	-2.1753070000	-1.2332100000
O	3.6027560000	-0.0779560000	-0.1645140000
O	3.8126260000	2.0480330000	0.6194560000
O	1.9421580000	1.4796370000	2.6979110000
O	0.3144210000	-0.8049690000	2.2115320000
O	1.6226420000	-2.9403790000	0.8782700000
O	2.7617580000	-1.6296880000	-2.2889100000
H	4.2014830000	0.3737520000	1.7578550000
H	1.4176580000	1.1203560000	0.7201310000
H	2.3206120000	-1.0921450000	2.6295690000
H	1.1753360000	-1.2225830000	-0.1945910000
H	3.9838820000	-1.8595190000	0.8407120000
H	4.6080980000	-2.1209930000	-1.4759540000
H	3.2553500000	-3.2239270000	-1.1297220000
H	4.7726730000	2.1515870000	0.5675650000
H	2.0014810000	2.4183190000	2.4725840000
H	0.1963520000	-0.3126360000	3.0358500000
H	0.7298050000	-3.0122210000	1.2451360000
H	2.9983160000	-0.6945320000	-2.3736600000
N	-4.2886640000	1.0409630000	-0.8554920000
H	-4.4703940000	1.6537770000	-0.0524070000
H	-5.0512190000	1.1900540000	-1.5203750000
H	-3.4156710000	1.3229360000	-1.3131730000
C	-4.2407910000	-0.3763160000	-0.3867900000
H	-4.3774170000	-1.0094860000	-1.2650140000
C	-2.8821500000	-0.6647680000	0.2694320000
C	-5.3869360000	-0.5999980000	0.6227810000

H	-2.7990670000	-0.0701890000	1.1881110000
H	-2.8938410000	-1.7176660000	0.5632020000
C	-1.7144610000	-0.3806850000	-0.6273850000
O	-5.9072740000	0.4299810000	1.1193660000
C	-1.1555450000	-1.2246030000	-1.5568210000
C	-0.9678410000	0.8501790000	-0.7018810000
H	-1.4130110000	-2.2471010000	-1.7988980000
N	-0.1270100000	-0.5918090000	-2.2118390000
C	0.0282560000	0.6716810000	-1.6972570000
C	-1.0364810000	2.0767580000	-0.0114220000
H	0.5371270000	-1.0532510000	-2.8203490000
C	0.9586970000	1.6726480000	-2.0101270000
C	-0.1215600000	3.0714630000	-0.3235890000
H	-1.7901920000	2.2378740000	0.7555910000
H	1.7190180000	1.5148200000	-2.7692190000
C	0.8683210000	2.8687190000	-1.3127890000
H	-0.1586200000	4.0208580000	0.2016580000
H	1.5757070000	3.6639170000	-1.5267420000
O	-5.6551060000	-1.7960760000	0.8780210000

Table S52. Cartesian coordinates of β -Glc-gt_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1711114			
ZPE / Hartree = 0.4222743			
BSSE / Hartree = 0.0033840289			
C	2.7582850000	-0.1340640000	0.7789150000
C	3.2224460000	-0.4545080000	-0.6372950000
C	2.0441550000	-0.9987130000	-1.4297580000
C	1.4142420000	-2.1848880000	-0.7138230000
C	1.0620510000	-1.7843710000	0.7165650000
C	0.5318040000	-2.9379410000	1.5438330000
O	2.2342350000	-1.3116510000	1.3788890000
O	3.8547200000	0.2899300000	1.5195470000
O	3.6731960000	0.7112720000	-1.3020330000
O	2.4274780000	-1.4406110000	-2.7211820000
O	0.2194680000	-2.5863580000	-1.3607460000
O	0.1713730000	-2.5052490000	2.8468820000
H	1.9763160000	0.6358050000	0.7534930000
H	4.0198220000	-1.2100540000	-0.5843250000
H	1.2855990000	-0.2040650000	-1.5131800000
H	2.1372730000	-3.0149600000	-0.6909170000
H	0.3096510000	-0.9814800000	0.6862200000
H	-0.3700110000	-3.3383300000	1.0769480000
H	1.2909750000	-3.7302310000	1.5905640000
H	3.5478880000	0.8202070000	2.2686110000
H	4.4825840000	1.0194090000	-0.8712050000
H	2.6792390000	-0.6703620000	-3.2488540000
H	0.4243530000	-2.7364410000	-2.2950220000
H	0.9552970000	-2.1078260000	3.2517240000
N	-3.8093260000	1.4351960000	0.6330760000
H	-3.7932060000	0.9580480000	1.5411410000
H	-4.6683670000	1.9895430000	0.6062930000
H	-3.0159670000	2.0810970000	0.5723710000
C	-3.7842640000	0.4170910000	-0.4594860000
H	-4.0566280000	0.9324360000	-1.3821760000
C	-2.3781790000	-0.1885580000	-0.5853250000
C	-4.8180780000	-0.6816720000	-0.1332010000

H	-2.1485840000	-0.7419960000	0.3354030000
H	-2.4257510000	-0.9188000000	-1.3973090000
C	-1.3034610000	0.8216660000	-0.8581970000
O	-5.2306590000	-0.7317550000	1.0521030000
C	-0.8767370000	1.2592710000	-2.0895750000
C	-0.5136290000	1.5334000000	0.1161490000
H	-1.2073860000	0.9628560000	-3.0759180000
N	0.1242190000	2.1871770000	-1.9393250000
C	0.3727400000	2.3769220000	-0.6026260000
C	-0.4504440000	1.5163270000	1.5247530000
H	0.6084190000	2.6478580000	-2.6972310000
C	1.3069750000	3.2020700000	0.0397980000
C	0.4720600000	2.3307770000	2.1638620000
H	-1.1097790000	0.8677390000	2.0977830000
H	1.9791800000	3.8354730000	-0.5306000000
C	1.3418880000	3.1677730000	1.4258560000
H	0.5337970000	2.3264310000	3.2476480000
H	2.0548520000	3.7914870000	1.9560960000
O	-5.1129270000	-1.4423210000	-1.0830230000

Table S53. Cartesian coordinates of β -Glc-gt_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1704102			
ZPE / Hartree = 0.4223406			
BSSE / Hartree = 0.0032364388			
C	3.1701370000	-0.5036200000	-0.5160580000
C	2.7658470000	0.2303150000	0.7583670000
C	2.2425430000	-0.7676070000	1.7804090000
C	1.1264350000	-1.6085140000	1.1775780000
C	1.6129990000	-2.2472660000	-0.1216580000
C	0.5181750000	-3.0093150000	-0.8441340000
O	2.0473750000	-1.2207150000	-1.0111800000
O	3.5397830000	0.4397790000	-1.4656730000
O	3.8651570000	0.9033880000	1.3439330000
O	1.7109830000	-0.1159210000	2.9217670000
O	0.7327670000	-2.6447010000	2.0591530000
O	0.9996920000	-3.5754470000	-2.0529990000
H	3.9903820000	-1.2103870000	-0.3155560000
H	1.9676620000	0.9384600000	0.5020920000
H	3.0643060000	-1.4371380000	2.0797470000
H	0.2733900000	-0.9493110000	0.9503290000
H	2.4531930000	-2.9272870000	0.0941180000
H	0.1685750000	-3.8319830000	-0.2180840000
H	-0.3204320000	-2.3286910000	-1.0414140000
H	4.0550120000	0.0101880000	-2.1623670000
H	4.0622880000	1.6882500000	0.8145310000
H	2.4272660000	0.3611710000	3.3633330000
H	0.4720520000	-2.2388790000	2.8983630000
H	1.3383980000	-2.8525460000	-2.6000080000
N	-3.8712690000	1.5904030000	0.0774840000
H	-3.9271250000	1.6132700000	1.1021960000
H	-4.7033400000	2.0665220000	-0.2777770000
H	-3.0497300000	2.1181810000	-0.2353510000
C	-3.8246530000	0.1664550000	-0.3692120000
H	-4.0995290000	0.1505300000	-1.4250850000
C	-2.4072920000	-0.3971450000	-0.1838530000
C	-4.8400890000	-0.6437480000	0.4652400000

H	-2.1845530000	-0.4430290000	0.8903640000
H	-2.4322070000	-1.4257870000	-0.5542440000
C	-1.3492000000	0.3975210000	-0.8908790000
O	-5.2392670000	-0.1135710000	1.5317670000
C	-0.9457920000	0.2703790000	-2.1988740000
C	-0.5686900000	1.4739220000	-0.3336040000
H	-1.2765050000	-0.4291950000	-2.9551010000
N	0.0261430000	1.1970830000	-2.4845760000
C	0.2821230000	1.9487840000	-1.3650220000
C	-0.4931900000	2.0646450000	0.9436460000
H	0.4985930000	1.2890190000	-3.3729970000
C	1.1915340000	2.9960190000	-1.1611980000
C	0.4098980000	3.0963390000	1.1510000000
H	-1.1261270000	1.7099500000	1.7537950000
H	1.8355550000	3.3418880000	-1.9636990000
C	1.2430410000	3.5586770000	0.1057640000
H	0.4843980000	3.5572220000	2.1311080000
H	1.9394210000	4.3683870000	0.3008290000
O	-5.1312460000	-1.7735950000	0.0114140000

Table S54. Cartesian coordinates of β -Glc-tg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.170065			
ZPE / Hartree = 0.4225603			
BSSE / Hartree = 0.0032579203			
C	-1.0239540000	-1.7828270000	-1.2837560000
C	-2.1272770000	-0.9754030000	-1.9629160000
C	-2.6469880000	0.0819990000	-1.0000360000
C	-3.0649800000	-0.5692130000	0.3084810000
C	-1.8975100000	-1.3794500000	0.8725810000
C	-2.2471850000	-2.1137030000	2.1616960000
O	-1.5204870000	-2.3632860000	-0.0847900000
O	-0.6485280000	-2.8059430000	-2.1443320000
O	-1.6332860000	-0.3071270000	-3.1083640000
O	-3.7753600000	0.7667890000	-1.5192770000
O	-3.4269780000	0.4062040000	1.2752540000
O	-2.3440190000	-1.2248570000	3.2641560000
H	-0.1712450000	-1.1294300000	-1.0394140000
H	-2.9419550000	-1.6639160000	-2.2318990000
H	-1.8381480000	0.7965770000	-0.7924330000
H	-3.9110310000	-1.2484200000	0.1224720000
H	-1.0502400000	-0.7037860000	1.0679480000
H	-3.1799730000	-2.6778230000	2.0249310000
H	-1.4442850000	-2.8192250000	2.3893040000
H	0.2215730000	-3.1408240000	-1.8869920000
H	-1.4131520000	-0.9677970000	-3.7795510000
H	-3.4766300000	1.3715580000	-2.2122440000
H	-4.1430950000	0.9461690000	0.9109610000
H	-2.9630010000	-0.5195570000	3.0194580000
N	4.0480470000	1.3548990000	-0.1531210000
H	4.1042860000	1.2218820000	-1.1689130000
H	4.8951670000	1.8529480000	0.1290450000
H	3.2444730000	1.9521100000	0.0680700000
C	3.9488280000	0.0216500000	0.5123400000
H	4.1720290000	0.1735090000	1.5697030000
C	2.5287080000	-0.5411940000	0.3463780000
C	4.9851370000	-0.9283330000	-0.1242290000

H	2.3492170000	-0.7316960000	-0.7197670000
H	2.5136110000	-1.5075460000	0.8571820000
C	1.4598340000	0.3593310000	0.8911840000
O	5.4752520000	-0.5728770000	-1.2247430000
C	1.0073840000	0.4193610000	2.1882170000
C	0.7140370000	1.3526570000	0.1591810000
H	1.3013870000	-0.1691800000	3.0469310000
N	0.0324270000	1.3795620000	2.3023650000
C	-0.1724030000	1.9693450000	1.0797780000
C	0.6994590000	1.7678940000	-1.1876480000
H	-0.4728320000	1.5968210000	3.1502250000
C	-1.0595560000	2.9860280000	0.6986120000
C	-0.1756190000	2.7737560000	-1.5683130000
H	1.3612930000	1.3035810000	-1.9152320000
H	-1.7321320000	3.4409330000	1.4191860000
C	-1.0462700000	3.3781680000	-0.6316250000
H	-0.2010300000	3.1012450000	-2.6030620000
H	-1.7216240000	4.1609490000	-0.9628220000
O	5.2039240000	-1.9864910000	0.5086770000

Table S55. Cartesian coordinates of β -Glc-tg_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.168933			
ZPE / Hartree = 0.422648			
BSSE / Hartree = 0.0030368492			
C	-3.5703320000	-0.6645740000	0.6735050000
C	-2.2191200000	-0.8569850000	1.3552330000
C	-1.6654760000	0.4912580000	1.7892890000
C	-1.6180120000	1.4180880000	0.5864360000
C	-3.0011080000	1.5172980000	-0.0585510000
C	-2.9894430000	2.3601030000	-1.3296890000
O	-3.4209490000	0.2113760000	-0.4371210000
O	-3.9912610000	-1.8997940000	0.1979090000
O	-2.3312310000	-1.6703830000	2.5079520000
O	-0.3461720000	0.3788880000	2.2962420000
O	-1.2000780000	2.7262530000	0.9498720000
O	-2.8537680000	3.7440430000	-1.0497540000
H	-4.3031050000	-0.2352520000	1.3742150000
H	-1.5349600000	-1.3087730000	0.6245610000
H	-2.3265450000	0.9265110000	2.5548400000
H	-0.9246010000	0.9953060000	-0.1538980000
H	-3.7152490000	1.9527970000	0.6586660000
H	-2.1823940000	2.0077370000	-1.9872990000
H	-3.9427140000	2.2283930000	-1.8470330000
H	-4.9415400000	-1.8710620000	0.0205620000
H	-2.4643410000	-2.5859130000	2.2261650000
H	-0.3698380000	-0.1688340000	3.0932140000
H	-0.2832430000	2.6783240000	1.2568390000
H	-2.0669550000	3.8521960000	-0.4928820000
N	4.2451450000	-1.1033380000	-0.6344120000
H	4.2854160000	-1.6057000000	0.2589280000
H	5.1043940000	-1.3286880000	-1.1413290000
H	3.4542010000	-1.4570030000	-1.1823090000
C	4.1240590000	0.3643190000	-0.3822510000
H	4.2862980000	0.8645950000	-1.3386320000
C	2.7199360000	0.6863580000	0.1524990000
C	5.2065770000	0.7881770000	0.6328830000

H	2.6064060000	0.2269230000	1.1424330000
H	2.6783220000	1.7700160000	0.2896060000
C	1.6143510000	0.2279860000	-0.7519130000
O	5.7758250000	-0.1329050000	1.2689420000
C	1.0716550000	0.9167390000	-1.8106900000
C	0.9228040000	-1.0363500000	-0.6978780000
H	1.3057150000	1.9063260000	-2.1797670000
N	0.0896290000	0.1647630000	-2.4077550000
C	-0.0279690000	-1.0354470000	-1.7511070000
C	1.0068670000	-2.1619640000	0.1465620000
H	-0.4656680000	0.4580730000	-3.1995060000
C	-0.8884560000	-2.1177820000	-1.9848650000
C	0.1630580000	-3.2373960000	-0.0854500000
H	1.7207470000	-2.1839430000	0.9664890000
H	-1.6139040000	-2.0920420000	-2.7920600000
C	-0.7764980000	-3.2138550000	-1.1426360000
H	0.2158910000	-4.1110440000	0.5568080000
H	-1.4280470000	-4.0691760000	-1.2926380000
O	5.3832520000	2.0230740000	0.7448250000

Complex Glc-Phe

Table S56. Cartesian coordinates of α -Glc-gg_Phe_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6272032			
ZPE / Hartree = 0.3932709			
BSSE / Hartree = 0.0020739934			
C	1.5180080000	0.9483640000	-0.1544120000
C	2.9561380000	1.1978590000	0.3028080000
C	3.8892350000	0.1438700000	-0.2863060000
C	3.3795220000	-1.2469850000	0.0550720000
C	1.9416930000	-1.3981760000	-0.4364220000
C	1.2996490000	-2.7129590000	-0.0307650000
O	1.1269520000	-0.3745880000	0.1415580000
O	1.4708990000	1.2161220000	-1.5318160000
O	3.3784610000	2.5062650000	-0.0308450000
O	5.1993790000	0.2598030000	0.2462240000
O	4.1586840000	-2.2487890000	-0.5756590000
O	1.2389730000	-2.8611870000	1.3801530000
H	0.8173970000	1.5882020000	0.3910020000
H	2.9879170000	1.1265950000	1.3948150000
H	3.9192470000	0.2510540000	-1.3810800000
H	3.4032380000	-1.3743150000	1.1473060000
H	1.9261620000	-1.3204160000	-1.5322900000
H	0.2952300000	-2.7616410000	-0.4692420000
H	1.8922610000	-3.5445640000	-0.4167840000
H	0.5507880000	1.3784600000	-1.7866730000
H	3.1868420000	2.6468750000	-0.9710330000
H	5.5726480000	1.1041240000	-0.0423200000
H	5.0806110000	-2.1177050000	-0.3121990000
H	0.7695660000	-2.0941240000	1.7383450000
H	-1.9493650000	-1.1313730000	-0.9255900000
H	-1.4663350000	-1.3703060000	0.7612520000
H	-2.9330830000	-3.1931090000	0.6686680000
H	-1.9725560000	1.0721340000	-1.8596910000
C	-2.1452800000	-0.8137720000	0.1052720000
C	-1.8243950000	1.4976200000	-0.8690860000
C	-1.8836230000	0.6639640000	0.2521410000

H	-1.5291070000	3.4994310000	-1.6067090000
C	-1.5785990000	2.8656310000	-0.7263340000
N	-3.7366140000	-2.6724660000	0.3080310000
C	-1.7031400000	1.2236500000	1.5219010000
H	-3.8482800000	-2.8697410000	-0.6945260000
H	-1.7431180000	0.5818410000	2.3991980000
C	-1.3944050000	3.4141530000	0.5436250000
C	-1.4622300000	2.5892560000	1.6690330000
C	-3.5864860000	-1.1942240000	0.4739900000
H	-1.1994120000	4.4760060000	0.6561910000
H	-4.5722610000	-3.0229810000	0.7826310000
H	-1.3186310000	3.0084910000	2.6602260000
C	-4.6072070000	-0.5117430000	-0.4661710000
O	-4.8525620000	-1.1245340000	-1.5367720000
H	-3.7988990000	-0.9523920000	1.5159270000
O	-5.0592670000	0.5928670000	-0.0928080000

Table S57. Cartesian coordinates of α -Glc-gg_Phe_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6285549			
ZPE / Hartree = 0.3934054			
BSSE / Hartree = 0.0022915527			
C	-1.3253320000	-0.2698300000	1.6473100000
C	-1.8027190000	1.0033070000	0.9480210000
C	-3.1248260000	0.7583070000	0.2294690000
C	-2.9809830000	-0.4302620000	-0.7066510000
C	-2.5200600000	-1.6499930000	0.0874060000
C	-2.2507770000	-2.8661770000	-0.7801240000
O	-1.2832160000	-1.3522840000	0.7427170000
O	-2.2051650000	-0.5089400000	2.7149410000
O	-1.8951840000	2.0820380000	1.8588080000
O	-3.4917410000	1.8776560000	-0.5627210000
O	-4.2157630000	-0.7541870000	-1.3214830000
O	-1.2338000000	-2.6183450000	-1.7394110000
H	-0.2980020000	-0.1518640000	2.0062020000
H	-1.0532370000	1.2871270000	0.2036360000
H	-3.9165850000	0.5422340000	0.9630220000
H	-2.2233040000	-0.1894220000	-1.4682450000
H	-3.2880770000	-1.9095540000	0.8290980000
H	-1.9753800000	-3.7067750000	-0.1322180000
H	-3.1561770000	-3.1286480000	-1.3305980000
H	-1.7927730000	-1.1196310000	3.3411600000
H	-2.4229130000	1.7852820000	2.6161460000
H	-3.6511530000	2.6299680000	0.0241180000
H	-4.5504690000	0.0452550000	-1.7523310000
H	-0.4321220000	-2.3687590000	-1.2582350000
H	2.2872980000	-0.5334210000	1.5173890000
H	1.4156780000	-1.5455960000	0.3517960000
H	3.2319110000	-3.0333370000	0.7340190000
H	2.0764470000	1.8275490000	1.4240410000
C	2.1264630000	-0.7161350000	0.4485910000
C	1.6178400000	1.7595070000	0.4403140000
C	1.5539220000	0.5194450000	-0.2023430000
H	1.1465170000	3.8582380000	0.3473000000
C	1.0945360000	2.9031280000	-0.1664580000

N	3.9666860000	-2.3469610000	0.5458990000
C	0.9580740000	0.4425120000	-1.4668400000
H	4.3769960000	-2.0336600000	1.4347490000
H	0.9062920000	-0.5164120000	-1.9777150000
C	0.4986830000	2.8164360000	-1.4252730000
C	0.4320480000	1.5814900000	-2.0754720000
C	3.4604660000	-1.1423210000	-0.1820270000
H	0.0844930000	3.7028860000	-1.8955400000
H	4.7064180000	-2.8197620000	0.0201390000
H	-0.0349190000	1.5045610000	-3.0528080000
C	4.5314530000	-0.0342320000	-0.0406720000
O	5.1654240000	-0.0311300000	1.0454300000
H	3.3282790000	-1.4187000000	-1.2286530000
O	4.6413520000	0.7639490000	-0.9969380000

Table S58. Cartesian coordinates of α -Glc-gg_Phe_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6288845			
ZPE / Hartree = 0.3933954			
BSSE / Hartree = 0.002517554			
C	-1.3253320000	-0.2698300000	1.6473100000
C	-1.8027190000	1.0033070000	0.9480210000
C	-3.1248260000	0.7583070000	0.2294690000
C	-2.9809830000	-0.4302620000	-0.7066510000
C	-2.5200600000	-1.6499930000	0.0874060000
C	-2.2507770000	-2.8661770000	-0.7801240000
O	-1.2832160000	-1.3522840000	0.7427170000
O	-2.2051650000	-0.5089400000	2.7149410000
O	-1.8951840000	2.0820380000	1.8588080000
O	-3.4917410000	1.8776560000	-0.5627210000
O	-4.2157630000	-0.7541870000	-1.3214830000
O	-1.2338000000	-2.6183450000	-1.7394110000
H	-0.2980020000	-0.1518640000	2.0062020000
H	-1.0532370000	1.2871270000	0.2036360000
H	-3.9165850000	0.5422340000	0.9630220000
H	-2.2233040000	-0.1894220000	-1.4682450000
H	-3.2880770000	-1.9095540000	0.8290980000
H	-1.9753800000	-3.7067750000	-0.1322180000
H	-3.1561770000	-3.1286480000	-1.3305980000
H	-1.7927730000	-1.1196310000	3.3411600000
H	-2.4229130000	1.7852820000	2.6161460000
H	-3.6511530000	2.6299680000	0.0241180000
H	-4.5504690000	0.0452550000	-1.7523310000
H	-0.4321220000	-2.3687590000	-1.2582350000
H	2.2872980000	-0.5334210000	1.5173890000
H	1.4156780000	-1.5455960000	0.3517960000
H	3.2319110000	-3.0333370000	0.7340190000
H	2.0764470000	1.8275490000	1.4240410000
C	2.1264630000	-0.7161350000	0.4485910000
C	1.6178400000	1.7595070000	0.4403140000
C	1.5539220000	0.5194450000	-0.2023430000
H	1.1465170000	3.8582380000	0.3473000000

C	1.0945360000	2.9031280000	-0.1664580000
N	3.9666860000	-2.3469610000	0.5458990000
C	0.9580740000	0.4425120000	-1.4668400000
H	4.3769960000	-2.0336600000	1.4347490000
H	0.9062920000	-0.5164120000	-1.9777150000
C	0.4986830000	2.8164360000	-1.4252730000
C	0.4320480000	1.5814900000	-2.0754720000
C	3.4604660000	-1.1423210000	-0.1820270000
H	0.0844930000	3.7028860000	-1.8955400000
H	4.7064180000	-2.8197620000	0.0201390000
H	-0.0349190000	1.5045610000	-3.0528080000
C	4.5314530000	-0.0342320000	-0.0406720000
O	5.1654240000	-0.0311300000	1.0454300000
H	3.3282790000	-1.4187000000	-1.2286530000
O	4.6413520000	0.7639490000	-0.9969380000

Table S59. Cartesian coordinates of α -Glc-gg_Phe_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6270297			
ZPE / Hartree = 0.3930715			
BSSE / Hartree = 0.0024164532			
C	1.9468510000	-2.0704050000	0.3313210000
C	1.6024450000	-1.4457610000	-1.0227880000
C	2.5004550000	-0.2431650000	-1.3026600000
C	2.4202970000	0.7351490000	-0.1407000000
C	2.8328230000	0.0067410000	1.1367200000
C	2.7664180000	0.8620670000	2.3873100000
O	1.9408130000	-1.0928750000	1.3505060000
O	3.2048110000	-2.6766440000	0.1908670000
O	1.6792750000	-2.4033220000	-2.0610770000
O	2.0933000000	0.4428600000	-2.4754430000
O	3.2986110000	1.8305870000	-0.3282880000
O	1.4681950000	1.3869860000	2.6141650000
H	1.1901930000	-2.8023070000	0.6268990000
H	0.5637530000	-1.1022560000	-0.9896330000
H	3.5436570000	-0.5770810000	-1.4109200000
H	1.3814820000	1.0884190000	-0.0389170000
H	3.8619540000	-0.3620540000	1.0262710000
H	3.0964980000	0.2565520000	3.2401980000
H	3.4416800000	1.7131900000	2.2799170000
H	3.3424370000	-3.3071770000	0.9109300000
H	2.5365570000	-2.8504380000	-1.9873430000
H	2.2411300000	-0.1361700000	-3.2358770000
H	3.0898460000	2.2306620000	-1.1847870000
H	0.8437090000	0.6475610000	2.6337830000
H	-1.8334460000	-1.4955990000	-0.2961010000
H	-1.3294590000	-1.0543470000	1.3455540000
H	-3.0456450000	-2.5529150000	1.9947810000
H	-1.4866160000	0.0524570000	-2.0693880000
C	-1.9559050000	-0.7494710000	0.4981800000
C	-1.3222770000	0.8546300000	-1.3531230000
C	-1.5145020000	0.6092090000	0.0095490000
H	-0.7591220000	2.2847290000	-2.8594290000

C	-0.9132520000	2.1125900000	-1.7984590000
N	-3.7750960000	-2.1310520000	1.4153210000
C	-1.3003790000	1.6499250000	0.9202470000
H	-3.9357510000	-2.7177110000	0.5869230000
H	-1.4484510000	1.4709650000	1.9831270000
C	-0.6926440000	3.1416150000	-0.8825680000
C	-0.8903270000	2.9074450000	0.4800700000
C	-3.4241440000	-0.7542520000	0.9497000000
H	-0.3680780000	4.1188110000	-1.2266510000
H	-4.6413240000	-2.1319690000	1.9593370000
H	-0.7175360000	3.7013120000	1.2005680000
C	-4.3721990000	-0.4073230000	-0.2234000000
O	-4.7236450000	-1.3788740000	-0.9404350000
H	-3.5800300000	-0.0721140000	1.7862000000
O	-4.6693260000	0.7988910000	-0.3651800000

Table S60. Cartesian coordinates of α -Glc-gg_Phe_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6281769			
ZPE / Hartree = 0.3933706			
BSSE / Hartree = 0.0023636874			
C	1.9468510000	-2.0704050000	0.3313210000
C	1.6024450000	-1.4457610000	-1.0227880000
C	2.5004550000	-0.2431650000	-1.3026600000
C	2.4202970000	0.7351490000	-0.1407000000
C	2.8328230000	0.0067410000	1.1367200000
C	2.7664180000	0.8620670000	2.3873100000
O	1.9408130000	-1.0928750000	1.3505060000
O	3.2048110000	-2.6766440000	0.1908670000
O	1.6792750000	-2.4033220000	-2.0610770000
O	2.0933000000	0.4428600000	-2.4754430000
O	3.2986110000	1.8305870000	-0.3282880000
O	1.4681950000	1.3869860000	2.6141650000
H	1.1901930000	-2.8023070000	0.6268990000
H	0.5637530000	-1.1022560000	-0.9896330000
H	3.5436570000	-0.5770810000	-1.4109200000
H	1.3814820000	1.0884190000	-0.0389170000
H	3.8619540000	-0.3620540000	1.0262710000
H	3.0964980000	0.2565520000	3.2401980000
H	3.4416800000	1.7131900000	2.2799170000
H	3.3424370000	-3.3071770000	0.9109300000
H	2.5365570000	-2.8504380000	-1.9873430000
H	2.2411300000	-0.1361700000	-3.2358770000
H	3.0898460000	2.2306620000	-1.1847870000
H	0.8437090000	0.6475610000	2.6337830000
H	-1.8334460000	-1.4955990000	-0.2961010000
H	-1.3294590000	-1.0543470000	1.3455540000
H	-3.0456450000	-2.5529150000	1.9947810000
H	-1.4866160000	0.0524570000	-2.0693880000
C	-1.9559050000	-0.7494710000	0.4981800000
C	-1.3222770000	0.8546300000	-1.3531230000
C	-1.5145020000	0.6092090000	0.0095490000
H	-0.7591220000	2.2847290000	-2.8594290000
C	-0.9132520000	2.1125900000	-1.7984590000

N	-3.7750960000	-2.1310520000	1.4153210000
C	-1.3003790000	1.6499250000	0.9202470000
H	-3.9357510000	-2.7177110000	0.5869230000
H	-1.4484510000	1.4709650000	1.9831270000
C	-0.6926440000	3.1416150000	-0.8825680000
C	-0.8903270000	2.9074450000	0.4800700000
C	-3.4241440000	-0.7542520000	0.9497000000
H	-0.3680780000	4.1188110000	-1.2266510000
H	-4.6413240000	-2.1319690000	1.9593370000
H	-0.7175360000	3.7013120000	1.2005680000
C	-4.3721990000	-0.4073230000	-0.2234000000
O	-4.7236450000	-1.3788740000	-0.9404350000
H	-3.5800300000	-0.0721140000	1.7862000000
O	-4.6693260000	0.7988910000	-0.3651800000

Table S61. Cartesian coordinates of α -Glc-gg_Phe_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6267441			
ZPE / Hartree = 0.3930209			
BSSE / Hartree = 0.0021947019			
C	3.0020820000	-0.4996440000	-1.5620660000
C	3.6238130000	-1.0215190000	-0.2651090000
C	2.6521560000	-0.8512000000	0.8998880000
C	2.1927360000	0.5954200000	0.9798200000
C	1.5737890000	0.9949300000	-0.3575010000
C	1.1231780000	2.4421110000	-0.4122650000
O	2.5448600000	0.8252390000	-1.3951970000
O	1.9609860000	-1.3799960000	-1.8983000000
O	4.0352890000	-2.3684590000	-0.4010520000
O	3.2708060000	-1.1747520000	2.1349310000
O	1.2111080000	0.7698080000	1.9866680000
O	2.1773360000	3.3481810000	-0.1219220000
H	3.7479460000	-0.4532590000	-2.3595000000
H	4.5259170000	-0.4372520000	-0.0572320000
H	1.7707230000	-1.4927710000	0.7432610000
H	3.0641670000	1.2360220000	1.1798180000
H	0.7047350000	0.3555690000	-0.5583420000
H	0.7019510000	2.6390290000	-1.4057250000
H	0.3401400000	2.6046400000	0.3336670000
H	1.7305260000	-1.2668520000	-2.8305980000
H	3.2894510000	-2.8687230000	-0.7670710000
H	3.5177760000	-2.1099670000	2.1174640000
H	1.5832320000	0.4529680000	2.8219590000
H	2.8644360000	3.2345380000	-0.7930920000
H	-1.0322250000	-1.2596390000	-0.5490860000
H	-0.7475780000	-0.9623750000	1.1748240000
H	-1.3103170000	-3.2512380000	1.3985340000
H	-1.8325670000	0.4920770000	-1.9499940000
C	-1.4933720000	-0.8878130000	0.3740750000
C	-2.0405180000	1.1072620000	-1.0770760000
C	-1.9055930000	0.5534860000	0.1992610000
H	-2.5292430000	2.8545360000	-2.2353620000

C	-2.4328260000	2.4371430000	-1.2375880000
N	-2.1763040000	-3.1977440000	0.8564750000
C	-2.1668260000	1.3547670000	1.3164910000
H	-2.0135580000	-3.5716020000	-0.0867620000
H	-2.0535220000	0.9343420000	2.3133070000
C	-2.6922050000	3.2288360000	-0.1186540000
C	-2.5580410000	2.6839470000	1.1607120000
C	-2.6809370000	-1.7963780000	0.7233890000
H	-2.9930860000	4.2647260000	-0.2409590000
H	-2.8650070000	-3.8036800000	1.3091240000
H	-2.7532090000	3.2959020000	2.0361390000
C	-3.7416140000	-1.7878930000	-0.4020540000
O	-3.5317110000	-2.5896350000	-1.3479360000
H	-3.1264120000	-1.5119000000	1.6772610000
O	-4.6793090000	-0.9693370000	-0.2815530000

Table S62. Cartesian coordinates of α -Glc-gt_Phe_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6263829			
ZPE / Hartree = 0.3929509			
BSSE / Hartree = 0.0019202445			
C	1.6182140000	0.6988780000	0.9651250000
C	1.2747460000	-0.7852670000	1.0929650000
C	2.4760170000	-1.6447580000	0.7113250000
C	2.9646010000	-1.2603280000	-0.6763120000
C	3.2671100000	0.2350940000	-0.7149480000
C	3.6244680000	0.7168190000	-2.1085450000
O	2.1052010000	0.9756820000	-0.3308530000
O	2.5599650000	0.9937800000	1.9638350000
O	0.8045470000	-1.0932590000	2.3910220000
O	2.1343120000	-3.0212660000	0.6724470000
O	4.1531890000	-1.9541410000	-1.0128790000
O	3.9331510000	2.1018070000	-2.1119060000
H	0.7228330000	1.3158090000	1.0780580000
H	0.4551000000	-1.0059820000	0.4011010000
H	3.2919090000	-1.4813330000	1.4310680000
H	2.1695700000	-1.4858690000	-1.4046520000
H	4.0922630000	0.4589490000	-0.0248290000
H	4.5120500000	0.1888650000	-2.4614770000
H	2.7889470000	0.5021520000	-2.7886830000
H	2.5779860000	1.9487050000	2.1150490000
H	1.4375780000	-0.7295930000	3.0297660000
H	1.9135390000	-3.3073000000	1.5697050000
H	3.9851320000	-2.9008890000	-0.9017630000
H	3.1572960000	2.5771710000	-1.7833740000
H	-1.7991600000	-1.3454660000	-0.7343200000
H	-1.9218520000	-1.5598750000	1.0225440000
H	-3.5076340000	-3.2226380000	0.3345910000
H	-1.3199990000	0.7970560000	-1.6737830000
C	-2.2743470000	-0.9600310000	0.1752600000
C	-1.4307720000	1.2566250000	-0.6942070000
C	-1.8944510000	0.4865200000	0.3769900000
H	-0.7473170000	3.1877690000	-1.3555690000

C	-1.1096240000	2.6032230000	-0.5152840000
N	-4.0666870000	-2.5898040000	-0.2424880000
C	-2.0222530000	1.0837930000	1.6360710000
H	-3.8565250000	-2.7598670000	-1.2342160000
H	-2.3713500000	0.4885590000	2.4767740000
C	-1.2482710000	3.1937700000	0.7415900000
C	-1.7035270000	2.4294610000	1.8188290000
C	-3.7936450000	-1.1479240000	0.0482860000
H	-0.9970290000	4.2403050000	0.8833560000
H	-5.0522260000	-2.8228460000	-0.0960040000
H	-1.8057470000	2.8802280000	2.8012400000
C	-4.3638320000	-0.3227070000	-1.1294930000
O	-4.2774970000	-0.8655130000	-2.2606380000
H	-4.3005140000	-0.8929900000	0.9793170000
O	-4.8209480000	0.8077450000	-0.8525750000

Table S63. Cartesian coordinates of α -Glc-gt_Phe_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6279686			
ZPE / Hartree = 0.393197			
BSSE / Hartree = 0.0023188824			
C	2.8680460000	0.7890540000	-0.7328880000
C	2.1211980000	1.2124750000	0.5319840000
C	2.1314170000	0.0891730000	1.5638810000
C	1.5975950000	-1.1903990000	0.9416370000
C	2.3976940000	-1.5274270000	-0.3121720000
C	1.8142730000	-2.7109550000	-1.0613270000
O	2.3511360000	-0.4282390000	-1.2257980000
O	4.2275300000	0.6928590000	-0.3981440000
O	2.6525350000	2.4105600000	1.0656240000
O	1.2935050000	0.3983590000	2.6676040000
O	1.7029920000	-2.2835200000	1.8370710000
O	2.5757220000	-3.0174190000	-2.2185110000
H	2.7115480000	1.5157930000	-1.5355540000
H	1.0837400000	1.4257040000	0.2592350000
H	3.1603940000	-0.0875800000	1.9118180000
H	0.5463120000	-1.0271860000	0.6584930000
H	3.4410170000	-1.7376120000	-0.0385700000
H	1.8318550000	-3.5948120000	-0.4214110000
H	0.7720110000	-2.4860440000	-1.3284840000
H	4.7596230000	0.6999920000	-1.2056430000
H	3.6113460000	2.2961100000	1.1550010000
H	1.6515580000	1.1778580000	3.1147380000
H	1.2560830000	-2.0362500000	2.6593670000
H	2.5829280000	-2.2311560000	-2.7822270000
H	-1.8468200000	-1.3695370000	0.2777730000
H	-1.7364610000	-0.4292550000	1.7767630000
H	-3.5687680000	-1.7457690000	2.4400270000
H	-1.0454900000	-0.4273730000	-1.7443640000
C	-2.1365080000	-0.4257950000	0.7553010000
C	-1.0406870000	0.5640160000	-1.2966120000
C	-1.5592000000	0.7397630000	-0.0104800000
H	-0.0991790000	1.4901930000	-2.9968680000
C	-0.5079570000	1.6446990000	-2.0026710000

N	-4.1367920000	-1.5652410000	1.6087890000
C	-1.5392610000	2.0189200000	0.5592510000
H	-4.1003630000	-2.3834750000	0.9876140000
H	-1.9315040000	2.1634820000	1.5633600000
C	-0.4945910000	2.9163050000	-1.4290700000
C	-1.0133330000	3.1014800000	-0.1446440000
C	-3.6693740000	-0.3733200000	0.8371230000
H	-0.0776030000	3.7569170000	-1.9750700000
H	-5.1074410000	-1.4604470000	1.9136680000
H	-1.0000790000	4.0870300000	0.3107390000
C	-4.3088300000	-0.4486180000	-0.5695560000
O	-4.4890570000	-1.6083070000	-1.0209680000
H	-4.0046990000	0.5187630000	1.3669610000
O	-4.5512820000	0.6413450000	-1.1328060000

Table S64. Cartesian coordinates of α -Glc-gt_Phe_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6286916			
ZPE / Hartree = 0.3932052			
BSSE / Hartree = 0.0025360913			
C	-2.4236700000	0.5582860000	1.7535210000
C	-2.6060790000	-0.9102260000	1.3563820000
C	-2.1261380000	-1.1392140000	-0.0742020000
C	-2.7862730000	-0.1538210000	-1.0247390000
C	-2.5232640000	1.2654250000	-0.5342830000
C	-3.2374780000	2.3148030000	-1.3638450000
O	-3.0237700000	1.4079660000	0.7979390000
O	-1.0444740000	0.7869250000	1.8703460000
O	-1.9442460000	-1.7671670000	2.2667710000
O	-2.4489680000	-2.4446840000	-0.5297460000
O	-2.2521000000	-0.2778330000	-2.3314370000
O	-2.9491680000	3.6233840000	-0.8962080000
H	-2.9368450000	0.7725210000	2.6944940000
H	-3.6721750000	-1.1514040000	1.4170260000
H	-1.0389830000	-0.9864850000	-0.1209140000
H	-3.8726050000	-0.3369150000	-1.0355020000
H	-1.4406800000	1.4594020000	-0.5460180000
H	-2.8933650000	2.2596760000	-2.3981660000
H	-4.3182790000	2.1207490000	-1.3378240000
H	-0.8957970000	1.6029620000	2.3675440000
H	-1.0111440000	-1.5014610000	2.2944470000
H	-1.7937800000	-3.0641650000	-0.1790940000
H	-2.2370680000	-1.2214280000	-2.5508560000
H	-3.2227530000	3.6706130000	0.0306210000
H	1.9183750000	1.6376290000	-0.3833420000
H	1.5301440000	1.2504100000	1.3031330000
H	3.3027380000	2.7456770000	1.8071760000
H	1.4986460000	0.0145470000	-2.0837590000
C	2.0946000000	0.9178670000	0.4245120000
C	1.3713730000	-0.7571970000	-1.3282410000
C	1.6214250000	-0.4546630000	0.0131930000
H	0.7637860000	-2.2567120000	-2.7493090000

C	0.9591910000	-2.0379290000	-1.7037510000
N	3.9837810000	2.3076170000	1.1821430000
C	1.4451280000	-1.4551760000	0.9772910000
H	4.0817160000	2.8768190000	0.3321100000
H	1.6271050000	-1.2257000000	2.0256360000
C	0.7965220000	-3.0318160000	-0.7383530000
C	1.0359990000	-2.7359810000	0.6065650000
C	3.5904790000	0.9231290000	0.7749700000
H	0.4785110000	-4.0288220000	-1.0290780000
H	4.8892940000	2.3135180000	1.6580840000
H	0.9013370000	-3.5013820000	1.3652960000
C	4.4546650000	0.5364320000	-0.4488650000
O	4.7452110000	1.4814940000	-1.2258080000
H	3.7965150000	0.2610070000	1.6166530000
O	4.7500110000	-0.6730700000	-0.5661420000

Table S65. Cartesian coordinates of α -Glc-gt_Phe_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6277836			
ZPE / Hartree = 0.3928945			
BSSE / Hartree = 0.0023248882			
C	1.9849990000	-1.2750290000	-1.4795170000
C	2.3591120000	0.2069540000	-1.5674130000
C	3.0815580000	0.6625220000	-0.3016460000
C	2.2642430000	0.2974180000	0.9272580000
C	1.9933870000	-1.2029330000	0.9141880000
C	1.1161200000	-1.6485860000	2.0686130000
O	1.2843200000	-1.5403520000	-0.2821580000
O	3.1802590000	-2.0051490000	-1.5683440000
O	3.1312560000	0.4695330000	-2.7238480000
O	3.2573240000	2.0709140000	-0.2917340000
O	2.9606070000	0.6112730000	2.1210930000
O	0.8451260000	-3.0402050000	2.0017840000
H	1.2975560000	-1.5502920000	-2.2839340000
H	1.4369910000	0.7873350000	-1.6672290000
H	4.0599790000	0.1627650000	-0.2342390000
H	1.3034700000	0.8352640000	0.8902970000
H	2.9448330000	-1.7521120000	0.9433460000
H	1.6341550000	-1.4651700000	3.0115730000
H	0.1844840000	-1.0678630000	2.0602340000
H	2.9841640000	-2.9203150000	-1.8112990000
H	3.8579140000	-0.1723800000	-2.7444230000
H	3.8607160000	2.3098940000	-1.0089840000
H	3.2086100000	1.5461680000	2.0810110000
H	0.4330820000	-3.2163970000	1.1440370000
H	-1.8648420000	-1.1915770000	-0.8193040000
H	-1.7977290000	-1.4972630000	0.9248750000
H	-3.6853940000	-2.8513440000	0.4765250000
H	-1.1295460000	0.8974570000	-1.7083210000
C	-2.1569980000	-0.7972380000	0.1606950000
C	-1.0625390000	1.3092990000	-0.7034970000
C	-1.5366890000	0.5612320000	0.3773010000
H	-0.1247510000	3.1354410000	-1.3524410000

C	-0.4989430000	2.5710030000	-0.5032790000
N	-4.2159160000	-2.1290000000	-0.0166260000
C	-1.4430360000	1.1005040000	1.6661350000
H	-4.1755800000	-2.3063060000	-1.0282180000
H	-1.8052550000	0.5232990000	2.5142900000
C	-0.4059700000	3.0990580000	0.7844400000
C	-0.8813470000	2.3600440000	1.8708510000
C	-3.6905220000	-0.7520780000	0.2331110000
H	0.0382450000	4.0769680000	0.9425430000
H	-5.1943430000	-2.2123420000	0.2689710000
H	-0.8092090000	2.7623500000	2.8767400000
C	-4.2756910000	0.1728380000	-0.8603370000
O	-4.4368810000	-0.3596620000	-1.9881510000
H	-4.0269890000	-0.4411680000	1.2227700000
O	-4.4976700000	1.3587160000	-0.5316240000

Table S66. Cartesian coordinates of α -Glc-gt_Phe_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6265183			
ZPE / Hartree = 0.393196			
BSSE / Hartree = 0.0025421589			
C	2.2463380000	-2.0117820000	-0.8185910000
C	1.8728900000	-2.1846410000	0.6559990000
C	1.4489870000	-0.8427560000	1.2429330000
C	2.5268530000	0.2033170000	1.0187970000
C	2.8250640000	0.2899580000	-0.4750710000
C	3.9752410000	1.2265100000	-0.7896050000
O	3.2166680000	-0.9964610000	-0.9637290000
O	1.0583110000	-1.7146220000	-1.5048020000
O	0.8548730000	-3.1550160000	0.8148680000
O	1.2140290000	-0.9269950000	2.6390770000
O	2.0903160000	1.4805550000	1.4508540000
O	4.2025620000	1.3105800000	-2.1879820000
H	2.7115040000	-2.9179820000	-1.2150600000
H	2.7495810000	-2.5553470000	1.1965040000
H	0.5394820000	-0.4998540000	0.7323490000
H	3.4400890000	-0.0945520000	1.5579550000
H	1.9216400000	0.6268020000	-1.0034910000
H	3.7310730000	2.2323890000	-0.4428110000
H	4.8774470000	0.8796280000	-0.2680450000
H	1.1862480000	-1.8600670000	-2.4522440000
H	0.1345730000	-2.9271570000	0.2062190000
H	0.4329700000	-1.4791330000	2.7842420000
H	1.7143030000	1.3812670000	2.3378250000
H	4.3907760000	0.4178090000	-2.5097280000
H	-1.2815550000	3.5732980000	2.3329980000
O	-4.4200660000	1.1133820000	-1.0202350000
H	-0.2891110000	4.4899480000	0.2456570000
H	-4.0622890000	-0.1934840000	1.1520380000
C	-1.2009240000	2.9489380000	1.4483090000
C	-0.6433290000	3.4641940000	0.2759540000
C	-4.0930770000	-0.0932920000	-1.0324470000
O	-4.0877910000	-0.8833030000	-2.0109710000
H	-2.0776080000	1.2271440000	2.4034180000

C	-1.6500660000	1.6291930000	1.4874630000
C	-0.5345270000	2.6513860000	-0.8527740000
C	-3.5897120000	-0.6896520000	0.3036390000
H	-0.0935100000	3.0413270000	-1.7653480000
H	-4.9973250000	-2.2316570000	0.5081110000
C	-1.5548110000	0.8110330000	0.3561070000
C	-0.9895620000	1.3324740000	-0.8115280000
H	-3.8036630000	-2.5337610000	-0.5913810000
N	-3.9947720000	-2.1288140000	0.3334740000
C	-2.0588330000	-0.6116210000	0.3997770000
H	-0.9030810000	0.6993140000	-1.6919840000
H	-1.7456850000	-1.0855640000	1.3385950000
H	-3.4995500000	-2.6667840000	1.0487210000
H	-1.6273090000	-1.1863790000	-0.4292610000

Table S67. Cartesian coordinates of α -Glc-gt_Phe_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6248461			
ZPE / Hartree = 0.3932003			
BSSE / Hartree = 0.001470314			
C	3.4607570000	-1.3885520000	1.1032520000
C	3.4888050000	-1.6224780000	-0.4089620000
C	3.5209350000	-0.2908900000	-1.1545840000
C	2.3697330000	0.5885780000	-0.6942240000
C	2.4311130000	0.7588160000	0.8201460000
C	1.2370600000	1.5211880000	1.3621440000
O	2.3971200000	-0.5264260000	1.4480500000
O	4.7109940000	-0.8608120000	1.4594880000
O	4.5776630000	-2.4465790000	-0.7787840000
O	3.3743890000	-0.4800590000	-2.5529940000
O	2.4361690000	1.8760230000	-1.2811080000
O	1.3182090000	1.6724410000	2.7715110000
H	3.2630120000	-2.3214200000	1.6373080000
H	2.5782550000	-2.1610810000	-0.6901810000
H	4.4687110000	0.2262880000	-0.9427610000
H	1.4207620000	0.0956700000	-0.9585530000
H	3.3589260000	1.2788420000	1.0959090000
H	1.2168510000	2.5238940000	0.9307110000
H	0.3131850000	0.9984350000	1.0766630000
H	4.8450560000	-0.9619600000	2.4116810000
H	5.3805230000	-2.0655620000	-0.3906540000
H	4.1455180000	-0.9637020000	-2.8797580000
H	2.4470100000	1.7646850000	-2.2425430000
H	1.3667740000	0.7872970000	3.1590270000
H	-2.5755510000	-1.6242860000	0.7275720000
H	-2.8933160000	-0.5135060000	2.0711060000
H	-4.7800450000	-1.8654730000	2.4601970000
H	-1.5097010000	-0.8270190000	-1.2704150000
C	-3.0258040000	-0.6617210000	0.9938940000
C	-1.6103780000	0.1971240000	-0.9179880000
C	-2.3472700000	0.4566290000	0.2410290000
H	-0.4279480000	1.0226790000	-2.5173100000

C	-1.0042700000	1.2395370000	-1.6221750000
N	-5.1228160000	-1.8456380000	1.4965690000
C	-2.4649050000	1.7785530000	0.6871780000
H	-4.8865220000	-2.7311960000	1.0315180000
H	-3.0298890000	1.9880920000	1.5926630000
C	-1.1292700000	2.5539700000	-1.1728750000
C	-1.8622360000	2.8216720000	-0.0145030000
C	-4.5318500000	-0.7273670000	0.6988090000
H	-0.6521190000	3.3637890000	-1.7164910000
H	-6.1432380000	-1.7835590000	1.5304560000
H	-1.9579170000	3.8415340000	0.3458110000
C	-4.7976880000	-1.0320650000	-0.7939650000
O	-4.7878250000	-2.2503170000	-1.1062980000
H	-5.0302960000	0.1945470000	1.0003500000
O	-4.9600590000	-0.0474570000	-1.5475330000

Table S68. Cartesian coordinates of α -Glc-tg_Phe_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6255793			
ZPE / Hartree = 0.3934119			
BSSE / Hartree = 0.0019389675			
C	1.4815700000	0.8238470000	0.9168790000
C	1.1219650000	-0.6630820000	0.9240960000
C	2.3728450000	-1.5192710000	0.7423590000
C	3.1144640000	-1.0693460000	-0.5041850000
C	3.4346670000	0.4218010000	-0.4053260000
C	4.0958770000	0.9675750000	-1.6667750000
O	2.2192320000	1.1519480000	-0.2424170000
O	2.2037580000	1.0747730000	2.0945410000
O	0.4237140000	-1.0140300000	2.1032660000
O	2.0382580000	-2.8870310000	0.5732600000
O	4.3414570000	-1.7684120000	-0.6608920000
O	5.4399480000	0.5317840000	-1.7945090000
H	0.5813150000	1.4418910000	0.8712200000
H	0.4429460000	-0.8556840000	0.0856690000
H	3.0348690000	-1.3982530000	1.6129200000
H	2.4710970000	-1.2352270000	-1.3819850000
H	4.0987100000	0.5958260000	0.4528680000
H	3.5016380000	0.6790680000	-2.5445220000
H	4.1171180000	2.0582650000	-1.6056640000
H	2.1781610000	2.0210080000	2.2914130000
H	0.9232950000	-0.6612170000	2.8560400000
H	1.6215150000	-3.2016370000	1.3876020000
H	4.1458910000	-2.7107570000	-0.7619500000
H	5.4407240000	-0.4357010000	-1.7289870000
O	-4.6681660000	-1.2456180000	-2.0570870000
O	-4.9853900000	0.6903370000	-0.9484160000
C	-4.5915470000	-0.4920320000	-1.0532490000
H	-4.0445770000	-2.9038780000	-0.7937220000
H	-5.0969680000	-2.7825930000	0.4715900000
H	-4.3020240000	-0.6920290000	1.1038500000
C	-3.8828970000	-1.0967740000	0.1819450000
N	-4.1423880000	-2.5688420000	0.1728320000

H	-3.5017810000	-3.0859880000	0.7795500000
H	-1.3817290000	0.6565030000	-1.9125090000
H	-0.7880970000	3.0631640000	-1.8609830000
C	-1.5060310000	1.2271580000	-0.9951680000
C	-1.1727930000	2.5831400000	-0.9662920000
C	-2.3647710000	-0.8733150000	0.1194550000
C	-1.9968690000	0.5899400000	0.1478440000
C	-1.3316620000	3.3172370000	0.2094350000
H	-1.0726970000	4.3711680000	0.2341660000
H	-1.9803180000	-1.3397370000	-0.7954560000
C	-2.1451180000	1.3319890000	1.3261000000
C	-1.8193500000	2.6872660000	1.3575600000
H	-2.5129270000	0.8416310000	2.2247500000
H	-1.9387430000	3.2502260000	2.2782740000
H	-1.9052810000	-1.3809580000	0.9760060000

Table S69. Cartesian coordinates of α -Glc-tg_Phe_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6270778			
ZPE / Hartree = 0.3935588			
BSSE / Hartree = 0.0023229316			
C	-2.8363360000	-0.9494190000	-0.8622360000
C	-2.1711920000	-1.2144320000	0.4884710000
C	-2.2441680000	0.0223100000	1.3787810000
C	-1.6680050000	1.2088230000	0.6280140000
C	-2.3995620000	1.4008620000	-0.6991140000
C	-1.7794310000	2.5059120000	-1.5484280000
O	-2.2964570000	0.2049060000	-1.4708830000
O	-4.2143620000	-0.8271020000	-0.6244800000
O	-2.7326010000	-2.3480260000	1.1222450000
O	-1.4701670000	-0.1472080000	2.5564740000
O	-1.7918040000	2.4114910000	1.3743890000
O	-2.0586990000	3.7968980000	-1.0312760000
H	-2.6290690000	-1.7656260000	-1.5605810000
H	-1.1180970000	-1.4479250000	0.3083900000
H	-3.2907000000	0.2365900000	1.6425900000
H	-0.6080720000	1.0056780000	0.4136840000
H	-3.4548680000	1.6398950000	-0.5062320000
H	-0.6959650000	2.3365860000	-1.6274730000
H	-2.2107220000	2.4617700000	-2.5513150000
H	-4.6969290000	-0.9338200000	-1.4558320000
H	-3.6963140000	-2.2403330000	1.1242300000
H	-1.8515040000	-0.8710970000	3.0726320000
H	-1.2994930000	2.3092040000	2.2015160000
H	-1.7920310000	3.8024470000	-0.0989000000
O	4.4734080000	1.4012660000	-1.1901120000
O	4.5688260000	-0.8312060000	-0.8983910000
C	4.2924220000	0.3364640000	-0.5463180000
H	4.0060510000	2.5145940000	0.6474020000
H	5.0091680000	1.7717610000	1.7278230000
H	3.9213780000	-0.2823260000	1.5177000000
C	3.6027820000	0.5008810000	0.8291260000
N	4.0422800000	1.8124320000	1.3968200000
H	3.4602250000	2.1220100000	2.1791200000

H	1.117200000	0.090560000	-1.832756000
H	0.251496000	-2.022662000	-2.796726000
C	1.091353000	-0.812388000	-1.226656000
C	0.604505000	-2.003090000	-1.769903000
C	2.073945000	0.520480000	0.682208000
C	1.538759000	-0.763641000	0.096688000
C	0.565904000	-3.161264000	-0.993001000
H	0.184956000	-4.087313000	-1.412449000
H	1.796630000	1.367476000	0.042792000
C	1.491354000	-1.929053000	0.871493000
C	1.011203000	-3.121461000	0.331044000
H	1.826471000	-1.898116000	1.905861000
H	0.976280000	-4.016941000	0.944062000
H	1.631599000	0.686508000	1.671983000

Table S70. Cartesian coordinates of α -Glc-tg_Phe_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6283631			
ZPE / Hartree = 0.3939175			
BSSE / Hartree = 0.0026622507			
C	3.3988710000	0.0382090000	-1.1966730000
C	3.3372040000	-0.8367200000	0.0614670000
C	2.0791480000	-0.5273500000	0.8693650000
C	1.9923200000	0.9659780000	1.1304110000
C	2.0136090000	1.7114260000	-0.2008520000
C	1.9714930000	3.2264260000	-0.0357950000
O	3.2327190000	1.4049730000	-0.8760080000
O	2.3963780000	-0.4215540000	-2.0634920000
O	3.4137430000	-2.2081360000	-0.2766600000
O	2.0909150000	-1.1847390000	2.1277200000
O	0.7911000000	1.3031600000	1.8079870000
O	0.6814190000	3.6793650000	0.3458740000
H	4.3831670000	-0.0293220000	-1.6668250000
H	4.2156030000	-0.6155500000	0.6763130000
H	1.1939870000	-0.8339950000	0.2970430000
H	2.8626940000	1.2819430000	1.7267320000
H	1.1528690000	1.3941370000	-0.8084530000
H	2.7317430000	3.5388560000	0.6928650000
H	2.2012730000	3.6905280000	-0.9978340000
H	2.5732710000	-0.1021540000	-2.9589090000
H	2.7123150000	-2.3913980000	-0.9217890000
H	1.7463020000	-2.0809090000	2.0111740000
H	0.7236350000	0.7433940000	2.5957820000
H	0.4243320000	3.1956920000	1.1459230000
O	-5.0612410000	0.4533800000	0.8914610000
O	-4.5454020000	-1.3297190000	-0.3859240000
C	-4.4505620000	-0.1320460000	-0.0391150000
H	-4.3177080000	2.3296460000	0.1293670000
H	-4.6798880000	2.2793530000	-1.4822180000
H	-3.3558720000	0.4093800000	-1.8522160000
C	-3.4265920000	0.7320120000	-0.8129350000
N	-3.9276410000	2.1408930000	-0.8031130000

H	-3.1951510000	2.8248020000	-1.0094050000
H	-1.7605040000	-0.9501440000	2.0123700000
H	-0.7151220000	-3.1977840000	2.0736320000
C	-1.3633340000	-1.3896370000	1.1003310000
C	-0.7722950000	-2.6541460000	1.1349740000
C	-2.0507890000	0.7081680000	-0.1315090000
C	-1.4378130000	-0.6702340000	-0.0963090000
C	-0.2462270000	-3.2123120000	-0.0313000000
H	0.2235680000	-4.1908480000	-0.0048710000
H	-2.1585670000	1.0967950000	0.8877290000
C	-0.9191210000	-1.2425380000	-1.2638860000
C	-0.3263360000	-2.5043760000	-1.2335570000
H	-0.9630910000	-0.6864940000	-2.1979110000
H	0.0852050000	-2.9301180000	-2.1440640000
H	-1.3850750000	1.3869480000	-0.6780210000

Table S71. Cartesian coordinates of α -Glc-tg_Phe_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6269306			
ZPE / Hartree = 0.3930205			
BSSE / Hartree = 0.0022522322			
C	1.854200000	-2.000900000	-0.699828000
C	2.143784000	-0.786811000	-1.586252000
C	2.930649000	0.275097000	-0.820822000
C	2.213259000	0.596547000	0.478715000
C	2.029914000	-0.685725000	1.287564000
C	1.272812000	-0.461485000	2.591748000
O	1.255239000	-1.605273000	0.517334000
O	3.076212000	-2.660627000	-0.497033000
O	2.813780000	-1.169296000	-2.772356000
O	3.026048000	1.475722000	-1.570229000
O	2.951955000	1.516505000	1.271567000
O	2.077980000	0.184453000	3.565655000
H	1.126503000	-2.663371000	-1.176129000
H	1.187784000	-0.351494000	-1.892864000
H	3.937481000	-0.104080000	-0.588036000
H	1.220612000	1.011138000	0.248131000
H	3.012672000	-1.120653000	1.518078000
H	0.360138000	0.115309000	2.390944000
H	0.987708000	-1.433265000	3.002629000
H	2.909102000	-3.564582000	-0.196669000
H	3.572428000	-1.717094000	-2.518144000
H	3.524545000	1.291402000	-2.378534000
H	3.005348000	2.356166000	0.793479000
H	2.415915000	1.001020000	3.166291000
O	-4.462548000	-1.342495000	-1.415833000
O	-4.585355000	0.855599000	-0.934970000
C	-4.316356000	-0.337319000	-0.674237000
H	-4.115705000	-2.601816000	0.349592000
H	-5.138105000	-1.932854000	1.461609000
H	-4.014831000	0.113877000	1.444022000
C	-3.683167000	-0.619772000	0.708553000
N	-4.163120000	-1.964472000	1.154671000

H	-3.6072520000	-2.3472270000	1.9239370000
H	-1.3131540000	-0.0408220000	-1.8915890000
H	-0.3332480000	2.0902070000	-2.6944590000
C	-1.1847380000	0.7920410000	-1.2033060000
C	-0.6355130000	1.9926820000	-1.6558880000
C	-2.1503300000	-0.6615780000	0.6207540000
C	-1.5640750000	0.6402140000	0.1334590000
C	-0.4624980000	3.0588310000	-0.7724440000
H	-0.0270050000	3.9905270000	-1.1202780000
H	-1.8612310000	-1.4744910000	-0.0554630000
C	-1.3961790000	1.7180850000	1.0106740000
C	-0.8480020000	2.9199440000	0.5631890000
H	-1.6864790000	1.6087010000	2.0534070000
H	-0.7151290000	3.7445490000	1.2569860000
H	-1.7552980000	-0.8956530000	1.6160050000

Table S72. Cartesian coordinates of α -Glc-tg_Phe_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6248165			
ZPE / Hartree = 0.393481			
BSSE / Hartree = 0.0018123806			
C	-3.9983630000	0.8526580000	1.1078960000
C	-4.3324320000	-0.2857180000	0.1395900000
C	-3.0660640000	-0.7856700000	-0.5520970000
C	-2.3519640000	0.3888430000	-1.1970960000
C	-2.0478640000	1.4433860000	-0.1353070000
C	-1.3706830000	2.6814010000	-0.7120660000
O	-3.2746610000	1.8743600000	0.4530510000
O	-3.2705720000	0.2833570000	2.1644510000
O	-5.0079590000	-1.3362790000	0.8034650000
O	-3.3669910000	-1.7193240000	-1.5762420000
O	-1.1217460000	-0.0018650000	-1.7878980000
O	-0.0003100000	2.4440580000	-0.9982110000
H	-4.9098100000	1.3323620000	1.4734810000
H	-5.0198850000	0.0987420000	-0.6206280000
H	-2.3954200000	-1.2446470000	0.1895950000
H	-3.0105490000	0.8339870000	-1.9589760000
H	-1.3937430000	1.0085170000	0.6329230000
H	-1.9098110000	3.0165010000	-1.6087200000
H	-1.4072040000	3.4796080000	0.0332270000
H	-3.2819510000	0.8804030000	2.9250380000
H	-4.4920380000	-1.5655480000	1.5919410000
H	-3.7427050000	-2.5118770000	-1.1684380000
H	-1.2964670000	-0.7062530000	-2.4284830000
H	0.0527880000	1.6474990000	-1.5498900000
O	5.8857740000	-0.3627590000	-0.5589510000
O	4.7811640000	-1.5276590000	1.0221630000
C	5.0343940000	-0.4997440000	0.3564880000
H	5.5541830000	1.8155150000	-0.4475970000
H	5.7237860000	2.0657310000	1.1757970000
H	3.8578330000	0.7624380000	1.6989110000
C	4.1735950000	0.7499750000	0.6550440000
N	5.0345820000	1.9513730000	0.4281170000
H	4.4948310000	2.8185170000	0.3711740000

H	2.6945990000	-1.4246420000	-1.8009830000
H	1.1589110000	-3.3352140000	-1.4285110000
C	2.0114400000	-1.4158150000	-0.9548160000
C	1.1485650000	-2.4929510000	-0.7432670000
C	2.9625600000	0.8318200000	-0.2863140000
C	2.0109040000	-0.3217860000	-0.0843790000
C	0.2740530000	-2.4854050000	0.3438390000
H	-0.4022720000	-3.3193970000	0.5065330000
H	3.3236990000	0.8492850000	-1.3207480000
C	1.1269730000	-0.3207870000	1.0007540000
C	0.2639680000	-1.3942850000	1.2157570000
H	1.1109020000	0.5323570000	1.6759100000
H	-0.4234120000	-1.3751470000	2.0570090000
H	2.4395830000	1.7750160000	-0.0941680000

Table S73. Cartesian coordinates of α -Glc-tg_Phe_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6259172			
ZPE / Hartree = 0.3931813			
BSSE / Hartree = 0.0020588513			
C	-1.5203210000	-1.6741520000	-1.0739440000
C	-1.7920370000	-1.9520360000	0.4055850000
C	-2.8793430000	-1.0198590000	0.9343410000
C	-2.4939980000	0.4186210000	0.6397050000
C	-2.2464900000	0.5970040000	-0.8576660000
C	-1.7395290000	1.9942150000	-1.2004690000
O	-1.2286860000	-0.3095540000	-1.2808990000
O	-2.6593070000	-2.0883840000	-1.7819050000
O	-2.1275790000	-3.3099300000	0.6167470000
O	-3.0239590000	-1.1463570000	2.3394940000
O	-3.5219080000	1.3239560000	1.0184280000
O	-2.7663190000	2.9700750000	-1.1102330000
H	-0.6316300000	-2.2139630000	-1.4134440000
H	-0.8694840000	-1.7651620000	0.9662600000
H	-3.8342690000	-1.2428610000	0.4355610000
H	-1.5649790000	0.6561880000	1.1803010000
H	-3.1788160000	0.4044340000	-1.4071650000
H	-0.8956430000	2.2459710000	-0.5432710000
H	-1.3849990000	1.9948920000	-2.2345860000
H	-2.4354990000	-2.1973560000	-2.7162220000
H	-2.8306390000	-3.5398490000	-0.0104610000
H	-3.3283110000	-2.0433790000	2.5355690000
H	-3.6484290000	1.2605760000	1.9756910000
H	-3.1593760000	2.8973010000	-0.2267740000
O	3.8347710000	-1.9101520000	1.4005610000
O	4.5654870000	0.1787450000	0.9783000000
C	4.0006310000	-0.8953440000	0.6762280000
H	3.2418440000	-3.0033350000	-0.3829400000
H	4.4325130000	-2.6523140000	-1.4727560000
H	3.9604740000	-0.3745390000	-1.4457310000
C	3.3895140000	-0.9815270000	-0.7423530000
N	3.4821520000	-2.4070810000	-1.1851750000

H	2.8554030000	−2.6206080000	−1.9647730000
H	0.9914340000	0.1971390000	1.7068280000
H	0.6699960000	2.5036250000	2.5564330000
C	1.2216620000	1.0482060000	1.0690040000
C	1.0420730000	2.3470760000	1.5482660000
C	1.9071430000	−0.5777130000	−0.7363440000
C	1.6924990000	0.8257460000	−0.2281110000
C	1.3357770000	3.4398640000	0.7317880000
H	1.1953250000	4.4508100000	1.1016970000
H	1.3584550000	−1.2888140000	−0.1074570000
C	1.9795060000	1.9272500000	−1.0423390000
C	1.8052700000	3.2264410000	−0.5665580000
H	2.3389110000	1.7634240000	−2.0558130000
H	2.0295230000	4.0719680000	−1.2098630000
H	1.5189800000	−0.6645090000	−1.7576090000

Table S74. Cartesian coordinates of β -Glc-gg_Phe_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6279281			
ZPE / Hartree = 0.3931105			
BSSE / Hartree = 0.0024416148			
C	-1.7397590000	0.7579730000	-0.9492590000
C	-3.1535160000	0.8564230000	-0.3883880000
C	-3.2321940000	0.0535460000	0.8996200000
C	-2.7781060000	-1.3766730000	0.6537280000
C	-1.3870430000	-1.3879840000	0.0188620000
C	-0.9361260000	-2.7817750000	-0.3833650000
O	-1.4007080000	-0.6042580000	-1.1727850000
O	-1.7057980000	1.4197030000	-2.1703450000
O	-3.4809210000	2.1970470000	-0.0754250000
O	-4.5550850000	-0.0093920000	1.4063350000
O	-2.7025100000	-2.1008150000	1.8688370000
O	-1.8247480000	-3.3816920000	-1.3137240000
H	-1.0240040000	1.1978970000	-0.2396280000
H	-3.8548350000	0.4424280000	-1.1272960000
H	-2.5648890000	0.5155190000	1.6445750000
H	-3.4877900000	-1.8568280000	-0.0352910000
H	-0.6613050000	-0.9710160000	0.7360670000
H	0.0757120000	-2.7200660000	-0.8002720000
H	-0.9140490000	-3.4234220000	0.4997260000
H	-0.7918990000	1.6743120000	-2.3656100000
H	-3.5422650000	2.7002450000	-0.8990960000
H	-4.8163050000	0.8723670000	1.7048250000
H	-3.5648440000	-2.0400570000	2.3042290000
H	-1.8556340000	-2.8203260000	-2.1010910000
O	4.5652760000	-1.1898290000	1.5737650000
O	4.6832840000	0.9448000000	0.8612420000
C	4.3950200000	-0.2657070000	0.7380650000
H	4.0777080000	-2.6218170000	-0.0026280000
H	5.0757490000	-2.1343730000	-1.2247020000
H	4.0447380000	-0.0536140000	-1.4083930000
C	3.7054140000	-0.6802840000	-0.5829380000
N	4.1134650000	-2.0879350000	-0.8804590000

H	3.5116690000	-2.5356560000	-1.5763360000
H	1.3661560000	0.3338850000	1.9598170000
H	0.5008810000	2.5972030000	2.4784890000
C	1.2809910000	1.0765430000	1.1696960000
C	0.7935540000	2.3517240000	1.4621780000
C	2.1753660000	-0.6408290000	-0.4549350000
C	1.6540390000	0.7378920000	-0.1346250000
C	0.6750220000	3.3047370000	0.4496370000
H	0.2893450000	4.2943840000	0.6735500000
H	1.8712830000	-1.3455910000	0.3281680000
C	1.5414980000	1.7030060000	-1.1430510000
C	1.0553430000	2.9789630000	-0.8548720000
H	1.8313520000	1.4487230000	-2.1607040000
H	0.9675870000	3.7156510000	-1.6480350000
H	1.7440470000	-0.9841380000	-1.4024610000

Table S75. Cartesian coordinates of β -Glc-gg_Phe_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6273707			
ZPE / Hartree = 0.3925139			
BSSE / Hartree = 0.0025278091			
C	-2.7248140000	-0.4625530000	-1.3807390000
C	-2.3384590000	-1.0683400000	-0.0365210000
C	-2.7789480000	-0.1419260000	1.0843680000
C	-2.1933800000	1.2440020000	0.8661880000
C	-2.5728360000	1.7534260000	-0.5248330000
C	-1.9272940000	3.0834980000	-0.8710610000
O	-2.1252180000	0.8201440000	-1.5060840000
O	-2.2183670000	-1.2793480000	-2.3832000000
O	-2.9622340000	-2.3217930000	0.1691000000
O	-2.3288030000	-0.5973060000	2.3497040000
O	-2.6927150000	2.1667470000	1.8173820000
O	-0.5101330000	3.0058590000	-0.8457030000
H	-3.8178060000	-0.3590660000	-1.4638080000
H	-1.2458980000	-1.1690450000	-0.0154470000
H	-3.8781640000	-0.0688190000	1.0818680000
H	-1.0966980000	1.1746780000	0.9344820000
H	-3.6671000000	1.8658900000	-0.5809680000
H	-2.2812620000	3.3988340000	-1.8596560000
H	-2.2220140000	3.8342590000	-0.1353930000
H	-2.6669180000	-1.0828320000	-3.2169630000
H	-2.5125670000	-2.9817190000	-0.3769390000
H	-2.7228540000	-1.4643150000	2.5206260000
H	-2.5153990000	1.8101090000	2.6994790000
H	-0.2395370000	2.3290400000	-1.4824190000
O	4.7575780000	0.7247300000	-1.2631950000
O	4.5805390000	-1.1469160000	-0.0213290000
C	4.3605480000	0.0581430000	-0.2735560000
H	4.1065690000	2.5440340000	-0.2066760000
H	4.8022140000	2.3317530000	1.2772610000
H	3.5627600000	0.4129260000	1.7295850000
C	3.4575890000	0.8211170000	0.7237900000
N	3.9249500000	2.2414410000	0.7585280000
H	3.2422420000	2.8700420000	1.1890350000

H	1.5648860000	−0.7453730000	−1.9323020000
H	0.7323480000	−3.0788500000	−2.0208490000
C	1.3021670000	−1.2636510000	−1.0129180000
C	0.8367600000	−2.5794160000	−1.0623520000
C	1.9890280000	0.8011390000	0.2735080000
C	1.4391460000	−0.6025700000	0.2114170000
C	0.5008820000	−3.2475590000	0.1157200000
H	0.1359550000	−4.2695370000	0.0787950000
H	1.9191460000	1.2763010000	−0.7113090000
C	1.0895840000	−1.2767750000	1.3878660000
C	0.6243090000	−2.5904870000	1.3425630000
H	1.1787350000	−0.7648140000	2.3436330000
H	0.3512280000	−3.0986230000	2.2626540000
H	1.4046290000	1.3998120000	0.9815810000

Table S76. Cartesian coordinates of β -Glc-gg_Phe_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6277712			
ZPE / Hartree = 0.3930865			
BSSE / Hartree = 0.0025024406			
C	2.9843100000	-0.2850530000	-1.1949820000
C	3.0908750000	-1.0139010000	0.1414430000
C	1.9182820000	-0.6161500000	1.0238190000
C	1.8490960000	0.8976630000	1.1553800000
C	1.7921740000	1.5277630000	-0.2358050000
C	1.8020000000	3.0453110000	-0.2122900000
O	2.9389330000	1.1175860000	-0.9780830000
O	4.1230500000	-0.5776760000	-1.9347200000
O	3.0384330000	-2.4157670000	-0.0440100000
O	2.0281820000	-1.1512080000	2.3337320000
O	0.6869550000	1.2917950000	1.8631890000
O	2.9549230000	3.5639590000	0.4329550000
H	2.0710230000	-0.5972970000	-1.7258830000
H	4.0348010000	-0.7171470000	0.6217580000
H	0.9895490000	-0.9691910000	0.5553990000
H	2.7517610000	1.2541540000	1.6731930000
H	0.8746810000	1.1887960000	-0.7440550000
H	1.7348260000	3.4130480000	-1.2430510000
H	0.9340840000	3.4032320000	0.3454030000
H	3.9601810000	-0.3852850000	-2.8683500000
H	3.8396120000	-2.6940140000	-0.5089230000
H	1.7804670000	-2.0854170000	2.3087520000
H	0.6455510000	0.7647030000	2.6747330000
H	3.7335870000	3.2614820000	-0.0548320000
O	-5.2589130000	0.5080890000	0.8209690000
O	-4.7065410000	-1.1159000000	-0.6398460000
C	-4.6167520000	0.0309750000	-0.1493090000
H	-4.4671350000	2.4815940000	0.2900630000
H	-4.8176380000	2.5585430000	-1.3220150000
H	-3.4375380000	0.7557230000	-1.8393360000
C	-3.5605640000	0.9702100000	-0.7772000000
N	-4.0692370000	2.3701790000	-0.6506070000

H	-3.337550000	3.070144000	-0.797552000
H	-2.115625000	-0.989223000	1.946757000
H	-1.161792000	-3.275945000	1.844602000
C	-1.666455000	-1.350053000	1.024417000
C	-1.129957000	-2.637896000	0.966514000
C	-2.218684000	0.876109000	-0.036365000
C	-1.628606000	-0.511319000	-0.093681000
C	-0.549238000	-3.100504000	-0.214995000
H	-0.124759000	-4.098734000	-0.260301000
H	-2.371660000	1.175220000	1.006836000
C	-1.042832000	-0.983064000	-1.274542000
C	-0.507164000	-2.269033000	-1.336994000
H	-0.998733000	-0.333383000	-2.146342000
H	-0.047315000	-2.618688000	-2.256658000
H	-1.524819000	1.593049000	-0.491889000

Table S77. Cartesian coordinates of β -Glc-gg_Phe_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6265145			
ZPE / Hartree = 0.3927871			
BSSE / Hartree = 0.0025195185			
C	1.9140850000	-2.1899490000	0.2518440000
C	1.5585860000	-1.5283500000	-1.0752880000
C	2.5280040000	-0.3927400000	-1.3641270000
C	2.5754460000	0.5694070000	-0.1854170000
C	2.9291690000	-0.2131080000	1.0793790000
C	2.9740470000	0.6333930000	2.3372960000
O	1.9335510000	-1.2149530000	1.2851510000
O	0.9242040000	-3.1198280000	0.5445480000
O	1.6465100000	-2.4495790000	-2.1454360000
O	2.1417680000	0.3490870000	-2.5088170000
O	3.5629660000	1.5648520000	-0.3820510000
O	1.7467790000	1.3009670000	2.5819020000
H	2.9042590000	-2.6669430000	0.1902570000
H	0.5410710000	-1.1214390000	-0.9909110000
H	3.5345840000	-0.8134480000	-1.5138780000
H	1.5832690000	1.0304450000	-0.0572580000
H	3.9154580000	-0.6858080000	0.9469520000
H	3.2416410000	-0.0136600000	3.1814510000
H	3.7406110000	1.4030730000	2.2286480000
H	1.2538570000	-3.7463710000	1.2035320000
H	0.9353360000	-3.0983520000	-2.0531400000
H	2.2603000000	-0.2059030000	-3.2917330000
H	3.3793430000	1.9990540000	-1.2277220000
H	1.0410000000	0.6387890000	2.6040770000
O	-4.6459280000	-1.0174630000	-1.0385180000
O	-4.5097130000	1.1238280000	-0.3501520000
C	-4.2709940000	-0.1006740000	-0.2637350000
H	-3.9867960000	-2.4680320000	0.4693120000
H	-4.6960200000	-1.8831220000	1.8407580000
H	-3.4987910000	0.1098320000	1.7700370000
C	-3.3704480000	-0.5500300000	0.9112870000
N	-3.8160760000	-1.9177580000	1.3202700000

H	-3.1300690000	-2.4011440000	1.9051440000
H	-1.3836440000	0.2699910000	-2.0494870000
H	-0.5204820000	2.4878730000	-2.7365040000
C	-1.1658300000	1.0246170000	-1.2966400000
C	-0.6805790000	2.2745660000	-1.6839230000
C	-1.8967580000	-0.6200330000	0.4838730000
C	-1.3666250000	0.7265120000	0.0544550000
C	-0.3931320000	3.2429590000	-0.7214550000
H	-0.0106500000	4.2138310000	-1.0209700000
H	-1.8062900000	-1.3446040000	-0.3342190000
C	-1.0817800000	1.7058980000	1.0124740000
C	-0.5983190000	2.9561800000	0.6297690000
H	-1.2365130000	1.4838470000	2.0665230000
H	-0.3731070000	3.7022260000	1.3859650000
H	-1.3061680000	-0.9930200000	1.3294920000

Table S78. Cartesian coordinates of β -Glc-gg_Phe_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6277444			
ZPE / Hartree = 0.3925033			
BSSE / Hartree = 0.002508497			
C	-1.4724290000	-1.2336200000	1.3856600000
C	-1.8959880000	-2.1387990000	0.2338850000
C	-1.8952560000	-1.3484250000	-1.0647920000
C	-2.7405440000	-0.0924030000	-0.9236450000
C	-2.2506520000	0.7132740000	0.2787020000
C	-3.0710180000	1.9595750000	0.5496470000
O	-2.3279430000	-0.1023550000	1.4482570000
O	-1.6052020000	-1.9516130000	2.5673590000
O	-0.9919220000	-3.2162650000	0.0740730000
O	-2.4294260000	-2.1031490000	-2.1394670000
O	-2.6235680000	0.7263980000	-2.0740730000
O	-4.4389800000	1.6644870000	0.7889020000
H	-0.4356230000	-0.8923210000	1.2405820000
H	-2.9119130000	-2.5062290000	0.4395000000
H	-0.8608070000	-1.0462870000	-1.2945930000
H	-3.7891870000	-0.3819320000	-0.7627650000
H	-1.2087120000	1.0163720000	0.1026120000
H	-2.6305100000	2.4894190000	1.4034910000
H	-3.0309970000	2.6128650000	-0.3248410000
H	-1.0913640000	-1.5211270000	3.2647020000
H	-1.0837810000	-3.8125790000	0.8298870000
H	-1.8345550000	-2.8435240000	-2.3218090000
H	-2.8505560000	0.1877030000	-2.8455750000
H	-4.4919150000	1.1004490000	1.5729900000
O	4.8697660000	-0.4822900000	1.2805480000
O	4.6019230000	1.3570420000	0.0067650000
C	4.4365300000	0.1488070000	0.2829500000
H	4.2815300000	-2.3446200000	0.2720010000
H	4.9574250000	-2.1399970000	-1.2220810000
H	3.6421830000	-0.2810080000	-1.7073910000
C	3.5585110000	-0.6706750000	-0.6922750000
N	4.0809410000	-2.0722140000	-0.6983810000
H	3.4213370000	-2.7381970000	-1.1080160000

H	1.6597570000	0.8943010000	1.9354130000
H	0.6712750000	3.1678570000	1.9877420000
C	1.3381200000	1.3689620000	1.0109880000
C	0.7822310000	2.6490570000	1.0403540000
C	2.0930410000	−0.6977720000	−0.2341900000
C	1.4823710000	0.6820910000	−0.1990850000
C	0.3644960000	3.2569920000	−0.1447920000
H	−0.0747230000	4.2497030000	−0.1236180000
H	2.0442340000	−1.1552850000	0.7610500000
C	1.0590090000	1.2982720000	−1.3821000000
C	0.5043660000	2.5780370000	−1.3573000000
H	1.1552330000	0.7660500000	−2.3260310000
H	0.1721090000	3.0405650000	−2.2818320000
H	1.5290690000	−1.3349550000	−0.9257120000

Table S79. Cartesian coordinates of β -Glc-gg_Phe_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6254142			
ZPE / Hartree = 0.392371			
BSSE / Hartree = 0.0021944721			
C	3.0099270000	-0.4906080000	-1.3989560000
C	3.5613870000	-1.0732820000	-0.1014670000
C	2.5147860000	-0.9611180000	0.9965190000
C	2.0362630000	0.4773440000	1.1208570000
C	1.5371870000	0.9611930000	-0.2409100000
C	1.0795060000	2.4078180000	-0.2411600000
O	2.6023540000	0.8530890000	-1.1839450000
O	4.0306390000	-0.4949060000	-2.3403110000
O	3.8747920000	-2.4454930000	-0.2473800000
O	3.0356770000	-1.3514110000	2.2556390000
O	0.9697910000	0.5829750000	2.0462610000
O	2.0962320000	3.2943290000	0.2014520000
H	2.1445980000	-1.0779300000	-1.7444100000
H	4.4526800000	-0.4953970000	0.1821140000
H	1.6542210000	-1.5968260000	0.7321400000
H	2.8801650000	1.1083710000	1.4347340000
H	0.6927400000	0.3315850000	-0.5618540000
H	0.7474480000	2.6683170000	-1.2536150000
H	0.2318800000	2.5188640000	0.4407960000
H	3.6537660000	-0.3942900000	-3.2253300000
H	4.6619270000	-2.5279660000	-0.8027160000
H	3.2650730000	-2.2902380000	2.2148210000
H	1.2791430000	0.2431540000	2.8979720000
H	2.8411420000	3.2287720000	-0.4120590000
O	-3.6612440000	-2.5783820000	-1.5430340000
O	-4.7905360000	-0.9513910000	-0.4672620000
C	-3.8674200000	-1.7864340000	-0.5881760000
H	-2.1695170000	-3.5948630000	-0.2931760000
H	-3.0246210000	-3.8453780000	1.0969730000
H	-3.2769050000	-1.5639180000	1.5040800000
C	-2.8212370000	-1.8296230000	0.5496290000
N	-2.3292800000	-3.2378340000	0.6572050000

H	-1.4647440000	-3.3102200000	1.1996210000
H	-1.8294380000	0.5736680000	-2.0310450000
H	-2.4726530000	2.9598250000	-2.2313790000
C	-2.0721300000	1.1480140000	-1.1396940000
C	-2.4347490000	2.4915990000	-1.2523920000
C	-1.6219610000	-0.9234830000	0.2375150000
C	-2.0117590000	0.5291510000	0.1119940000
C	-2.7396650000	3.2311470000	-0.1098720000
H	-3.0174580000	4.2771950000	-0.1946710000
H	-1.1588290000	-1.2682950000	-0.6949380000
C	-2.3195520000	1.2787260000	1.2535550000
C	-2.6818630000	2.6203710000	1.1455680000
H	-2.2641160000	0.8077670000	2.2325280000
H	-2.9134980000	3.1911220000	2.0397310000
H	-0.8820340000	-1.0338520000	1.0398360000

Table S80. Cartesian coordinates of β -Glc-gt_Phe_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6279368			
ZPE / Hartree = 0.3924296			
BSSE / Hartree = 0.0025697318			
C	2.2348380000	1.1461010000	-0.0732940000
C	2.4827060000	0.6032810000	-1.4760220000
C	1.8289770000	-0.7645420000	-1.6012770000
C	2.3097080000	-1.6918460000	-0.4939280000
C	2.1005670000	-1.0232250000	0.8632690000
C	2.6740560000	-1.8314660000	2.0104290000
O	2.7674370000	0.2367910000	0.8808310000
O	2.8980050000	2.3600860000	0.0527620000
O	1.9030860000	1.4403780000	-2.4584860000
O	2.1352680000	-1.3887070000	-2.8363600000
O	1.5786110000	-2.9053050000	-0.4994950000
O	2.4139230000	-1.2057660000	3.2573330000
H	1.1578170000	1.2630360000	0.1036510000
H	3.5682320000	0.5113450000	-1.6285190000
H	0.7380820000	-0.6405550000	-1.5019580000
H	3.3834720000	-1.8892400000	-0.6362480000
H	1.0220370000	-0.8691780000	1.0276830000
H	2.2005050000	-2.8143130000	2.0385750000
H	3.7535340000	-1.9610280000	1.8553400000
H	2.4844650000	2.8773120000	0.7584810000
H	2.3560370000	2.2948720000	-2.4399960000
H	1.7043080000	-0.8950950000	-3.5475950000
H	1.6614630000	-3.2978530000	-1.3804830000
H	2.8087920000	-0.3229020000	3.2325530000
O	-4.7494250000	-0.6730200000	-1.3633690000
O	-4.6454850000	0.9041510000	0.2427360000
C	-4.3549030000	-0.1999360000	-0.2669500000
H	-3.9308410000	-2.5974470000	-0.7550730000
H	-4.5451890000	-2.7924200000	0.7657390000
H	-3.4435630000	-0.9148230000	1.5883860000
C	-3.3541260000	-1.0838630000	0.5147940000
N	-3.7114170000	-2.5094920000	0.2450770000

H	-2.9580730000	-3.1588860000	0.4841680000
H	-1.6868700000	1.2144240000	-1.7329950000
H	-0.9412520000	3.5356750000	-1.2833350000
C	-1.4013060000	1.5077810000	-0.7253390000
C	-0.9814260000	2.8152730000	-0.4719070000
C	-1.9141390000	-0.8474620000	0.0370220000
C	-1.4508420000	0.5635840000	0.3042300000
C	-0.6057490000	3.1918470000	0.8181500000
H	-0.2737380000	4.2064930000	1.0156790000
H	-1.8605900000	-1.0653820000	-1.0359200000
C	-1.0712550000	0.9495710000	1.5959540000
C	-0.6506090000	2.2541400000	1.8534420000
H	-1.0958470000	0.2181270000	2.4011300000
H	-0.3534630000	2.5374340000	2.8586600000
H	-1.2597390000	-1.5574440000	0.5574900000

Table S81. Cartesian coordinates of β -Glc-gt_Phe_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6273057			
ZPE / Hartree = 0.3928202			
BSSE / Hartree = 0.0025942233			
C	2.2846000000	-0.1303060000	1.5838990000
C	2.2735970000	-1.0816430000	0.3915590000
C	2.8905640000	-0.3927000000	-0.8152880000
C	2.1874720000	0.9296940000	-1.0851400000
C	2.1878420000	1.7803120000	0.1830910000
C	1.3949790000	3.0637440000	0.0258650000
O	1.5687550000	1.0489570000	1.2390100000
O	1.6296760000	-0.7478140000	2.6410100000
O	3.0287520000	-2.2502220000	0.6508230000
O	2.7679460000	-1.1796320000	-1.9885510000
O	2.8453960000	1.6586810000	-2.1053050000
O	1.4256470000	3.8347330000	1.2163170000
H	3.3159950000	0.1410860000	1.8571740000
H	1.2293970000	-1.3348020000	0.1685380000
H	3.9532700000	-0.1904720000	-0.6082230000
H	1.1447730000	0.7194720000	-1.3726180000
H	3.2264320000	2.0215100000	0.4610430000
H	1.8365180000	3.6728080000	-0.7647410000
H	0.3614280000	2.8165490000	-0.2513400000
H	1.8699230000	-0.3110670000	3.4696970000
H	2.5273690000	-2.8096720000	1.2600490000
H	3.2734640000	-1.9953620000	-1.8661400000
H	2.9090560000	1.0880520000	-2.8846900000
H	1.0712420000	3.2861880000	1.9303140000
O	-4.4917560000	0.9165310000	1.2344760000
O	-4.6026160000	-0.9991220000	0.0525530000
C	-4.2386560000	0.1816270000	0.2462140000
H	-3.7396760000	2.6436210000	0.0310720000
H	-4.6026520000	2.4038970000	-1.3551160000
H	-3.5251440000	0.3672890000	-1.8115250000
C	-3.3332360000	0.8147030000	-0.8356850000
N	-3.6863560000	2.2651400000	-0.9222530000
H	-3.0025230000	2.8025780000	-1.4603670000

H	-1.6831690000	-0.8043520000	1.8007100000
H	-0.9579610000	-3.1639640000	2.0126580000
C	-1.3782740000	-1.3601620000	0.9166620000
C	-0.9693360000	-2.6889620000	1.0362340000
C	-1.8469700000	0.7044680000	-0.4627840000
C	-1.3908130000	-0.7276190000	-0.3308050000
C	-0.5652320000	-3.4009240000	-0.0944790000
H	-0.2399790000	-4.4326270000	-0.0022490000
H	-1.6833170000	1.2386520000	0.4806830000
C	-0.9842270000	-1.4487060000	-1.4591840000
C	-0.5726440000	-2.7767720000	-1.3438420000
H	-0.9786670000	-0.9607210000	-2.4314330000
H	-0.2501270000	-3.3205410000	-2.2266550000
H	-1.2635310000	1.2084680000	-1.2416530000

Table S82. Cartesian coordinates of β -Glc-gt_Phe_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6280019			
ZPE / Hartree = 0.3931237			
BSSE / Hartree = 0.0025780685			
C	3.0789910000	0.0221960000	-1.0310410000
C	3.1771130000	-0.9191730000	0.1665020000
C	1.9601730000	-0.7254470000	1.0581530000
C	1.8077860000	0.7389800000	1.4417070000
C	1.7723640000	1.5879350000	0.1730180000
C	1.7124410000	3.0743580000	0.4632370000
O	2.9663560000	1.3622980000	-0.5727100000
O	4.2510910000	-0.0930020000	-1.7668670000
O	3.1889670000	-2.2713620000	-0.2499460000
O	2.0526700000	-1.4725020000	2.2603600000
O	0.6020280000	0.9541060000	2.1527110000
O	1.6531120000	3.8302320000	-0.7361710000
H	2.1957790000	-0.2273330000	-1.6405210000
H	4.0919270000	-0.6714450000	0.7245510000
H	1.0659700000	-1.0311230000	0.4983240000
H	2.6726220000	1.0431810000	2.0520520000
H	0.8996860000	1.2953010000	-0.4338890000
H	0.8066660000	3.2981130000	1.0300080000
H	2.5869720000	3.3605560000	1.0627590000
H	4.1096820000	0.2525070000	-2.6591410000
H	4.0171180000	-2.4430540000	-0.7189000000
H	1.8772420000	-2.4020000000	2.0592430000
H	0.5460110000	0.2808770000	2.8470050000
H	2.4401720000	3.6180830000	-1.2573980000
O	-5.1553760000	0.2221780000	0.9054480000
O	-4.6248670000	-1.1819570000	-0.7753760000
C	-4.5398920000	-0.1080540000	-0.1401410000
H	-4.4153180000	2.2904240000	0.6052010000
H	-4.8691940000	2.5198760000	-0.9645910000
H	-3.4232610000	0.8548620000	-1.7538930000
C	-3.5268580000	0.9329050000	-0.6710680000
N	-4.0740100000	2.2905770000	-0.3635610000

H	-3.3762010000	3.0296730000	-0.4796860000
H	-2.0825200000	-1.3311960000	1.7266860000
H	-1.0602270000	-3.5577840000	1.3419890000
C	-1.5904640000	-1.5477220000	0.7811920000
C	-1.0147270000	-2.8008870000	0.5647240000
C	-2.1646950000	0.7933650000	0.0260450000
C	-1.5355490000	-0.5581330000	-0.2054420000
C	-0.3749920000	-3.0764920000	-0.6447900000
H	0.0814270000	-4.0472610000	-0.8121720000
H	-2.3033070000	0.9601030000	1.1003050000
C	-0.8920460000	-0.8429380000	-1.4152830000
C	-0.3147130000	-2.0934760000	-1.6353570000
H	-0.8330850000	-0.0741080000	-2.1829400000
H	0.1910080000	-2.2973630000	-2.5745810000
H	-1.5025130000	1.5806260000	-0.3538000000

Table S83. Cartesian coordinates of β -Glc-gt_Phe_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6273883			
ZPE / Hartree = 0.3927913			
BSSE / Hartree = 0.0025400934			
C	1.9056470000	-2.0952520000	0.0261990000
C	1.5433800000	-1.4223280000	-1.2938280000
C	2.4381140000	-0.2130540000	-1.5215290000
C	2.3887170000	0.7165460000	-0.3173640000
C	2.7293380000	-0.0715800000	0.9451870000
C	2.6132110000	0.7597360000	2.2080680000
O	1.8040210000	-1.1495780000	1.0813400000
O	0.9860420000	-3.1110520000	0.2556670000
O	1.7286370000	-2.3028900000	-2.3856230000
O	2.0270160000	0.5356110000	-2.6534440000
O	3.3240020000	1.7724120000	-0.4502100000
O	2.9579020000	-0.0011930000	3.3555800000
H	2.9333070000	-2.4882570000	-0.0102380000
H	0.4965780000	-1.0908940000	-1.2311360000
H	3.4748640000	-0.5585420000	-1.6563720000
H	1.3693470000	1.1174040000	-0.2197180000
H	3.7522460000	-0.4735410000	0.8644710000
H	3.3077030000	1.6001540000	2.1577770000
H	1.5899990000	1.1490630000	2.2900620000
H	1.3465310000	-3.7335400000	0.9021810000
H	1.0677990000	-3.0068190000	-2.3289290000
H	2.1950080000	0.0107580000	-3.4480460000
H	3.1227190000	2.2423170000	-1.2723680000
H	2.3680910000	-0.7674850000	3.3881710000
O	-4.7869040000	-0.8179120000	-0.9767660000
O	-4.5097440000	1.1954360000	-0.0041680000
C	-4.3121020000	-0.0343990000	-0.1153680000
H	-4.0230880000	-2.4908110000	0.2133690000
H	-4.6208450000	-2.1186170000	1.7049200000
H	-3.3777260000	-0.1536470000	1.8568180000
C	-3.3334500000	-0.6727940000	0.8988110000
N	-3.7795980000	-2.0820750000	1.1240300000

H	-3.0645320000	-2.6575650000	1.5753300000
H	-1.5310740000	0.5557450000	-2.0492710000
H	-0.6646870000	2.8412000000	-2.4573000000
C	-1.2473550000	1.1866320000	-1.2097980000
C	-0.7598090000	2.4745100000	-1.4396910000
C	-1.8995420000	-0.6965950000	0.3494130000
C	-1.3663420000	0.6917840000	0.0921520000
C	-0.3883110000	3.2839870000	-0.3656000000
H	-0.0050520000	4.2841890000	-0.5424980000
H	-1.8909190000	-1.2846080000	-0.5764570000
C	-0.9898030000	1.5098620000	1.1636330000
C	-0.5054660000	2.7979580000	0.9388640000
H	-1.0682950000	1.1292150000	2.1798630000
H	-0.2094480000	3.4178600000	1.7799800000
H	-1.2564960000	-1.2058210000	1.0772720000

Table S84. Cartesian coordinates of β -Glc-gt_Phe_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6270997			
ZPE / Hartree = 0.3923513			
BSSE / Hartree = 0.0022393413			
C	3.1789090000	0.6163050000	-1.0883790000
C	4.0275390000	-0.1945520000	-0.1127990000
C	3.1312980000	-0.8502100000	0.9275940000
C	2.2362610000	0.1869520000	1.5907780000
C	1.4751840000	0.9570570000	0.5141050000
C	0.6131810000	2.0697520000	1.0811720000
O	2.4174710000	1.5723650000	-0.3642440000
O	4.0371860000	1.2923800000	-1.9454690000
O	4.7287590000	-1.2271860000	-0.7789380000
O	3.8855710000	-1.4742660000	1.9528850000
O	1.2940100000	-0.4293800000	2.4496590000
O	-0.0067910000	2.8153880000	0.0453860000
H	2.4939860000	-0.0433740000	-1.6441850000
H	4.7248890000	0.4941700000	0.3859810000
H	2.4910250000	-1.5928060000	0.4254390000
H	2.8661680000	0.8916460000	2.1556450000
H	0.8455700000	0.2607850000	-0.0588730000
H	-0.1852600000	1.6364060000	1.6887760000
H	1.2290280000	2.7226920000	1.7149950000
H	3.5528890000	1.5703590000	-2.7351310000
H	5.4086510000	-0.8277040000	-1.3386120000
H	4.3416670000	-2.2402080000	1.5784860000
H	1.7822300000	-0.9762710000	3.0817780000
H	0.6922250000	3.1299250000	-0.5457330000
O	-5.3275620000	-0.9300730000	1.1504180000
O	-4.6171780000	-1.6791970000	-0.8525030000
C	-4.7925500000	-0.8001150000	0.0200060000
H	-5.3118630000	1.2996460000	1.3293560000
H	-6.0649650000	1.6486210000	-0.0963320000
H	-4.2835650000	0.8029780000	-1.3756390000
C	-4.2506560000	0.6118090000	-0.3023040000
N	-5.1514080000	1.6037250000	0.3618470000
H	-4.7590120000	2.5483780000	0.3651360000

H	-1.7618820000	-1.4419730000	1.3666410000
H	-0.1408790000	-3.0228070000	0.3590980000
C	-1.3999910000	-1.2760400000	0.3545530000
C	-0.4876960000	-2.1677150000	-0.2136540000
C	-2.8306990000	0.8040510000	0.2510020000
C	-1.8450480000	-0.1608910000	-0.3600560000
C	-0.0135630000	-1.9526970000	-1.5077720000
H	0.7036960000	-2.6392820000	-1.9476100000
H	-2.8595840000	0.6708020000	1.3386570000
C	-1.3669990000	0.0457910000	-1.6599770000
C	-0.4577940000	-0.8429710000	-2.2319790000
H	-1.7017270000	0.9163380000	-2.2196570000
H	-0.0880220000	-0.6660010000	-3.2375780000
H	-2.5113710000	1.8321890000	0.0451380000

Table S85. Cartesian coordinates of β -Glc-gt_Phe_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6269772			
ZPE / Hartree = 0.3927311			
BSSE / Hartree = 0.0025033975			
C	-2.2955090000	-0.8518420000	-1.4143080000
C	-2.3564830000	-1.6688590000	-0.1260840000
C	-2.9952840000	-0.8467910000	0.9826170000
C	-2.2967710000	0.4980900000	1.1189000000
C	-2.2820360000	1.2045860000	-0.2346320000
C	-1.5267370000	2.5214450000	-0.1882920000
O	-1.6132260000	0.3705560000	-1.1772020000
O	-1.5684140000	-1.5829470000	-2.3463840000
O	-3.1412700000	-2.8339210000	-0.2974880000
O	-2.9019160000	-1.4987330000	2.2383170000
O	-2.9681110000	1.3273480000	2.0488920000
O	-1.4559370000	3.1219800000	-1.4719140000
H	-3.3113730000	-0.6356310000	-1.7798120000
H	-1.3289450000	-1.9306120000	0.1637760000
H	-4.0517550000	-0.6687640000	0.7297410000
H	-1.2542310000	0.3277310000	1.4355120000
H	-3.3160380000	1.3842240000	-0.5705750000
H	-2.0564750000	3.2180620000	0.4640420000
H	-0.5205070000	2.3512260000	0.2162230000
H	-1.7419330000	-1.2402750000	-3.2340670000
H	-2.6690070000	-3.4433490000	-0.8811110000
H	-3.4739320000	-2.2783130000	2.2277630000
H	-3.0450840000	0.8376600000	2.8804860000
H	-0.9358730000	2.5357250000	-2.0400590000
O	3.7573470000	-2.3061330000	1.4150440000
O	4.6182780000	-0.5647500000	0.2732440000
C	3.7960460000	-1.4884670000	0.4603140000
H	2.2824950000	-3.4529550000	0.2872520000
H	2.9991650000	-3.5991370000	-1.1928120000
H	2.9926800000	-1.2994300000	-1.5635150000
C	2.6570670000	-1.6217400000	-0.5771490000
N	2.2985870000	-3.0712990000	-0.6669320000

H	1.3902700000	-3.2290190000	-1.1113400000
H	1.7521660000	0.6186360000	2.1336230000
H	2.1623930000	3.0568830000	2.3282090000
C	1.8145590000	1.2329250000	1.2383060000
C	2.0456590000	2.6055660000	1.3476190000
C	1.4064090000	-0.8455930000	-0.1402120000
C	1.6552860000	0.6361570000	-0.0155500000
C	2.1204990000	3.3956990000	0.1998750000
H	2.2950760000	4.4639160000	0.2833470000
H	1.0598810000	-1.2492340000	0.8193770000
C	1.7318140000	1.4362270000	-1.1621230000
C	1.9646680000	2.8067250000	-1.0573220000
H	1.5973090000	0.9805050000	-2.1410000000
H	2.0145470000	3.4166480000	-1.9543970000
H	0.6199340000	-1.0173630000	-0.8839580000

Table S86. Cartesian coordinates of β -Glc-tg_Phe_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6269086			
ZPE / Hartree = 0.3930151			
BSSE / Hartree = 0.0026001615			
C	-2.2977790000	1.2607830000	-0.2039310000
C	-2.5298120000	0.8782370000	1.2539540000
C	-1.8443590000	-0.4492460000	1.5396260000
C	-2.3002450000	-1.4972380000	0.5372950000
C	-2.0904010000	-0.9883900000	-0.8902500000
C	-2.6132810000	-1.9565080000	-1.9455140000
O	-2.8000310000	0.2339060000	-1.0515020000
O	-2.9991600000	2.4304070000	-0.4651600000
O	-1.9723970000	1.8389990000	2.1302820000
O	-2.1530520000	-0.9374560000	2.8336420000
O	-1.5617990000	-2.7017210000	0.6852410000
O	-1.7831760000	-3.1008280000	-2.0681480000
H	-1.2236970000	1.3891750000	-0.3958100000
H	-3.6126870000	0.7777680000	1.4187980000
H	-0.7560710000	-0.3117080000	1.4363250000
H	-3.3730940000	-1.6910370000	0.6870220000
H	-1.0150310000	-0.8213960000	-1.0612410000
H	-3.6463480000	-2.2407470000	-1.7034450000
H	-2.6094490000	-1.4521780000	-2.9147290000
H	-2.6132880000	2.8688130000	-1.2364920000
H	-2.4654900000	2.6656960000	2.0353560000
H	-1.7679340000	-0.3392200000	3.4887180000
H	-1.7248970000	-3.0531270000	1.5721770000
H	-1.6843760000	-3.4870110000	-1.1841080000
O	4.5884770000	-0.5155180000	1.5431320000
O	4.6074850000	0.8495710000	-0.2491820000
C	4.2597910000	-0.1748910000	0.3780470000
H	3.7374500000	-2.4989420000	1.1290460000
H	4.4537320000	-2.8611940000	-0.3137860000
H	3.4113900000	-1.0881370000	-1.4183880000
C	3.2721690000	-1.1268540000	-0.3375480000
N	3.5891130000	-2.5173960000	0.1123310000

H	2.8471500000	−3.1862870000	−0.1092870000
H	1.5617160000	1.4088660000	1.6146710000
H	0.9205520000	3.7017140000	0.9252430000
C	1.3434830000	1.6210240000	0.5703580000
C	0.9825590000	2.9127600000	0.1817610000
C	1.8188370000	−0.8056120000	0.0442390000
C	1.4191230000	0.5896220000	−0.3699990000
C	0.6933840000	3.1860460000	−1.1555690000
H	0.4076620000	4.1887340000	−1.4583180000
H	1.7070850000	−0.9221390000	1.1286380000
C	1.1267040000	0.8722320000	−1.7100590000
C	0.7660610000	2.1609420000	−2.1025910000
H	1.1732540000	0.0729880000	−2.4467270000
H	0.5370160000	2.3641390000	−3.1442960000
H	1.1634000000	−1.5393300000	−0.4410260000

Table S87. Cartesian coordinates of β -Glc-tg_Phe_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6262422			
ZPE / Hartree = 0.3926459			
BSSE / Hartree = 0.0025062398			
C	-3.0510670000	-0.7647730000	-0.7010060000
C	-2.2991450000	-1.0561970000	0.5938110000
C	-2.2354300000	0.2051480000	1.4402300000
C	-1.6427730000	1.3392370000	0.6212130000
C	-2.4125340000	1.5166140000	-0.6885820000
C	-1.7722710000	2.5580400000	-1.6010410000
O	-2.3966870000	0.2856550000	-1.4011490000
O	-3.0094300000	-1.9067950000	-1.4897640000
O	-2.9502180000	-2.0534360000	1.3581080000
O	-1.4074520000	0.0328410000	2.5785030000
O	-1.6868300000	2.5692530000	1.3296610000
O	-1.9664600000	3.8786550000	-1.1214100000
H	-4.0885370000	-0.4631060000	-0.4885550000
H	-1.2794000000	-1.3690510000	0.3311820000
H	-3.2547420000	0.4820660000	1.7517610000
H	-0.6024110000	1.0827440000	0.3749850000
H	-3.4501320000	1.8147440000	-0.4676020000
H	-0.7027580000	2.3302650000	-1.7143320000
H	-2.2449150000	2.5007510000	-2.5843310000
H	-3.6910900000	-1.8511370000	-2.1734710000
H	-2.8456880000	-2.9026320000	0.9069110000
H	-1.8120290000	-0.6287920000	3.1565230000
H	-1.1614810000	2.4754550000	2.1373690000
H	-1.6627070000	3.9043160000	-0.2007970000
O	4.3337300000	1.2393280000	-1.3554480000
O	4.4714150000	-0.9561940000	-0.8667580000
C	4.1923220000	0.2355460000	-0.6112090000
H	3.9626060000	2.5029330000	0.4012380000
H	4.9892740000	1.8490430000	1.5181790000
H	3.8874740000	-0.2084600000	1.5084590000
C	3.5508840000	0.5178600000	0.7680500000
N	4.0145670000	1.8696610000	1.2092970000
H	3.4534570000	2.2501340000	1.9759290000

H	1.1057090000	−0.0748970000	−1.8197320000
H	0.2104160000	−2.2416940000	−2.6247650000
C	1.0394220000	−0.9219870000	−1.1402500000
C	0.5369340000	−2.1425160000	−1.5939170000
C	2.0180870000	0.5409310000	0.6720860000
C	1.4543820000	−0.7720020000	0.1866420000
C	0.4438460000	−3.2280470000	−0.7218450000
H	0.0476100000	−4.1763750000	−1.0718150000
H	1.7264410000	1.3478560000	−0.0110140000
C	1.3520700000	−1.8635090000	1.0565920000
C	0.8516860000	−3.0854030000	0.6066330000
H	1.6609600000	−1.7511900000	2.0934610000
H	0.7739090000	−3.9231150000	1.2930680000
H	1.6130350000	0.7744070000	1.6638890000

Table S88. Cartesian coordinates of β -Glc-tg_Phe_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6268202			
ZPE / Hartree = 0.393307			
BSSE / Hartree = 0.0026428427			
C	-2.1479770000	0.4132870000	1.7251810000
C	-2.8915290000	-0.6804390000	0.9624450000
C	-2.3575370000	-0.7561100000	-0.4601890000
C	-2.4243650000	0.6149140000	-1.1123840000
C	-1.6821420000	1.6324650000	-0.2451420000
C	-1.7487640000	3.0499160000	-0.8020320000
O	-2.2824970000	1.6544370000	1.0443970000
O	-2.7318240000	0.5371210000	2.9788160000
O	-2.6892510000	-1.9449590000	1.5640440000
O	-3.1085810000	-1.6503380000	-1.2646090000
O	-1.8167190000	0.6022750000	-2.3952590000
O	-0.9173230000	3.2050740000	-1.9413750000
H	-1.0780880000	0.1609170000	1.8024840000
H	-3.9602080000	-0.4213140000	0.9435090000
H	-1.3068570000	-1.0759920000	-0.4260980000
H	-3.4770250000	0.9261090000	-1.1962530000
H	-0.6250570000	1.3322150000	-0.1637600000
H	-2.7914150000	3.3059320000	-1.0343620000
H	-1.3819610000	3.7425240000	-0.0407560000
H	-2.1238640000	0.9951870000	3.5755090000
H	-3.1572730000	-1.9637630000	2.4099260000
H	-2.8772740000	-2.5559650000	-1.0168400000
H	-2.2595570000	-0.0692790000	-2.9339820000
H	-1.1635530000	2.5186900000	-2.5807270000
O	4.7163910000	1.0266710000	-0.7960760000
O	4.5355190000	-1.1426410000	-0.2132410000
C	4.3111260000	0.0797350000	-0.0746970000
H	4.0338240000	2.4128030000	0.7555760000
H	4.7135820000	1.7645920000	2.1131440000
H	3.4882580000	-0.2154010000	1.9286260000
C	3.3899970000	0.4867270000	1.0999360000
N	3.8434380000	1.8285630000	1.5794410000

H	3.1501880000	2.2927610000	2.1712030000
H	1.5567780000	-0.0050780000	-1.9793130000
H	0.7183780000	-2.1265450000	-2.9502580000
C	1.2812440000	-0.8302140000	-1.3262360000
C	0.8093470000	-2.0250030000	-1.8729500000
C	1.9266040000	0.6078570000	0.6465930000
C	1.3969620000	-0.6769980000	0.0587160000
C	0.4479360000	-3.0817680000	-1.0362970000
H	0.0766410000	-4.0102780000	-1.4591100000
H	1.8606780000	1.4113970000	-0.0962660000
C	1.0267340000	-1.7396580000	0.8911360000
C	0.5566560000	-2.9355500000	0.3488780000
H	1.1010970000	-1.6243600000	1.9703980000
H	0.2666750000	-3.7494230000	1.0065780000
H	1.3204950000	0.8982420000	1.5133590000

Table S89. Cartesian coordinates of β -Glc-tg_Phe_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6267274			
ZPE / Hartree = 0.3930463			
BSSE / Hartree = 0.0025356666			
C	1.6231630000	2.2631800000	-0.4883770000
C	1.3394870000	1.8111610000	0.9410310000
C	2.3508080000	0.7570850000	1.3670980000
C	2.3900550000	-0.3648700000	0.3414980000
C	2.6610440000	0.2131970000	-1.0485070000
C	2.6539520000	-0.8475390000	-2.1441980000
O	1.6251260000	1.1391370000	-1.3585460000
O	0.5976880000	3.1157600000	-0.8772240000
O	1.4413820000	2.8922510000	1.8479380000
O	2.0114130000	0.1839550000	2.6185470000
O	3.4138070000	-1.3030730000	0.6425340000
O	3.8088880000	-1.6702330000	-2.0917120000
H	2.6019120000	2.7638600000	-0.5464210000
H	0.3312800000	1.3729640000	0.9660000000
H	3.3475820000	1.2213110000	1.4231190000
H	1.4127250000	-0.8679230000	0.3227520000
H	3.6380670000	0.7236980000	-1.0518280000
H	1.7373530000	-1.4470000000	-2.0642820000
H	2.6596840000	-0.3466190000	-3.1152600000
H	0.8868430000	3.6467740000	-1.6321080000
H	0.7074290000	3.5011610000	1.6870930000
H	2.1122640000	0.8584460000	3.3041450000
H	3.1896230000	-1.7393530000	1.4769550000
H	3.8689530000	-2.0298010000	-1.1928880000
O	-4.7569320000	0.7144050000	0.9151430000
O	-4.4495100000	-1.4236220000	0.2734070000
C	-4.3034940000	-0.1866250000	0.1639820000
H	-4.1709960000	2.1796020000	-0.5980860000
H	-4.8241990000	1.5410240000	-1.9729170000
H	-3.4932980000	-0.3757920000	-1.8579450000
C	-3.4237100000	0.3055620000	-1.0091950000
N	-3.9548740000	1.6346060000	-1.4422760000

H	-3.2927430000	2.1558980000	-2.0223650000
H	-1.5337480000	-0.2622380000	2.0143490000
H	-0.4838930000	-2.3516790000	2.8341340000
C	-1.1895190000	-1.0117210000	1.3048200000
C	-0.5978790000	-2.1882390000	1.7667240000
C	-1.9645660000	0.4979680000	-0.5690320000
C	-1.3327260000	-0.7764020000	-0.0662080000
C	-0.1450570000	-3.1466450000	0.8586600000
H	0.3209650000	-4.0598640000	1.2157180000
H	-1.9408590000	1.2637770000	0.2151830000
C	-0.8775480000	-1.7431830000	-0.9695830000
C	-0.2883890000	-2.9219180000	-0.5123460000
H	-0.9745570000	-1.5631950000	-2.0381400000
H	0.0686940000	-3.6589640000	-1.2255850000
H	-1.3935950000	0.8769630000	-1.4245840000

Table S90. Cartesian coordinates of β -Glc-tg_Phe_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6261901			
ZPE / Hartree = 0.3927435			
BSSE / Hartree = 0.0020956893			
C	2.8262590000	-1.1083250000	-0.9152160000
C	4.0678790000	-0.4816630000	-0.2901010000
C	3.6424710000	0.5164230000	0.7756990000
C	2.6754250000	1.5274760000	0.1811920000
C	1.5002010000	0.8089560000	-0.4856400000
C	0.5663900000	1.7672680000	-1.2170400000
O	2.0029520000	-0.0902910000	-1.4677250000
O	3.2335800000	-1.9459210000	-1.9451930000
O	4.8731490000	-1.4592560000	0.3398220000
O	4.7461140000	1.2392090000	1.2926140000
O	2.1469720000	2.3811490000	1.1860810000
O	-0.1897790000	2.5690460000	-0.3251040000
H	2.2545640000	-1.6594510000	-0.1534090000
H	4.6282070000	0.0393330000	-1.0800940000
H	3.1320880000	-0.0260410000	1.5872530000
H	3.2050540000	2.1209100000	-0.5793290000
H	0.9296360000	0.2568470000	0.2786160000
H	1.1542360000	2.3892140000	-1.9063530000
H	-0.1435040000	1.1771340000	-1.8035630000
H	2.5206680000	-2.5647950000	-2.1567630000
H	5.2613740000	-2.0254280000	-0.3414200000
H	5.3216930000	0.6242650000	1.7678440000
H	2.8795770000	2.8639700000	1.5943550000
H	0.4281330000	2.9754570000	0.3026180000
O	-5.6140130000	0.4881740000	1.0725650000
O	-4.7633220000	-1.5861270000	0.8467470000
C	-4.9475410000	-0.4027360000	0.4864060000
H	-5.4489020000	1.7145370000	-0.7419990000
H	-5.9327780000	0.6436460000	-1.9005960000
H	-4.1417510000	-0.7922780000	-1.5081450000
C	-4.2405010000	0.0439190000	-0.8149440000
N	-5.1101710000	1.0709510000	-1.4676120000
H	-4.6192680000	1.6014960000	-2.1916110000

H	-2.0883080000	0.5187990000	2.0880460000
H	-0.5451170000	-1.1265420000	3.1169090000
C	-1.6276630000	-0.2514690000	1.4740060000
C	-0.7597680000	-1.1791900000	2.0538700000
C	-2.8741280000	0.6800590000	-0.5185950000
C	-1.9140960000	-0.3016720000	0.1068800000
C	-0.1678260000	-2.1682440000	1.2679040000
H	0.5118560000	-2.8874590000	1.7151510000
H	-3.0223370000	1.5389500000	0.1454280000
C	-1.3102230000	-1.2931910000	-0.6756960000
C	-0.4444370000	-2.2220890000	-0.1006780000
H	-1.5174030000	-1.3321990000	-1.7430980000
H	0.0223730000	-2.9820120000	-0.7213720000
H	-2.4587790000	1.0539850000	-1.4619090000

Table S91. Cartesian coordinates of β -Glc-tg_Phe_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6253141			
ZPE / Hartree = 0.3931307			
BSSE / Hartree = 0.0023365917			
C	-2.3441970000	-1.1224090000	-1.4323650000
C	-2.2174950000	-1.8210240000	-0.0811540000
C	-2.7681990000	-0.9338130000	1.0249120000
C	-2.1294260000	0.4431670000	0.9515330000
C	-2.3137800000	1.0281260000	-0.4490420000
C	-1.6501280000	2.3925070000	-0.6060600000
O	-1.7061660000	0.1470080000	-1.3868320000
O	-1.6914370000	-1.9047280000	-2.3769460000
O	-2.9535130000	-3.0295910000	-0.0611320000
O	-2.4880730000	-1.4675390000	2.3078520000
O	-2.7183650000	1.3379030000	1.8827910000
O	-2.3930850000	3.4158070000	0.0396040000
H	-3.4047380000	-0.9833140000	-1.6925990000
H	-1.1517280000	-2.0124150000	0.1062070000
H	-3.8553560000	-0.8271390000	0.8885030000
H	-1.0495900000	0.3488280000	1.1472000000
H	-3.3896140000	1.1292060000	-0.6668070000
H	-0.6233440000	2.3487450000	-0.2207970000
H	-1.6127750000	2.6437660000	-1.6692420000
H	-1.9952230000	-1.6635840000	-3.2629270000
H	-2.5153180000	-3.6692270000	-0.6391590000
H	-2.9733230000	-2.2979800000	2.4085310000
H	-2.5694160000	0.9959430000	2.7757450000
H	-2.4973310000	3.1560850000	0.9679520000
O	3.7220000000	-1.9408380000	1.6602690000
O	4.6134660000	-0.3061660000	0.3915820000
C	3.8147170000	-1.2410930000	0.6193020000
H	2.4200950000	-3.3028930000	0.5493870000
H	3.2953230000	-3.5685620000	-0.8250870000
H	3.1922840000	-1.3301450000	-1.4740620000
C	2.7836020000	-1.5598850000	-0.4894930000
N	2.5155220000	-3.0315700000	-0.4375860000

H	1.6699180000	−3.3024180000	−0.9462430000
H	1.5795580000	0.8380330000	1.9057790000
H	1.8976200000	3.2972610000	1.9286430000
C	1.6851990000	1.3818150000	0.9695580000
C	1.8645510000	2.7659520000	0.9823140000
C	1.4600710000	−0.8164750000	−0.2541870000
C	1.6353750000	0.6814060000	−0.2398020000
C	1.9975520000	3.4643510000	−0.2188350000
H	2.1339280000	4.5413450000	−0.2111070000
H	1.0380990000	−1.1499800000	0.7017290000
C	1.7667680000	1.3896750000	−1.4394460000
C	1.9487470000	2.7723000000	−1.4309720000
H	1.7189290000	0.8529750000	−2.3843900000
H	2.0450220000	3.3103380000	−2.3691900000
H	0.7595660000	−1.0963330000	−1.0500590000

Complex Glc-His

Table S92. Cartesian coordinates of α -Glc-gg_His_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6232898			
ZPE / Hartree = 0.3644632			
BSSE / Hartree = 0.00168198892			
C	1.0235510000	0.1945100000	0.0080650000
C	1.9598800000	1.2190340000	-0.6359290000
C	3.1381990000	0.5134230000	-1.3006390000
C	3.8302090000	-0.3961520000	-0.2997300000
C	2.8177630000	-1.3802320000	0.2814640000
C	3.3949320000	-2.2534420000	1.3815000000
O	1.7359820000	-0.6580210000	0.8776570000
O	0.4091440000	-0.5093880000	-1.0402330000
O	1.2660930000	2.0373340000	-1.5586020000
O	4.1028760000	1.4452390000	-1.7638510000
O	4.8590510000	-1.1498240000	-0.9178240000
O	3.8795110000	-1.4856210000	2.4729000000
H	0.2781190000	0.6893420000	0.6356430000
H	2.3397390000	1.8813120000	0.1490290000
H	2.7736590000	-0.0969360000	-2.1405100000
H	4.2417960000	0.2199630000	0.5130530000
H	2.4416680000	-2.0271230000	-0.5229880000
H	2.6220350000	-2.9560070000	1.7149480000
H	4.2400330000	-2.8216530000	0.9882310000
H	-0.3947840000	-0.9382540000	-0.7156560000
H	0.7554640000	1.4548180000	-2.1424140000
H	3.6992000000	1.9827730000	-2.4592310000
H	5.4532720000	-0.5292140000	-1.3632990000
H	3.1401570000	-0.9704090000	2.8248420000
N	-4.8803520000	0.5438100000	-0.6646800000
H	-5.7114980000	0.1434720000	-0.2117990000
H	-5.1322810000	0.7296290000	-1.6381670000
H	-4.6420890000	1.4390660000	-0.2282800000
C	-3.7739360000	-0.4567860000	-0.5654370000
H	-3.0814700000	-0.2703580000	-1.3886880000
C	-3.0705570000	-0.3243510000	0.7824130000

C	−4.3838680000	−1.8724080000	−0.7132920000
H	−3.8089500000	−0.4265830000	1.5874440000
H	−2.3782320000	−1.1676380000	0.8756870000
C	−2.3275150000	0.9672470000	0.9307190000
O	−5.6306730000	−1.9584050000	−0.5983990000
N	−1.7869170000	1.3608100000	2.1305850000
C	−1.9862400000	1.9667520000	0.0486120000
H	−1.8430220000	0.8527490000	3.0047160000
C	−1.1530720000	2.5443690000	1.9399820000
N	−1.2549180000	2.9461040000	0.6890310000
H	−2.2147070000	2.0339100000	−1.0071250000
H	−0.6441540000	3.0637990000	2.7391440000
O	−3.5588240000	−2.7930030000	−0.9023350000

Table S93. Cartesian coordinates of α -Glc-gg_His_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6276981			
ZPE / Hartree = 0.3654229			
BSSE / Hartree = 0.00274491082			
C	-0.7124050000	-0.9074170000	1.3385480000
C	-1.5146350000	0.3892890000	1.4488020000
C	-2.9022390000	0.2055300000	0.8444910000
C	-2.7891300000	-0.3090160000	-0.5811790000
C	-1.9447730000	-1.5826350000	-0.6146550000
C	-1.6482070000	-2.0581000000	-2.0281090000
O	-0.6791180000	-1.3629150000	0.0063750000
O	-1.3122320000	-1.8369390000	2.2035510000
O	-1.5892550000	0.8305990000	2.7912790000
O	-3.6081850000	1.4359490000	0.7928710000
O	-4.0649690000	-0.6341860000	-1.1079780000
O	-0.8024740000	-1.1484820000	-2.7306130000
H	0.3350400000	-0.7383590000	1.6116650000
H	-0.9858540000	1.1708990000	0.8938050000
H	-3.4683990000	-0.5271540000	1.4394510000
H	-2.3127270000	0.4651580000	-1.1982160000
H	-2.4946960000	-2.3761420000	-0.0883850000
H	-1.1829100000	-3.0470610000	-1.9873740000
H	-2.5869150000	-2.1349050000	-2.5814330000
H	-0.6910970000	-2.5559990000	2.3837220000
H	-1.8910380000	0.0835010000	3.3309400000
H	-3.7398600000	1.7516190000	1.6978280000
H	-4.6183150000	0.1579420000	-1.0562720000
H	0.1135880000	-1.4206100000	-2.5855300000
N	4.2618490000	1.1768860000	-0.0063250000
H	5.0041220000	0.7019560000	-0.5403010000
H	4.6979580000	1.5776400000	0.8275160000
H	3.8792770000	1.9488920000	-0.5585020000
C	3.2403710000	0.1390170000	0.3431980000
H	2.8345360000	0.3833580000	1.3270080000
C	2.1305590000	0.1017710000	-0.7016850000
C	3.9566090000	-1.2337910000	0.4132160000
H	2.5735390000	-0.0135190000	-1.6997610000

H	1.5299840000	-0.7931340000	-0.5112030000
C	1.2470910000	1.3098600000	-0.6616600000
O	5.1156160000	-1.2854410000	-0.0674730000
N	0.1620900000	1.4471470000	-1.4921240000
C	1.2602450000	2.4601540000	0.0943920000
H	-0.2004840000	0.7286430000	-2.1176000000
C	-0.4315460000	2.6334370000	-1.2122830000
N	0.2090890000	3.2814060000	-0.2589530000
H	1.9568590000	2.7415380000	0.8729140000
H	-1.3223850000	2.9694780000	-1.7242760000
O	3.2889840000	-2.1611380000	0.9204090000

Table S94. Cartesian coordinates of α -Glc-gg_His_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6290496			
ZPE / Hartree = 0.3651065			
BSSE / Hartree = 0.00260633864			
C	3.2258200000	-1.2286510000	0.6296820000
C	2.0174750000	-0.7863130000	1.4602170000
C	1.1478710000	0.1752020000	0.6522020000
C	1.9869150000	1.3267780000	0.1223160000
C	3.1661730000	0.7811850000	-0.6784020000
C	4.1271540000	1.8600920000	-1.1446530000
O	3.9316760000	-0.1041710000	0.1433070000
O	2.7476190000	-2.0356990000	-0.4118110000
O	1.2853180000	-1.8965980000	1.9358320000
O	0.1152460000	0.7414080000	1.4466960000
O	1.2220380000	2.1519910000	-0.7400400000
O	4.6838130000	2.5857360000	-0.0588040000
H	3.9430360000	-1.7729860000	1.2500370000
H	2.3933790000	-0.2575730000	2.3426030000
H	0.7112220000	-0.3543880000	-0.2070050000
H	2.3673050000	1.9100540000	0.9737440000
H	2.7843810000	0.2449140000	-1.5583970000
H	4.9173580000	1.3916150000	-1.7433310000
H	3.5918060000	2.5778530000	-1.7693130000
H	3.4848210000	-2.5269430000	-0.7993280000
H	0.8928790000	-2.3654180000	1.1760150000
H	-0.5920530000	0.0879140000	1.5449480000
H	0.4176600000	2.4064170000	-0.2647230000
H	5.1483720000	1.9573720000	0.5115510000
N	-4.7404390000	-0.8138410000	0.1330630000
H	-5.4210550000	-0.5207310000	-0.5781810000
H	-5.2665780000	-0.9889880000	0.9921800000
H	-4.3033020000	-1.6958270000	-0.1501510000
C	-3.7466930000	0.2871020000	0.3181270000
H	-3.2806720000	0.1510850000	1.2959220000
C	-2.7038050000	0.2443650000	-0.7962320000
C	-4.5009580000	1.6385230000	0.2843150000

H	-3.2044690000	0.3147450000	-1.7693490000
H	-2.0762840000	1.1356380000	-0.6881100000
C	-1.8485290000	-0.9827480000	-0.7481670000
O	-5.6696140000	1.6143290000	-0.1723240000
N	-1.0696940000	-1.3761120000	-1.8096320000
C	-1.5761400000	-1.8956260000	0.2434790000
H	-1.0239790000	-0.9221520000	-2.7138160000
C	-0.3642290000	-2.4692400000	-1.4351320000
N	-0.6411590000	-2.8148930000	-0.1928860000
H	-1.9914830000	-1.9433400000	1.2420120000
H	0.3356540000	-2.9624520000	-2.0939290000
O	-3.8480060000	2.6258910000	0.6879300000

Table S95. Cartesian coordinates of α -Glc-gg_His_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6266150			
ZPE / Hartree = 0.3647330			
BSSE / Hartree = 0.00243694122			
C	-3.4693320000	-0.2089010000	-1.0108260000
C	-2.4099340000	-1.3073260000	-0.8912450000
C	-2.0292220000	-1.5405560000	0.5678180000
C	-1.6498060000	-0.2211280000	1.2205560000
C	-2.8086830000	0.7611670000	1.0746460000
C	-2.5372210000	2.1260100000	1.6816210000
O	-3.0712460000	0.9555480000	-0.3198490000
O	-4.6650190000	-0.7414430000	-0.5022650000
O	-2.8435310000	-2.5026480000	-1.5123560000
O	-0.9044510000	-2.4009900000	0.6715490000
O	-1.3807510000	-0.3877250000	2.6009130000
O	-1.2850110000	2.6766720000	1.3166520000
H	-3.5910370000	0.0993470000	-2.0528800000
H	-1.5160670000	-0.9821340000	-1.4309730000
H	-2.8833330000	-1.9733770000	1.1099180000
H	-0.7658870000	0.1868180000	0.7032340000
H	-3.7018650000	0.3458500000	1.5618260000
H	-3.3615530000	2.7919700000	1.3952830000
H	-2.5341790000	2.0314970000	2.7700270000
H	-5.4112500000	-0.2078180000	-0.8075910000
H	-3.7318790000	-2.7012950000	-1.1781240000
H	-1.1638450000	-3.2852980000	0.3784860000
H	-0.7135140000	-1.0836150000	2.6891680000
H	-1.1425410000	2.6106820000	0.3546120000
N	4.5973420000	1.1387940000	-0.6825690000
H	5.2380420000	0.6063100000	-1.2832340000
H	5.1708000000	1.7916810000	-0.1432480000
H	3.9577810000	1.6904050000	-1.2618160000
C	3.8765410000	0.1835540000	0.2126140000
H	3.5132120000	0.7502790000	1.0713330000
C	2.7204120000	-0.4748600000	-0.5371530000
C	4.8814100000	-0.8931000000	0.6896590000
H	3.1089040000	-0.9880220000	-1.4250570000

H	2.3043590000	-1.2421880000	0.1232500000
C	1.6512250000	0.4932550000	-0.9390400000
O	5.9658600000	-0.9630770000	0.0618820000
N	0.7958630000	0.2468200000	-1.9868240000
C	1.2430700000	1.7026370000	-0.4301360000
H	0.8138280000	-0.5672600000	-2.5897100000
C	-0.0820120000	1.2741550000	-2.0668760000
N	0.1584090000	2.1799180000	-1.1393040000
H	1.6552050000	2.2486830000	0.4075830000
H	-0.8686680000	1.3110490000	-2.8073290000
O	4.4895860000	-1.6065530000	1.6392600000

Table S96. Cartesian coordinates of α -Glc-gg_His_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6262145			
ZPE / Hartree = 0.3640428			
BSSE / Hartree = 0.00217617295			
C	3.5320350000	0.3720840000	-0.3183640000
C	3.3843720000	-1.1065290000	-0.6818130000
C	1.9153130000	-1.5184400000	-0.6387300000
C	1.3224510000	-1.1675580000	0.7156920000
C	1.5144670000	0.3252760000	0.9751370000
C	1.0311730000	0.7675440000	2.3437760000
O	2.9088440000	0.6446400000	0.9183840000
O	2.9629120000	1.1048670000	-1.3713800000
O	3.9603790000	-1.3836260000	-1.9440740000
O	1.7697110000	-2.9175020000	-0.8223790000
O	-0.0685630000	-1.4361060000	0.7551420000
O	1.6952660000	0.0828300000	3.3951770000
H	4.5832710000	0.6375400000	-0.1791940000
H	3.9383490000	-1.6999810000	0.0526970000
H	1.3568160000	-0.9775720000	-1.4186270000
H	1.8461000000	-1.7419180000	1.4939310000
H	0.9708280000	0.8926510000	0.2083720000
H	1.1736020000	1.8519170000	2.4328510000
H	-0.0348210000	0.5473050000	2.4396100000
H	3.2482530000	2.0273670000	-1.3165380000
H	3.6067760000	-0.7396330000	-2.5770410000
H	2.0966710000	-3.1444320000	-1.7041500000
H	-0.2015340000	-2.3682180000	0.5308980000
H	2.6420090000	0.2670600000	3.3203370000
N	-4.0460640000	0.3279680000	-1.5418190000
H	-4.9912460000	0.4255940000	-1.1489610000
H	-4.1354550000	-0.1998720000	-2.4131460000
H	-3.6662040000	1.2502900000	-1.7736290000
C	-3.2078850000	-0.4048380000	-0.5425510000
H	-2.4215170000	-0.9302060000	-1.0880550000
C	-2.6075980000	0.5716510000	0.4642780000
C	-4.1084940000	-1.4320170000	0.1859700000

H	-3.4121010000	1.1363410000	0.9516190000
H	-2.1109760000	-0.0301260000	1.2315690000
C	-1.6210520000	1.5106170000	-0.1547740000
O	-5.3481240000	-1.2758700000	0.0614130000
N	-1.0971000000	2.5758940000	0.5344430000
C	-1.0128760000	1.5591670000	-1.3887050000
H	-1.3192500000	2.8363320000	1.4874800000
C	-0.2123350000	3.2095080000	-0.2747660000
N	-0.1379010000	2.6242820000	-1.4533930000
H	-1.1474940000	0.8874930000	-2.2265370000
H	0.3384300000	4.0837630000	0.0415320000
O	-3.5017370000	-2.2976690000	0.8539010000

Table S97. Cartesian coordinates of α -Glc-gg_His_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6261932			
ZPE / Hartree = 0.3642129			
BSSE / Hartree = 0.00229966380			
C	2.4594220000	-0.7742180000	1.5300870000
C	3.3327830000	0.2317860000	0.7755120000
C	2.5319960000	0.9091560000	-0.3338200000
C	1.9016080000	-0.1440770000	-1.2297890000
C	1.0377280000	-1.0625120000	-0.3718670000
C	0.3815860000	-2.1900370000	-1.1457240000
O	1.8483690000	-1.6770640000	0.6334390000
O	1.5132630000	-0.0329880000	2.2564410000
O	3.8964170000	1.1797480000	1.6615100000
O	3.3600230000	1.7216680000	-1.1502440000
O	1.0661040000	0.4471830000	-2.2095770000
O	1.3345610000	-3.0251980000	-1.7860680000
H	3.0662950000	-1.3916680000	2.1972430000
H	4.1691720000	-0.3108280000	0.3231520000
H	1.7303290000	1.5189160000	0.1101550000
H	2.6989680000	-0.7317080000	-1.7086870000
H	0.2510090000	-0.4632060000	0.1040660000
H	-0.2462940000	-2.7701120000	-0.4562690000
H	-0.2562110000	-1.7698440000	-1.9275020000
H	1.1340040000	-0.5889620000	2.9512610000
H	3.1774430000	1.5412640000	2.2026720000
H	3.6601570000	2.4790600000	-0.6293120000
H	1.5666220000	1.1587900000	-2.6346750000
H	1.9074210000	-3.4010370000	-1.1029750000
N	-3.2799060000	1.7343130000	1.2274560000
H	-3.9535630000	2.3251190000	0.7241170000
H	-3.0664820000	2.2081170000	2.1080470000
H	-3.7081610000	0.8316560000	1.4542980000
C	-2.0630320000	1.5908830000	0.3724910000
H	-1.2188670000	1.3678400000	1.0291570000
C	-2.2739160000	0.4777750000	-0.6529740000
C	-1.8176050000	2.9375140000	-0.3519680000
H	-3.1428150000	0.7199080000	-1.2769920000

H	-1.3942620000	0.4719110000	-1.3085470000
C	-2.4623600000	-0.8670560000	-0.0211210000
O	-2.7877930000	3.7333900000	-0.3879650000
N	-3.0217370000	-1.9249860000	-0.6946510000
C	-2.1416010000	-1.3722760000	1.2182670000
H	-3.3705810000	-1.9096410000	-1.6452000000
C	-3.0137180000	-3.0012980000	0.1286210000
N	-2.4900980000	-2.7041110000	1.3017170000
H	-1.6763940000	-0.8552170000	2.0474940000
H	-3.4028680000	-3.9632730000	-0.1723010000
O	-0.6834560000	3.0760820000	-0.8596800000

Table S98. Cartesian coordinates of α -Glc-gt_His_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6214966			
ZPE / Hartree = 0.3647328			
BSSE / Hartree = 0.00153749958			
C	-1.1752400000	-0.0555090000	-0.0616910000
C	-1.9301830000	-1.3336930000	-0.4281330000
C	-3.2598380000	-0.9875660000	-1.0910850000
C	-4.0567510000	-0.0386040000	-0.2095900000
C	-3.2129060000	1.1952470000	0.1081200000
C	-3.9139930000	2.1232290000	1.0839620000
O	-1.9864500000	0.7924490000	0.7199400000
O	-0.7737690000	0.5457040000	-1.2661730000
O	-1.1459470000	-2.1733640000	-1.2539470000
O	-4.0564410000	-2.1446100000	-1.2914980000
O	-5.2371620000	0.3911970000	-0.8658720000
O	-3.1724590000	3.3093220000	1.3286090000
H	-0.3100380000	-0.2850180000	0.5631210000
H	-2.1264390000	-1.8923490000	0.4932790000
H	-3.0699270000	-0.4923610000	-2.0552760000
H	-4.3074520000	-0.5543880000	0.7307900000
H	-3.0011800000	1.7347410000	-0.8265000000
H	-4.9129750000	2.3551630000	0.7012700000
H	-4.0157140000	1.6151580000	2.0477770000
H	-0.0518270000	1.1645160000	-1.0902600000
H	-0.7900930000	-1.6288610000	-1.9732910000
H	-3.6081230000	-2.7189800000	-1.9275460000
H	-5.7216000000	-0.3977050000	-1.1487420000
H	-3.1939250000	3.8585450000	0.5336780000
N	5.1559510000	-0.7400880000	0.3006090000
H	5.8017730000	-0.0668840000	0.7306810000
H	5.7220210000	-1.3716420000	-0.2708910000
H	4.7021340000	-1.3006810000	1.0280050000
C	4.1720890000	0.0154340000	-0.5324940000
H	3.7672480000	-0.6768310000	-1.2720910000
C	3.0630190000	0.5813690000	0.3539080000
C	4.9182270000	1.1664840000	-1.2489280000

H	3.5058680000	1.2347060000	1.1149360000
H	2.4299040000	1.2083090000	-0.2817020000
C	2.2458840000	-0.4850840000	1.0161020000
O	6.0555070000	1.4572840000	-0.8047230000
N	1.6148050000	-0.2896830000	2.2207530000
C	1.9097630000	-1.7679910000	0.6491100000
H	1.6463650000	0.5543060000	2.7795060000
C	0.9338980000	-1.4206510000	2.5290800000
N	1.0911280000	-2.3422140000	1.5988900000
H	2.2067680000	-2.3046900000	-0.2415880000
H	0.3514440000	-1.5177420000	3.4339390000
O	4.2890680000	1.7133420000	-2.1814630000

Table S99. Cartesian coordinates of α -Glc-gt_His_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6247185			
ZPE / Hartree = 0.3641846			
BSSE / Hartree = 0.00229328744			
C	0.6867330000	0.4811980000	1.3527070000
C	1.5053450000	-0.8058990000	1.2560980000
C	2.9131900000	-0.5025010000	0.7565670000
C	2.8432410000	0.2664560000	-0.5528170000
C	1.9971540000	1.5258130000	-0.3674080000
C	1.7822410000	2.2521080000	-1.6834040000
O	0.7036820000	1.1723430000	0.1250600000
O	1.2330820000	1.2391920000	2.4009340000
O	1.5269460000	-1.4935200000	2.4923090000
O	3.6394750000	-1.6950500000	0.5018170000
O	4.1356540000	0.6621340000	-0.9784700000
O	1.0714340000	3.4700340000	-1.5210980000
H	-0.3679340000	0.2548180000	1.5438180000
H	1.0151220000	-1.4705920000	0.5381090000
H	3.4472650000	0.1105450000	1.4978750000
H	2.3689530000	-0.3758180000	-1.3128510000
H	2.4987250000	2.1936030000	0.3486830000
H	2.7524140000	2.4225120000	-2.1609760000
H	1.1732410000	1.6208750000	-2.3387230000
H	0.5930680000	1.9077740000	2.6808820000
H	1.7768990000	-0.8575080000	3.1803600000
H	3.7810410000	-2.1540660000	1.3412660000
H	4.6961780000	-0.1271720000	-0.9879500000
H	1.6451940000	4.1065260000	-1.0743770000
N	-4.3408900000	-1.0942580000	-0.1500600000
H	-5.0092060000	-0.5652100000	-0.7245650000
H	-4.8648700000	-1.4698950000	0.6440130000
H	-3.9765230000	-1.8864770000	-0.6863920000
C	-3.2694020000	-0.1494440000	0.2944900000
H	-2.8546330000	-0.5342460000	1.2285630000
C	-2.1905490000	-0.0301390000	-0.7765370000
C	-3.9178380000	1.2333260000	0.5507490000

H	-2.6608650000	0.2150550000	-1.7375840000
H	-1.5490110000	0.8151450000	-0.5075130000
C	-1.3527670000	-1.2633510000	-0.9102790000
O	-5.0688380000	1.4080190000	0.0815680000
N	-0.3575250000	-1.3652750000	-1.8512810000
C	-1.3188830000	-2.4618950000	-0.2349430000
H	-0.0982910000	-0.6519220000	-2.5221240000
C	0.2288930000	-2.5804500000	-1.7172550000
N	-0.3301630000	-3.2772900000	-0.7479770000
H	-1.9398640000	-2.7825220000	0.5910080000
H	1.0487910000	-2.9003210000	-2.3444040000
O	-3.2064090000	2.0487660000	1.1779170000

Table S100. Cartesian coordinates of α -Glc-gt_His_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6273032			
ZPE / Hartree = 0.3656392			
BSSE / Hartree = 0.00259382317			
C	-3.3040130000	1.1919080000	0.6320050000
C	-2.0950780000	0.9190110000	1.5319110000
C	-1.1940760000	-0.1347770000	0.8929300000
C	-1.9941990000	-1.3796720000	0.5432130000
C	-3.1804260000	-0.9961320000	-0.3392830000
C	-4.0813030000	-2.1839350000	-0.6247900000
O	-3.9746450000	-0.0147010000	0.3283030000
O	-2.8384680000	1.8418040000	-0.5199250000
O	-1.3946830000	2.1071740000	1.8351600000
O	-0.1547570000	-0.5405560000	1.7714450000
O	-1.1878360000	-2.3031150000	-0.1686290000
O	-5.1274440000	-1.8625260000	-1.5297500000
H	-4.0417180000	1.8061730000	1.1554630000
H	-2.4703530000	0.5261900000	2.4829870000
H	-0.7627800000	0.2619970000	-0.0378680000
H	-2.3695950000	-1.8352460000	1.4734050000
H	-2.8009060000	-0.5865020000	-1.2872490000
H	-3.4723470000	-3.0100950000	-1.0058350000
H	-4.5603370000	-2.5004600000	0.3066980000
H	-3.5849110000	2.2547120000	-0.9755670000
H	-0.9781970000	2.4486150000	1.0219050000
H	0.5445330000	0.1282470000	1.7491520000
H	-0.3693380000	-2.4215010000	0.3358140000
H	-4.7474970000	-1.7353040000	-2.4092520000
N	4.8043560000	0.8851540000	-0.5185400000
H	5.2940800000	0.4224630000	-1.2931460000
H	5.5225340000	1.2699630000	0.0990790000
H	4.2507300000	1.6686620000	-0.8777280000
C	3.9652420000	-0.1273730000	0.1887210000
H	3.7437360000	0.2662980000	1.1820110000
C	2.6823010000	-0.3827960000	-0.6019050000
C	4.7795410000	-1.4371340000	0.3172900000

H	2.9407890000	-0.7317050000	-1.6083620000
H	2.1490950000	-1.1982870000	-0.1021350000
C	1.8009020000	0.8243750000	-0.6972420000
O	5.7989830000	-1.5339090000	-0.4081370000
N	0.9958940000	1.0640030000	-1.7850880000
C	1.5314790000	1.8567230000	0.1713540000
H	0.9421470000	0.4960890000	-2.6222050000
C	0.2809680000	2.1873720000	-1.5447490000
N	0.5746370000	2.6971610000	-0.3636060000
H	1.9653410000	2.0414910000	1.1455600000
H	-0.4372900000	2.5812080000	-2.2488810000
O	4.3126060000	-2.2820030000	1.1127920000

Table S101. Cartesian coordinates of α -Glc-gt_His_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6242002			
ZPE / Hartree = 0.3644056			
BSSE / Hartree = 0.00240269905			
C	3.6770080000	-0.6375640000	0.5939870000
C	2.4252630000	-1.4730960000	0.8730880000
C	1.5041410000	-1.4618250000	-0.3424240000
C	1.2044440000	-0.0285110000	-0.7497520000
C	2.5116690000	0.7174740000	-1.0059170000
C	2.2704940000	2.1853240000	-1.3080310000
O	3.3260730000	0.6601670000	0.1678960000
O	4.4221040000	-1.3330020000	-0.3725490000
O	2.7674110000	-2.7919840000	1.2536580000
O	0.2605510000	-2.0849280000	-0.0589390000
O	0.4199660000	0.0111450000	-1.9299060000
O	3.4688160000	2.8702850000	-1.6412570000
H	4.2606220000	-0.4949250000	1.5073150000
H	1.8935810000	-1.0275640000	1.7209220000
H	1.9956990000	-1.9743580000	-1.1828170000
H	0.6741930000	0.4697800000	0.0747640000
H	3.0408490000	0.2483430000	-1.8482980000
H	1.5332210000	2.2683850000	-2.1129750000
H	1.8690720000	2.6711300000	-0.4129980000
H	5.3310430000	-1.0031340000	-0.3777960000
H	3.3887770000	-3.1359520000	0.5933860000
H	0.4067330000	-3.0353070000	0.0426870000
H	-0.3409020000	-0.5727550000	-1.7928570000
H	3.7631130000	2.5704680000	-2.5115970000
N	-4.6113000000	1.0785140000	0.4990670000
H	-5.3394990000	0.4559570000	0.8717950000
H	-5.0873510000	1.8000130000	-0.0472210000
H	-4.1229440000	1.5438650000	1.2695730000
C	-3.6926080000	0.2616230000	-0.3539490000
H	-3.2382010000	0.9305880000	-1.0869270000
C	-2.6273990000	-0.4070990000	0.5108000000
C	-4.5322790000	-0.8134200000	-1.0858550000

H	-3.1142590000	-1.0051240000	1.2914350000
H	-2.0728300000	-1.1040340000	-0.1255030000
C	-1.6798510000	0.5699680000	1.1338950000
O	-5.6894900000	-1.0162440000	-0.6436520000
N	-0.8354260000	0.2161930000	2.1573220000
C	-1.3809980000	1.8878000000	0.8730570000
H	-0.7784310000	-0.6960900000	2.5932670000
C	-0.0705570000	1.2923070000	2.4652450000
N	-0.3763050000	2.3288920000	1.7098120000
H	-1.8262590000	2.5385300000	0.1324200000
H	0.6808750000	1.2661500000	3.2414330000
O	-3.9519110000	-1.3950700000	-2.0287840000

Table S102. Cartesian coordinates of α -Glc-gt_His_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6251346			
ZPE / Hartree = 0.3650851			
BSSE / Hartree = 0.00248997512			
C	3.5851860000	-0.0016290000	-0.1717190000
C	3.2540200000	-1.4853260000	-0.3463910000
C	1.7452270000	-1.7035670000	-0.2745550000
C	1.1920600000	-1.0964530000	1.0049230000
C	1.5690780000	0.3840730000	1.0572570000
C	1.1027510000	1.0475540000	2.3399380000
O	2.9921570000	0.5046450000	1.0038930000
O	3.1260480000	0.6526180000	-1.3259270000
O	3.7926810000	-1.9916550000	-1.5529150000
O	1.4228330000	-3.0849620000	-0.2620280000
O	-0.2190400000	-1.2061820000	1.0520600000
O	1.4591540000	2.4209390000	2.3974380000
H	4.6605770000	0.1448530000	-0.0405260000
H	3.7284330000	-2.0425610000	0.4677070000
H	1.2594210000	-1.2121360000	-1.1318730000
H	1.6451320000	-1.6093370000	1.8683190000
H	1.1234540000	0.9021110000	0.1950130000
H	0.0179990000	0.9183070000	2.4285270000
H	1.5861180000	0.5659200000	3.1956450000
H	3.5244870000	1.5321190000	-1.3793460000
H	3.5285050000	-1.3916690000	-2.2676060000
H	1.6761810000	-3.4673400000	-1.1134380000
H	-0.4492200000	-2.1382370000	0.9264210000
H	0.9760210000	2.8953440000	1.7072840000
N	-3.8748380000	-0.0868310000	-1.6464200000
H	-4.8182540000	0.1896000000	-1.3485150000
H	-3.9876050000	-0.8649970000	-2.3000710000
H	-3.4311480000	0.6852230000	-2.1519260000
C	-3.1059350000	-0.4996260000	-0.4332210000
H	-2.2932600000	-1.1520470000	-0.7580700000
C	-2.5584720000	0.7295930000	0.2853710000
C	-4.0600740000	-1.2820590000	0.5011400000
H	-3.3844890000	1.4127590000	0.5190200000

H	-2.1338620000	0.3816090000	1.2313860000
C	-1.5083440000	1.4441570000	-0.5053330000
O	-5.2885700000	-1.1659500000	0.2692480000
N	-1.0314320000	2.6783730000	-0.1383270000
C	-0.7990090000	1.1174800000	-1.6381340000
H	-1.3599050000	3.2336430000	0.6426940000
C	-0.0778940000	3.0453910000	-1.0329250000
N	0.0892840000	2.1234710000	-1.9589140000
H	-0.8715260000	0.2157190000	-2.2322270000
H	0.4486920000	3.9866760000	-0.9631660000
O	-3.5050640000	-1.9279760000	1.4172650000

Table S103. Cartesian coordinates of α -Glc-gt_His_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6297514			
ZPE / Hartree = 0.3648079			
BSSE / Hartree = 0.00216583063			
C	3.8228750000	0.4153730000	0.3797730000
C	3.2817740000	-0.9025010000	0.9317800000
C	2.1928800000	-1.4607350000	0.0204190000
C	1.1135000000	-0.4157570000	-0.2258950000
C	1.7615850000	0.8658340000	-0.7553030000
C	0.7483790000	1.9870050000	-0.8944490000
O	2.7662290000	1.3206530000	0.1541270000
O	4.5287490000	0.1113780000	-0.7956390000
O	4.3189290000	-1.8473950000	1.1227230000
O	1.5806250000	-2.5955720000	0.6115560000
O	0.1724260000	-0.8570750000	-1.1797330000
O	1.3195610000	3.1718810000	-1.4308560000
H	4.4744210000	0.9042370000	1.1088750000
H	2.8501450000	-0.7086670000	1.9190630000
H	2.6345400000	-1.7362980000	-0.9497510000
H	0.6218050000	-0.1866730000	0.7355080000
H	2.2179940000	0.6577230000	-1.7342740000
H	-0.0859510000	1.6390030000	-1.5105590000
H	0.3626080000	2.2469920000	0.0980620000
H	5.1121590000	0.8492410000	-1.0194620000
H	4.8245030000	-1.8993680000	0.2967230000
H	2.2710270000	-3.2518000000	0.7829750000
H	-0.3473030000	-1.6183830000	-0.8269140000
H	1.5122570000	3.0249840000	-2.3663460000
N	-4.4559880000	-0.7629820000	-0.5586220000
H	-4.9515310000	-1.4932730000	-0.0314860000
H	-4.7403590000	-0.8553230000	-1.5374340000
H	-4.7597530000	0.1584810000	-0.2331320000
C	-2.9864470000	-0.9846200000	-0.3944500000
H	-2.4887630000	-0.5751790000	-1.2759480000
C	-2.4755760000	-0.3078300000	0.8747800000
C	-2.7306830000	-2.5081750000	-0.3306860000

H	-3.1288410000	-0.5727740000	1.7161660000
H	-1.4907100000	-0.7295410000	1.0984870000
C	-2.3686330000	1.1783650000	0.7387340000
O	-3.7232200000	-3.2483070000	-0.1669650000
N	-1.9020870000	1.9743720000	1.7566750000
C	-2.6471770000	2.0497270000	-0.2874580000
H	-1.6017310000	1.6588900000	2.6705950000
C	-1.9098040000	3.2590470000	1.3234120000
N	-2.3576630000	3.3453170000	0.0867280000
H	-3.0265030000	1.8186950000	-1.2739970000
H	-1.5822150000	4.0809010000	1.9436910000
O	-1.5237610000	-2.8509610000	-0.4262440000

Table S104. Cartesian coordinates of α -Glc-tg_His_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6219014			
ZPE / Hartree = 0.3649309			
BSSE / Hartree = 0.00158733798			
C	-1.0563390000	-0.1832750000	0.0434800000
C	-1.9046200000	-1.3218230000	-0.5276770000
C	-3.2021020000	-0.7818510000	-1.1241010000
C	-3.9190130000	0.0710640000	-0.0925870000
C	-2.9910620000	1.1861360000	0.3870370000
C	-3.6113950000	2.0328670000	1.4939530000
O	-1.8108940000	0.6048310000	0.9401880000
O	-0.5797820000	0.5604760000	-1.0474610000
O	-1.1799420000	-2.0722080000	-1.4830960000
O	-4.0734840000	-1.8380190000	-1.4926140000
O	-5.0840510000	0.6772900000	-0.6350530000
O	-4.6303900000	2.8877280000	1.0008100000
H	-0.2284760000	-0.5782160000	0.6364800000
H	-2.1516790000	-2.0077480000	0.2898900000
H	-2.9723910000	-0.1593510000	-2.0020300000
H	-4.1878030000	-0.5592110000	0.7685890000
H	-2.7322590000	1.8365240000	-0.4602170000
H	-3.9959060000	1.3747430000	2.2850890000
H	-2.8351860000	2.6721300000	1.9212780000
H	0.1934340000	1.0733600000	-0.7744940000
H	-0.7777180000	-1.4456260000	-2.1045480000
H	-3.6360210000	-2.3684340000	-2.1732070000
H	-5.7070990000	-0.0206330000	-0.8819970000
H	-5.2622490000	2.3371560000	0.5127210000
N	5.1328000000	-0.6169270000	-0.2913690000
H	5.8531510000	-0.1797930000	0.2958380000
H	5.5916530000	-0.9109220000	-1.1567420000
H	4.7716010000	-1.4563960000	0.1718110000
C	4.0626710000	0.3915420000	-0.5557410000
H	3.5227420000	0.0735290000	-1.4491280000
C	3.1243540000	0.4849820000	0.6462500000
C	4.7323660000	1.7628240000	-0.8143250000
H	3.7030090000	0.7553260000	1.5377450000

H	2.4295160000	1.3082720000	0.4522590000
C	2.3744290000	-0.7862860000	0.8978450000
O	5.9368810000	1.8694710000	-0.4788250000
N	1.8258320000	-1.0855820000	2.1209920000
C	2.0469780000	-1.8553880000	0.0960460000
H	1.8768500000	-0.5119810000	2.9539730000
C	1.2001500000	-2.2845840000	2.0206190000
N	1.3149730000	-2.7842980000	0.8062480000
H	2.2920710000	-2.0047100000	-0.9470480000
H	0.6868960000	-2.7413040000	2.8545570000
O	3.9856750000	2.6383910000	-1.3047890000

Table S105. Cartesian coordinates of α -Glc-tg_His_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6249700			
ZPE / Hartree = 0.3646482			
BSSE / Hartree = 0.00216841790			
C	-0.6671260000	-0.4276520000	1.4638380000
C	-1.4060090000	0.9013620000	1.3051450000
C	-2.8355890000	0.6685160000	0.8251380000
C	-2.8089570000	-0.1740440000	-0.4375720000
C	-2.0561530000	-1.4789520000	-0.1814520000
C	-1.8881390000	-2.3152270000	-1.4462060000
O	-0.7360570000	-1.1826290000	0.2729520000
O	-1.2508880000	-1.0962760000	2.5501810000
O	-1.3759020000	1.6491720000	2.5054710000
O	-3.4742680000	1.8938900000	0.5044700000
O	-4.1207780000	-0.5080780000	-0.8696310000
O	-3.1072820000	-2.9114550000	-1.8581060000
H	0.4006990000	-0.2567770000	1.6377790000
H	-0.8789020000	1.4971630000	0.5532710000
H	-3.4082480000	0.1357510000	1.5989610000
H	-2.2847970000	0.3881690000	-1.2256990000
H	-2.5945330000	-2.0687400000	0.5737500000
H	-1.4667750000	-1.6867610000	-2.2437100000
H	-1.1871730000	-3.1272000000	-1.2384750000
H	-0.6518470000	-1.7886440000	2.8615040000
H	-1.6653300000	1.0662940000	3.2244180000
H	-3.5447010000	2.4228940000	1.3113450000
H	-4.5886260000	0.3106860000	-1.0869400000
H	-3.7711290000	-2.2070800000	-1.9199650000
N	4.4936490000	0.8624940000	-0.5202030000
H	5.0783670000	0.2461660000	-1.0990920000
H	5.1168730000	1.3314990000	0.1406400000
H	4.0622800000	1.5831150000	-1.1062990000
C	3.4856760000	0.0125490000	0.1869240000
H	3.2171120000	0.5179230000	1.1165350000
C	2.2592450000	-0.1956370000	-0.6961620000
C	4.1420760000	-1.3512460000	0.5143700000

H	2.5750870000	-0.6051510000	-1.6641990000
H	1.6323540000	-0.9554680000	-0.2192480000
C	1.4690730000	1.0583270000	-0.9073500000
O	5.2191680000	-1.6110250000	-0.0756410000
N	0.4498980000	1.1296110000	-1.8250140000
C	1.5138880000	2.3107560000	-0.3377090000
H	0.1368350000	0.3746960000	-2.4233730000
C	-0.0744010000	2.3789910000	-1.7796340000
N	0.5481860000	3.1272240000	-0.8904460000
H	2.1817550000	2.6700340000	0.4338230000
H	-0.8987720000	2.6846700000	-2.4080400000
O	3.5079870000	-2.0704750000	1.3173890000

Table S106. Cartesian coordinates of α -Glc-tg_His_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6281007			
ZPE / Hartree = 0.3657911			
BSSE / Hartree = 0.00256111827			
C	-3.2949970000	-1.2849750000	-0.6308030000
C	-2.0457980000	-1.0323690000	-1.4812430000
C	-1.1666580000	0.0311440000	-0.8242350000
C	-1.9919890000	1.2746500000	-0.5425460000
C	-3.2074560000	0.9135790000	0.3084910000
C	-4.1351400000	2.1009010000	0.5443620000
O	-3.9787710000	-0.0715030000	-0.3766740000
O	-2.8803090000	-1.9103790000	0.5524230000
O	-1.3421120000	-2.2298130000	-1.7336440000
O	-0.0948090000	0.4206860000	-1.6691080000
O	-1.2304070000	2.2423860000	0.1657770000
O	-3.5794180000	3.0352720000	1.4562710000
H	-4.0110920000	-1.9075070000	-1.1738200000
H	-2.3767280000	-0.6539760000	-2.4544340000
H	-0.7736950000	-0.3463830000	0.1313750000
H	-2.3415130000	1.6945290000	-1.4984960000
H	-2.8687170000	0.5242840000	1.2790390000
H	-4.3699180000	2.5781840000	-0.4167880000
H	-5.0652190000	1.7360240000	0.9866870000
H	-3.6460020000	-2.3087960000	0.9887380000
H	-0.9634940000	-2.5612050000	-0.8978570000
H	0.5974240000	-0.2533500000	-1.6135500000
H	-0.4425800000	2.4469890000	-0.3589260000
H	-2.6972340000	3.2738640000	1.1322480000
N	4.6589010000	-0.8845590000	0.0089060000
H	5.3629050000	-0.5083490000	0.6559230000
H	5.1578560000	-1.1799220000	-0.8339540000
H	4.2200760000	-1.7142180000	0.4186670000
C	3.6739550000	0.1988820000	-0.2918220000
H	3.2105440000	-0.0332610000	-1.2525920000
C	2.6251440000	0.2819410000	0.8133470000
C	4.4401870000	1.5400550000	-0.4003460000
H	3.1206110000	0.4476770000	1.7775610000

H	2.0090260000	1.1642660000	0.6091740000
C	1.7541160000	-0.9326060000	0.8854250000
O	5.6124360000	1.5515190000	0.0475890000
N	0.9266450000	-1.1756070000	1.9549970000
C	1.5083100000	-1.9647810000	0.0104430000
H	0.8517410000	-0.6081080000	2.7907950000
C	0.2208530000	-2.3015730000	1.6975190000
N	0.5425950000	-2.8100550000	0.5239510000
H	1.9653430000	-2.1491310000	-0.9539020000
H	-0.5122240000	-2.6975600000	2.3851220000
O	3.7924840000	2.4866310000	-0.8985760000

Table S107. Cartesian coordinates of α -Glc-tg_His_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6245118			
ZPE / Hartree = 0.3653139			
BSSE / Hartree = 0.00220443591			
C	3.7813980000	-0.5316390000	0.4803690000
C	2.6967740000	-1.5397490000	0.0916600000
C	1.8702890000	-1.0156640000	-1.0801110000
C	1.3509750000	0.3723250000	-0.7507420000
C	2.5116320000	1.2982650000	-0.3951610000
C	2.0400290000	2.6795350000	0.0483520000
O	3.2220830000	0.7445710000	0.7124040000
O	4.7178830000	-0.5173350000	-0.5645320000
O	3.2579070000	-2.8062570000	-0.1940120000
O	0.7418520000	-1.8411650000	-1.3241230000
O	0.6519600000	0.9413710000	-1.8494250000
O	1.5533960000	3.4506390000	-1.0389690000
H	4.2536300000	-0.8146910000	1.4245850000
H	2.0330280000	-1.6787000000	0.9512640000
H	2.4979720000	-0.9593900000	-1.9820600000
H	0.6848280000	0.3049010000	0.1215850000
H	3.1799670000	1.4039060000	-1.2609370000
H	1.2740930000	2.5668140000	0.8281460000
H	2.8897270000	3.2213540000	0.4706170000
H	5.5455190000	-0.1284990000	-0.2500780000
H	3.9721000000	-2.6736420000	-0.8362780000
H	1.0507810000	-2.6970010000	-1.6517410000
H	-0.0853840000	0.3561630000	-2.0753490000
H	0.8718990000	2.9266370000	-1.4876690000
N	-4.5996150000	0.1659000000	1.2263210000
H	-5.1702160000	-0.6868660000	1.1903000000
H	-5.2468280000	0.9537230000	1.3019340000
H	-4.0195170000	0.1598990000	2.0705790000
C	-3.7829380000	0.2469660000	-0.0216050000
H	-3.4811140000	1.2876900000	-0.1499740000
C	-2.5647290000	-0.6678690000	0.0959550000
C	-4.6649290000	-0.1887180000	-1.2161260000

H	-2.8983530000	-1.6931170000	0.2975320000
H	-2.0698380000	-0.6767190000	-0.8803360000
C	-1.6058090000	-0.2297300000	1.1591690000
O	-5.7344760000	-0.7818480000	-0.9343400000
N	-0.7389070000	-1.1025310000	1.7691750000
C	-1.3142310000	0.9969510000	1.7108600000
H	-0.6727680000	-2.0972650000	1.5909380000
C	0.0307590000	-0.3974530000	2.6343550000
N	-0.2922270000	0.8808730000	2.6299660000
H	-1.7767460000	1.9506430000	1.4955050000
H	0.7980390000	-0.8609860000	3.2381020000
O	-4.1994660000	0.0707900000	-2.3478450000

Table S108. Cartesian coordinates of α -Glc-tg_His_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6302324			
ZPE / Hartree = 0.3656027			
BSSE / Hartree = 0.00312741433			
C	3.2407880000	-0.7878110000	-0.6333580000
C	2.3272080000	-2.0088900000	-0.5023110000
C	0.9322240000	-1.5790020000	-0.0541140000
C	1.0463150000	-0.7794570000	1.2319280000
C	1.9613970000	0.4219300000	0.9822800000
C	2.1877650000	1.2609230000	2.2353100000
O	3.2465920000	-0.0352090000	0.5612950000
O	2.7626700000	-0.0452690000	-1.7244670000
O	2.2731670000	-2.7398590000	-1.7127670000
O	0.1005240000	-2.7003250000	0.1889840000
O	-0.1948780000	-0.2731900000	1.6772210000
O	1.0422930000	2.0292810000	2.5711100000
H	4.2791920000	-1.0911060000	-0.7900690000
H	2.7509860000	-2.6807110000	0.2508660000
H	0.4869670000	-0.9387560000	-0.8312060000
H	1.5016360000	-1.4179690000	2.0064090000
H	1.5110230000	1.0585040000	0.2042970000
H	2.4813910000	0.6061280000	3.0675180000
H	3.0023090000	1.9639980000	2.0438670000
H	3.4373130000	0.5870750000	-2.0072450000
H	2.0768600000	-2.1140940000	-2.4272940000
H	0.0326480000	-3.2084590000	-0.6319740000
H	-0.9207800000	-0.9377140000	1.6500260000
H	0.2814270000	1.4259230000	2.5689980000
N	-3.5087100000	-0.3403770000	-1.6408630000
H	-4.4924050000	-0.3111580000	-1.3450930000
H	-3.3865390000	-1.2001790000	-2.1816910000
H	-3.3166900000	0.4481830000	-2.2642520000
C	-2.6524910000	-0.3386160000	-0.4140820000
H	-1.7090780000	-0.8219350000	-0.6746570000
C	-2.4198800000	1.0918060000	0.0740160000
C	-3.3558490000	-1.1874920000	0.6699850000
H	-3.3562180000	1.6586870000	-0.0080840000

H	-2.1634230000	1.0464450000	1.1353740000
C	-1.3098170000	1.7813420000	-0.6573220000
O	-4.5630850000	-1.4562310000	0.4895940000
N	-0.7812610000	2.9706240000	-0.2188030000
C	-0.5792240000	1.4670250000	-1.7792070000
H	-1.0721090000	3.4844180000	0.6037820000
C	0.2225360000	3.3224680000	-1.0600260000
N	0.3728160000	2.4360250000	-2.0235890000
H	-0.6806560000	0.6002570000	-2.4196110000
H	0.8021340000	4.2242850000	-0.9241050000
O	-2.6337490000	-1.5080840000	1.6488230000

Table S109. Cartesian coordinates of α -Glc-tg_His_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6222591			
ZPE / Hartree = 0.3641624			
BSSE / Hartree = 0.00139407338			
C	3.8513280000	1.2505870000	0.1467700000
C	4.4284020000	-0.0465090000	0.7181740000
C	3.8172640000	-1.2581690000	0.0188700000
C	2.3026320000	-1.1720550000	0.0890130000
C	1.8298830000	0.1507810000	-0.5131380000
C	0.3239100000	0.3501230000	-0.3796260000
O	2.4394240000	1.2317140000	0.1923240000
O	4.3379510000	1.3712120000	-1.1633400000
O	5.8402820000	-0.0601240000	0.6315680000
O	4.2086500000	-2.4659580000	0.6502800000
O	1.6867230000	-2.2247260000	-0.6398840000
O	-0.4052600000	-0.4882200000	-1.2607360000
H	4.1481340000	2.1086780000	0.7550580000
H	4.1797110000	-0.0938400000	1.7832720000
H	4.1235610000	-1.2691080000	-1.0378260000
H	1.9911380000	-1.2114780000	1.1439550000
H	2.1058450000	0.1879370000	-1.5761320000
H	0.0279120000	0.1798780000	0.6658590000
H	0.0788200000	1.3842310000	-0.6404870000
H	4.2551080000	2.2892200000	-1.4552320000
H	6.0816580000	0.1537460000	-0.2830080000
H	5.1682510000	-2.5556160000	0.5674600000
H	1.9334460000	-3.0665000000	-0.2315510000
H	-0.0994110000	-1.3979290000	-1.1197210000
N	-5.2918180000	0.1181670000	-0.2891500000
H	-5.8828190000	-0.2489430000	0.4671250000
H	-5.8033670000	-0.0247720000	-1.1628150000
H	-5.1581650000	1.1266270000	-0.1684030000
C	-4.0019350000	-0.6368830000	-0.2792610000
H	-3.5778170000	-0.5836600000	-1.2835030000
C	-3.0493920000	-0.0315720000	0.7476940000
C	-4.3026930000	-2.1125140000	0.0787200000

H	-3.5246310000	-0.0436570000	1.7363490000
H	-2.1723360000	-0.6856440000	0.7964880000
C	-2.6259770000	1.3602730000	0.3982580000
O	-5.4396280000	-2.3528220000	0.5537000000
N	-1.9865060000	2.1776440000	1.2972960000
C	-2.6837410000	2.0943220000	-0.7631740000
H	-1.7697530000	1.9507560000	2.2598790000
C	-1.6766080000	3.3367560000	0.6668940000
N	-2.0883070000	3.3262570000	-0.5855000000
H	-3.1086100000	1.8035910000	-1.7148390000
H	-1.1642870000	4.1475300000	1.1645420000
O	-3.3611940000	-2.9131220000	-0.1139310000

Table S110. Cartesian coordinates of β -Glc-gg_His_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6247389			
ZPE / Hartree = 0.3639584			
BSSE / Hartree = 0.00235726178			
C	-0.9662200000	-0.4419430000	0.7803210000
C	-1.3940360000	-1.5761560000	-0.1430370000
C	-2.4201280000	-1.0447710000	-1.1308570000
C	-3.5750060000	-0.3843370000	-0.3922150000
C	-3.0412300000	0.6741540000	0.5741110000
C	-4.1239550000	1.2983330000	1.4362090000
O	-2.1037540000	0.0673280000	1.4618010000
O	-0.0715760000	-0.9471880000	1.7146910000
O	-0.2977320000	-2.0676850000	-0.8909680000
O	-2.9691170000	-2.0765450000	-1.9333010000
O	-4.4526950000	0.2582550000	-1.2998940000
O	-4.8042420000	0.3329130000	2.2234360000
H	-0.5117900000	0.3702240000	0.1986160000
H	-1.8421290000	-2.3741010000	0.4668060000
H	-1.9321700000	-0.2901850000	-1.7691230000
H	-4.1121760000	-1.1525780000	0.1824890000
H	-2.5471530000	1.4717620000	-0.0045940000
H	-3.6676390000	2.0662070000	2.0717460000
H	-4.8695160000	1.7711180000	0.7940450000
H	0.4866370000	-0.2286490000	2.0444160000
H	0.3060590000	-2.5217710000	-0.2869480000
H	-2.2691970000	-2.4349910000	-2.4961700000
H	-4.7390180000	-0.3987740000	-1.9505290000
H	-4.1596940000	-0.0799020000	2.8148680000
N	4.6857590000	1.3886690000	0.0294330000
H	5.4144820000	1.0616190000	-0.6172550000
H	5.1621220000	1.8361870000	0.8156700000
H	4.1071300000	2.0996030000	-0.4275470000
C	3.8901210000	0.2034120000	0.4719060000
H	3.4492050000	0.4420230000	1.4415100000
C	2.8066160000	-0.1140450000	-0.5562180000
C	4.8502870000	-1.0020000000	0.6202350000

H	3.2731670000	-0.3183780000	-1.5275580000
H	2.3143160000	-1.0368640000	-0.2325820000
C	1.7979420000	0.9825250000	-0.6974870000
O	5.9800050000	-0.8853420000	0.0856610000
N	0.9464840000	1.0614480000	-1.7717970000
C	1.4478440000	2.0440140000	0.1060070000
H	0.9192340000	0.4256190000	-2.5597150000
C	0.1282690000	2.1263020000	-1.5845040000
N	0.4045880000	2.7503310000	-0.4562810000
H	1.8829430000	2.3335340000	1.0533350000
H	-0.6399540000	2.3984260000	-2.2943180000
O	4.3833970000	-1.9862610000	1.2343920000

Table S111. Cartesian coordinates of β -Glc-gg_His_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6273537			
ZPE / Hartree = 0.3645725			
BSSE / Hartree = 0.00295549492			
C	-1.0030740000	-0.6881060000	1.7037880000
C	-1.7381960000	0.6136010000	1.4062480000
C	-3.0643830000	0.2972230000	0.7357180000
C	-2.8510830000	-0.5690670000	-0.4964650000
C	-2.0055000000	-1.7964520000	-0.1496690000
C	-1.6012700000	-2.5980500000	-1.3775480000
O	-0.8003620000	-1.3999860000	0.4939000000
O	0.2401680000	-0.3631900000	2.2330100000
O	-2.0216520000	1.3291250000	2.5935400000
O	-3.7338870000	1.4730760000	0.3111520000
O	-4.0891430000	-1.0367430000	-1.0039230000
O	-0.6916160000	-1.8782190000	-2.2068380000
H	-1.5854490000	-1.3113050000	2.4009110000
H	-1.1108530000	1.2123920000	0.7296430000
H	-3.6948380000	-0.2573440000	1.4485380000
H	-2.3332900000	0.0280880000	-1.2584600000
H	-2.5967430000	-2.4465700000	0.5154920000
H	-1.1526190000	-3.5444690000	-1.0616650000
H	-2.4914240000	-2.8123730000	-1.9729290000
H	0.6346880000	-1.1468520000	2.6406800000
H	-1.1895350000	1.6622930000	2.9569450000
H	-3.9730450000	1.9904030000	1.0926380000
H	-4.6373290000	-0.2658330000	-1.2079600000
H	0.2018260000	-2.0324760000	-1.8704650000
N	4.1659300000	1.1933180000	-0.5674750000
H	4.7853170000	0.6053340000	-1.1404390000
H	4.7647430000	1.7546850000	0.0416130000
H	3.6431970000	1.8362220000	-1.1688660000
C	3.2744300000	0.2869120000	0.2200520000
H	2.9956140000	0.8072260000	1.1382900000
C	2.0374790000	-0.0763190000	-0.5954740000
C	4.0723300000	-0.9929980000	0.5705480000
H	2.3503700000	-0.5294710000	-1.5452620000

H	1.4866210000	−0.8348030000	−0.0304820000
C	1.1426170000	1.0951290000	−0.8546910000
O	5.1326660000	−1.1848940000	−0.0738800000
N	0.0663800000	1.0163550000	−1.7034400000
C	1.1254110000	2.3879000000	−0.3824210000
H	−0.2614420000	0.1695710000	−2.1648400000
C	−0.5551630000	2.2211320000	−1.7050970000
N	0.0615630000	3.0831310000	−0.9204940000
H	1.8110750000	2.8542000000	0.3125230000
H	−1.4445440000	2.4129700000	−2.2889070000
O	3.5561940000	−1.7250370000	1.4434040000

Table S112. Cartesian coordinates of β -Glc-gg_His_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6331597			
ZPE / Hartree = 0.3648377			
BSSE / Hartree = 0.00311033181			
C	0.5129060000	-1.1583220000	0.7421420000
C	1.2422010000	-0.1866510000	1.6658580000
C	1.9908910000	0.8245720000	0.8165580000
C	2.9257440000	0.1031780000	-0.1436420000
C	2.1520240000	-0.9402340000	-0.9533100000
C	3.0479640000	-1.8001380000	-1.8277680000
O	1.4689440000	-1.8286210000	-0.0715740000
O	-0.1759520000	-2.0896990000	1.4931050000
O	0.3234350000	0.5193970000	2.4780970000
O	2.7833960000	1.7064440000	1.5962540000
O	3.5058890000	1.0128250000	-1.0623950000
O	3.9951960000	-2.5302830000	-1.0630850000
H	-0.1629580000	-0.5945600000	0.0817910000
H	1.9510220000	-0.7584910000	2.2833660000
H	1.2584530000	1.4008860000	0.2287940000
H	3.7077270000	-0.4039850000	0.4400510000
H	1.4252980000	-0.4189340000	-1.5979500000
H	2.4182900000	-2.4787300000	-2.4152280000
H	3.6106400000	-1.1615140000	-2.5114920000
H	-1.0913210000	-2.2076150000	1.1306830000
H	-0.1503060000	-0.1266940000	3.0218360000
H	2.1955090000	2.3017570000	2.0812950000
H	3.9321870000	1.7165250000	-0.5526020000
H	3.5077730000	-3.0943670000	-0.4463940000
N	-3.8449090000	0.0902910000	-1.6228130000
H	-4.7882290000	0.0130280000	-1.2221730000
H	-3.8391050000	-0.4618640000	-2.4840990000
H	-3.6587790000	1.0648250000	-1.8758740000
C	-2.8658200000	-0.4438720000	-0.6284170000
H	-1.9922710000	-0.7887380000	-1.1854160000
C	-2.4895080000	0.6412440000	0.3788750000
C	-3.5076390000	-1.6535920000	0.0860290000

H	-3.4035540000	1.0995420000	0.7771300000
H	-1.9850130000	0.1579400000	1.2235170000
C	-1.5913690000	1.6854420000	-0.2088200000
O	-4.7422780000	-1.7922420000	-0.0284140000
N	-1.2025330000	2.7986630000	0.4944140000
C	-0.9529550000	1.7973150000	-1.4226430000
H	-1.4795090000	3.0326330000	1.4398500000
C	-0.3665800000	3.5223020000	-0.2899920000
N	-0.1928780000	2.9478790000	-1.4637680000
H	-0.9932330000	1.1167720000	-2.2630130000
H	0.0796440000	4.4492770000	0.0405440000
O	-2.7145270000	-2.3806940000	0.7406810000

Table S113. Cartesian coordinates of β -Glc-gg_His_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6291725			
ZPE / Hartree = 0.3646080			
BSSE / Hartree = 0.00281016952			
C	-2.2832910000	-1.8878130000	-0.8473170000
C	-0.8253410000	-1.6448020000	-0.4687670000
C	-0.7424740000	-1.2532590000	0.9971950000
C	-1.6371200000	-0.0449890000	1.2411500000
C	-3.0645640000	-0.3543230000	0.7940700000
C	-4.0058410000	0.8301510000	0.9200980000
O	-3.0449680000	-0.7177530000	-0.5864530000
O	-2.3309460000	-2.1436440000	-2.2120760000
O	-0.0409800000	-2.8067150000	-0.6516000000
O	0.5623180000	-0.8949210000	1.3986080000
O	-1.6669530000	0.2964070000	2.6154780000
O	-3.5508580000	1.9574490000	0.1874880000
H	-2.6989960000	-2.7265630000	-0.2683920000
H	-0.4568890000	-0.8184330000	-1.0941590000
H	-1.1085290000	-2.0970580000	1.6057120000
H	-1.2533110000	0.7985040000	0.6454980000
H	-3.4631530000	-1.1862130000	1.3962660000
H	-5.0026430000	0.5227050000	0.5820650000
H	-4.0683290000	1.1334060000	1.9669600000
H	-3.1669710000	-2.5767850000	-2.4324060000
H	0.0162430000	-2.9954360000	-1.5985500000
H	1.2423050000	-1.5174410000	1.0624430000
H	-0.7515820000	0.4207770000	2.9055740000
H	-3.4580020000	1.6968450000	-0.7398000000
N	4.2283500000	1.3484990000	0.2465370000
H	5.0244870000	0.9527280000	-0.2694110000
H	4.5616090000	1.5656700000	1.1886980000
H	3.9397540000	2.2272980000	-0.1910970000
C	3.1366330000	0.3278810000	0.2765120000
H	2.5551430000	0.4926240000	1.1842630000
C	2.2474100000	0.4497020000	-0.9587950000
C	3.7782130000	-1.0779590000	0.3431020000
H	2.8732050000	0.5973920000	-1.8481410000

H	1.7411290000	-0.5118320000	-1.0888520000
C	1.2255660000	1.5377930000	-0.8397100000
O	5.0055590000	-1.1554190000	0.1149230000
N	0.2546930000	1.7335930000	-1.7925320000
C	0.9616510000	2.4798900000	0.1260720000
H	0.1457210000	1.2064810000	-2.6503470000
C	-0.5402270000	2.7526270000	-1.3818570000
N	-0.1401070000	3.2346140000	-0.2224080000
H	1.4960510000	2.6538240000	1.0504670000
H	-1.3849220000	3.0978510000	-1.9608620000
O	2.9810070000	-2.0157380000	0.5989300000

Table S114. Cartesian coordinates of β -Glc-gg_His_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6247854			
ZPE / Hartree = 0.3640338			
BSSE / Hartree = 0.00223548014			
C	-1.2535430000	-1.5546310000	-0.5098440000
C	-2.7636700000	-1.5288250000	-0.7231970000
C	-3.2823500000	-0.1112180000	-0.5367380000
C	-2.8457990000	0.4416700000	0.8120130000
C	-1.3278560000	0.3271360000	0.9368280000
C	-0.7859150000	0.7732730000	2.2815830000
O	-0.9442450000	-1.0373120000	0.7748150000
O	-0.8350900000	-2.8780690000	-0.5614550000
O	-3.1031250000	-1.9341330000	-2.0356750000
O	-4.6983100000	-0.0616300000	-0.5789040000
O	-3.1863900000	1.8114520000	0.9319660000
O	-1.3501770000	0.0414510000	3.3590540000
H	-0.7468570000	-0.9444820000	-1.2745730000
H	-3.2261080000	-2.1901250000	0.0236360000
H	-2.8598610000	0.5268570000	-1.3294540000
H	-3.3215080000	-0.1447930000	1.6109750000
H	-0.8655580000	0.9451760000	0.1529950000
H	0.3063290000	0.6655310000	2.2663210000
H	-1.0317360000	1.8253250000	2.4418280000
H	0.1229160000	-2.9103760000	-0.6924630000
H	-2.9310200000	-2.8816110000	-2.1226530000
H	-4.9890600000	-0.3077280000	-1.4678600000
H	-4.1410810000	1.8940360000	0.7964770000
H	-1.1101150000	-0.8891180000	3.2482750000
N	4.4854440000	0.9183840000	-0.4366930000
H	4.9924510000	0.3721830000	-1.1436270000
H	5.1824150000	1.2763080000	0.2201060000
H	4.0329160000	1.7243610000	-0.8785010000
C	3.5037890000	0.0183170000	0.2408360000
H	3.2825390000	0.4484290000	1.2190710000
C	2.2343360000	-0.1005300000	-0.6018150000
C	4.1518740000	-1.3756950000	0.4169540000

H	2.4858580000	-0.5147690000	-1.5856220000
H	1.5826820000	-0.8228020000	-0.0978030000
C	1.5184880000	1.2037400000	-0.7653340000
O	5.1902620000	-1.5980420000	-0.2519920000
N	0.6870370000	1.4590770000	-1.8287820000
C	1.4311510000	2.3266890000	0.0246530000
H	0.5176810000	0.8425100000	-2.6144270000
C	0.1297060000	2.6809270000	-1.6449030000
N	0.5603740000	3.2403450000	-0.5306310000
H	1.9353340000	2.5210940000	0.9617130000
H	-0.5667220000	3.1124730000	-2.3492870000
O	3.5467320000	-2.1534990000	1.1873660000

Table S115. Cartesian coordinates of β -Glc-gg_His_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6222295			
ZPE / Hartree = 0.3638675			
BSSE / Hartree = 0.00153343191			
C	2.9531220000	-1.2686570000	-0.5362400000
C	4.2994860000	-0.5521130000	-0.5422910000
C	4.2856870000	0.5510080000	0.5049360000
C	3.0959780000	1.4746230000	0.2881180000
C	1.8057410000	0.6559490000	0.2397500000
C	0.5767900000	1.4832670000	-0.0901460000
O	1.9184750000	-0.3300320000	-0.7839300000
O	2.9524590000	-2.2035270000	-1.5631080000
O	5.3540350000	-1.4363540000	-0.2153150000
O	5.4561870000	1.3490150000	0.4448250000
O	2.9797430000	2.4068300000	1.3482550000
O	0.6897320000	2.1290040000	-1.3497170000
H	2.7804590000	-1.7479800000	0.4406700000
H	4.4498150000	-0.1122990000	-1.5388020000
H	4.1962250000	0.0906530000	1.5010630000
H	3.2238590000	1.9973780000	-0.6707160000
H	1.6487640000	0.1695380000	1.2158710000
H	-0.3024550000	0.8273950000	-0.0666930000
H	0.4509110000	2.2645230000	0.6622030000
H	2.2506570000	-2.8509660000	-1.4075300000
H	5.4738140000	-2.0595700000	-0.9449950000
H	6.2103590000	0.8126040000	0.7251290000
H	3.8203480000	2.8811710000	1.4192860000
H	0.7985780000	1.4457900000	-2.0260260000
N	-5.2204490000	-0.8237410000	1.1462650000
H	-5.8725410000	-1.3619140000	0.5643360000
H	-5.7642020000	-0.4349730000	1.9201520000
H	-4.5131180000	-1.4486470000	1.5438810000
C	-4.6147590000	0.2557540000	0.3105000000
H	-4.2357520000	1.0218390000	0.9890510000
C	-3.4905770000	-0.3160760000	-0.5497200000
C	-5.7204360000	0.8592970000	-0.5887230000
H	-3.8920680000	-1.1087260000	-1.1926860000

H	-3.144760000	0.489157000	-1.205830000
C	-2.347908000	-0.845616000	0.259893000
O	-6.786191000	0.203194000	-0.681187000
N	-1.386365000	-1.665612000	-0.278326000
C	-1.959093000	-0.660168000	1.566099000
H	-1.359098000	-2.004651000	-1.232057000
C	-0.473959000	-1.935111000	0.687294000
N	-0.788696000	-1.345498000	1.822898000
H	-2.448686000	-0.071042000	2.330112000
H	0.385686000	-2.566176000	0.511089000
O	-5.420524000	1.931608000	-1.158596000

Table S116. Cartesian coordinates of β -Glc-gt_His_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6236479			
ZPE / Hartree = 0.3643936			
BSSE / Hartree = 0.00246168958			
C	0.9491410000	-0.3129990000	-0.8469250000
C	1.3631010000	-1.6713250000	-0.2923140000
C	2.4834470000	-1.4643900000	0.7140030000
C	3.6295210000	-0.6804950000	0.0891760000
C	3.1002430000	0.6112450000	-0.5388660000
C	4.1866400000	1.3600850000	-1.2891190000
O	2.0705830000	0.2945740000	-1.4700430000
O	-0.0426560000	-0.5066420000	-1.7999170000
O	0.2938100000	-2.3012880000	0.3877000000
O	3.0182890000	-2.6927700000	1.1766500000
O	4.5915170000	-0.3342000000	1.0695290000
O	3.7272330000	2.6000770000	-1.8054560000
H	0.5961240000	0.3391470000	-0.0363370000
H	1.7192450000	-2.2944330000	-1.1252370000
H	2.0860160000	-0.8841640000	1.5625910000
H	4.0889360000	-1.2965090000	-0.6994560000
H	2.6907510000	1.2541950000	0.2589900000
H	5.0455800000	1.5026920000	-0.6256310000
H	4.5018510000	0.7612670000	-2.1489000000
H	-0.5721270000	0.2999300000	-1.8785630000
H	-0.3682200000	-2.5712250000	-0.2634970000
H	2.3374380000	-3.1520640000	1.6874570000
H	4.8670490000	-1.1483450000	1.5148410000
H	3.5831820000	3.2087350000	-1.0684740000
N	-4.6502770000	1.2998350000	0.5132960000
H	-5.3824420000	0.7378480000	0.9659250000
H	-5.1244340000	2.0115810000	-0.0469210000
H	-4.0921740000	1.7834830000	1.2227160000
C	-3.8294660000	0.3878100000	-0.3409230000
H	-3.4065570000	0.9832500000	-1.1519020000
C	-2.7266020000	-0.2658900000	0.4885080000
C	-4.7625040000	-0.6985360000	-0.9302220000

H	-3.1748250000	-0.8158150000	1.3250310000
H	-2.2343180000	-1.0010510000	-0.1566050000
C	-1.7191370000	0.7140840000	1.0030420000
O	-5.8968430000	-0.8068690000	-0.4035390000
N	-0.8896320000	0.4253470000	2.0586710000
C	-1.3377140000	1.9708820000	0.5911780000
H	-0.8881690000	-0.4329550000	2.5962590000
C	-0.0523410000	1.4762630000	2.2376790000
N	-0.2962310000	2.4364750000	1.3670520000
H	-1.7480230000	2.5597700000	-0.2181520000
H	0.7035040000	1.4901410000	3.0098740000
O	-4.2721060000	-1.3813150000	-1.8559790000

Table S117. Cartesian coordinates of β -Glc-gt_His_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6244228			
ZPE / Hartree = 0.3642671			
BSSE / Hartree = 0.00250760450			
C	1.0028410000	0.5304350000	1.6131210000
C	1.6908660000	-0.7936840000	1.3020230000
C	3.0443160000	-0.5183460000	0.6683910000
C	2.8964860000	0.3934240000	-0.5414390000
C	2.1062790000	1.6486400000	-0.1638210000
C	1.8020680000	2.5039210000	-1.3811860000
O	0.8604230000	1.2709230000	0.4115350000
O	-0.2632070000	0.2492970000	2.1115210000
O	1.9161410000	-1.5523450000	2.4748570000
O	3.6682580000	-1.7097680000	0.2188350000
O	4.1660040000	0.7991970000	-1.0218510000
O	1.1483940000	3.7166450000	-1.0409590000
H	1.5960210000	1.1164380000	2.3330560000
H	1.0572330000	-1.3472920000	0.5944320000
H	3.6855860000	-0.0153060000	1.4090480000
H	2.3469320000	-0.1510080000	-1.3248690000
H	2.6911680000	2.2328860000	0.5662200000
H	2.7314390000	2.6956700000	-1.9268270000
H	1.1176480000	1.9531090000	-2.0349500000
H	-0.6303120000	1.0411650000	2.5285380000
H	1.0631320000	-1.8644960000	2.8071320000
H	3.8726100000	-2.2593510000	0.9880900000
H	4.6877300000	0.0014300000	-1.1904750000
H	1.7841650000	4.3009200000	-0.6069910000
N	-4.2694770000	-1.1292370000	-0.5515360000
H	-4.8690610000	-0.5444710000	-1.1478470000
H	-4.8859760000	-1.6313910000	0.0907130000
H	-3.7821940000	-1.8242440000	-1.1243870000
C	-3.3311540000	-0.2258080000	0.1830080000
H	-3.0543920000	-0.7195540000	1.1163820000
C	-2.0980940000	0.0601980000	-0.6687860000
C	-4.0763230000	1.0944120000	0.4973000000
H	-2.4102790000	0.4894090000	-1.6292080000

H	-1.5066670000	0.8167890000	-0.1441310000
C	-1.2551330000	-1.1543750000	-0.9005670000
O	-5.1396090000	1.3012400000	-0.1376200000
N	-0.2356110000	-1.1681530000	-1.8200820000
C	-1.2271010000	-2.4062890000	-0.3296160000
H	0.0290530000	-0.4001400000	-2.4248600000
C	0.3615500000	-2.3846860000	-1.7722960000
N	-0.2155160000	-3.1661290000	-0.8811420000
H	-1.8692560000	-2.7990600000	0.4473200000
H	1.2006480000	-2.6431750000	-2.4024710000
O	-3.5202300000	1.8384670000	1.3347580000

Table S118. Cartesian coordinates of β -Glc-gt_His_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6318408			
ZPE / Hartree = 0.3644775			
BSSE / Hartree = 0.00313229745			
C	0.5038060000	-1.0593550000	1.0146650000
C	1.2715810000	0.0033600000	1.7961750000
C	2.0934070000	0.8251000000	0.8197940000
C	2.9932920000	-0.0839880000	-0.0062960000
C	2.1704120000	-1.2030240000	-0.6526530000
C	3.0585140000	-2.2113260000	-1.3591180000
O	1.4354250000	-1.9009980000	0.3473740000
O	-0.2557160000	-1.8186240000	1.8831510000
O	0.3828120000	0.8791290000	2.4635560000
O	2.9329730000	1.7659370000	1.4707560000
O	3.6265250000	0.6484910000	-1.0409680000
O	2.3091860000	-3.2071650000	-2.0385730000
H	-0.1255930000	-0.5712140000	0.2552600000
H	1.9338500000	-0.5034440000	2.5139800000
H	1.4050890000	1.3474680000	0.1363730000
H	3.7456430000	-0.5352500000	0.6595600000
H	1.4702120000	-0.7521870000	-1.3772770000
H	3.7255950000	-1.6817320000	-2.0467120000
H	3.6649590000	-2.7322740000	-0.6119750000
H	-1.1643460000	-1.9432430000	1.5093620000
H	-0.1467850000	0.3519590000	3.0792160000
H	2.3827900000	2.4753690000	1.8298560000
H	4.0597660000	1.4143150000	-0.6369350000
H	1.8889200000	-2.8057960000	-2.8106590000
N	-3.7372740000	0.0817630000	-1.6556200000
H	-4.6934370000	0.0642460000	-1.2774170000
H	-3.7166110000	-0.5575930000	-2.4539530000
H	-3.5261910000	1.0193840000	-2.0081540000
C	-2.8013210000	-0.3528920000	-0.5737580000
H	-1.9383050000	-0.8182840000	-1.0547020000
C	-2.3859480000	0.8478320000	0.2749160000
C	-3.5202560000	-1.4122010000	0.2917790000

H	-3.2823970000	1.4101170000	0.5649060000
H	-1.9379170000	0.4722050000	1.2018080000
C	-1.4088890000	1.7430340000	-0.4241510000
O	-4.7582440000	-1.5044360000	0.1635310000
N	-0.9668300000	2.9177750000	0.1325920000
C	-0.7366390000	1.6489720000	-1.6214160000
H	-1.2497600000	3.2960150000	1.0283180000
C	-0.0688090000	3.4756530000	-0.7160860000
N	0.0950550000	2.7357060000	-1.7948790000
H	-0.8025990000	0.8642650000	-2.3635980000
H	0.4271270000	4.4112150000	-0.5008750000
O	-2.7819080000	-2.0747370000	1.0669050000

Table S119. Cartesian coordinates of β -Glc-gt_His_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6242739			
ZPE / Hartree = 0.3642598			
BSSE / Hartree = 0.00236303034			
C	2.4447300000	1.8333690000	-0.7587990000
C	0.9965520000	1.8109380000	-0.2797760000
C	0.9413420000	1.2295390000	1.1234230000
C	1.6086510000	-0.1366700000	1.1493990000
C	3.0276650000	-0.0345240000	0.5886280000
C	3.6873250000	-1.3977300000	0.4846480000
O	2.9698440000	0.5149330000	-0.7250990000
O	2.4518110000	2.2715870000	-2.0772640000
O	0.4422720000	3.1106250000	-0.2239740000
O	-0.3907340000	1.0546140000	1.5750850000
O	1.6805450000	-0.6387880000	2.4718410000
O	5.0311720000	-1.3136250000	0.0351920000
H	3.0559770000	2.4866810000	-0.1168890000
H	0.4274010000	1.1704220000	-0.9696090000
H	1.4843590000	1.9017790000	1.8064460000
H	1.0293030000	-0.8212710000	0.5123730000
H	3.6300760000	0.6209050000	1.2397670000
H	3.6258420000	-1.9000160000	1.4552690000
H	3.1460560000	-1.9963660000	-0.2547730000
H	3.3444000000	2.5535100000	-2.3201500000
H	0.3264530000	3.4384940000	-1.1263500000
H	-0.8163770000	1.9214890000	1.6320640000
H	0.7839780000	-0.6314320000	2.8375340000
H	5.5704920000	-0.9334880000	0.7413060000
N	-4.2704800000	-1.4998150000	0.0046160000
H	-4.9789180000	-1.2249970000	-0.6872680000
H	-4.7732260000	-1.7866810000	0.8478940000
H	-3.7481460000	-2.3108600000	-0.3393490000
C	-3.3914110000	-0.3185850000	0.2657800000
H	-2.9525550000	-0.4430850000	1.2576580000
C	-2.3043190000	-0.2232240000	-0.7996990000
C	-4.2692760000	0.9565110000	0.2420570000

H	-2.7679740000	-0.1835990000	-1.7933750000
H	-1.7898630000	0.7292620000	-0.6383820000
C	-1.3197730000	-1.3489660000	-0.7347900000
O	-5.4196180000	0.8349100000	-0.2455030000
N	-0.3530540000	-1.5289350000	-1.6939630000
C	-1.1027270000	-2.3597030000	0.1735900000
H	-0.2155480000	-0.9539510000	-2.5163350000
C	0.3953370000	-2.6037830000	-1.3436730000
N	-0.0313980000	-3.1376440000	-0.2163760000
H	-1.6466320000	-2.5661280000	1.0859990000
H	1.2269090000	-2.9496650000	-1.9408830000
O	-3.7230510000	1.9908340000	0.6850170000

Table S120. Cartesian coordinates of β -Glc-gt_His_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6244473			
ZPE / Hartree = 0.3649667			
BSSE / Hartree = 0.00251306003			
C	-1.3689420000	-1.6138440000	-0.3469310000
C	-2.8790170000	-1.5555880000	-0.5482790000
C	-3.3484220000	-0.1172990000	-0.3942420000
C	-2.8821640000	0.4667120000	0.9320060000
C	-1.3704080000	0.2849920000	1.0726910000
C	-0.8617160000	0.7398370000	2.4281180000
O	-1.0445660000	-1.0941940000	0.9320520000
O	-0.9751970000	-2.9449810000	-0.3908790000
O	-3.2448740000	-1.9814450000	-1.8468830000
O	-4.7619680000	-0.0177110000	-0.4225890000
O	-3.1658990000	1.8532750000	0.9942300000
O	0.5498300000	0.6283090000	2.5337230000
H	-0.8571380000	-1.0205240000	-1.1224730000
H	-3.3524080000	-2.1836930000	0.2199060000
H	-2.9127620000	0.4833700000	-1.2086510000
H	-3.3859400000	-0.0666100000	1.7528730000
H	-0.8722990000	0.8669220000	0.2798340000
H	-1.1904840000	1.7695640000	2.6040950000
H	-1.2858160000	0.0964780000	3.2049160000
H	-0.0154520000	-2.9928420000	-0.5061750000
H	-3.1000200000	-2.9351090000	-1.9134340000
H	-5.0713570000	-0.2690320000	-1.3037070000
H	-4.1117720000	1.9709780000	0.8255410000
H	0.9496530000	1.2464440000	1.9042820000
N	4.4246230000	0.6199060000	-0.6364460000
H	4.8661110000	-0.0370950000	-1.2917280000
H	5.1625940000	0.9655640000	-0.0186280000
H	4.0486440000	1.4231110000	-1.1491810000
C	3.3697200000	-0.1187790000	0.1220190000
H	3.2501730000	0.3738700000	1.0889840000
C	2.0562700000	-0.1121080000	-0.6557300000
C	3.8490120000	-1.5743760000	0.3439320000
H	2.2039140000	-0.5807330000	-1.6364280000

H	1.3537750000	−0.7378180000	−0.0927720000
C	1.4834110000	1.2609110000	−0.8220960000
O	4.8520120000	−1.9416200000	−0.3152260000
N	0.5150080000	1.5454570000	−1.7524510000
C	1.6663760000	2.4409010000	−0.1360340000
H	0.1323980000	0.9010280000	−2.4335020000
C	0.1434700000	2.8399740000	−1.5931510000
N	0.8224970000	3.4182370000	−0.6236890000
H	2.3660040000	2.6459800000	0.6648590000
H	−0.6127580000	3.3044600000	−2.2095200000
O	3.1599710000	−2.2463220000	1.1424730000

Table S121. Cartesian coordinates of β -Glc-gt_His_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6297007			
ZPE / Hartree = 0.3649596			
BSSE / Hartree = 0.00204142103			
C	3.9180250000	0.7985020000	0.0311700000
C	3.7572870000	-0.6925760000	0.2984290000
C	2.5900210000	-1.2344230000	-0.5119280000
C	1.3221710000	-0.4249280000	-0.2605160000
C	1.6131560000	1.0677560000	-0.4571230000
C	0.4236400000	1.9258940000	-0.0654730000
O	2.7095130000	1.4604040000	0.3641770000
O	4.9253410000	1.2792850000	0.8594550000
O	4.9092760000	-1.4195420000	-0.0885400000
O	2.3225500000	-2.5856950000	-0.1773980000
O	0.2964710000	-0.8099860000	-1.1496890000
O	0.6497060000	3.3090970000	-0.2986980000
H	4.1533190000	0.9790820000	-1.0293650000
H	3.5538870000	-0.8255830000	1.3709200000
H	2.8404160000	-1.1547960000	-1.5819490000
H	1.0092250000	-0.5853350000	0.7848100000
H	1.8638330000	1.2458180000	-1.5166800000
H	-0.4623400000	1.5769610000	-0.6055350000
H	0.2434830000	1.8147460000	1.0094390000
H	5.2235510000	2.1410210000	0.5374000000
H	5.6255510000	-1.2190150000	0.5292000000
H	3.1243650000	-3.1000790000	-0.3467270000
H	-0.1582790000	-1.6049170000	-0.7738020000
H	0.6126630000	3.4734310000	-1.2504370000
N	-4.3411400000	-1.6180940000	-0.2119350000
H	-4.6189740000	-2.1833550000	0.5989660000
H	-4.6449580000	-2.1253060000	-1.0467570000
H	-4.8407450000	-0.7240190000	-0.1925550000
C	-2.8582560000	-1.4422320000	-0.1917300000
H	-2.5459000000	-1.1831500000	-1.2055120000
C	-2.4701540000	-0.3452980000	0.7968540000
C	-2.2132770000	-2.7843030000	0.2169620000

H	-2.9168630000	-0.5607400000	1.7754660000
H	-1.3823580000	-0.3873980000	0.9242070000
C	-2.8635670000	1.0189320000	0.3281820000
O	-2.9561350000	-3.6377020000	0.7428200000
N	-2.7655570000	2.1236590000	1.1366230000
C	-3.2766260000	1.5083990000	-0.8884220000
H	-2.4743420000	2.1278600000	2.1061880000
C	-3.1036820000	3.2126620000	0.4036860000
N	-3.4246090000	2.8795560000	-0.8303550000
H	-3.4673140000	0.9562830000	-1.7988300000
H	-3.1044940000	4.2108920000	0.8171900000
O	-0.9750990000	-2.8731810000	0.0020600000

Table S122. Cartesian coordinates of β -Glc-tg_His_H1 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6238332			
ZPE / Hartree = 0.3645971			
BSSE / Hartree = 0.00234966727			
C	0.8153800000	-0.5240440000	-0.7543480000
C	1.3184070000	-1.6940320000	0.0848580000
C	2.5062200000	-1.2341020000	0.9166770000
C	3.5610920000	-0.6100580000	0.0161720000
C	2.9406630000	0.4956060000	-0.8414410000
C	3.9268270000	1.0845260000	-1.8448700000
O	1.8645690000	-0.0547900000	-1.5914690000
O	-0.2265330000	-0.9704770000	-1.5559120000
O	0.3219850000	-2.1468570000	0.9819440000
O	3.1191510000	-2.3097920000	1.6056790000
O	4.6100780000	-0.0318810000	0.7790670000
O	4.9054860000	1.8952900000	-1.2146170000
H	0.4906760000	0.2982170000	-0.1021700000
H	1.6317230000	-2.5010090000	-0.5930490000
H	2.1594020000	-0.4737450000	1.6348300000
H	3.9625540000	-1.3872460000	-0.6512730000
H	2.5702210000	1.3003530000	-0.1850010000
H	4.3946040000	0.2709380000	-2.4160190000
H	3.3777490000	1.7249380000	-2.5391250000
H	-0.7912830000	-0.2214910000	-1.7965710000
H	-0.3703190000	-2.5927250000	0.4748720000
H	2.5020720000	-2.6391110000	2.2734450000
H	5.0432560000	-0.7327770000	1.2864130000
H	5.3091120000	1.3707330000	-0.5056210000
N	-4.6550710000	1.4673030000	0.0165480000
H	-5.4434090000	1.0986100000	0.5640730000
H	-5.0528140000	1.9815020000	-0.7729180000
H	-4.1193130000	2.1316770000	0.5821060000
C	-3.8330040000	0.3058560000	-0.4427310000
H	-3.3140260000	0.6042690000	-1.3554310000
C	-2.8372540000	-0.0962240000	0.6421980000
C	-4.7870600000	-0.8732750000	-0.7530180000
H	-3.3771630000	-0.3161260000	1.5712980000

H	-2.3608980000	-1.0261580000	0.3152000000
C	-1.7930650000	0.9480620000	0.8863320000
O	-5.9556730000	-0.7789950000	-0.3045260000
N	-0.9398930000	0.8947240000	1.9605640000
C	-1.3994750000	2.0634750000	0.1822090000
H	-0.9359230000	0.1858220000	2.6837520000
C	-0.0791220000	1.9384520000	1.8693360000
N	-0.3294360000	2.6737420000	0.8038730000
H	-1.8201860000	2.4554980000	-0.7343840000
H	0.6979670000	2.1138850000	2.5995570000
O	-4.2791710000	-1.8177340000	-1.3963050000

Table S123. Cartesian coordinates of β -Glc-tg_His_H2 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6291788			
ZPE / Hartree = 0.3647520			
BSSE / Hartree = 0.00298747779			
C	-0.5835720000	-0.4769510000	1.5606300000
C	-1.3685510000	0.8274800000	1.4444910000
C	-2.7945050000	0.5412120000	1.0029980000
C	-2.7835080000	-0.2905560000	-0.2690730000
C	-1.9288560000	-1.5452290000	-0.0752940000
C	-1.7802340000	-2.3582790000	-1.3573600000
O	-0.6182080000	-1.1519800000	0.3080760000
O	0.7276460000	-0.1601620000	1.8629220000
O	-1.4341260000	1.5078940000	2.6840940000
O	-3.5054250000	1.7352250000	0.7195920000
O	-4.0946840000	-0.7033200000	-0.6269320000
O	-2.9829780000	-3.0189230000	-1.7148750000
H	-1.0332120000	-1.1349260000	2.3242640000
H	-0.8684070000	1.4481430000	0.6844380000
H	-3.3089670000	-0.0259190000	1.7940480000
H	-2.3428870000	0.3104720000	-1.0792550000
H	-2.3810120000	-2.1779670000	0.7053250000
H	-1.4355420000	-1.6984950000	-2.1662890000
H	-1.0245070000	-3.1306210000	-1.1954980000
H	1.3316170000	-0.9377890000	1.7417570000
H	-0.5527130000	1.8431810000	2.8986770000
H	-3.5892390000	2.2444370000	1.5376040000
H	-4.6274910000	0.0859600000	-0.7993410000
H	-3.6899030000	-2.3550530000	-1.7275190000
N	4.4875420000	0.5578440000	-0.5275630000
H	5.0221810000	-0.2024530000	-0.9661820000
H	5.0826840000	0.9603100000	0.2009260000
H	4.3094250000	1.2885320000	-1.2210030000
C	3.2320650000	-0.0199480000	0.0452340000
H	2.9251510000	0.6185590000	0.8745590000
C	2.1347380000	-0.0911190000	-1.0172210000
C	3.5524420000	-1.4312500000	0.5904980000

H	2.5754090000	-0.3957360000	-1.9750650000
H	1.4318490000	-0.8750240000	-0.7223550000
C	1.3689180000	1.1875610000	-1.1633350000
O	4.6335920000	-1.9485310000	0.2409870000
N	0.2450560000	1.2694320000	-1.9489590000
C	1.4922550000	2.4355490000	-0.5995980000
H	-0.1536340000	0.5190280000	-2.4998140000
C	-0.2611300000	2.5224250000	-1.8341950000
N	0.4715520000	3.2619390000	-1.0256710000
H	2.2515450000	2.7824290000	0.0882910000
H	-1.1539010000	2.8362670000	-2.3561590000
O	2.6644500000	-1.9393550000	1.3270470000

Table S124. Cartesian coordinates of β -Glc-tg_His_H3 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6322335			
ZPE / Hartree = 0.3657752			
BSSE / Hartree = 0.00312147952			
C	0.3716180000	-1.2036890000	0.9658520000
C	1.1379020000	-0.2265910000	1.8545970000
C	2.0214380000	0.6457310000	0.9792200000
C	2.9173490000	-0.2354160000	0.1223320000
C	2.0815080000	-1.2537150000	-0.6579750000
C	2.9405630000	-2.2417470000	-1.4403460000
O	1.3012750000	-2.0162520000	0.2549800000
O	-0.4340120000	-2.0088000000	1.7446620000
O	0.2455060000	0.6192290000	2.5547970000
O	2.8672540000	1.4954700000	1.7371050000
O	3.6479100000	0.5405710000	-0.8163380000
O	3.5667790000	-1.6347040000	-2.5593750000
H	-0.2187020000	-0.6384630000	0.2292650000
H	1.7587600000	-0.8055780000	2.5546280000
H	1.3784270000	1.2473230000	0.3172110000
H	3.6102080000	-0.7821530000	0.7801700000
H	1.4217620000	-0.7156160000	-1.3589910000
H	3.6833460000	-2.6899580000	-0.7664610000
H	2.2967260000	-3.0362100000	-1.8250080000
H	-1.3218660000	-2.1053940000	1.3142760000
H	-0.3220510000	0.0619210000	3.1067640000
H	2.3315210000	2.1998440000	2.1263960000
H	4.1865470000	1.1791030000	-0.3272580000
H	4.0379000000	-0.8483810000	-2.2425090000
N	-3.6934620000	0.2249370000	-1.7908360000
H	-4.6623370000	0.2491900000	-1.4495500000
H	-3.6828700000	-0.3738450000	-2.6205040000
H	-3.4107010000	1.1647310000	-2.0835740000
C	-2.8236920000	-0.3227140000	-0.7062180000
H	-1.9399830000	-0.7507760000	-1.1846430000
C	-2.4458330000	0.7902180000	0.2699990000
C	-3.5952640000	-1.4477570000	0.0176770000
H	-3.3528000000	1.3304880000	0.5692010000

H	-2.0418420000	0.3271490000	1.1775920000
C	-1.4361520000	1.7350100000	-0.3043750000
O	-4.8259010000	-1.5099800000	-0.1779070000
N	-1.0184520000	2.8585240000	0.3646350000
C	-0.7106670000	1.7332380000	-1.4735420000
H	-1.3423030000	3.1658300000	1.2733280000
C	-0.0813810000	3.4774090000	-0.3945800000
N	0.1306640000	2.8256100000	-1.5207190000
H	-0.7418170000	1.0091810000	-2.2768550000
H	0.4059640000	4.3900470000	-0.0828350000
O	-2.9024930000	-2.1907580000	0.7623200000

Table S125. Cartesian coordinates of β -Glc-tg_His_H4 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6281771			
ZPE / Hartree = 0.3645033			
BSSE / Hartree = 0.00276281989			
C	-2.2484610000	2.1070590000	0.6869650000
C	-0.7981520000	1.8680000000	0.2734610000
C	-0.7694640000	1.1198350000	-1.0497790000
C	-1.5826600000	-0.1589470000	-0.9032660000
C	-3.0026900000	0.1564380000	-0.4340860000
C	-3.8184430000	-1.1039650000	-0.1642670000
O	-2.9244670000	0.8623180000	0.8001040000
O	-2.2406250000	2.7115420000	1.9370970000
O	-0.1009870000	3.0849930000	0.0986840000
O	0.5339130000	0.7575530000	-1.4518340000
O	-1.6616370000	-0.8651170000	-2.1335040000
O	-4.1822960000	-1.7689880000	-1.3631040000
H	-2.7640210000	2.7328160000	-0.0574360000
H	-0.3283590000	1.2553450000	1.0578750000
H	-1.2377820000	1.7544990000	-1.8204510000
H	-1.1042550000	-0.7920310000	-0.1417460000
H	-3.5183390000	0.7694270000	-1.1905300000
H	-3.2448710000	-1.7677340000	0.4981700000
H	-4.7449320000	-0.8226330000	0.3419840000
H	-3.0965020000	3.1312920000	2.0997160000
H	0.0144060000	3.5025060000	0.9635320000
H	1.2093470000	1.4115700000	-1.1706260000
H	-0.7714140000	-1.1690210000	-2.3628670000
H	-3.3702070000	-1.9133760000	-1.8737540000
N	4.2240170000	-1.3807240000	-0.2235200000
H	5.0225680000	-0.9657920000	0.2723220000
H	4.5522660000	-1.6310440000	-1.1592410000
H	3.9403640000	-2.2439480000	0.2475470000
C	3.1272200000	-0.3668440000	-0.2853270000
H	2.5218640000	-0.5905010000	-1.1643780000
C	2.2731860000	-0.4157650000	0.9795080000
C	3.7576000000	1.0351820000	-0.4532790000

H	2.9237080000	−0.4997490000	1.8594030000
H	1.7593040000	0.5463550000	1.0604120000
C	1.2571300000	−1.5143330000	0.9604630000
O	4.9874230000	1.1350650000	−0.2489660000
N	0.3157000000	−1.6505110000	1.9513950000
C	0.9677130000	−2.5148120000	0.0625150000
H	0.2271070000	−1.0668530000	2.7741770000
C	−0.4892070000	−2.6933720000	1.6286050000
N	−0.1226920000	−3.2457540000	0.4890600000
H	1.4745320000	−2.7449980000	−0.8652550000
H	−1.3147800000	−3.0029830000	2.2532380000
O	2.9497000000	1.9494980000	−0.7571900000

Table S126. Cartesian coordinates of β -Glc-tg_His_H5 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6241787			
ZPE / Hartree = 0.3645529			
BSSE / Hartree = 0.00228533724			
C	1.3617320000	-1.5989550000	0.4462430000
C	2.8851110000	-1.6203900000	0.3642360000
C	3.4096770000	-0.2067290000	0.1628350000
C	2.7274800000	0.4374880000	-1.0338810000
C	1.2093750000	0.3699820000	-0.8617850000
C	0.4414940000	0.9082020000	-2.0635450000
O	0.8271210000	-0.9934960000	-0.7218220000
O	0.9194260000	-2.9143070000	0.4977840000
O	3.4540420000	-2.1195170000	1.5592760000
O	4.8044190000	-0.1933390000	-0.0870850000
O	3.0957600000	1.8033240000	-1.1557380000
O	0.5633970000	2.3146700000	-2.1957750000
H	1.0321320000	-1.0298460000	1.3291810000
H	3.1712040000	-2.2423270000	-0.4963390000
H	3.1800890000	0.3886860000	1.0602390000
H	3.0054210000	-0.1131710000	-1.9450050000
H	0.9225400000	0.9425380000	0.0355840000
H	0.7846360000	0.3934910000	-2.9715720000
H	-0.6207070000	0.6875640000	-1.9179040000
H	0.0074100000	-2.9379420000	0.8190330000
H	3.2475740000	-3.0616070000	1.6299750000
H	5.2661530000	-0.4795420000	0.7128310000
H	4.0539830000	1.8514490000	-1.2827640000
H	1.5073850000	2.5346910000	-2.1616790000
N	-4.4812060000	0.6679090000	0.4242480000
H	-5.0738990000	-0.0313170000	0.8901480000
H	-5.0805990000	1.1842880000	-0.2234510000
H	-4.1221000000	1.3354400000	1.1129310000
C	-3.3912180000	-0.0591040000	-0.2970430000
H	-3.0810650000	0.5603220000	-1.1403720000
C	-2.2194560000	-0.3237000000	0.6447910000
C	-3.9609870000	-1.3995330000	-0.8206920000
H	-2.5703460000	-0.8898250000	1.5163420000

H	-1.5086710000	-0.9573780000	0.1031770000
C	-1.5334830000	0.9307830000	1.0869410000
O	-5.0551520000	-1.7714610000	-0.3304120000
N	-0.7066090000	0.9692100000	2.1837050000
C	-1.4723550000	2.1988690000	0.5582530000
H	-0.5245550000	0.2043000000	2.8218600000
C	-0.1798340000	2.2153780000	2.2710180000
N	-0.6238190000	2.9917780000	1.3021930000
H	-1.9780660000	2.5788230000	-0.3193050000
H	0.5057920000	2.5007050000	3.0559050000
O	-3.2475240000	-1.9927930000	-1.6592360000

Table S127. Cartesian coordinates of β -Glc-tg_His_H6 optimized at the M06- 2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6207438			
ZPE / Hartree = 0.3640923			
BSSE / Hartree = 0.00136416649			
C	-3.1710620000	1.2630760000	-0.5713940000
C	-3.8417720000	0.0354350000	-1.1801610000
C	-3.9568510000	-1.0604010000	-0.1310380000
C	-2.5948860000	-1.3324850000	0.4874510000
C	-1.9891630000	-0.0325180000	1.0205170000
C	-0.5745820000	-0.2197040000	1.5592670000
O	-1.9002360000	0.9020610000	-0.0483040000
O	-2.9762370000	2.1921740000	-1.5851910000
O	-5.1500510000	0.3338200000	-1.6275290000
O	-4.4191480000	-2.2768340000	-0.6923340000
O	-2.6951430000	-2.2456470000	1.5702120000
O	-0.5615150000	-0.9242240000	2.7901160000
H	-3.7901460000	1.6779720000	0.2385840000
H	-3.2146690000	-0.3187640000	-2.0110890000
H	-4.6440410000	-0.7243580000	0.6604080000
H	-1.9263040000	-1.7369640000	-0.2872770000
H	-2.6309910000	0.3673660000	1.8218960000
H	0.0362070000	-0.7318450000	0.8023330000
H	-0.1375940000	0.7648960000	1.7475870000
H	-2.8315320000	3.0670360000	-1.1990410000
H	-5.0887490000	0.9084910000	-2.4028320000
H	-5.3332760000	-2.1544800000	-0.9830740000
H	-3.0298730000	-3.0879230000	1.2310020000
H	-1.0579790000	-1.7475020000	2.6625060000
N	5.1966660000	0.6225510000	-0.4097670000
H	5.4761270000	0.5719110000	-1.3963250000
H	6.0505320000	0.5408570000	0.1471160000
H	4.7836400000	1.5392980000	-0.2116540000
C	4.2485890000	-0.4949730000	-0.1204440000
H	4.2677640000	-0.6696530000	0.9566900000
C	2.8427210000	-0.1222710000	-0.5883990000
C	4.7382680000	-1.7617490000	-0.8621010000

H	2.8578650000	0.0637380000	−1.6691590000
H	2.2053030000	−0.9961910000	−0.4195270000
C	2.2889360000	1.0748060000	0.1198210000
O	5.6063420000	−1.5888810000	−1.7520660000
N	1.2918010000	1.8476300000	−0.4210130000
C	2.5585990000	1.6535410000	1.3388190000
H	0.8453120000	1.7011940000	−1.3179340000
C	0.9948040000	2.8321640000	0.4614670000
N	1.7462860000	2.7502820000	1.5417060000
H	3.2873670000	1.3433530000	2.0756030000
H	0.2329990000	3.5734570000	0.2666010000
O	4.1881300000	−2.8305530000	−0.5163710000

Table S128. Cartesian coordinates of α -Gal-gg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1715012			
ZPE / Hartree = 0.4235385			
BSSE / Hartree = 0.0026794018			
C	-3.0669260000	-2.0900920000	0.6788060000
C	-2.0601230000	-2.3182100000	-0.4507950000
C	-1.2418660000	-1.0528820000	-0.6817190000
C	-2.1590820000	0.1350330000	-0.9345350000
C	-3.1558240000	0.2544660000	0.2152490000
C	-4.1740860000	1.3700060000	0.0280850000
O	-3.8750120000	-0.9671060000	0.4080990000
O	-2.3221280000	-1.9376050000	1.8620240000
O	-1.2172280000	-3.4219370000	-0.1708590000
O	-0.3916770000	-1.1884950000	-1.8089630000
O	-2.8745920000	-0.0314690000	-2.1561480000
O	-5.0916890000	1.1413430000	-1.0305750000
H	-3.7565410000	-2.9343220000	0.7608160000
H	-2.6115610000	-2.5680650000	-1.3615290000
H	-0.6472170000	-0.8446550000	0.2181130000
H	-1.5583280000	1.0545170000	-0.9742700000
H	-2.5783250000	0.4869480000	1.1206780000
H	-4.7685490000	1.4652150000	0.9401120000
H	-3.6201710000	2.3068400000	-0.1224930000
H	-2.8960170000	-2.0895860000	2.6250810000
H	-0.8469660000	-3.2914210000	0.7161480000
H	0.1112640000	-2.0100660000	-1.7105030000
H	-2.2311680000	-0.1969060000	-2.8607750000
H	-4.5767840000	0.8978980000	-1.8155710000
H	5.2593140000	1.6475130000	0.6829930000
H	4.4666360000	-0.4056320000	1.4306230000
N	4.4375770000	1.2840120000	0.1948360000
H	3.6167690000	1.7878020000	0.5460930000
H	4.5664910000	1.4894010000	-0.8025720000
C	4.3044850000	-0.1928610000	0.3727930000

O	5.9041470000	-0.2027340000	-1.3981570000
C	5.3787610000	-0.8911600000	-0.4881830000
O	5.5889230000	-2.0950520000	-0.2158570000
H	1.4965230000	-1.1938460000	2.5278560000
H	-0.2784330000	0.4709070000	3.1262820000
C	1.2581300000	-0.3403440000	1.9074790000
N	0.2733240000	0.5405630000	2.2825770000
C	1.7970420000	0.0407780000	0.7015560000
C	2.8985430000	-0.6458000000	-0.0502370000
C	0.1522900000	1.5214500000	1.3296240000
H	-1.4270840000	2.8204030000	2.0603450000
C	1.0970480000	1.2387760000	0.3093410000
H	2.8561740000	-1.7262530000	0.1112870000
C	-0.7105580000	2.6249290000	1.2681090000
C	1.1591070000	2.0845210000	-0.8166820000
C	-0.6199130000	3.4430320000	0.1523800000
H	2.7817100000	-0.4716000000	-1.1272710000
H	1.8651030000	1.8833210000	-1.6188210000
C	0.3046840000	3.1744120000	-0.8836610000
H	-1.2761780000	4.3038600000	0.0685180000
H	0.3408270000	3.8338060000	-1.7451810000

Table S129. Cartesian coordinates of α -Gal-gg_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1698584			
ZPE / Hartree = 0.423793			
BSSE / Hartree = 0.002610926			
C	1.1419980000	-0.9018190000	-1.2326090000
C	1.7500210000	0.4929720000	-1.1056360000
C	3.2689190000	0.4205370000	-1.2054260000
C	3.8087460000	-0.5539920000	-0.1636280000
C	3.1078410000	-1.9043110000	-0.3020590000
C	3.4951740000	-2.9031630000	0.7812690000
O	1.6851600000	-1.7676390000	-0.2629210000
O	1.3916680000	-1.3431880000	-2.5443200000
O	1.2106310000	1.3811350000	-2.0679330000
O	3.8503790000	1.6885450000	-0.9428850000
O	3.5877030000	-0.0491360000	1.1489230000
O	3.0054090000	-2.5680330000	2.0708400000
H	0.0670560000	-0.8713220000	-1.0303540000
H	1.4816830000	0.8941140000	-0.1244740000
H	3.5599620000	0.0667570000	-2.2045750000
H	4.8840580000	-0.7046560000	-0.3295240000
H	3.4113490000	-2.3306920000	-1.2677520000
H	3.0691970000	-3.8780030000	0.5321120000
H	4.5892850000	-2.9950470000	0.7844680000
H	0.7929050000	-2.0719080000	-2.7570960000
H	1.2877620000	0.9593800000	-2.9379090000
H	3.3613970000	2.3538690000	-1.4490910000
H	3.8628220000	0.8799730000	1.1653780000
H	3.2397740000	-1.6427120000	2.2417140000
H	-4.9712060000	0.1333330000	1.9557100000
H	-4.9007530000	0.5708460000	-0.3267010000
N	-4.0973810000	-0.1085110000	1.4822910000
H	-3.4122680000	0.6247990000	1.6918910000
H	-3.7782220000	-0.9984820000	1.8806800000
C	-4.2964580000	-0.2728190000	0.0110090000
O	-5.0786420000	-2.4162640000	0.7118860000
C	-5.0400130000	-1.6012170000	-0.2429100000

O	-5.5002600000	-1.7474290000	-1.3982840000
H	-2.8142690000	2.4465660000	-1.9449280000
H	-1.1767200000	4.0093340000	-0.8714640000
C	-2.1976870000	2.1637390000	-1.1024730000
N	-1.3226310000	3.0637400000	-0.5468610000
C	-2.1244420000	0.9624600000	-0.4380950000
C	-2.9368680000	-0.2699930000	-0.7045870000
C	-0.6518210000	2.4656730000	0.4903520000
H	0.7185400000	3.9818890000	1.2236410000
C	-1.1357370000	1.1361540000	0.5964450000
H	-3.1471250000	-0.3693000000	-1.7725860000
C	0.3560740000	2.9639690000	1.3277370000
C	-0.5910030000	0.2848690000	1.5787620000
C	0.8746710000	2.1022820000	2.2833730000
H	-2.3767060000	-1.1625000000	-0.3972170000
H	-0.9372950000	-0.7417810000	1.6737270000
C	0.4052460000	0.7740640000	2.4094080000
H	1.6612340000	2.4518700000	2.9451540000
H	0.8432770000	0.1267270000	3.1631650000

Table S130. Cartesian coordinates of α -Gal-gt_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1712727			
ZPE / Hartree = 0.4227011			
BSSE / Hartree = 0.0027199662			
C	-3.1228930000	-2.0738430000	0.5578770000
C	-2.0279410000	-2.3954740000	-0.4623840000
C	-1.1809830000	-1.1567810000	-0.7370960000
C	-2.0623750000	0.0106290000	-1.1622980000
C	-3.1257130000	0.2281040000	-0.0938670000
C	-4.1241720000	1.3090830000	-0.4579120000
O	-3.8852870000	-0.9663510000	0.1312550000
O	-2.4816180000	-1.8368190000	1.7859580000
O	-1.2192430000	-3.4726100000	-0.0234300000
O	-0.2494500000	-1.3976020000	-1.7798290000
O	-2.6995190000	-0.2566390000	-2.4042100000
O	-5.0153510000	1.5691450000	0.6176600000
H	-3.8306090000	-2.9026310000	0.6428510000
H	-2.5062950000	-2.7208470000	-1.3904870000
H	-0.6528970000	-0.8745840000	0.1839760000
H	-1.4465700000	0.9184590000	-1.2376330000
H	-2.6183660000	0.5119770000	0.8379580000
H	-3.5849170000	2.2387790000	-0.6590970000
H	-4.6772290000	1.0174210000	-1.3579030000
H	-3.1236290000	-1.9179640000	2.5044160000
H	-0.9157410000	-3.2653270000	0.8742260000
H	0.2410770000	-2.2045600000	-1.5655030000
H	-2.0156090000	-0.5461600000	-3.0257500000
H	-5.5055790000	0.7553700000	0.7993860000
H	5.2431170000	1.6945320000	0.8164090000
H	4.4004450000	-0.3331410000	1.5981210000
N	4.4311900000	1.3220520000	0.3186830000
H	3.6034820000	1.8331610000	0.6417080000
H	4.5812020000	1.5077360000	-0.6793170000
C	4.2907610000	-0.1498430000	0.5280340000
O	5.9791610000	-0.2032700000	-1.1574580000
C	5.4060740000	-0.8693160000	-0.2598390000

O	5.5989690000	-2.0669150000	0.0509380000
H	1.3872480000	-1.0244470000	2.5883340000
H	-0.4399440000	0.6420450000	2.9871120000
C	1.1701290000	-0.2161480000	1.9029890000
N	0.1535310000	0.6690180000	2.1695680000
C	1.7661640000	0.0980640000	0.7047120000
C	2.9088270000	-0.6173150000	0.0464620000
C	0.0681680000	1.5850970000	1.1503190000
H	-1.5714980000	2.8963060000	1.7071860000
C	1.0706390000	1.2562650000	0.2018730000
H	2.8555600000	-1.6908630000	0.2465900000
C	-0.8079370000	2.6653160000	0.9702290000
C	1.1857190000	2.0317690000	-0.9690250000
C	-0.6668860000	3.4132300000	-0.1888500000
H	2.8532970000	-0.4856420000	-1.0413890000
H	1.9394650000	1.7945790000	-1.7158920000
C	0.3200340000	3.0991360000	-1.1523110000
H	-1.3312890000	4.2539480000	-0.3637330000
H	0.3952480000	3.7050180000	-2.0498670000

Table S131. Cartesian coordinates of α -Gal-gt_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1693046			
ZPE / Hartree = 0.4233954			
BSSE / Hartree = 0.0025509387			
C	-1.2170120000	0.8757190000	-1.0591930000
C	-1.7576730000	-0.5516540000	-1.0071340000
C	-3.2813240000	-0.5534010000	-1.0732560000
C	-3.8541960000	0.3325240000	0.0296690000
C	-3.2297930000	1.7194410000	-0.0711830000
C	-3.6329590000	2.6342870000	1.0699680000
O	-1.7985860000	1.6541310000	-0.0369990000
O	-1.4979370000	1.3785910000	-2.3407920000
O	-1.2010080000	-1.3534730000	-2.0332670000
O	-3.7844260000	-1.8657880000	-0.8739100000
O	-3.5706870000	-0.2120020000	1.3097810000
O	-3.1288310000	3.9482050000	0.8772200000
H	-0.1405210000	0.8871520000	-0.8630000000
H	-1.4478400000	-0.9981650000	-0.0583920000
H	-3.6112300000	-0.1623750000	-2.0462590000
H	-4.9401600000	0.4279180000	-0.1104270000
H	-3.5472240000	2.1703370000	-1.0205790000
H	-4.7224560000	2.7107050000	1.1041440000
H	-3.2761920000	2.2186540000	2.0191360000
H	-0.9344690000	2.1441570000	-2.5170290000
H	-1.3180280000	-0.8827170000	-2.8731410000
H	-3.2597710000	-2.4727000000	-1.4166560000
H	-3.7562710000	-1.1623560000	1.2691490000
H	-2.1634910000	3.8924320000	0.8543230000
H	4.9985790000	-0.0909490000	1.9116870000
H	4.9242610000	-0.4327350000	-0.3941790000
N	4.1073630000	0.1125300000	1.4527190000
H	3.4762630000	-0.6765310000	1.6263990000
H	3.7285730000	0.9556780000	1.8974190000
C	4.2864460000	0.3644070000	-0.0084760000
O	4.9725410000	2.5034950000	0.7989080000
C	4.9674310000	1.7366080000	-0.1957680000

O	5.4146870000	1.9625190000	-1.3434270000
H	2.8512760000	-2.2931570000	-2.1252240000
H	1.2948360000	-3.9752690000	-1.1137040000
C	2.2508110000	-2.0862220000	-1.2496970000
N	1.4201130000	-3.0484720000	-0.7315490000
C	2.1595360000	-0.9337540000	-0.5059620000
C	2.9219490000	0.3409510000	-0.7141030000
C	0.7607320000	-2.5411850000	0.3598740000
H	-0.5402060000	-4.1457980000	1.0294120000
C	1.2064440000	-1.2064290000	0.5406570000
H	3.1184110000	0.5022710000	-1.7770940000
C	-0.2057860000	-3.1256790000	1.1905060000
C	0.6676080000	-0.4402180000	1.5936770000
C	-0.7205230000	-2.3461210000	2.2162890000
H	2.3296130000	1.1938960000	-0.3582460000
H	0.9873880000	0.5879640000	1.7479440000
C	-0.2874180000	-1.0149450000	2.4180680000
H	-1.4754080000	-2.7640010000	2.8753220000
H	-0.7199480000	-0.4342150000	3.2270690000

Table S132. Cartesian coordinates of α -Gal-tg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1700469			
ZPE / Hartree = 0.4231957			
BSSE / Hartree = 0.0030203869			
C	-3.0221820000	-2.2331500000	0.6231860000
C	-1.9441310000	-2.4229390000	-0.4460170000
C	-1.2296360000	-1.1013680000	-0.7039210000
C	-2.2261490000	-0.0067770000	-1.0608000000
C	-3.2820740000	0.0740330000	0.0348180000
C	-4.4217740000	1.0285020000	-0.3027490000
O	-3.9036440000	-1.1947380000	0.2582610000
O	-2.3562100000	-1.9652310000	1.8317610000
O	-1.0204930000	-3.4301930000	-0.0711190000
O	-0.3119660000	-1.2190560000	-1.7798420000
O	-2.8654930000	-0.2828450000	-2.2987560000
O	-3.9455130000	2.3262190000	-0.6186850000
H	-3.6447060000	-3.1272410000	0.7130200000
H	-2.4252290000	-2.7659400000	-1.3662680000
H	-0.7027850000	-0.8032730000	0.2116330000
H	-1.6962640000	0.9557690000	-1.1092140000
H	-2.7814190000	0.4076080000	0.9556640000
H	-4.9488360000	0.6629430000	-1.1869640000
H	-5.1239260000	1.0554040000	0.5380140000
H	-2.9572110000	-2.1234790000	2.5724170000
H	-0.6974880000	-3.2172530000	0.8184690000
H	0.2729370000	-1.9685850000	-1.5956610000
H	-2.1743380000	-0.4940990000	-2.9431650000
H	-3.5325170000	2.7089790000	0.1675090000
H	5.1707330000	1.7136800000	0.7084460000
H	4.4010120000	-0.3502420000	1.4569750000
N	4.3525880000	1.3395940000	0.2222780000
H	3.5257470000	1.8309960000	0.5767910000
H	4.4754780000	1.5492560000	-0.7749110000
C	4.2411480000	-0.1391770000	0.3984380000
O	5.8528000000	-0.1238800000	-1.3619770000
C	5.3302810000	-0.8210170000	-0.4570620000

O	5.5545270000	-2.0226420000	-0.1856720000
H	1.4360570000	-1.2062880000	2.5313820000
H	-0.3790700000	0.4163540000	3.1257750000
C	1.1857950000	-0.3528290000	1.9156080000
N	0.1794770000	0.5046190000	2.2883630000
C	1.7275330000	0.0491800000	0.7177540000
C	2.8448340000	-0.6126950000	-0.0328840000
C	0.0452100000	1.4889340000	1.3408920000
H	-1.5621550000	2.7539090000	2.0704150000
C	1.0059350000	1.2349890000	0.3281450000
H	2.8199530000	-1.6948670000	0.1212330000
C	-0.8382630000	2.5759350000	1.2805060000
C	1.0599370000	2.0893310000	-0.7915370000
C	-0.7512380000	3.4063860000	0.1734540000
H	2.7299210000	-0.4335050000	-1.1093850000
H	1.7766740000	1.9078930000	-1.5888750000
C	0.1854320000	3.1630240000	-0.8576820000
H	-1.4191730000	4.2589810000	0.0928550000
H	0.2161340000	3.8302810000	-1.7133160000

Table S133. Cartesian coordinates of α -Gal-tg_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1677713			
ZPE / Hartree = 0.4234427			
BSSE / Hartree = 0.002580916			
C	1.1251210000	-0.8827690000	-1.0908250000
C	1.6632460000	0.5452750000	-1.0351900000
C	3.1860010000	0.5459210000	-1.1079250000
C	3.7617140000	-0.3449790000	-0.0111520000
C	3.1381830000	-1.7331370000	-0.1148660000
C	3.5352900000	-2.6533960000	1.0336560000
O	1.7101360000	-1.6692920000	-0.0771100000
O	1.4011280000	-1.3778500000	-2.3769540000
O	1.0998030000	1.3487690000	-2.0565870000
O	3.6921600000	1.8574570000	-0.9074520000
O	3.4790720000	0.1915830000	1.2722520000
O	4.9421560000	-2.8137560000	1.1105210000
H	0.0496070000	-0.8972430000	-0.8904440000
H	1.3569770000	0.9887830000	-0.0838580000
H	3.5108070000	0.1579180000	-2.0839640000
H	4.8466950000	-0.4371440000	-0.1534260000
H	3.4620400000	-2.1788080000	-1.0656730000
H	3.2137010000	-2.2137220000	1.9805090000
H	3.0310600000	-3.6174060000	0.9053090000
H	0.8363350000	-2.1417820000	-2.5559790000
H	1.2152680000	0.8809560000	-2.8982990000
H	3.1694780000	2.4657410000	-1.4504750000
H	3.6719020000	1.1405720000	1.2398810000
H	5.2385810000	-3.3331990000	0.3513180000
H	-5.0416180000	-0.0454740000	1.9755790000
H	-5.0037420000	0.2806700000	-0.3364370000
N	-4.1499230000	-0.2209580000	1.5060290000
H	-3.5461950000	0.5926950000	1.6621170000
H	-3.7341260000	-1.0446590000	1.9538820000
C	-4.3401070000	-0.4945690000	0.0501900000
O	-4.9468310000	-2.6466380000	0.8860170000
C	-4.9851040000	-1.8868140000	-0.1133630000
O	-5.4494380000	-2.1338820000	-1.2498740000

H	-2.993060000	2.164264000	-2.131575000
H	-1.466570000	3.901383000	-1.168985000
C	-2.379120000	1.988383000	-1.258593000
N	-1.565878000	2.979452000	-0.768029000
C	-2.253602000	0.853008000	-0.493757000
C	-2.985194000	-0.444138000	-0.672434000
C	-0.882810000	2.508565000	0.325102000
H	0.389504000	4.154756000	0.947153000
C	-1.295946000	1.167907000	0.536692000
H	-3.189982000	-0.626473000	-1.730472000
C	0.079976000	3.130843000	1.132108000
C	-0.728466000	0.435113000	1.598032000
C	0.623243000	2.383452000	2.167203000
H	-2.366642000	-1.276098000	-0.311372000
H	-1.023079000	-0.596789000	1.775765000
C	0.221987000	1.047462000	2.400401000
H	1.375688000	2.830925000	2.809392000
H	0.676008000	0.492785000	3.215853000

Table S134. Cartesian coordinates of β -Gal-gg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1706582			
ZPE / Hartree = 0.4227393			
BSSE / Hartree = 0.0029716792			
C	1.1876800000	-1.4003000000	1.3425250000
C	2.2416840000	-0.4428990000	1.8878730000
C	2.5675110000	0.6026640000	0.8322080000
C	2.9613510000	-0.0513900000	-0.4858240000
C	1.8973830000	-1.0712560000	-0.8853690000
C	2.2238190000	-1.8364010000	-2.1587060000
O	1.6767270000	-2.0148960000	0.1609630000
O	0.9674110000	-2.3884420000	2.2946400000
O	1.7682900000	0.2567430000	3.0254810000
O	3.6444010000	1.4303720000	1.2395800000
O	4.2177670000	-0.7100120000	-0.3714190000
O	3.3175300000	-2.7310450000	-2.0262320000
H	0.2583120000	-0.8542950000	1.1101040000
H	3.1409240000	-1.0246640000	2.1331210000
H	1.6664160000	1.2076600000	0.6587630000
H	3.0097560000	0.7221640000	-1.2655780000
H	0.9697040000	-0.5117300000	-1.0703040000
H	1.3574690000	-2.4416570000	-2.4381800000
H	2.4044310000	-1.1032590000	-2.9565870000
H	0.1392080000	-2.8472050000	2.0954730000
H	1.7220870000	-0.3561510000	3.7718180000
H	3.4496370000	1.7634820000	2.1274810000
H	4.8498190000	-0.0883080000	0.0188040000
H	4.0527620000	-2.2382520000	-1.6301420000
H	-5.1810540000	1.4002080000	-0.3329210000
H	-4.3063030000	-0.4229970000	-1.4920360000
N	-4.2644730000	1.0663720000	-0.0245180000
H	-3.5526880000	1.6953050000	-0.4097740000
H	-4.2556880000	1.1268850000	0.9996370000
C	-4.0343020000	-0.3503520000	-0.4375540000
O	-5.4289260000	-0.7596800000	1.4546710000
C	-4.9364840000	-1.2663110000	0.4163190000

O	-5.0534220000	-2.4427760000	0.0039100000
H	-1.4448860000	-0.6413350000	-3.0213200000
H	0.1395510000	1.2510190000	-3.4523070000
C	-1.1918300000	0.0953370000	-2.2706980000
N	-0.3162370000	1.1132540000	-2.5609310000
C	-1.6071460000	0.1901940000	-0.9634930000
C	-2.5567560000	-0.7203360000	-0.2432140000
C	-0.1436370000	1.8980100000	-1.4469540000
H	1.2692200000	3.4329310000	-2.0500490000
C	-0.9501570000	1.3506780000	-0.4159280000
H	-2.4438730000	-1.7491720000	-0.5948880000
C	0.6539160000	3.0345690000	-1.2493220000
C	-0.9593110000	1.9704460000	0.8496600000
C	0.6221340000	3.6244740000	0.0056890000
H	-2.3314350000	-0.7157980000	0.8310860000
H	-1.5664610000	1.5670810000	1.6567800000
C	-0.1784140000	3.0990080000	1.0468540000
H	1.2273110000	4.5056260000	0.1950180000
H	-0.1721230000	3.5861440000	2.0170060000

Table S135. Cartesian coordinates of β -Gal-gg_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1686966			
ZPE / Hartree = 0.4232148			
BSSE / Hartree = 0.0029873335			
C	-1.4825760000	-1.3995490000	-1.5369810000
C	-1.2906170000	-1.7123540000	-0.0586280000
C	-2.6364550000	-2.0411720000	0.5670850000
C	-3.6280330000	-0.9065950000	0.3296450000
C	-3.6575800000	-0.5310520000	-1.1534530000
C	-4.5053400000	0.7029370000	-1.4421280000
O	-2.3475460000	-0.2804050000	-1.6547700000
O	-0.2474730000	-1.0578600000	-2.0737590000
O	-0.4477070000	-2.8310650000	0.1469370000
O	-2.5143000000	-2.2114720000	1.9698350000
O	-3.2600730000	0.2384720000	1.0875900000
O	-3.9224230000	1.9129950000	-0.9832290000
H	-1.9224140000	-2.2589270000	-2.0677060000
H	-0.8724370000	-0.8167400000	0.4179820000
H	-3.0300830000	-2.9578520000	0.1032950000
H	-4.6331090000	-1.2402130000	0.6209940000
H	-4.1055250000	-1.3795450000	-1.6940290000
H	-4.6233680000	0.8069740000	-2.5232800000
H	-5.4976860000	0.5463560000	-0.9992710000
H	-0.2919540000	-1.1043980000	-3.0387340000
H	0.4712490000	-2.5444120000	0.0499490000
H	-1.7497460000	-2.7825410000	2.1362570000
H	-2.9827020000	-0.0560430000	1.9686280000
H	-3.6410980000	1.7765560000	-0.0647160000
H	5.0871560000	1.8438490000	0.5537430000
H	4.4549120000	-0.2479050000	1.3640510000
N	4.2570050000	1.4274130000	0.1258420000
H	3.4336470000	1.8789100000	0.5365240000
H	4.2991780000	1.6408780000	-0.8769320000
C	4.2324050000	-0.0543090000	0.3134470000
O	5.7716040000	0.0389940000	-1.5093130000
C	5.3136750000	-0.6844650000	-0.5904430000

O	5.5977530000	-1.8774240000	-0.3368310000
H	1.5696980000	-1.2842940000	2.5713530000
H	-0.2728120000	0.2708260000	3.2634950000
C	1.2592570000	-0.4368560000	1.9748350000
N	0.2457410000	0.3851080000	2.4037080000
C	1.7276870000	-0.0085530000	0.7547160000
C	2.8452680000	-0.6093130000	-0.0459530000
C	0.0328620000	1.3716620000	1.4718850000
H	-1.5915180000	2.5642070000	2.2793120000
C	0.9492960000	1.1565720000	0.4117180000
H	2.8955890000	-1.6897440000	0.1154900000
C	-0.8949790000	2.4225060000	1.4587070000
C	0.9234530000	2.0214500000	-0.7014150000
C	-0.8944370000	3.2581890000	0.3531480000
H	2.6678500000	-0.4471450000	-1.1168290000
H	1.6103250000	1.8717940000	-1.5310980000
C	0.0059240000	3.0595880000	-0.7198730000
H	-1.6033760000	4.0791980000	0.3061020000
H	-0.0285470000	3.7325520000	-1.5709690000

Table S136. Cartesian coordinates of β -Gal-gt_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1708584			
ZPE / Hartree = 0.4223645			
BSSE / Hartree = 0.0030337424			
C	1.2318250000	-1.3453910000	1.4249120000
C	2.3203390000	-0.3818200000	1.8860930000
C	2.6881330000	0.5535540000	0.7427930000
C	3.0651520000	-0.2270260000	-0.5112270000
C	1.9579560000	-1.2280640000	-0.8211340000
C	2.2798280000	-2.1388000000	-1.9895730000
O	1.7037710000	-2.0740180000	0.3019880000
O	0.9771670000	-2.2397240000	2.4572500000
O	1.8727930000	0.4347070000	2.9539440000
O	3.7925240000	1.3748000000	1.0864010000
O	4.2884050000	-0.9235140000	-0.3313850000
O	1.1739750000	-2.9728070000	-2.3049360000
H	0.3227960000	-0.7904780000	1.1411250000
H	3.1965770000	-0.9724720000	2.1870500000
H	1.8110480000	1.1729460000	0.5108520000
H	3.1448360000	0.4761590000	-1.3536720000
H	1.0448910000	-0.6614510000	-1.0527740000
H	2.4855460000	-1.5304760000	-2.8741520000
H	3.1660900000	-2.7407950000	-1.7585310000
H	0.1225800000	-2.6678480000	2.3087590000
H	1.8075820000	-0.1047290000	3.7535410000
H	3.6062460000	1.7865000000	1.9427310000
H	4.9155520000	-0.3089580000	0.0778180000
H	0.9716850000	-3.5016900000	-1.5204940000
H	-4.9997710000	1.6716420000	-0.2757500000
H	-4.2789700000	-0.2702700000	-1.3379900000
N	-4.1088190000	1.2884290000	0.0484280000
H	-3.3576650000	1.8485080000	-0.3670290000
H	-4.0918330000	1.3949870000	1.0691360000
C	-3.9786020000	-0.1595010000	-0.2947360000
O	-5.3363980000	-0.3851330000	1.6545900000
C	-4.9166830000	-0.9695490000	0.6251510000

O	-5.1325710000	-2.1504690000	0.2689010000
H	-1.4779550000	-0.8390570000	-2.8994520000
H	0.1898170000	0.9184170000	-3.5371830000
C	-1.1660130000	-0.0529400000	-2.2252180000
N	-0.2480540000	0.8860790000	-2.6270270000
C	-1.5398410000	0.1800310000	-0.9229890000
C	-2.5220370000	-0.6107340000	-0.1099680000
C	-0.0047970000	1.7572020000	-1.5935800000
H	1.4611070000	3.1578450000	-2.3705940000
C	-0.8077890000	1.3473710000	-0.4974920000
H	-2.4841400000	-1.6676960000	-0.3868570000
C	0.8516780000	2.8650480000	-1.5213150000
C	-0.7467100000	2.0777920000	0.7066870000
C	0.8854800000	3.5674370000	-0.3256590000
H	-2.2655680000	-0.5422570000	0.9552230000
H	-1.3460510000	1.7791610000	1.5636120000
C	0.0931500000	3.1786020000	0.7795360000
H	1.5370040000	4.4308890000	-0.2337980000
H	0.1529530000	3.7495630000	1.7009230000

Table S137. Cartesian coordinates of β -Gal-gt_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1681896			
ZPE / Hartree = 0.4226876			
BSSE / Hartree = 0.0028508909			
C	-1.6129100000	-1.3529370000	-1.3179290000
C	-1.3539390000	-1.5779440000	0.1666840000
C	-2.6680690000	-1.8394160000	0.8876850000
C	-3.6664690000	-0.7153770000	0.6218630000
C	-3.7749900000	-0.4824290000	-0.8834870000
C	-4.6303130000	0.7209230000	-1.2345090000
O	-2.4908860000	-0.2464780000	-1.4614130000
O	-0.4045600000	-1.0383500000	-1.9265710000
O	-0.5236770000	-2.7019610000	0.3965640000
O	-2.4646850000	-1.9078660000	2.2897670000
O	-3.2449090000	0.4866270000	1.2459820000
O	-4.7941650000	0.8404980000	-2.6399340000
H	-2.0710790000	-2.2430340000	-1.7774180000
H	-0.8923420000	-0.6651250000	0.5647530000
H	-3.0937150000	-2.7833500000	0.5166370000
H	-4.6528700000	-1.0156970000	1.0020070000
H	-4.2164620000	-1.3825400000	-1.3390960000
H	-5.6266760000	0.5950120000	-0.8042410000
H	-4.1753760000	1.6272810000	-0.8192370000
H	-0.4878370000	-1.1484770000	-2.8838170000
H	0.3949040000	-2.4412200000	0.2399600000
H	-1.6902020000	-2.4667640000	2.4519430000
H	-2.8947310000	0.2549800000	2.1198120000
H	-3.9174540000	0.9658430000	-3.0288590000
H	5.2448500000	1.6223880000	0.5529040000
H	4.5442810000	-0.5007320000	1.1706830000
N	4.3973660000	1.2851760000	0.0905470000
H	3.5949050000	1.7401980000	0.5376100000
H	4.4554590000	1.5787300000	-0.8909650000
C	4.2971940000	-0.2039430000	0.1500180000
O	5.7791170000	-0.0295760000	-1.7132590000
C	5.3114300000	-0.8073130000	-0.8449350000
O	5.5368030000	-2.0313390000	-0.7071680000

H	1.7455790000	-1.3117730000	2.5006000000
H	0.0322910000	0.3151740000	3.3388310000
C	1.4290410000	-0.4466030000	1.9332680000
N	0.4901980000	0.4162940000	2.4436230000
C	1.8249390000	-0.0262360000	0.6845910000
C	2.8676680000	-0.6486910000	-0.1969660000
C	0.2565200000	1.4234740000	1.5390000000
H	-1.2412370000	2.6851460000	2.4756230000
C	1.0806170000	1.1781680000	0.4118030000
H	2.8528300000	-1.7386520000	-0.1090750000
C	-0.6148860000	2.5195350000	1.6044470000
C	1.0217400000	2.0599340000	-0.6857720000
C	-0.6513440000	3.3702480000	0.5106390000
H	2.6642420000	-0.4029640000	-1.2465970000
H	1.6400110000	1.8898170000	-1.5637150000
C	0.1588580000	3.1427570000	-0.6264130000
H	-1.3169740000	4.2277070000	0.5250870000
H	0.0998300000	3.8304350000	-1.4642960000

Table S138. Cartesian coordinates of β -Gal-tg_Trp_bottom optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1694747			
ZPE / Hartree = 0.4226382			
BSSE / Hartree = 0.0031802098			
C	-1.2037010000	-1.5759140000	-1.3631410000
C	-2.3109110000	-0.6660510000	-1.8835360000
C	-2.6420530000	0.3781430000	-0.8280060000
C	-2.9747490000	-0.2738370000	0.5087190000
C	-1.8562960000	-1.2414400000	0.8827050000
C	-2.1487170000	-2.0465240000	2.1423080000
O	-1.6322100000	-2.1906760000	-0.1576970000
O	-0.9797790000	-2.5688330000	-2.3091600000
O	-1.9025850000	0.0372960000	-3.0440390000
O	-3.7582310000	1.1643000000	-1.2144990000
O	-4.1998700000	-0.9862920000	0.4390140000
O	-2.3624510000	-1.1991470000	3.2599690000
H	-0.2873970000	-0.9942280000	-1.1673350000
H	-3.1938600000	-1.2854180000	-2.0933590000
H	-1.7586150000	1.0157830000	-0.6893400000
H	-3.0306340000	0.5094540000	1.2780050000
H	-0.9412530000	-0.6499080000	1.0380670000
H	-3.0630470000	-2.6281070000	2.0040680000
H	-1.3158580000	-2.7360550000	2.3200560000
H	-0.1268720000	-2.9915920000	-2.1366750000
H	-1.8544130000	-0.5829680000	-3.7840750000
H	-3.6016570000	1.4875780000	-2.1135620000
H	-4.8471070000	-0.4096970000	0.0070430000
H	-1.5218840000	-0.7869410000	3.5019730000
H	4.9954300000	1.6877800000	0.0669540000
H	4.3035520000	-0.0453500000	1.4436760000
N	4.1364780000	1.2143940000	-0.2215610000
H	3.3473860000	1.8187370000	0.0293990000
H	4.1794740000	1.1111600000	-1.2421000000
C	4.0222780000	-0.1418400000	0.3938590000
O	5.3972040000	-0.7242210000	-1.4677770000
C	4.9881570000	-1.0972360000	-0.3399470000

O	5.2324700000	-2.1746570000	0.2488110000
H	1.4674060000	-0.3929710000	3.0390890000
H	-0.2020610000	1.4563260000	3.3238690000
C	1.1677050000	0.2587270000	2.2292380000
N	0.2395120000	1.2496360000	2.4385800000
C	1.5693300000	0.2602200000	0.9144660000
C	2.5762150000	-0.6496110000	0.2758540000
C	0.0216380000	1.9264100000	1.2639070000
H	-1.4500490000	3.4456700000	1.7544700000
C	0.8462860000	1.3310670000	0.2742450000
H	2.5521160000	-1.6364400000	0.7455440000
C	-0.8255510000	3.0077830000	0.9820350000
C	0.8108590000	1.8375480000	-1.0407540000
C	-0.8306540000	3.4907260000	-0.3182030000
H	2.3358330000	-0.7865350000	-0.7864490000
H	1.4243030000	1.3915780000	-1.8205590000
C	-0.0206850000	2.9108690000	-1.3222650000
H	-1.4742440000	4.3269830000	-0.5729510000
H	-0.0597660000	3.3105470000	-2.3308270000

Table S139. Cartesian coordinates of β -Gal-tg_Trp_upper optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1373.1665996			
ZPE / Hartree = 0.4230462			
BSSE / Hartree = 0.0028375581			
C	-1.5251920000	-1.3396780000	-1.4430530000
C	-1.2900320000	-1.5741610000	0.0436860000
C	-2.6163460000	-1.8566460000	0.7323230000
C	-3.6168510000	-0.7367730000	0.4593150000
C	-3.6965350000	-0.4797530000	-1.0448950000
C	-4.5370750000	0.7438890000	-1.3938070000
O	-2.4049220000	-0.2354190000	-1.5953830000
O	-0.3085210000	-1.0182180000	-2.0307280000
O	-0.4506950000	-2.6901650000	0.2791850000
O	-2.4436860000	-1.9439610000	2.1379200000
O	-3.2172430000	0.4592440000	1.1077920000
O	-5.8525360000	0.6418960000	-0.8747620000
H	-1.9730560000	-2.2281570000	-1.9158360000
H	-0.8470270000	-0.6597490000	0.4590540000
H	-3.0253290000	-2.7991400000	0.3390030000
H	-4.6076430000	-1.0488300000	0.8148990000
H	-4.1356110000	-1.3734370000	-1.5172190000
H	-4.0849190000	1.6306580000	-0.9434510000
H	-4.5463410000	0.8686280000	-2.4819170000
H	-0.3778530000	-1.1190300000	-2.9901140000
H	0.4664320000	-2.4193700000	0.1322270000
H	-1.6722460000	-2.5041030000	2.3095730000
H	-2.8947190000	0.2195080000	1.9898240000
H	-6.3349610000	-0.0316370000	-1.3724740000
H	5.2654980000	1.7334430000	0.4483070000
H	4.5642260000	-0.3047790000	1.3272110000
N	4.4262040000	1.3290760000	0.0266940000
H	3.6147130000	1.8239900000	0.4103620000
H	4.4861750000	1.5020650000	-0.9830040000
C	4.3479230000	-0.1432690000	0.2699260000
O	5.8828090000	-0.1756530000	-1.5582460000
C	5.4053230000	-0.8452550000	-0.6090330000

O	5.6515820000	-2.0353250000	-0.3069040000
H	1.6540850000	-1.1604680000	2.5817220000
H	-0.1053910000	0.5075170000	3.2184290000
C	1.3753890000	-0.3284940000	1.9487950000
N	0.4075920000	0.5594640000	2.3493740000
C	1.8498190000	0.0207120000	0.7059820000
C	2.9403240000	-0.6605740000	-0.0675630000
C	0.2306680000	1.5116420000	1.3749670000
H	-1.3202810000	2.8202130000	2.1455140000
C	1.1226030000	1.2041970000	0.3162870000
H	2.9486720000	-1.7336900000	0.1428980000
C	-0.6431750000	2.6064790000	1.3242740000
C	1.1257560000	2.0192760000	-0.8339470000
C	-0.6156550000	3.3911030000	0.1819970000
H	2.7688610000	-0.5392550000	-1.1446850000
H	1.7942790000	1.7993090000	-1.6629860000
C	0.2602020000	3.0999850000	-0.8898850000
H	-1.2810360000	4.2455450000	0.1067050000
H	0.2497260000	3.7357180000	-1.7697370000

Table S140. Cartesian coordinates of α -Gal-gg_Phe_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6272696			
ZPE / Hartree = 0.3935528			
BSSE / Hartree = 0.0020328427			
C	-1.7606170000	0.6186380000	-1.1588490000
C	-1.3063160000	-0.8384980000	-1.0795810000
C	-2.4732120000	-1.7412980000	-0.6955720000
C	-3.1046960000	-1.2437840000	0.5998890000
C	-3.4882440000	0.2266890000	0.4512750000
C	-4.0465100000	0.8438350000	1.7266480000
O	-2.3680600000	1.0176890000	0.0480860000
O	-2.6372480000	0.7143790000	-2.2545190000
O	-0.7061980000	-1.2569000000	-2.2918570000
O	-2.0309890000	-3.0708270000	-0.4730320000
O	-2.1881090000	-1.3744870000	1.6820560000
O	-3.0867300000	0.9883340000	2.7623470000
H	-0.9016510000	1.2837550000	-1.2876740000
H	-0.5371300000	-0.9143350000	-0.3059430000
H	-3.2337510000	-1.7194920000	-1.4886060000
H	-4.0149740000	-1.8219070000	0.8074150000
H	-4.2749340000	0.2815320000	-0.3133610000
H	-4.4141450000	1.8479670000	1.5021420000
H	-4.8954060000	0.2307220000	2.0565360000
H	-2.7154250000	1.6403880000	-2.5216350000
H	-1.3130400000	-1.0324600000	-3.0145440000
H	-1.4750050000	-3.3324710000	-1.2213090000
H	-1.8572520000	-2.2847300000	1.6892940000
H	-2.6371480000	0.1355010000	2.8666430000
H	3.6016270000	-2.9232090000	-0.9015750000
H	1.8647210000	-1.3304520000	-1.2408240000
N	4.1024260000	-2.3652560000	-0.2058100000
C	2.1989950000	-0.8105220000	-0.3350740000
H	5.1037730000	-2.4967130000	-0.3670220000
H	3.8969350000	-2.7249250000	0.7343430000

H	1.7615970000	−1.3240710000	0.5296810000
H	2.3304780000	0.9291940000	−2.4211270000
C	3.7287310000	−0.9179040000	−0.2435780000
C	1.8824060000	1.3841380000	−1.5405210000
H	4.2068490000	−0.4750820000	−1.1179950000
C	1.7279880000	0.6231640000	−0.3756420000
C	1.4630870000	2.7135550000	−1.5807650000
H	1.5882670000	3.2921480000	−2.4909580000
C	1.1354160000	1.2132850000	0.7446840000
C	4.2544180000	−0.2683120000	1.0584500000
O	4.2571740000	−1.0147350000	2.0704630000
H	1.0016850000	0.6255910000	1.6503260000
C	0.8750810000	3.2966260000	−0.4553140000
C	0.7096920000	2.5422660000	0.7067680000
O	4.5891550000	0.9345900000	0.9895060000
H	0.5431800000	4.3297200000	−0.4871010000
H	0.2445010000	2.9844930000	1.5826450000

Table S141. Cartesian coordinates of α -Gal-gg_Phe_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6289284			
ZPE / Hartree = 0.3942662			
BSSE / Hartree = 0.0022993614			
C	1.3743770000	0.2079840000	1.6146850000
C	1.9626210000	-0.9732530000	0.8468190000
C	3.3123700000	-0.5933380000	0.2486110000
C	3.1747840000	0.6591590000	-0.6108980000
C	2.4974590000	1.7710120000	0.1885750000
C	2.1807590000	3.0071370000	-0.6441210000
O	1.2691800000	1.3343090000	0.7754090000
O	2.2080430000	0.4408190000	2.7225310000
O	2.0723640000	-2.1222150000	1.6671750000
O	3.8014710000	-1.6294340000	-0.5887700000
O	2.4024120000	0.3809590000	-1.7731420000
O	1.1439150000	2.8058610000	-1.5928380000
H	0.3529380000	-0.0135370000	1.9380260000
H	1.2718700000	-1.2314190000	0.0380770000
H	4.0272990000	-0.3868090000	1.0575950000
H	4.1742860000	1.0081230000	-0.9040330000
H	3.1972960000	2.0734890000	0.9792680000
H	1.8413670000	3.8048240000	0.0209530000
H	3.1072880000	3.3355820000	-1.1330960000
H	1.7296740000	0.9654200000	3.3790110000
H	2.5523210000	-1.8688170000	2.4708460000
H	3.7064770000	-2.4689760000	-0.1154530000
H	2.7189180000	-0.4527230000	-2.1529060000
H	1.3588210000	2.0044030000	-2.0951840000
H	-3.2463390000	3.0851070000	0.3049720000
H	-1.3905530000	1.6415650000	-0.1063840000
N	-3.9390090000	2.3338110000	0.3598470000
C	-2.0181390000	0.8073240000	0.2262510000
H	-4.7945530000	2.6686980000	-0.0903570000
H	-4.1641600000	2.1501520000	1.3453660000
H	-2.0159940000	0.7973150000	1.3229000000
H	-0.8863100000	0.3435450000	-2.2018870000
C	-3.4549850000	1.0599490000	-0.2564110000

C	-0.9242580000	-0.5569140000	-1.5924870000
H	-3.4879880000	1.1814800000	-1.3397180000
C	-1.4598360000	-0.4909920000	-0.3022140000
C	-0.4269140000	-1.7599680000	-2.0949780000
H	-0.0056860000	-1.7939320000	-3.0954110000
C	-1.4884250000	-1.6515170000	0.4789190000
C	-4.4118910000	-0.0667920000	0.1970750000
O	-4.8705580000	0.0502370000	1.3623300000
H	-1.8988360000	-1.6073550000	1.4855400000
C	-0.4606920000	-2.9137700000	-1.3092110000
C	-0.9930460000	-2.8566450000	-0.0196160000
O	-4.6111450000	-0.9945570000	-0.6172520000
H	-0.0691810000	-3.8491780000	-1.6969870000
H	-1.0164560000	-3.7477240000	0.6003800000

Table S142. Cartesian coordinates of α -Gal-gg_Phe_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6294548			
ZPE / Hartree = 0.3938958			
BSSE / Hartree = 0.0023286959			
C	3.3449860000	-0.2055710000	-1.0797830000
C	3.2428170000	-0.8680450000	0.2957960000
C	1.8582060000	-0.6395820000	0.8921610000
C	1.5243720000	0.8463060000	0.9105620000
C	1.6973240000	1.4257610000	-0.4902640000
C	1.4715350000	2.9298770000	-0.5619540000
O	3.0050840000	1.1601510000	-1.0035710000
O	2.4928330000	-0.9173470000	-1.9416900000
O	3.5394570000	-2.2512440000	0.2215490000
O	1.7962310000	-1.1056450000	2.2307330000
O	2.3806560000	1.5431270000	1.8105740000
O	2.4689730000	3.6938830000	0.0979160000
H	4.3751180000	-0.2301130000	-1.4448930000
H	3.9966830000	-0.4205530000	0.9498380000
H	1.1107090000	-1.1555360000	0.2736580000
H	0.4759990000	0.9765480000	1.2147820000
H	0.9443130000	0.9476820000	-1.1332330000
H	1.4842730000	3.2407270000	-1.6095060000
H	0.4751020000	3.1413680000	-0.1509730000
H	2.7358240000	-0.7327520000	-2.8593300000
H	2.9882620000	-2.6339280000	-0.4791720000
H	2.1043290000	-2.0233460000	2.2456000000
H	2.3475140000	1.0918580000	2.6669230000
H	2.5753730000	3.3280570000	0.9896950000
H	-3.1917860000	3.0706000000	-0.6963360000
H	-1.4288030000	1.5099050000	-0.6119330000
N	-3.9341790000	2.4081980000	-0.4590140000
C	-2.0918560000	0.8366510000	-0.0551150000
H	-4.7480320000	2.6309280000	-1.0368510000
H	-4.2106750000	2.5425070000	0.5217870000
H	-2.1015760000	1.1639540000	0.9912020000
H	-1.1094520000	-0.4455960000	-2.2445680000

C	-3.5106380000	0.9839740000	-0.6263260000
C	-1.1133060000	-1.0863260000	-1.3651950000
H	-3.5311050000	0.7512480000	-1.6916220000
C	-1.5763700000	-0.5784530000	-0.1455930000
C	-0.6487110000	-2.3978480000	-1.4570690000
H	-0.2855110000	-2.7767270000	-2.4077180000
C	-1.5629340000	-1.4061360000	0.9814610000
C	-4.5232260000	0.1064660000	0.1469690000
O	-4.9999850000	0.6241350000	1.1891530000
H	-1.9156170000	-1.0169210000	1.9338450000
C	-0.6364760000	-3.2174210000	-0.3256370000
C	-1.0958000000	-2.7184480000	0.8941680000
O	-4.7431040000	-1.0346890000	-0.3144160000
H	-0.2680840000	-4.2363550000	-0.3946200000
H	-1.0843000000	-3.3471490000	1.7794440000

Table S143. Cartesian coordinates of α -Gal-gg_Phe_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6275071			
ZPE / Hartree = 0.3940978			
BSSE / Hartree = 0.0017839342			
C	-3.9748600000	0.7515400000	0.9556730000
C	-4.0898180000	-0.3898300000	-0.0565690000
C	-2.7113570000	-0.9686600000	-0.3573790000
C	-1.7624400000	0.1364760000	-0.8050180000
C	-1.7514850000	1.2542620000	0.2332900000
C	-0.8966590000	2.4472180000	-0.1712670000
O	-3.0725410000	1.7335820000	0.4990180000
O	-3.5674270000	0.1790460000	2.1730280000
O	-4.9768280000	-1.3954430000	0.3989070000
O	-2.7758480000	-1.9238230000	-1.4039630000
O	-2.1767980000	0.6704460000	-2.0596540000
O	-1.4222720000	3.1910980000	-1.2595060000
H	-4.9332500000	1.2650750000	1.0692140000
H	-4.5203050000	0.0113260000	-0.9785440000
H	-2.3045790000	-1.4299900000	0.5540040000
H	-0.7450990000	-0.2697440000	-0.8881770000
H	-1.3175050000	0.8374250000	1.1524280000
H	-0.8255540000	3.1380410000	0.6725100000
H	0.1112770000	2.0730710000	-0.3979210000
H	-3.7522880000	0.7950220000	2.8951100000
H	-4.6972820000	-1.6560700000	1.2901720000
H	-3.4984150000	-2.5380980000	-1.2086570000
H	-2.2990380000	-0.0688770000	-2.6734070000
H	-1.6296940000	2.5639310000	-1.9694900000
H	4.4929220000	2.7945530000	0.8121050000
H	2.3838680000	1.7781260000	0.4469490000
N	5.0301120000	1.9542380000	0.5824540000
C	2.8840030000	0.9201540000	-0.0162680000
H	5.8503650000	1.9322730000	1.1932860000
H	5.3750340000	2.0232000000	-0.3821490000
H	3.0885640000	1.1713740000	-1.0632150000
H	1.2884180000	0.1592080000	2.0477040000

C	4.2224770000	0.7017160000	0.7055730000
C	1.2461450000	-0.5467270000	1.2208580000
H	4.0677180000	0.5116550000	1.7682860000
C	1.9917090000	-0.2943960000	0.0633750000
C	0.4482680000	-1.6863800000	1.3178540000
H	-0.1318180000	-1.8645900000	2.2188890000
C	1.9172070000	-1.1998020000	-0.9998050000
C	5.0354790000	-0.4425530000	0.0560940000
O	5.7173900000	-0.1163120000	-0.9485700000
H	2.4910170000	-1.0100410000	-1.9039020000
C	0.3842200000	-2.5883820000	0.2535340000
C	1.1184610000	-2.3412010000	-0.9070160000
O	4.9122510000	-1.5776020000	0.5666300000
H	-0.2441270000	-3.4712350000	0.3245750000
H	1.0674620000	-3.0338390000	-1.7416330000

Table S144. Cartesian coordinates of α -Gal-gg_Phe_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6289923			
ZPE / Hartree = 0.3936664			
BSSE / Hartree = 0.0020004167			
C	3.3199950000	-0.0004040000	-1.4453190000
C	4.0529970000	-0.2171160000	-0.1204210000
C	3.0542350000	-0.4163140000	1.0153220000
C	2.0644330000	0.7414450000	1.0558810000
C	1.4180740000	0.9064160000	-0.3159850000
C	0.4697260000	2.0943350000	-0.4006590000
O	2.4046440000	1.0655470000	-1.3400950000
O	2.6901730000	-1.2155290000	-1.7649420000
O	4.9530180000	-1.3076580000	-0.2016920000
O	3.7161870000	-0.4582040000	2.2692260000
O	2.7242700000	1.9533860000	1.4083640000
O	1.1221050000	3.3540340000	-0.3495000000
H	4.0210390000	0.2925680000	-2.2316520000
H	4.6565860000	0.6711790000	0.0869170000
H	2.4922280000	-1.3471690000	0.8483800000
H	1.2742700000	0.5175390000	1.7859030000
H	0.8313850000	-0.0009740000	-0.5097290000
H	-0.0651330000	2.0558620000	-1.3542560000
H	-0.2667670000	1.9968920000	0.4089650000
H	2.4287550000	-1.2076680000	-2.6960970000
H	4.4629180000	-2.0704780000	-0.5459100000
H	4.4577550000	-1.0766740000	2.1978840000
H	3.2291220000	1.7953740000	2.2197380000
H	1.7137210000	3.3442250000	0.4189040000
H	-4.8501970000	2.1427510000	-1.5033630000
H	-2.6253920000	1.3177290000	-1.3860600000
N	-5.2230140000	1.4896250000	-0.8099030000
C	-2.8983910000	0.7632410000	-0.4809190000
H	-6.1649480000	1.2255370000	-1.1080390000
H	-5.3126070000	1.9689870000	0.0938780000
H	-2.8387550000	1.4539860000	0.3682880000
H	-1.8932490000	-0.9109190000	-2.3704800000
C	-4.3525070000	0.2888820000	-0.6229590000

C	-1.5246270000	-1.1538460000	-1.3764160000
H	-4.4735910000	-0.3475750000	-1.5002570000
C	-1.9367640000	-0.3828370000	-0.2830800000
C	-0.6423750000	-2.2197080000	-1.2016650000
H	-0.3241550000	-2.8043240000	-2.0596770000
C	-1.4476900000	-0.6963500000	0.9887150000
C	-4.8326630000	-0.4397950000	0.6537810000
O	-5.2642290000	0.3041750000	1.5710470000
H	-1.7563740000	-0.0973140000	1.8426910000
C	-0.1568670000	-2.5247200000	0.0720700000
C	-0.5618530000	-1.7605290000	1.1671640000
O	-4.7148940000	-1.6847840000	0.6655210000
H	0.5404520000	-3.3460830000	0.2075940000
H	-0.1804760000	-1.9847690000	2.1592040000

Table S145. Cartesian coordinates of α -Gal-gg_Phe_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6268503			
ZPE / Hartree = 0.3939559			
BSSE / Hartree = 0.0020528915			
C	-1.9847470000	-0.7025300000	1.5282890000
C	-3.2331990000	-1.2433200000	0.8298730000
C	-3.0953310000	-1.1061970000	-0.6828790000
C	-2.7838330000	0.3393330000	-1.0525400000
C	-1.5583330000	0.8126940000	-0.2748220000
C	-1.2113520000	2.2768190000	-0.5060000000
O	-1.7274560000	0.6254190000	1.1323210000
O	-0.9275950000	-1.5709080000	1.2030480000
O	-3.4870210000	-2.5870990000	1.1971860000
O	-4.3028370000	-1.4642890000	-1.3350050000
O	-3.8886150000	1.1818020000	-0.7416820000
O	-2.1682320000	3.1849170000	0.0182140000
H	-2.1341080000	-0.6618820000	2.6102600000
H	-4.0953190000	-0.6593340000	1.1642800000
H	-2.2693740000	-1.7419270000	-1.0329350000
H	-2.5571850000	0.3994110000	-2.1255310000
H	-0.7047370000	0.2162660000	-0.6256750000
H	-0.2644220000	2.4976950000	-0.0057610000
H	-1.0732640000	2.4248740000	-1.5859560000
H	-0.2237410000	-1.4818070000	1.8599630000
H	-2.6645470000	-3.0870450000	1.0767410000
H	-4.6026140000	-2.3103880000	-0.9715820000
H	-4.6807070000	0.7995790000	-1.1477460000
H	-3.0422040000	2.9034330000	-0.2935120000
H	2.2592510000	-2.7200330000	-2.4637410000
H	1.3625400000	-0.5995330000	-1.9115970000
N	2.8818460000	-2.7647900000	-1.6529810000
C	1.8348680000	-0.6690900000	-0.9248900000
H	3.7388690000	-3.2394690000	-1.9480550000
H	2.4498220000	-3.3430360000	-0.9227950000
H	1.1787680000	-1.2636910000	-0.2777330000
H	2.4208520000	1.6347260000	-2.2486870000

C	3.1687010000	-1.4135310000	-1.0800330000
C	2.3229850000	1.7953210000	-1.1774590000
H	3.8322040000	-0.8946150000	-1.7727000000
C	2.0099350000	0.7140250000	-0.3466640000
C	2.5036280000	3.0720910000	-0.6446770000
H	2.7427900000	3.9025550000	-1.3019700000
C	1.8757830000	0.9345650000	1.0281090000
C	3.8552040000	-1.6253020000	0.2891470000
O	3.4369670000	-2.6073210000	0.9542580000
H	1.6358220000	0.0998970000	1.6827190000
C	2.3695250000	3.2823320000	0.7290850000
C	2.0546240000	2.2097480000	1.5652200000
O	4.7270150000	-0.7907080000	0.6161360000
H	2.5051310000	4.2760860000	1.1444380000
H	1.9447030000	2.3655310000	2.6340880000

Table S146. Cartesian coordinates of α -Gal-gt_Phe_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6269885			
ZPE / Hartree = 0.3931441			
BSSE / Hartree = 0.0020091356			
C	1.7387520000	0.4965690000	1.0465110000
C	1.2137630000	-0.9378140000	0.9933290000
C	2.3309690000	-1.9083850000	0.6222910000
C	2.9873450000	-1.4712170000	-0.6843520000
C	3.4480790000	-0.0250120000	-0.5482370000
C	4.0021720000	0.5455220000	-1.8400200000
O	2.3644370000	0.8332890000	-0.1715310000
O	2.6196210000	0.5730490000	2.1390730000
O	0.5955050000	-1.3065340000	2.2125340000
O	1.8126060000	-3.2147160000	0.4262050000
O	2.0690640000	-1.5638680000	-1.7633380000
O	4.5208660000	1.8529470000	-1.6413310000
H	0.9143860000	1.2062870000	1.1596230000
H	0.4399180000	-0.9876120000	0.2220370000
H	3.0931380000	-1.9150910000	1.4140620000
H	3.8660400000	-2.1023860000	-0.8773080000
H	4.2263650000	0.0156620000	0.2250790000
H	4.8294850000	-0.0789910000	-2.1856560000
H	3.2182150000	0.5522540000	-2.6056190000
H	2.7361520000	1.4988410000	2.3924470000
H	1.2116880000	-1.0976190000	2.9319810000
H	1.2321530000	-3.4230650000	1.1728510000
H	1.6469080000	-2.4342080000	-1.7120320000
H	3.7949170000	2.4133130000	-1.3334440000
H	-5.2243990000	-2.3702190000	0.2829650000
H	-3.7146790000	-2.8754200000	0.7210040000
N	-4.2270710000	-2.2588370000	0.0857220000
H	-4.2490750000	-0.4187020000	1.1022580000
H	-4.0734650000	-2.5625780000	-0.8839650000
C	-3.8065970000	-0.8279780000	0.1934990000
H	-1.9338070000	-1.3418440000	1.1242170000
H	-2.2852040000	0.8732570000	2.4158120000

C	-2.2726380000	-0.7726700000	0.2501640000
C	-1.8519270000	1.3548420000	1.5419920000
C	-4.3439060000	-0.0940000000	-1.0586280000
H	-1.8737060000	-1.2611930000	-0.6472040000
O	-4.3810610000	-0.7804370000	-2.1116080000
C	-1.7558360000	0.6428820000	0.3403900000
O	-4.6531570000	1.1089050000	-0.9140390000
H	-1.4733980000	3.2094640000	2.5652540000
C	-1.3931880000	2.6690520000	1.6269600000
C	-1.1817190000	1.2659920000	-0.7715450000
C	-0.8240130000	3.2856550000	0.5097130000
H	-1.0942250000	0.7162590000	-1.7061100000
C	-0.7164750000	2.5797380000	-0.6891230000
H	-0.4620550000	4.3069540000	0.5760300000
H	-0.2675870000	3.0483730000	-1.5597190000

Table S147. Cartesian coordinates of α -Gal-gt_Phe_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6280082			
ZPE / Hartree = 0.3934321			
BSSE / Hartree = 0.0022175656			
C	1.3612070000	0.3818110000	1.4427650000
C	1.8228480000	-0.9749230000	0.9141030000
C	3.2130640000	-0.8647580000	0.2949900000
C	3.2371710000	0.2266810000	-0.7722210000
C	2.7115450000	1.5251320000	-0.1711990000
C	2.5518650000	2.6316260000	-1.1967840000
O	1.4161740000	1.3464610000	0.4155410000
O	2.1886920000	0.7085600000	2.5296040000
O	1.7942990000	-1.9626800000	1.9285020000
O	3.5748930000	-2.0846630000	-0.3339780000
O	2.4279070000	-0.1346200000	-1.8804460000
O	2.1694720000	3.8516670000	-0.5775570000
H	0.3124990000	0.3392000000	1.7519400000
H	1.1153100000	-1.2984350000	0.1446770000
H	3.9430600000	-0.6066460000	1.0754440000
H	4.2746760000	0.3884600000	-1.0971370000
H	3.4159160000	1.8533460000	0.6043820000
H	3.5099300000	2.8087440000	-1.6914670000
H	1.8132700000	2.3323240000	-1.9492460000
H	1.7616680000	1.3907740000	3.0651320000
H	2.2932530000	-1.6239240000	2.6880150000
H	3.3660740000	-2.8092770000	0.2739040000
H	2.6034570000	-1.0671850000	-2.0776710000
H	1.3243670000	3.7014020000	-0.1314080000
H	-4.6277100000	2.8753370000	-0.4165980000
H	-3.0586880000	3.1963960000	-0.0117060000
N	-3.8162080000	2.5165330000	0.0927730000
H	-3.3868380000	1.1835830000	-1.4729350000
H	-4.0840380000	2.4528970000	1.0818490000
C	-3.4276300000	1.1537470000	-0.3835270000
H	-1.3396310000	1.5831650000	-0.0972020000
H	-0.9385530000	0.1490330000	-2.1742950000
C	-2.0543200000	0.8113610000	0.2124130000

C	-1.0163940000	-0.7097430000	-1.5108890000
C	-4.5118560000	0.1624550000	0.0993920000
H	-2.1326910000	0.8434370000	1.3054720000
O	-5.0400550000	0.4361220000	1.2071570000
C	-1.5571140000	-0.5428280000	-0.2311750000
O	-4.7331830000	-0.8257080000	-0.6344620000
H	-0.1374180000	-2.0719610000	-2.9259630000
C	-0.5632460000	-1.9594000000	-1.9332890000
C	-1.6339280000	-1.6493970000	0.6207100000
C	-0.6425360000	-3.0591390000	-1.0759100000
H	-2.0476010000	-1.5270880000	1.6192530000
C	-1.1792490000	-2.9010270000	0.2029170000
H	-0.2830410000	-4.0307040000	-1.4006240000
H	-1.2379740000	-3.7493160000	0.8781220000

Table S148. Cartesian coordinates of α -Gal-gt_Phe_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6289741			
ZPE / Hartree = 0.3930903			
BSSE / Hartree = 0.0024558843			
C	-2.4547550000	0.8056710000	1.6100910000
C	-3.0594420000	-0.4742270000	1.0281640000
C	-2.3031460000	-0.9039540000	-0.2257460000
C	-2.2322660000	0.2403420000	-1.2304570000
C	-1.6354740000	1.4584810000	-0.5386510000
C	-1.6005660000	2.6942280000	-1.4162680000
O	-2.3918400000	1.8132140000	0.6251210000
O	-1.1845600000	0.4695020000	2.1071290000
O	-3.0743670000	-1.5163370000	1.9877600000
O	-2.9572970000	-1.9908810000	-0.8618450000
O	-3.5241730000	0.5689520000	-1.7196740000
O	-0.9355690000	3.7657030000	-0.7616180000
H	-3.0888540000	1.2092880000	2.4037540000
H	-4.1027880000	-0.2730680000	0.7686780000
H	-1.2777750000	-1.1855140000	0.0512680000
H	-1.5720330000	-0.0519190000	-2.0597120000
H	-0.6096690000	1.2081030000	-0.2370830000
H	-1.0353460000	2.4733680000	-2.3253390000
H	-2.6205660000	2.9834130000	-1.6936240000
H	-0.8848480000	1.1566220000	2.7179240000
H	-2.1739350000	-1.6057620000	2.3377720000
H	-3.1184030000	-2.6772030000	-0.1980440000
H	-3.9552600000	-0.2582010000	-1.9806320000
H	-1.4299760000	3.9697060000	0.0444230000
H	4.8450580000	1.8045810000	1.8280740000
H	3.2800600000	2.3140670000	1.9519750000
N	3.9520460000	1.8551080000	1.3320550000
H	3.6627600000	-0.1932570000	1.7038220000
H	4.0995990000	2.4369210000	0.4977590000
C	3.4981790000	0.5036300000	0.8813450000
H	1.4527430000	0.9239960000	1.3999040000
H	1.4476170000	-1.6068390000	2.0227800000

C	2.0083880000	0.5872110000	0.5161600000
C	1.2328830000	-1.7716670000	0.9691240000
C	4.3529000000	0.1117490000	-0.3476470000
H	1.8851950000	1.3441810000	-0.2677510000
O	4.7206550000	1.0666140000	-1.0786490000
C	1.4551830000	-0.7377330000	0.0509960000
O	4.5643930000	-1.1092990000	-0.5149380000
H	0.5561270000	-3.7918320000	1.2699980000
C	0.7282390000	-3.0007310000	0.5463760000
C	1.1602410000	-0.9566770000	-1.2974980000
C	0.4384170000	-3.2113920000	-0.8044960000
H	1.3220980000	-0.1562410000	-2.0164110000
C	0.6536810000	-2.1859600000	-1.7250270000
H	0.0393460000	-4.1657850000	-1.1340150000
H	0.4218280000	-2.3379690000	-2.7749950000

Table S149. Cartesian coordinates of α -Gal-gt_Phe_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6289293			
ZPE / Hartree = 0.3940198			
BSSE / Hartree = 0.0020521008			
C	-3.3909010000	-1.4811720000	-0.6643210000
C	-3.8916790000	-0.0503480000	-0.4559430000
C	-2.7193610000	0.9003530000	-0.2283420000
C	-1.8506450000	0.4001150000	0.9210150000
C	-1.4259820000	-1.0318120000	0.6246670000
C	-0.6358300000	-1.6655500000	1.7531090000
O	-2.5631220000	-1.8759080000	0.4070860000
O	-2.7157000000	-1.5049520000	-1.8962280000
O	-4.6920350000	0.3771420000	-1.5432210000
O	-3.1801750000	2.1969530000	0.1168130000
O	-2.5693520000	0.4274880000	2.1463970000
O	-0.1511940000	-2.9490220000	1.3843630000
H	-4.2258710000	-2.1866240000	-0.6650060000
H	-4.5352160000	-0.0391400000	0.4283420000
H	-2.1019640000	0.9455230000	-1.1377570000
H	-0.9509770000	1.0267840000	0.9931530000
H	-0.8075950000	-1.0216810000	-0.2830820000
H	0.2361970000	-1.0430220000	1.9737730000
H	-1.2596960000	-1.7302340000	2.6517950000
H	-2.6437940000	-2.4182850000	-2.2057700000
H	-4.1953600000	0.2113340000	-2.3595630000
H	-3.8642460000	2.4541290000	-0.5183700000
H	-2.9781050000	1.3023420000	2.2221180000
H	-0.9164030000	-3.5096690000	1.1949140000
H	4.8279290000	-2.3488220000	-1.6647990000
H	3.3723490000	-2.9135070000	-1.1294490000
N	4.1042090000	-2.2206010000	-0.9531300000
H	3.4083940000	-0.5211030000	-1.9765440000
H	4.5379440000	-2.4078020000	-0.0405100000
C	3.5842660000	-0.8188260000	-0.9422620000
H	1.5653540000	-1.4749210000	-0.6121610000
H	0.8322920000	0.5222140000	-2.0209340000

C	2.2792450000	−0.7949440000	−0.1315950000
C	0.9736000000	1.1234420000	−1.1249990000
C	4.6683070000	0.0736190000	−0.2930690000
H	2.4868060000	−1.1814900000	0.8734930000
O	5.3441950000	−0.4712970000	0.6167280000
C	1.6841660000	0.5893340000	−0.0436950000
O	4.7457880000	1.2510430000	−0.7071950000
H	−0.1185710000	2.8076320000	−1.9009140000
C	0.4380750000	2.4094130000	−1.0575950000
C	1.8445730000	1.3644270000	1.1092140000
C	0.6054380000	3.1777170000	0.0964970000
H	2.3912610000	0.9556280000	1.9559740000
C	1.3099300000	2.6519200000	1.1805980000
H	0.1834850000	4.1764420000	0.1521380000
H	1.4398540000	3.2407910000	2.0834530000

Table S150. Cartesian coordinates of α -Gal-gt_Phe_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6293227			
ZPE / Hartree = 0.3938133			
BSSE / Hartree = 0.0022938758			
C	2.2344810000	-1.1131750000	-1.6114630000
C	2.4464840000	-2.0505510000	-0.4214500000
C	1.8997680000	-1.4229030000	0.8579550000
C	2.5024700000	-0.0385630000	1.0732010000
C	2.2633370000	0.8007220000	-0.1749340000
C	2.9261940000	2.1630130000	-0.1121850000
O	2.7889680000	0.1546000000	-1.3425110000
O	0.8496620000	-1.0546430000	-1.8410160000
O	1.8597580000	-3.3186810000	-0.6526770000
O	2.2287700000	-2.2152590000	1.9876210000
O	3.8988210000	-0.1279600000	1.3155690000
O	2.5844000000	2.9518390000	-1.2431500000
H	2.7608470000	-1.4824570000	-2.4957530000
H	3.5207590000	-2.2201550000	-0.3053530000
H	0.8087380000	-1.3151670000	0.7715420000
H	1.9978950000	0.4456960000	1.9216260000
H	1.1806250000	0.9350780000	-0.2957560000
H	2.5654880000	2.6964090000	0.7715970000
H	4.0132510000	2.0442940000	-0.0371580000
H	0.6831960000	-0.6835380000	-2.7184870000
H	0.9412820000	-3.1729260000	-0.9281060000
H	2.0139380000	-3.1369440000	1.7825010000
H	4.0327440000	-0.8111970000	1.9891000000
H	2.8767630000	2.4754050000	-2.0326820000
H	-4.8816420000	-2.5802550000	0.7365150000
H	-3.3660830000	-3.0810530000	0.3186340000
N	-4.0627020000	-2.3468940000	0.1698020000
H	-3.4986730000	-0.9004380000	1.5842070000
H	-4.3628820000	-2.3518740000	-0.8125470000
C	-3.5410930000	-0.9844860000	0.4976680000
H	-1.5029940000	-1.6292670000	0.2817380000
H	-1.0522060000	0.0272590000	2.2183480000
C	-2.1428050000	-0.8349100000	-0.1207210000

C	-1.0257490000	0.7963210000	1.4488500000
C	-4.5310110000	0.0471150000	-0.0922790000
H	-2.2191560000	-0.9829060000	-1.2037610000
O	-5.0972280000	-0.2963130000	-1.1612400000
C	-1.5322120000	0.5132060000	0.1750020000
O	-4.6477240000	1.1279410000	0.5260010000
H	-0.0863040000	2.2518020000	2.7258550000
C	-0.4818380000	2.0485280000	1.7349690000
C	-1.4778060000	1.5043070000	-0.8099900000
C	-0.4341690000	3.0332900000	0.7460160000
H	-1.8651210000	1.2905410000	-1.8035450000
C	-0.9316010000	2.7576260000	-0.5282390000
H	-0.0019590000	4.0052080000	0.9645510000
H	-0.8897120000	3.5153230000	-1.3048550000

Table S151. Cartesian coordinates of α -Gal-gt_Phe_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6278148			
ZPE / Hartree = 0.3936324			
BSSE / Hartree = 0.0020897052			
C	3.2210710000	-0.3378190000	-1.3622940000
C	3.5258310000	-1.0190620000	-0.0269510000
C	2.3033040000	-0.9798920000	0.8865620000
C	1.8073350000	0.4540840000	1.0459820000
C	1.5618180000	1.0461980000	-0.3360610000
C	1.1654310000	2.5095930000	-0.2961110000
O	2.7412060000	0.9708260000	-1.1462610000
O	2.2866180000	-1.1452910000	-2.0314150000
O	3.9740950000	-2.3487890000	-0.2159160000
O	2.6255730000	-1.4676060000	2.1791120000
O	2.7688610000	1.2458970000	1.7270160000
O	0.8848640000	2.9970140000	-1.6006380000
H	4.1318820000	-0.2225800000	-1.9558010000
H	4.3463950000	-0.4783140000	0.4531420000
H	1.4982680000	-1.5830950000	0.4422360000
H	0.8577900000	0.4516780000	1.6006300000
H	0.7579550000	0.4743670000	-0.8185820000
H	0.2484840000	2.6170380000	0.2920550000
H	1.9624140000	3.0978850000	0.1729430000
H	2.2753350000	-0.9142680000	-2.9703280000
H	3.3322330000	-2.7994690000	-0.7863390000
H	3.1157470000	-2.2964430000	2.0758300000
H	3.0532660000	0.7477390000	2.5076610000
H	1.6878780000	2.8939940000	-2.1303540000
H	-3.0101000000	-3.9556130000	0.8358220000
H	-1.4846950000	-3.4588060000	1.2287350000
N	-2.2618020000	-3.3071950000	0.5798720000
H	-3.2647200000	-1.7140090000	1.5148530000
H	-1.9632800000	-3.5530590000	-0.3714010000
C	-2.7392390000	-1.8895780000	0.5754890000
H	-0.8496150000	-1.1822170000	1.3030860000
H	-1.8545220000	0.6888410000	2.5736680000

C	-1.5096130000	-0.9770570000	0.4518490000
C	-2.0202760000	1.1980650000	1.6268810000
C	-3.6943610000	-1.7229930000	-0.6290160000
H	-0.9708090000	-1.2453300000	-0.4655610000
O	-3.3853570000	-2.3788540000	-1.6562290000
C	-1.8715710000	0.4878440000	0.4305190000
O	-4.6533570000	-0.9344530000	-0.4793780000
H	-2.4763360000	3.0889450000	2.5484340000
C	-2.3692140000	2.5489210000	1.6126000000
C	-2.0714390000	1.1554610000	-0.7821070000
C	-2.5742280000	3.2052080000	0.3972310000
H	-1.9454840000	0.6134060000	-1.7171620000
C	-2.4249670000	2.5046890000	-0.8007470000
H	-2.8422470000	4.2571530000	0.3841590000
H	-2.5725400000	3.0105740000	-1.7501000000

Table S152. Cartesian coordinates of α -Gal-tg_Phe_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6245056			
ZPE / Hartree = 0.3933221			
BSSE / Hartree = 0.0017460806			
C	-1.4612140000	-0.4573540000	0.4777090000
C	-1.5250180000	1.0701880000	0.4999210000
C	-2.9537120000	1.5389240000	0.7567470000
C	-3.9047880000	0.9186010000	-0.2614780000
C	-3.7417810000	-0.5972400000	-0.2385660000
C	-4.5411590000	-1.3007070000	-1.3296220000
O	-2.3811840000	-0.9783670000	-0.4557680000
O	-1.7198480000	-0.9014740000	1.7860370000
O	-0.6337240000	1.6081360000	1.4607470000
O	-3.0503700000	2.9492630000	0.6318280000
O	-3.6206410000	1.3929050000	-1.5688010000
O	-5.9237940000	-0.9971660000	-1.2439330000
H	-0.4795130000	-0.7979500000	0.1408900000
H	-1.1948790000	1.4418720000	-0.4749260000
H	-3.2626440000	1.2242550000	1.7640840000
H	-4.9386610000	1.1639380000	0.0151570000
H	-4.0727970000	-0.9574170000	0.7455940000
H	-4.2012630000	-0.9549280000	-2.3084040000
H	-4.3649040000	-2.3795030000	-1.2580190000
H	-1.3424030000	-1.7849040000	1.9010420000
H	-0.7764600000	1.1312620000	2.2933070000
H	-2.3356450000	3.3463580000	1.1505260000
H	-3.5546800000	2.3578910000	-1.5197920000
H	-6.2904800000	-1.4220400000	-0.4570790000
H	2.5744020000	1.2540450000	-1.1724170000
H	2.2869780000	1.7294280000	0.5119690000
H	2.1612250000	-0.9913740000	-1.8995410000
H	4.1459540000	3.1706310000	0.0702950000
C	2.7744970000	0.9864010000	-0.1289850000
C	1.9649820000	-1.2886980000	-0.8720830000
C	2.2174450000	-0.3846690000	0.1649070000
H	4.7942760000	2.4726430000	-1.3047910000

H	1.2643710000	-3.2507470000	-1.4142340000
C	1.4612980000	-2.5615270000	-0.5987940000
N	4.7572130000	2.4284970000	-0.2787610000
C	1.9613250000	-0.7776070000	1.4835790000
H	2.1468720000	-0.0777360000	2.2953130000
C	1.2076000000	-2.9451960000	0.7194120000
C	1.4621520000	-2.0500110000	1.7614780000
C	4.2902760000	1.0625990000	0.1101790000
H	0.8127690000	-3.9335140000	0.9339110000
H	1.2636920000	-2.3398430000	2.7892180000
H	5.7015200000	2.6136830000	0.0675000000
O	5.2975330000	0.4270950000	-1.9454830000
H	4.5299940000	0.9147240000	1.1636280000
C	5.0502140000	0.0453280000	-0.7730400000
O	5.3144120000	-1.0609480000	-0.2533880000

Table S153. Cartesian coordinates of α -Gal-tg_Phe_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6264794			
ZPE / Hartree = 0.3936980			
BSSE / Hartree = 0.0022621626			
C	1.2580220000	0.1829280000	1.5834140000
C	1.7140910000	-1.1072020000	0.9048210000
C	3.1193630000	-0.9430990000	0.3350430000
C	3.1804880000	0.2695580000	-0.5893250000
C	2.6560010000	1.4956140000	0.1509390000
C	2.5126980000	2.7172550000	-0.7501310000
O	1.3497150000	1.2668710000	0.6860410000
O	2.0619350000	0.3625280000	2.7214690000
O	1.6464990000	-2.2101680000	1.7907920000
O	3.4825550000	-2.0821180000	-0.4310500000
O	2.3899030000	0.0587430000	-1.7484860000
O	3.7391980000	3.0533830000	-1.3769860000
H	0.2012270000	0.1203700000	1.8605050000
H	1.0215980000	-1.3232440000	0.0860030000
H	3.8337550000	-0.7942630000	1.1572810000
H	4.2256730000	0.4533560000	-0.8719000000
H	3.3544520000	1.7222800000	0.9684810000
H	1.7989330000	2.4953550000	-1.5470240000
H	2.1267200000	3.5527170000	-0.1559320000
H	1.6336260000	0.9881160000	3.3217310000
H	2.1376000000	-1.9770240000	2.5938890000
H	3.2557020000	-2.8731120000	0.0795380000
H	2.5656860000	-0.8414280000	-2.0611370000
H	4.3441470000	3.4075690000	-0.7118240000
H	-2.2849800000	0.7485970000	1.4374900000
H	-1.3606110000	1.6335230000	0.2097140000
H	-2.2017770000	-1.6279190000	1.4780400000
H	-3.0351070000	3.2818170000	0.4300480000
C	-2.1222860000	0.8591690000	0.3590030000
C	-1.7649950000	-1.6419100000	0.4820780000
C	-1.6400510000	-0.4444890000	-0.2292290000
H	-4.2288870000	2.4448570000	1.2512080000
H	-1.4292550000	-3.7681270000	0.4936260000

C	-1.3313660000	-2.8470350000	-0.0729330000
N	-3.8237760000	2.6385430000	0.3268080000
C	-1.0695460000	-0.4720650000	-1.5068280000
H	-0.9535170000	0.4567470000	-2.0615490000
C	-0.7679990000	-2.8664870000	-1.3497430000
C	-0.6382670000	-1.6744260000	-2.0663430000
C	-3.4316260000	1.3340190000	-0.2888920000
H	-0.4267850000	-3.8021350000	-1.7818550000
H	-0.1910170000	-1.6794210000	-3.0559850000
H	-4.5428850000	3.1120580000	-0.2255860000
O	-5.1925140000	0.4904270000	1.0650050000
H	-3.3011930000	1.4976220000	-1.3591570000
C	-4.5814520000	0.3337510000	-0.0229140000
O	-4.7691820000	-0.5486170000	-0.8889130000

Table S154. Cartesian coordinates of α -Gal-tg_Phe_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6262559			
ZPE / Hartree = 0.3933981			
BSSE / Hartree = 0.0022192151			
C	-2.6916860000	-1.9268430000	0.6673840000
C	-3.5411590000	-1.3042640000	-0.4423300000
C	-2.8534000000	-0.0671410000	-1.0128770000
C	-2.5140330000	0.9112220000	0.1062820000
C	-1.6979040000	0.1835300000	1.1666550000
C	-1.3912340000	1.0462220000	2.3837400000
O	-2.3893060000	-0.9679610000	1.6563030000
O	-1.5359140000	-2.4458500000	0.0579240000
O	-3.8272670000	-2.2457350000	-1.4608400000
O	-3.7034880000	0.6055610000	-1.9286420000
O	-3.6938720000	1.4255330000	0.7051970000
O	-0.7423120000	2.2508430000	2.0106770000
H	-3.2464340000	-2.7152900000	1.1827880000
H	-4.5023780000	-1.0096650000	-0.0115430000
H	-1.9188740000	-0.3658890000	-1.5107300000
H	-1.9056880000	1.7287740000	-0.3035800000
H	-0.7532690000	-0.1287840000	0.7032000000
H	-2.3231360000	1.3284250000	2.8794400000
H	-0.7818770000	0.4653670000	3.0860710000
H	-1.1145240000	-3.0799780000	0.6543330000
H	-2.9875990000	-2.6392490000	-1.7445600000
H	-4.0654050000	-0.0494110000	-2.5430030000
H	-4.2732200000	1.7296270000	-0.0086780000
H	0.1180510000	2.0397040000	1.6162290000
H	2.6390860000	-0.5638530000	1.5618790000
H	1.4309920000	-1.4656490000	0.6282230000
H	2.8464470000	1.8036400000	1.2782890000
H	2.9776190000	-3.2413140000	0.7660350000
C	2.2704450000	-0.7640840000	0.5495300000
C	2.1904930000	1.7604530000	0.4118910000
C	1.7985990000	0.5166120000	-0.0932890000
H	4.3497950000	-2.4332660000	1.2781360000

H	2.0522930000	3.9012420000	0.2203850000
C	1.7447800000	2.9427090000	-0.1863500000
N	3.7855320000	-2.6936050000	0.4600610000
C	0.9584950000	0.4742870000	-1.2123060000
H	0.6419740000	-0.4902490000	-1.6049590000
C	0.9011020000	2.8901360000	-1.2961610000
C	0.5098920000	1.6510070000	-1.8093460000
C	3.3904240000	-1.4414310000	-0.2538380000
H	0.5472000000	3.8073090000	-1.7563190000
H	-0.1543140000	1.6017360000	-2.6675760000
H	4.3658620000	-3.2952800000	-0.1291850000
O	5.4398470000	-0.6243590000	0.6285170000
H	3.0448680000	-1.7214640000	-1.2496630000
C	4.6441740000	-0.5389440000	-0.3411160000
O	4.7272980000	0.2079570000	-1.3407420000

Table S155. Cartesian coordinates of α -Gal-tg_Phe_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6271281			
ZPE / Hartree = 0.3939877			
BSSE / Hartree = 0.0024688112			
C	2.7307190000	-1.8748180000	-0.7711390000
C	2.9854460000	-1.4519940000	0.6759600000
C	2.0081310000	-0.3535590000	1.0814230000
C	2.0822070000	0.8149050000	0.1038200000
C	1.8744880000	0.2964660000	-1.3146450000
C	2.1140710000	1.3596430000	-2.3811750000
O	2.7882000000	-0.7581110000	-1.6289110000
O	1.4747420000	-2.5047590000	-0.7997030000
O	2.9042320000	-2.5572390000	1.5582230000
O	2.3159130000	0.1478340000	2.3724380000
O	3.3487660000	1.4520050000	0.1816000000
O	1.3098000000	2.5080530000	-2.1731260000
H	3.5133360000	-2.5529310000	-1.1214690000
H	4.0077840000	-1.0700080000	0.7477160000
H	0.9863830000	-0.7581660000	1.0655850000
H	1.2793120000	1.5293570000	0.3366120000
H	0.8411840000	-0.0743270000	-1.3880250000
H	3.1541140000	1.6899320000	-2.3329840000
H	1.9314360000	0.9182660000	-3.3673430000
H	1.3963670000	-3.0264610000	-1.6101360000
H	2.0685970000	-3.0166080000	1.3813930000
H	2.4605600000	-0.6063510000	2.9624390000
H	3.5368120000	1.6054090000	1.1192810000
H	0.3808480000	2.2631560000	-2.2833280000
H	-1.6315410000	-1.0369570000	-1.0595270000
H	-1.0955890000	-1.6061210000	0.5305930000
H	-1.8383770000	1.3193900000	-1.5184740000
H	-2.6003200000	-3.3821620000	0.1328840000
C	-1.7890500000	-0.9277880000	0.0202090000
C	-1.5863090000	1.5403110000	-0.4827520000
C	-1.5134920000	0.4944540000	0.4423200000
H	-3.5370440000	-2.7800220000	-1.1162300000

H	-1.3979750000	3.6581420000	-0.8203310000
C	-1.3415790000	2.8568030000	-0.0892670000
N	-3.3988960000	-2.7856250000	-0.0977540000
C	-1.1925470000	0.7891410000	1.7720170000
H	-1.1246420000	-0.0197570000	2.4966280000
C	-1.0160390000	3.1407560000	1.2376030000
C	-0.9427940000	2.1024150000	2.1688880000
C	-3.2212590000	-1.3710770000	0.3568890000
H	-0.8174650000	4.1631230000	1.5437570000
H	-0.6849140000	2.3143700000	3.2021400000
H	-4.2309440000	-3.2104170000	0.3188290000
O	-4.5423160000	-0.8830920000	-1.5575660000
H	-3.3938940000	-1.3442130000	1.4333920000
C	-4.2700030000	-0.5108760000	-0.3875290000
O	-4.7172990000	0.4820640000	0.2264390000

Table S156. Cartesian coordinates of α -Gal-tg_Phe_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6285049			
ZPE / Hartree = 0.3936805			
BSSE / Hartree = 0.0025311930			
C	-3.1093610000	-0.6371900000	1.3948040000
C	-2.6744670000	-1.8584620000	0.5834890000
C	-1.4820660000	-1.5046190000	-0.2994390000
C	-1.8110680000	-0.3017230000	-1.1765790000
C	-2.2743900000	0.8474540000	-0.2894040000
C	-2.7782040000	2.0494980000	-1.0799930000
O	-3.3694120000	0.4558050000	0.5435700000
O	-2.0774110000	-0.3666550000	2.3092000000
O	-2.3748200000	-2.9571980000	1.4252280000
O	-1.1464900000	-2.5852180000	-1.1551980000
O	-2.8409840000	-0.6179280000	-2.1007240000
O	-1.8057280000	2.5175200000	-1.9992490000
H	-4.0505140000	-0.8318530000	1.9158430000
H	-3.5113950000	-2.1682790000	-0.0486970000
H	-0.6278740000	-1.2460750000	0.3432520000
H	-0.9040660000	0.0152200000	-1.7105040000
H	-1.4225710000	1.1511210000	0.3370710000
H	-3.6538500000	1.7592820000	-1.6651200000
H	-3.0713100000	2.8367340000	-0.3757110000
H	-2.4092820000	0.2159080000	3.0062900000
H	-1.7517230000	-2.6501170000	2.1020450000
H	-1.1114710000	-3.3921280000	-0.6208900000
H	-2.5969400000	-1.4480880000	-2.5356450000
H	-1.0419470000	2.8411240000	-1.4999370000
H	1.7671520000	-1.4837080000	0.1340360000
H	1.3725340000	-0.8606720000	-1.4776580000
H	1.2333840000	-0.1729030000	2.0212100000
H	3.1024850000	-2.3340510000	-2.1389460000
C	1.9445620000	-0.6569390000	-0.5640150000
C	1.1597080000	0.7201900000	1.4046000000
C	1.4807310000	0.6434520000	0.0468450000
H	3.9291510000	-2.6244330000	-0.7120890000
H	0.4817430000	1.9635130000	3.0263690000

C	0.7373310000	1.9245690000	1.9717290000
N	3.8065910000	-1.9679150000	-1.4937350000
C	1.3781690000	1.7983960000	-0.7384510000
H	1.6186400000	1.7502490000	-1.7984130000
C	0.6439160000	3.0719540000	1.1848460000
C	0.9732780000	3.0070880000	-0.1723120000
C	3.4382940000	-0.6366120000	-0.9222410000
H	0.3203660000	4.0110520000	1.6227500000
H	0.9159010000	3.9005930000	-0.7888820000
H	4.6963180000	-1.9283660000	-1.9967670000
O	4.6194640000	-1.4580040000	0.9705500000
H	3.6522960000	0.1211360000	-1.6765020000
C	4.3109890000	-0.4166400000	0.3365580000
O	4.5944190000	0.7676340000	0.6204270000

Table S157. Cartesian coordinates of α -Gal-tg_Phe_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6234491			
ZPE / Hartree = 0.3935222			
BSSE / Hartree = 0.0015696715			
C	2.3944480000	-1.8637780000	0.0239920000
C	3.4847720000	-1.2370310000	-0.8461810000
C	4.1763630000	-0.1030330000	-0.0960990000
C	3.1462170000	0.9120620000	0.3869560000
C	2.0825020000	0.1940840000	1.2100100000
C	0.9253130000	1.1044710000	1.6032190000
O	1.4907130000	-0.8795620000	0.4731760000
O	3.0427860000	-2.5162880000	1.0860910000
O	4.4203720000	-2.2079720000	-1.2787510000
O	5.0854070000	0.5799590000	-0.9454100000
O	2.5199730000	1.5526530000	-0.7142770000
O	1.3690960000	2.2150760000	2.3656570000
H	1.7933710000	-2.5689430000	-0.5563130000
H	3.0142350000	-0.8336990000	-1.7475200000
H	4.7046160000	-0.5118330000	0.7770420000
H	3.6424240000	1.6538630000	1.0267640000
H	2.5642350000	-0.2008590000	2.1156110000
H	0.4574540000	1.5060640000	0.7014010000
H	0.1789140000	0.5165600000	2.1507860000
H	2.4385750000	-3.1558060000	1.4874550000
H	4.7259800000	-2.6934380000	-0.4968860000
H	5.6306690000	-0.0806500000	-1.3969610000
H	3.2195740000	1.8350800000	-1.3217200000
H	1.6576160000	1.9040830000	3.2340260000
H	-2.4677470000	-1.4455560000	0.7380320000
H	-2.7855590000	-0.2370960000	1.9947860000
H	-1.3696940000	-0.8151030000	-1.2805520000
H	-4.6658580000	-1.6035980000	2.4665330000
C	-2.9208830000	-0.4669540000	0.9318800000
C	-1.4828970000	0.2356020000	-1.0234240000
C	-2.2449440000	0.5900350000	0.0932420000
H	-4.7765540000	-2.5412550000	1.0845080000

H	-0.2663730000	0.9233710000	-2.6608470000
C	-0.8629240000	1.2147380000	-1.8014130000
N	-5.0120690000	-1.6331270000	1.5043460000
C	-2.3798710000	1.9442200000	0.4192100000
H	-2.9646230000	2.2288080000	1.2911080000
C	-1.0015130000	2.5627270000	-1.4692220000
C	-1.7630480000	2.9258630000	-0.3557410000
C	-4.4270400000	-0.5584540000	0.6444840000
H	-0.5144910000	3.3253650000	-2.0691460000
H	-1.8710430000	3.9726540000	-0.0882100000
H	-6.0323670000	-1.5697880000	1.5396810000
O	-4.6744770000	-2.1826760000	-1.0721230000
H	-4.9303690000	0.3763760000	0.8934760000
C	-4.6934900000	-0.9490760000	-0.8284200000
O	-4.8659380000	-0.0093840000	-1.6354160000

Table S158. Cartesian coordinates of β -Gal-gg_Phe_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6277129			
ZPE / Hartree = 0.3935837			
BSSE / Hartree = 0.0024735990			
C	-2.0246970000	1.3077960000	-0.0501610000
C	-2.2683540000	0.7927120000	1.3630400000
C	-1.6472610000	-0.5886830000	1.5035700000
C	-2.1613070000	-1.5282790000	0.4178800000
C	-1.9994850000	-0.8762110000	-0.9554050000
C	-2.5817150000	-1.7008530000	-2.0958370000
O	-2.6071950000	0.4121680000	-0.9855750000
O	-2.6452930000	2.5450090000	-0.1772850000
O	-1.6497610000	1.6216240000	2.3307050000
O	-1.9607240000	-1.1731350000	2.7558980000
O	-3.5362020000	-1.8290540000	0.6272140000
O	-3.9984340000	-1.7766690000	-2.0833270000
H	-0.9460890000	1.3854840000	-0.2454960000
H	-3.3527330000	0.7358860000	1.5317150000
H	-0.5568240000	-0.4878020000	1.3896190000
H	-1.5678150000	-2.4526050000	0.4347900000
H	-0.9181300000	-0.7775860000	-1.1408190000
H	-2.3043070000	-1.2348370000	-3.0444150000
H	-2.1306030000	-2.7012710000	-2.0571620000
H	-2.2421780000	3.0290230000	-0.9116580000
H	-2.1105870000	2.4714930000	2.3511520000
H	-1.7649830000	-0.5273080000	3.4501290000
H	-3.6445770000	-2.1173400000	1.5456160000
H	-4.2688480000	-2.0536330000	-1.1942920000
H	1.9260700000	-1.1181540000	1.0957560000
H	1.2312890000	-1.6334470000	-0.4517340000
H	1.8664940000	1.1768070000	1.6948890000
H	2.7727670000	-3.3956650000	-0.3452240000
C	1.9685330000	-0.9654290000	0.0110950000
C	1.6363190000	1.4527880000	0.6683820000
C	1.6385210000	0.4684780000	-0.3236870000
H	3.7989090000	-2.8649600000	0.8651250000

H	1.3280740000	3.5314360000	1.1368830000
C	1.3330340000	2.7792700000	0.3537840000
N	3.5851280000	-2.8091520000	-0.1383560000
C	1.3312860000	0.8334120000	-1.6405770000
H	1.3201230000	0.0720870000	-2.4177960000
C	1.0287780000	3.1345180000	-0.9605970000
C	1.0284400000	2.1567080000	-1.9591770000
C	3.3630730000	-1.3727090000	-0.4871830000
H	0.7881730000	4.1644060000	-1.2058460000
H	0.7871910000	2.4241410000	-2.9834840000
H	4.3864580000	-3.1988820000	-0.6406170000
O	4.8657430000	-0.9986320000	1.3152610000
H	3.4355700000	-1.2785760000	-1.5712040000
C	4.4683300000	-0.5461970000	0.2115120000
O	4.8305790000	0.5026190000	-0.3650490000

Table S159. Cartesian coordinates of β -Gal-gg_Phe_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6274182			
ZPE / Hartree = 0.3936014			
BSSE / Hartree = 0.0023355928			
C	-1.7878680000	-0.8459480000	1.6469300000
C	-1.5878970000	0.6021560000	1.2154690000
C	-2.9220170000	1.2019500000	0.8011590000
C	-3.5829810000	0.3435180000	-0.2720850000
C	-3.6423900000	-1.1122000000	0.1930780000
C	-4.1974910000	-2.0642020000	-0.8588470000
O	-2.3513300000	-1.5810710000	0.5714620000
O	-0.5404660000	-1.3847450000	1.9371340000
O	-1.0800530000	1.3983220000	2.2710690000
O	-2.7486590000	2.5017090000	0.2615560000
O	-2.8442090000	0.4131770000	-1.4858960000
O	-3.3394760000	-2.2450470000	-1.9745680000
H	-2.4599540000	-0.9034650000	2.5183120000
H	-0.9006500000	0.6091340000	0.3592130000
H	-3.5834410000	1.2379640000	1.6794180000
H	-4.6088890000	0.6994020000	-0.4364510000
H	-4.3201220000	-1.1483110000	1.0605370000
H	-4.3322430000	-3.0500580000	-0.4075800000
H	-5.1808320000	-1.6891000000	-1.1712790000
H	-0.6520490000	-2.1965610000	2.4507730000
H	-0.1205460000	1.2794510000	2.3112930000
H	-2.0951070000	2.9674940000	0.8046950000
H	-2.5889190000	1.3377010000	-1.6299790000
H	-3.0790030000	-1.3663640000	-2.2911340000
H	2.5789920000	-0.9871100000	1.2850450000
H	1.8249180000	-1.9279530000	-0.0146070000
H	2.3058680000	1.3956130000	1.4008150000
H	3.8085650000	-3.2256810000	0.2633430000
C	2.4370300000	-1.0449690000	0.1998350000
C	1.7704840000	1.3783520000	0.4534570000
C	1.7316570000	0.1946240000	-0.2914240000
H	4.8099670000	-2.1685490000	1.0858400000
H	1.1618730000	3.4394670000	0.5856680000

C	1.1307300000	2.5303970000	-0.0076440000
N	4.4545680000	-2.4388410000	0.1603370000
C	1.0440230000	0.1835750000	-1.5105310000
H	1.0018310000	-0.7343790000	-2.0923080000
C	0.4469230000	2.5101890000	-1.2240610000
C	0.4077750000	1.3340400000	-1.9764090000
C	3.8113190000	-1.2393240000	-0.4586990000
H	-0.0575290000	3.4028750000	-1.5812280000
H	-0.1278890000	1.3098440000	-2.9208420000
H	5.2539090000	-2.7627200000	-0.3891620000
O	5.3398220000	-0.0401480000	0.9080010000
H	3.7127950000	-1.4267410000	-1.5283540000
C	4.7382520000	-0.0290050000	-0.1964170000
O	4.7745180000	0.8529310000	-1.0821660000

Table S160. Cartesian coordinates of β -Gal-gg_Phe_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6275410			
ZPE / Hartree = 0.3932786			
BSSE / Hartree = 0.0024080320			
C	1.9294860000	-0.5379700000	1.6294620000
C	2.6006300000	0.7467180000	1.1561760000
C	2.0964770000	1.0899670000	-0.2365360000
C	2.2857110000	-0.0808520000	-1.1919170000
C	1.6881600000	-1.3479980000	-0.5807380000
C	1.9127390000	-2.5966530000	-1.4230040000
O	2.2193360000	-1.5872970000	0.7200860000
O	2.4626150000	-0.8709620000	2.8687530000
O	2.2709750000	1.8402980000	1.9943580000
O	2.7869040000	2.2029760000	-0.7794260000
O	3.6674860000	-0.3008210000	-1.4544250000
O	3.2666430000	-3.0181860000	-1.4736040000
H	0.8373310000	-0.3975870000	1.6883690000
H	3.6866640000	0.5819200000	1.1364650000
H	1.0220810000	1.3056550000	-0.1676990000
H	1.7541900000	0.1358770000	-2.1290550000
H	0.6003560000	-1.1885810000	-0.5110860000
H	1.3459330000	-3.4233200000	-0.9880150000
H	1.5205920000	-2.4002790000	-2.4296750000
H	1.8825290000	-1.5062690000	3.3105840000
H	2.7315440000	1.7363790000	2.8380000000
H	2.7428760000	2.9267150000	-0.1379330000
H	4.0590840000	0.5397790000	-1.7338500000
H	3.8032710000	-2.2485620000	-1.7188070000
H	-1.9376290000	-1.5537830000	-0.2859380000
H	-1.5086430000	-1.0777110000	1.3678860000
H	-1.5330930000	-0.0431110000	-2.0778810000
H	-3.2544550000	-2.5639980000	1.9658970000
C	-2.0935840000	-0.7905580000	0.4858000000
C	-1.4033960000	0.7770420000	-1.3751510000
C	-1.6345430000	0.5580380000	-0.0137130000
H	-4.0923790000	-2.7488130000	0.5288890000

H	-0.8300990000	2.1887860000	-2.8962470000
C	-1.0094970000	2.0349500000	-1.8364170000
N	-3.9583800000	-2.1477840000	1.3517750000
C	-1.4548350000	1.6184630000	0.8826920000
H	-1.6175910000	1.4543160000	1.9457520000
C	-0.8444760000	3.0894800000	-0.9375780000
C	-1.0655850000	2.8771870000	0.4254970000
C	-3.5803420000	-0.7824490000	0.8736060000
H	-0.5365870000	4.0675610000	-1.2941520000
H	-0.9270830000	3.6893430000	1.1327920000
H	-4.8441130000	-2.1322300000	1.8631280000
O	-4.7965820000	-1.4403760000	-1.0599390000
H	-3.7683900000	-0.0824890000	1.6883860000
C	-4.4769630000	-0.4562910000	-0.3451190000
O	-4.7683270000	0.7469250000	-0.5203780000

Table S161. Cartesian coordinates of β -Gal-gg_Phe_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6274929			
ZPE / Hartree = 0.3936724			
BSSE / Hartree = 0.0019810085			
C	-3.2903730000	-1.1716950000	-1.0686080000
C	-3.7397740000	0.2308900000	-0.6714220000
C	-2.5276270000	1.0602600000	-0.2777640000
C	-1.7215910000	0.3538720000	0.8056330000
C	-1.4044040000	-1.0733200000	0.3624440000
C	-0.6697730000	-1.8868470000	1.4200810000
O	-2.5949950000	-1.7737350000	0.0112050000
O	-4.4290310000	-1.9247480000	-1.3296900000
O	-4.3674030000	0.8986020000	-1.7510590000
O	-2.9092600000	2.3266070000	0.2313890000
O	-2.4547160000	0.3024830000	2.0256420000
O	-1.4692570000	-2.2167960000	2.5449240000
H	-2.6297330000	-1.1280630000	-1.9492220000
H	-4.4239170000	0.1414810000	0.1833030000
H	-1.8858000000	1.1827400000	-1.1635460000
H	-0.7766180000	0.8917220000	0.9576340000
H	-0.7436780000	-1.0003700000	-0.5163830000
H	-0.3450970000	-2.8330670000	0.9795850000
H	0.2226290000	-1.3207750000	1.7211120000
H	-4.1850550000	-2.7186210000	-1.8251600000
H	-5.2336300000	0.4973470000	-1.9037370000
H	-3.5332560000	2.7284350000	-0.3901280000
H	-2.7471540000	1.2006530000	2.2393400000
H	-1.8790880000	-1.3970780000	2.8623310000
H	2.6057300000	-1.3862340000	0.7633110000
H	1.6785020000	-1.5593040000	-0.7377930000
H	2.5112620000	0.6467270000	2.0039210000
H	3.4656850000	-3.0281630000	-1.2870740000
C	2.4119050000	-0.9323720000	-0.2155130000
C	2.0070580000	1.1387370000	1.1752660000
C	1.8594340000	0.4609710000	-0.0389650000
H	4.6545390000	-2.5804760000	-0.1985130000

H	1.6309200000	2.9470620000	2.2810410000
C	1.5124060000	2.4349420000	1.3310560000
N	4.2114750000	-2.3541140000	-1.0980480000
C	1.2037580000	1.1019490000	-1.0967390000
H	1.0732760000	0.5775150000	-2.0411830000
C	0.8630830000	3.0677700000	0.2701410000
C	0.7101940000	2.3973800000	-0.9455550000
C	3.7182720000	-0.9445160000	-1.0250250000
H	0.4727900000	4.0736030000	0.3907180000
H	0.1971710000	2.8798710000	-1.7723980000
H	4.9231680000	-2.4694950000	-1.8239240000
O	5.4821520000	-0.7095840000	0.5506210000
H	3.5522340000	-0.5948650000	-2.0444210000
C	4.8183620000	-0.1059940000	-0.3306840000
O	4.9186630000	1.0891700000	-0.6841010000

Table S162. Cartesian coordinates of β -Gal-gg_Phe_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6282367			
ZPE / Hartree = 0.3935208			
BSSE / Hartree = 0.0023736962			
C	-1.5010340000	-1.1972850000	1.3308200000
C	-1.9261280000	-2.0341900000	0.1291520000
C	-1.8075460000	-1.2033980000	-1.1395860000
C	-2.5637990000	0.1136940000	-1.0041390000
C	-2.1447010000	0.8191970000	0.2840860000
C	-2.8997000000	2.1131000000	0.5481090000
O	-2.3127070000	-0.0375080000	1.4122610000
O	-1.7029960000	-1.9587680000	2.4756160000
O	-1.0862650000	-3.1628350000	-0.0385140000
O	-2.3437900000	-1.8888700000	-2.2580950000
O	-3.9680260000	-0.1154460000	-0.9740670000
O	-4.2722600000	1.9253430000	0.8564330000
H	-0.4454260000	-0.8954500000	1.2335250000
H	-2.9702090000	-2.3424960000	0.2776340000
H	-0.7439800000	-0.9741400000	-1.3048040000
H	-2.3055250000	0.7614370000	-1.8536340000
H	-1.0822590000	1.0794150000	0.1769280000
H	-2.4505220000	2.6138110000	1.4101250000
H	-2.7741760000	2.7617660000	-0.3297810000
H	-1.2034030000	-1.5745650000	3.2093800000
H	-1.2631090000	-3.7920680000	0.6740530000
H	-1.9666610000	-2.7801390000	-2.2788380000
H	-4.1956400000	-0.6836530000	-1.7249540000
H	-4.6494620000	1.3483100000	0.1745140000
H	2.1574960000	-0.9933700000	1.0532750000
H	1.4916780000	-1.4328900000	-0.5282920000
H	1.7875190000	1.1746590000	1.9252460000
H	3.3012510000	-2.9355330000	-0.5685310000
C	2.1348170000	-0.7133880000	-0.0064440000
C	1.4583560000	1.5251300000	0.9498670000
C	1.5676860000	0.6769380000	-0.1563040000
H	4.3165890000	-2.3321690000	0.6187970000
H	0.8420990000	3.4541140000	1.6817840000

C	0.9262330000	2.8089670000	0.8125200000
N	4.0243970000	-2.2419430000	-0.3625910000
C	1.1369710000	1.1361950000	-1.4071200000
H	1.2102550000	0.4803820000	-2.2722520000
C	0.4961750000	3.2571400000	-0.4369120000
C	0.6037450000	2.4169270000	-1.5482810000
C	3.5563970000	-0.8376070000	-0.5755430000
H	0.0743920000	4.2517480000	-0.5445980000
H	0.2656310000	2.7568960000	-2.5225770000
H	4.8382330000	-2.4600430000	-0.9420370000
O	5.0523490000	-0.3774260000	1.2130500000
H	3.5692690000	-0.6390930000	-1.6478120000
C	4.5403830000	0.0971640000	0.1670600000
O	4.7034490000	1.2374060000	-0.3195250000

Table S163. Cartesian coordinates of β -Gal-gg_Phe_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6257694			
ZPE / Hartree = 0.3937053			
BSSE / Hartree = 0.0020742959			
C	-1.6641690000	-1.2218240000	0.7708320000
C	-3.1206470000	-1.4693500000	0.3955960000
C	-3.4238090000	-0.7731650000	-0.9217950000
C	-3.0728560000	0.7081180000	-0.8374140000
C	-1.6396140000	0.8827250000	-0.3320250000
C	-1.2528540000	2.3379740000	-0.0966670000
O	-1.4296090000	0.1721850000	0.8854840000
O	-1.4335970000	-1.8057090000	2.0104350000
O	-3.3798960000	-2.8484160000	0.2054180000
O	-4.7998190000	-0.8655780000	-1.2483190000
O	-3.9622500000	1.3758720000	0.0504850000
O	-1.9279900000	2.9433860000	0.9949390000
H	-0.9982050000	-1.6441810000	0.0016770000
H	-3.7567610000	-1.0578170000	1.1907740000
H	-2.8116390000	-1.2350080000	-1.7106180000
H	-3.1420250000	1.1511460000	-1.8396000000
H	-0.9685830000	0.4880440000	-1.1129420000
H	-0.1865100000	2.3848470000	0.1349010000
H	-1.4290160000	2.8906120000	-1.0297170000
H	-0.4806860000	-1.8889140000	2.1549470000
H	-3.3824290000	-3.2870990000	1.0670600000
H	-5.0722510000	-1.7899550000	-1.1551560000
H	-4.8681820000	1.1448060000	-0.2030930000
H	-2.8770870000	2.7837050000	0.8785200000
H	1.4517490000	-1.3007400000	0.5341270000
H	0.9674210000	-1.0210420000	-1.1511820000
H	2.1039810000	0.5344500000	1.9087140000
H	1.8098220000	-3.1950380000	-1.4643850000
C	1.7610460000	-0.8462940000	-0.4150710000
C	2.1459690000	1.1843110000	1.0376590000
C	1.9715590000	0.6362600000	-0.2362910000
H	2.7485280000	-3.4344530000	-0.1004470000

H	2.5048320000	2.9652630000	2.1926830000
C	2.3726610000	2.5526830000	1.1971620000
N	2.7235520000	-3.0179910000	-1.0396420000
C	2.0188830000	1.4814090000	-1.3512610000
H	1.8746520000	1.0634690000	-2.3452590000
C	2.4259960000	3.3873440000	0.0801390000
C	2.2463760000	2.8483290000	-1.1961110000
C	3.0284780000	-1.5605470000	-0.9079190000
H	2.6000330000	4.4518650000	0.2024700000
H	2.2785190000	3.4932790000	-2.0690240000
H	3.4281080000	-3.4990020000	-1.6034910000
O	4.1974290000	-2.2651410000	1.0373890000
H	3.3276490000	-1.1917500000	-1.8895860000
C	4.1868860000	-1.4185380000	0.1076030000
O	4.9744530000	-0.4637440000	-0.0708940000

Table S164. Cartesian coordinates of β -Gal-gt_Phe_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6277968			
ZPE / Hartree = 0.3926855			
BSSE / Hartree = 0.0025301122			
C	2.1043220000	1.1669180000	-0.1329960000
C	2.3946790000	0.5139150000	-1.4792320000
C	1.7771640000	-0.8773070000	-1.5068110000
C	2.2573860000	-1.7107930000	-0.3216820000
C	2.0266770000	-0.9267950000	0.9660260000
C	2.5862980000	-1.6125440000	2.1974200000
O	2.6453330000	0.3585140000	0.9022440000
O	2.7300980000	2.4070640000	-0.0993490000
O	1.8125030000	1.2413500000	-2.5462650000
O	2.1311400000	-1.5724810000	-2.6898710000
O	3.6389770000	-2.0100320000	-0.4410650000
O	2.2345980000	-0.9022930000	3.3763040000
H	1.0209730000	1.2676910000	0.0161410000
H	3.4839790000	0.4423170000	-1.6040900000
H	0.6829700000	-0.7701540000	-1.4377380000
H	1.6686700000	-2.6379600000	-0.2768870000
H	0.9408070000	-0.7970830000	1.0941620000
H	2.1551200000	-2.6127430000	2.2838340000
H	3.6748610000	-1.7012620000	2.1080280000
H	2.2977800000	2.9630170000	0.5644210000
H	2.2884870000	2.0766630000	-2.6493790000
H	1.9684980000	-0.9876780000	-3.4442390000
H	3.7909500000	-2.3257010000	-1.3442310000
H	2.5939700000	-0.0074030000	3.2978730000
H	-1.9138140000	-1.1627320000	-1.0656000000
H	-1.2868070000	-1.6073110000	0.5321430000
H	-1.8095170000	1.1025460000	-1.8024510000
H	-2.9238310000	-3.2807690000	0.4677150000
C	-1.9715590000	-0.9320460000	0.0043450000
C	-1.5364420000	1.4242930000	-0.8000730000
C	-1.5609820000	0.4994240000	0.2478500000
H	-3.9133100000	-2.7618280000	-0.7765980000

H	-1.1353590000	3.4537610000	-1.3969480000
C	-1.1561690000	2.7484320000	-0.5716850000
N	-3.7006980000	-2.6614420000	0.2238390000
C	-1.1978260000	0.9219480000	1.5327360000
H	-1.2035480000	0.2064810000	2.3525420000
C	-0.7943650000	3.1608160000	0.7113880000
C	-0.8152640000	2.2428820000	1.7650110000
C	-3.3988660000	-1.2220500000	0.4891900000
H	-0.4920550000	4.1882490000	0.8895760000
H	-0.5290820000	2.5544190000	2.7650560000
H	-4.5249960000	-2.9743050000	0.7428830000
O	-4.8188900000	-0.8697950000	-1.3829910000
H	-3.4908710000	-1.0538250000	1.5626950000
C	-4.4356990000	-0.3787610000	-0.2905960000
O	-4.7631490000	0.7158890000	0.2171030000

Table S165. Cartesian coordinates of β -Gal-gt_Phe_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6277806			
ZPE / Hartree = 0.3933285			
BSSE / Hartree = 0.0024402863			
C	2.6356690000	0.2808520000	1.5230160000
C	1.3567740000	-0.4060320000	1.0581750000
C	1.6962990000	-1.7087100000	0.3492160000
C	2.6819770000	-1.4592190000	-0.7885360000
C	3.8828870000	-0.6873420000	-0.2469650000
C	4.8632300000	-0.2790160000	-1.3305340000
O	3.4674130000	0.5172990000	0.3968840000
O	2.2883280000	1.5066020000	2.0770480000
O	0.5111980000	-0.7335080000	2.1464930000
O	0.5329570000	-2.2964130000	-0.2104930000
O	2.0730120000	-0.7024060000	-1.8227950000
O	6.0071170000	0.3519140000	-0.7740070000
H	3.1758620000	-0.3473460000	2.2486040000
H	0.8462870000	0.2709660000	0.3605570000
H	2.1600010000	-2.3955920000	1.0725920000
H	3.0317640000	-2.4252760000	-1.1782080000
H	4.4014290000	-1.3277560000	0.4834590000
H	5.2121560000	-1.1701460000	-1.8577560000
H	4.3642130000	0.3845010000	-2.0456880000
H	3.0229200000	1.8389200000	2.6108340000
H	0.0254740000	0.0612400000	2.4085870000
H	-0.1741990000	-2.2453860000	0.4499390000
H	1.1701830000	-1.0377080000	-1.9370160000
H	5.7068310000	1.1419510000	-0.3034910000
H	-2.6738980000	-1.5391330000	-0.1813570000
H	-2.4279280000	-1.0256180000	1.4970660000
H	-1.6081020000	-0.3403660000	-1.9350430000
H	-4.5287980000	-1.9656200000	1.8947300000
C	-2.7677540000	-0.6926550000	0.5089650000
C	-1.3822760000	0.4767220000	-1.2534830000
C	-1.9017580000	0.4517880000	0.0435950000
H	-5.1209850000	-2.1568900000	0.3405860000
H	-0.1684740000	1.5339320000	-2.6832880000

C	-0.5713540000	1.5328420000	-1.6748740000
N	-5.0050750000	-1.4972210000	1.1195420000
C	-1.6019560000	1.5077480000	0.9135360000
H	-2.0012240000	1.4965610000	1.9260720000
C	-0.2681520000	2.5747950000	-0.7987480000
C	-0.7874820000	2.5605560000	0.4987810000
C	-4.2506520000	-0.3083740000	0.6160390000
H	0.3711890000	3.3907670000	-1.1211150000
H	-0.5518570000	3.3654420000	1.1884310000
H	-5.9423310000	-1.2410540000	1.4390870000
O	-5.2719570000	-0.8911770000	-1.4500100000
H	-4.3943240000	0.5030900000	1.3303220000
C	-4.8334500000	0.0685390000	-0.7660540000
O	-4.7796530000	1.2772010000	-1.0828010000

Table S166. Cartesian coordinates of β -Gal-gt_Phe_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6273468			
ZPE / Hartree = 0.3925612			
BSSE / Hartree = 0.0023732978			
C	-1.4872130000	-1.4129660000	-0.8832040000
C	-1.8098680000	-0.1762660000	-1.7148300000
C	-1.9535650000	1.0269460000	-0.7939090000
C	-2.9780900000	0.7591000000	0.3030200000
C	-2.6325480000	-0.5525440000	1.0018010000
C	-3.6751750000	-0.9756750000	2.0190360000
O	-2.5270360000	-1.6214440000	0.0597650000
O	-1.4357280000	-2.5090350000	-1.7350210000
O	-0.7681700000	0.1241510000	-2.6272050000
O	-2.3817210000	2.1735470000	-1.5105760000
O	-4.2873770000	0.6647930000	-0.2363600000
O	-3.2648690000	-2.1421610000	2.7172640000
H	-0.5337410000	-1.2779110000	-0.3471320000
H	-2.7535100000	-0.3575790000	-2.2475180000
H	-0.9813920000	1.2162000000	-0.3194940000
H	-2.9269030000	1.5719340000	1.0416820000
H	-1.6641790000	-0.4226350000	1.5098550000
H	-3.7980690000	-0.1831190000	2.7610570000
H	-4.6338110000	-1.1423430000	1.5153310000
H	-0.9819860000	-3.2393510000	-1.2918490000
H	-0.7801820000	-0.5288130000	-3.3401090000
H	-1.7980070000	2.2854390000	-2.2749900000
H	-4.4090600000	1.4149950000	-0.8369920000
H	-3.1571780000	-2.8513510000	2.0682580000
H	2.0000210000	-1.4992040000	-0.0077780000
H	1.9042660000	-0.7296010000	-1.6013610000
H	1.1396670000	-0.3628660000	1.8830840000
H	3.7950840000	-2.0550670000	-2.0933630000
C	2.2826090000	-0.6073210000	-0.5793710000
C	1.1255880000	0.5746870000	1.3317940000
C	1.6676050000	0.6218000000	0.0444420000
H	4.2804930000	-2.5363680000	-0.5668710000

H	0.1337580000	1.6590150000	2.9058070000
C	0.5593930000	1.7140740000	1.9082110000
N	4.3290520000	-1.7832530000	-1.2644200000
C	1.6379370000	1.8327500000	-0.6587520000
H	2.0470560000	1.8768980000	-1.6657150000
C	0.5357320000	2.9165990000	1.2014720000
C	1.0783350000	2.9735840000	-0.0853050000
C	3.8156070000	-0.5285600000	-0.6349790000
H	0.0929800000	3.8024720000	1.6462410000
H	1.0572910000	3.9043940000	-0.6440050000
H	5.3086930000	-1.6908500000	-1.5433630000
O	4.6220100000	-1.5360380000	1.3608860000
H	4.1436780000	0.3095030000	-1.2506810000
C	4.4240310000	-0.4363510000	0.7843020000
O	4.6265660000	0.7136650000	1.2323060000

Table S167. Cartesian coordinates of β -Gal-gt_Phe_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6275597			
ZPE / Hartree = 0.3928445			
BSSE / Hartree = 0.0021615545			
C	-2.7271440000	-1.6301730000	0.3207270000
C	-3.0046460000	-0.9525480000	-1.0176620000
C	-1.9411590000	0.1029160000	-1.2859020000
C	-1.8386570000	1.0823110000	-0.1206330000
C	-1.6565430000	0.2969240000	1.1740650000
C	-1.6506270000	1.1779200000	2.4080710000
O	-2.7104980000	-0.6508240000	1.3469990000
O	-3.7625650000	-2.5202720000	0.5761810000
O	-2.9485300000	-1.8773560000	-2.0889460000
O	-2.2415540000	0.8531190000	-2.4499700000
O	-3.0142160000	1.8721170000	-0.0185850000
O	-1.3541150000	0.4236170000	3.5741780000
H	-1.7532850000	-2.1457040000	0.2965900000
H	-3.9942480000	-0.4790700000	-0.9619360000
H	-0.9711290000	-0.4046850000	-1.3994320000
H	-0.9596240000	1.7247220000	-0.2706160000
H	-0.6963690000	-0.2396840000	1.1154390000
H	-0.8667950000	1.9330510000	2.3054400000
H	-2.6186320000	1.6818450000	2.5066550000
H	-3.4925420000	-3.1382840000	1.2697270000
H	-3.7316220000	-2.4431720000	-2.0537300000
H	-2.4402230000	0.2342720000	-3.1675550000
H	-3.2073300000	2.2199890000	-0.9016260000
H	-2.0474520000	-0.2426780000	3.6791780000
H	1.6372140000	-1.2987100000	0.8350560000
H	1.0884700000	-1.5107450000	-0.8380770000
H	1.8262900000	0.8959280000	1.7649790000
H	2.4835840000	-3.4238470000	-0.8192540000
C	1.8183670000	-0.9941760000	-0.2025150000
C	1.6923830000	1.3334910000	0.7777840000
C	1.6521630000	0.4992310000	-0.3433050000
H	3.3958010000	-3.1472180000	0.5562160000

H	1.5819210000	3.3506390000	1.5210270000
C	1.5542360000	2.7159150000	0.6403410000
N	3.3041940000	-2.9404080000	-0.4462480000
C	1.4679240000	1.0716840000	-1.6074760000
H	1.4233080000	0.4282810000	-2.4838400000
C	1.3732360000	3.2784360000	-0.6236260000
C	1.3292270000	2.4517160000	-1.7491790000
C	3.2258600000	-1.4566060000	-0.6107180000
H	1.2610480000	4.3527510000	-0.7317830000
H	1.1802440000	2.8812540000	-2.7351980000
H	4.1288590000	-3.3265900000	-0.9122670000
O	4.5152620000	-1.4435510000	1.3838490000
H	3.4245190000	-1.2270370000	-1.6580630000
C	4.3071460000	-0.8333110000	0.3040670000
O	4.8422230000	0.2237960000	-0.0958860000

Table S168. Cartesian coordinates of β -Gal-gt_Phe_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6281539			
ZPE / Hartree = 0.3934719			
BSSE / Hartree = 0.0023144522			
C	-1.7477050000	-1.0963490000	1.3941590000
C	-2.0788940000	-2.0225010000	0.2287380000
C	-1.8209660000	-1.3036680000	-1.0877160000
C	-2.5532000000	0.0349640000	-1.1388420000
C	-2.2346020000	0.8312680000	0.1219530000
C	-3.0134570000	2.1285640000	0.2201050000
O	-2.5425130000	0.0742680000	1.2945150000
O	-2.0723020000	-1.7555120000	2.5730970000
O	-1.2597000000	-3.1782320000	0.2333650000
O	-2.2683660000	-2.0758950000	-2.1893480000
O	-3.9559720000	-0.1613510000	-1.2224610000
O	-2.6220810000	2.8731750000	1.3643200000
H	-0.6817780000	-0.8143590000	1.3726420000
H	-3.1404220000	-2.2963360000	0.3025210000
H	-0.7414700000	-1.1104650000	-1.1704290000
H	-2.1935510000	0.6020780000	-2.0097210000
H	-1.1599260000	1.0618040000	0.1181890000
H	-2.7930920000	2.7450470000	-0.6557690000
H	-4.0884480000	1.9165940000	0.2447260000
H	-1.6356220000	-1.3187310000	3.3174950000
H	-1.5291900000	-3.7479130000	0.9666950000
H	-1.9368300000	-2.9791100000	-2.0818420000
H	-4.1141300000	-0.8373210000	-1.8982930000
H	-2.7883990000	2.3233520000	2.1428450000
H	2.1288830000	-0.9785050000	1.1640440000
H	1.4456740000	-1.5520080000	-0.3662900000
H	1.7641230000	1.2669400000	1.8462780000
H	3.2649510000	-3.0457670000	-0.3919990000
C	2.0915670000	-0.7889820000	0.0852070000
C	1.4291070000	1.5297130000	0.8456400000
C	1.5220890000	0.5835960000	-0.1796650000
H	4.2620960000	-2.3854850000	0.7795160000
H	0.8381100000	3.5239110000	1.4022370000

C	0.9100880000	2.8016110000	0.5947670000
N	3.9803810000	-2.3383620000	-0.2073550000
C	1.0869540000	0.9325540000	-1.4641810000
H	1.1487790000	0.2009040000	-2.2672680000
C	0.4759560000	3.1397020000	-0.6872810000
C	0.5661560000	2.2009250000	-1.7181500000
C	3.5050460000	-0.9503460000	-0.4939500000
H	0.0635920000	4.1251460000	-0.8817300000
H	0.2244800000	2.4543010000	-2.7173150000
H	4.8023640000	-2.5758770000	-0.7677730000
O	5.0204830000	-0.3714230000	1.2436520000
H	3.5012450000	-0.8189630000	-1.5765840000
C	4.4984040000	0.0299230000	0.1723680000
O	4.6600300000	1.1329030000	-0.3945890000

Table S169. Cartesian coordinates of β -Gal-gt_Phe_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6247452			
ZPE / Hartree = 0.3926386			
BSSE / Hartree = 0.0015879680			
C	4.2889380000	-0.0604870000	-0.7496920000
C	4.0009460000	-1.2143600000	0.2059470000
C	2.5332040000	-1.6080620000	0.1142740000
C	1.6328390000	-0.3965120000	0.3370730000
C	2.0597090000	0.7246880000	-0.6051350000
C	1.2885130000	2.0100840000	-0.3771090000
O	3.4427710000	1.0333330000	-0.4323860000
O	5.6077570000	0.3337160000	-0.5612960000
O	4.7569560000	-2.3648530000	-0.1258090000
O	2.2023720000	-2.5723470000	1.0996200000
O	1.7301670000	0.0628280000	1.6756180000
O	1.6355570000	2.9971490000	-1.3374710000
H	4.1098170000	-0.3687350000	-1.7915900000
H	4.2307410000	-0.8770090000	1.2257680000
H	2.3410810000	-2.0084970000	-0.8921030000
H	0.5945260000	-0.6727350000	0.1042110000
H	1.8910750000	0.3857590000	-1.6392770000
H	0.2194700000	1.8109160000	-0.4918270000
H	1.4707610000	2.3763020000	0.6400190000
H	5.9017340000	0.8501270000	-1.3241900000
H	5.6828330000	-2.2066550000	0.1027930000
H	2.8623680000	-3.2797330000	1.0645450000
H	1.6556380000	-0.7112260000	2.2535980000
H	2.5782270000	3.1894620000	-1.2379000000
H	-2.5912130000	-0.8729550000	-1.6445220000
H	-1.5867320000	-1.5626190000	-0.3581550000
H	-2.9893640000	1.4853910000	-1.7134150000
H	-2.9181430000	-3.4816980000	-0.5480380000
C	-2.4592640000	-0.9299170000	-0.5584440000
C	-2.5732940000	1.5922570000	-0.7145130000
C	-2.2313830000	0.4482990000	0.0126420000
H	-4.1708450000	-2.8972850000	-1.4922070000

H	-2.6573890000	3.7434150000	-0.7441130000
C	-2.3886930000	2.8637340000	-0.1671680000
N	-3.8113010000	-2.9825930000	-0.5339190000
C	-1.6941080000	0.5979520000	1.2968220000
H	-1.4125840000	-0.2868880000	1.8643780000
C	-1.8596160000	3.0028840000	1.1163250000
C	-1.5096790000	1.8653090000	1.8473010000
C	-3.6932410000	-1.6121130000	0.0516230000
H	-1.7123620000	3.9908430000	1.5416150000
H	-1.0854770000	1.9655360000	2.8419510000
H	-4.4771610000	-3.5572340000	-0.0116570000
O	-5.5252530000	-1.1410770000	-1.3881700000
H	-3.5834940000	-1.7234810000	1.1310500000
C	-4.9907790000	-0.8428950000	-0.2897200000
O	-5.3626950000	0.0189990000	0.5367870000

Table S170. Cartesian coordinates of β -Gal-tg_Phe_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6262745			
ZPE / Hartree = 0.3937002			
BSSE / Hartree = 0.0024808984			
C	-2.0997050000	1.3429850000	-0.2127950000
C	-2.3740850000	0.9483570000	1.2332260000
C	-1.7502220000	-0.4128760000	1.5018440000
C	-2.2317580000	-1.4485400000	0.4905050000
C	-2.0480110000	-0.9110130000	-0.9269780000
C	-2.6829870000	-1.8057620000	-1.9869970000
O	-2.6620800000	0.3661310000	-1.0769750000
O	-2.7181990000	2.5622700000	-0.4611830000
O	-1.7804070000	1.8591930000	2.1410380000
O	-2.0873460000	-0.8915000000	2.7930410000
O	-3.6040760000	-1.7533070000	0.6843110000
O	-2.1951260000	-3.1354210000	-1.9076240000
H	-1.0175160000	1.4046350000	-0.3915380000
H	-3.4618770000	0.9004490000	1.3815100000
H	-0.6581400000	-0.3131770000	1.4037610000
H	-1.6214780000	-2.3551840000	0.6061820000
H	-0.9671780000	-0.8248760000	-1.1165310000
H	-3.7721000000	-1.7767080000	-1.8792780000
H	-2.4196160000	-1.4222910000	-2.9752980000
H	-2.2947970000	2.9843910000	-1.2219040000
H	-2.2497810000	2.7027720000	2.0860710000
H	-1.9040200000	-0.1901930000	3.4347820000
H	-3.7364210000	-1.9164360000	1.6298500000
H	-2.6576000000	-3.5933940000	-1.1929580000
H	1.7760580000	-1.0014290000	1.1594900000
H	1.1889960000	-1.6127870000	-0.3968010000
H	1.7492050000	1.3414050000	1.6062420000
H	2.7512560000	-3.3517740000	-0.0916810000
C	1.8883240000	-0.9099600000	0.0727540000
C	1.5399340000	1.5468080000	0.5587960000
C	1.5645850000	0.4977090000	-0.3646940000
H	3.6885200000	-2.7354150000	1.1506880000

H	1.2182670000	3.6509560000	0.8801000000
C	1.2408770000	2.8479160000	0.1495870000
N	3.5371860000	-2.7369490000	0.1344150000
C	1.2842240000	0.7724280000	-1.7089160000
H	1.2906700000	-0.0398810000	-2.4325890000
C	0.9624570000	3.1129190000	-1.1917540000
C	0.9847920000	2.0703550000	-2.1220020000
C	3.3173870000	-1.3254730000	-0.3091560000
H	0.7241940000	4.1230050000	-1.5105920000
H	0.7637480000	2.2673400000	-3.1666350000
H	4.3749630000	-3.1374010000	-0.2950280000
O	4.6958960000	-0.8240490000	1.5610940000
H	3.4591880000	-1.2928310000	-1.3899740000
C	4.3664580000	-0.4436490000	0.4087420000
O	4.7565300000	0.5734640000	-0.2051710000

Table S171. Cartesian coordinates of β -Gal-tg_Phe_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6258937			
ZPE / Hartree = 0.3931113			
BSSE / Hartree = 0.0022964605			
C	1.7308160000	1.6683200000	0.7624100000
C	1.3382910000	0.2624190000	1.1997720000
C	2.5881970000	-0.5493670000	1.4998090000
C	3.5422400000	-0.5376330000	0.3098130000
C	3.7915010000	0.9017440000	-0.1352180000
C	4.5768530000	0.9848700000	-1.4415370000
O	2.5641360000	1.5822530000	-0.3832220000
O	0.5723260000	2.3492590000	0.4075480000
O	0.5599320000	0.2791980000	2.3835580000
O	2.2585970000	-1.9021570000	1.7711040000
O	3.0004660000	-1.2613490000	-0.7838590000
O	5.8014630000	0.2738670000	-1.3639400000
H	2.2702650000	2.1910360000	1.5678650000
H	0.7838340000	-0.2068100000	0.3769340000
H	3.1012020000	-0.1008950000	2.3637330000
H	4.4971120000	-0.9817080000	0.6227320000
H	4.3471260000	1.4130960000	0.6656610000
H	3.9521400000	0.6089180000	-2.2584240000
H	4.8214990000	2.0303240000	-1.6416030000
H	0.7524460000	3.2990860000	0.3821820000
H	-0.3545090000	0.4930480000	2.1505550000
H	1.4786690000	-1.9107260000	2.3459960000
H	2.6137920000	-2.0771240000	-0.4304510000
H	5.6220850000	-0.6680150000	-1.4865420000
H	-2.9278190000	1.1187420000	1.0971780000
H	-2.2833020000	1.9552060000	-0.3276340000
H	-2.3456320000	-1.1678900000	1.5547150000
H	-4.4385220000	2.9912580000	-0.2536970000
C	-2.7745770000	1.0378710000	0.0147650000
C	-1.8037300000	-1.2161350000	0.6123930000
C	-1.9027880000	-0.1546920000	-0.2927470000
H	-5.3200990000	1.9384600000	0.7005130000
H	-0.9387620000	-3.1419270000	1.0360670000

C	-1.0147010000	-2.3300600000	0.3188440000
N	-4.9694140000	2.1169960000	-0.2488580000
C	-1.2000210000	-0.2274790000	-1.5018710000
H	-1.2638280000	0.5982590000	-2.2068010000
C	-0.3223040000	-2.3964150000	-0.8905780000
C	-0.4173920000	-1.3418200000	-1.8019610000
C	-4.1474160000	0.9393820000	-0.6682020000
H	0.2958530000	-3.2598350000	-1.1186220000
H	0.1275100000	-1.3827940000	-2.7403010000
H	-5.7834300000	2.2437800000	-0.8562130000
O	-5.5293760000	-0.2389850000	0.8627920000
H	-4.0472400000	0.9721200000	-1.7535650000
C	-4.9077840000	-0.3337690000	-0.2263220000
O	-4.8072440000	-1.3343340000	-0.9695450000

Table S172. Cartesian coordinates of β -Gal-tg_Phe_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6257863			
ZPE / Hartree = 0.3927741			
BSSE / Hartree = 0.0021268464			
C	3.5659860000	-0.7287340000	-0.4101070000
C	2.9397830000	-1.0058040000	0.9523480000
C	1.5497870000	-0.3908420000	0.9961470000
C	1.5890700000	1.0894590000	0.6383150000
C	2.3350860000	1.2750590000	-0.6803970000
C	2.5704950000	2.7408540000	-1.0297680000
O	3.6255100000	0.6725490000	-0.6239240000
O	4.8629240000	-1.2267710000	-0.3990220000
O	2.7814100000	-2.3957160000	1.1756970000
O	0.9731230000	-0.5032960000	2.2870420000
O	2.2460800000	1.8472280000	1.6429790000
O	1.3488060000	3.4595360000	-1.0993450000
H	2.9659090000	-1.1933530000	-1.2093510000
H	3.5794410000	-0.5554720000	1.7236390000
H	0.9250940000	-0.9073800000	0.2542640000
H	0.5551010000	1.4406230000	0.5127480000
H	1.7374030000	0.8008860000	-1.4741240000
H	3.2505090000	3.1859040000	-0.2962760000
H	3.0353670000	2.7968770000	-2.0166010000
H	5.1853580000	-1.3080970000	-1.3072830000
H	3.6525100000	-2.7902500000	1.3175980000
H	1.0051700000	-1.4339910000	2.5517750000
H	1.8674480000	1.5914690000	2.4968750000
H	1.0740100000	3.6970290000	-0.2038180000
H	-2.5673390000	0.4665260000	1.5249250000
H	-1.8806030000	1.6504000000	0.3973150000
H	-2.1782620000	-1.8839990000	1.2225550000
H	-3.8596770000	2.8491090000	0.8560090000
C	-2.4558520000	0.7193480000	0.4644190000
C	-1.6856680000	-1.6804200000	0.2745540000
C	-1.7241290000	-0.3865880000	-0.2554920000
H	-4.8206950000	1.6709740000	1.5558080000

H	-0.9890970000	-3.7024090000	0.0291110000
C	-1.0163470000	-2.7043040000	-0.3974940000
N	-4.4967920000	2.0710570000	0.6666090000
C	-1.0810480000	-0.1340000000	-1.4724310000
H	-1.0945260000	0.8728920000	-1.8849610000
C	-0.3776680000	-2.4436770000	-1.6114350000
C	-0.4122450000	-1.1548790000	-2.1483360000
C	-3.8504840000	0.9799250000	-0.1261980000
H	0.1489340000	-3.2373860000	-2.1324520000
H	0.0903740000	-0.9419120000	-3.0872280000
H	-5.3174300000	2.4493870000	0.1871390000
O	-5.3465150000	-0.4163860000	1.0804230000
H	-3.7803460000	1.3180100000	-1.1606290000
C	-4.7521010000	-0.2718090000	-0.0181620000
O	-4.7757250000	-1.0314910000	-1.0112320000

Table S173. Cartesian coordinates of β -Gal-tg_Phe_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6256707			
ZPE / Hartree = 0.3931341			
BSSE / Hartree = 0.0021593125			
C	3.1070440000	-1.5699590000	-0.9555520000
C	2.4515610000	-1.9121980000	0.3773100000
C	1.3427990000	-0.9122500000	0.6665340000
C	1.8628950000	0.5206080000	0.6023790000
C	2.6104660000	0.7373340000	-0.7116130000
C	3.3358130000	2.0787580000	-0.7703540000
O	3.6222860000	-0.2497300000	-0.8952910000
O	4.1675580000	-2.4456020000	-1.1515180000
O	1.8529710000	-3.1956290000	0.3513910000
O	0.8006260000	-1.1125610000	1.9605650000
O	2.7487730000	0.7883330000	1.6791630000
O	2.4453360000	3.1698760000	-0.6097470000
H	2.3750960000	-1.6383680000	-1.7756290000
H	3.2199550000	-1.8552950000	1.1602010000
H	0.5613120000	-1.0321860000	-0.1001160000
H	1.0026880000	1.2040740000	0.6383330000
H	1.8757770000	0.6784270000	-1.5302570000
H	4.1253400000	2.0948670000	-0.0116010000
H	3.7956450000	2.1846130000	-1.7552710000
H	4.4321250000	-2.4283380000	-2.0815770000
H	2.5499410000	-3.8655220000	0.3653250000
H	0.5998360000	-2.0545200000	2.0608950000
H	2.3160830000	0.4886490000	2.4923090000
H	2.1813700000	3.2298090000	0.3186290000
H	-1.9297840000	-1.4044490000	-0.7114930000
H	-1.7344830000	-1.4550160000	1.0505530000
H	-1.4022840000	0.5787830000	-1.8979830000
H	-3.4456000000	-3.0779600000	0.8963060000
C	-2.2196000000	-0.9174930000	0.2267850000
C	-1.3827290000	1.1447490000	-0.9693220000
C	-1.7641840000	0.5209630000	0.2225040000
H	-4.0638210000	-2.8065500000	-0.6341870000

H	-0.6768310000	2.9499110000	-1.9063250000
C	-0.9772100000	2.4803010000	-0.9743750000
N	-4.0884120000	-2.5026530000	0.3470650000
C	-1.7281970000	1.2553650000	1.4132140000
H	-2.0114270000	0.7739410000	2.3466370000
C	-0.9493390000	3.2071410000	0.2164290000
C	-1.3250600000	2.5906000000	1.4121610000
C	-3.7404070000	-1.0494640000	0.3926430000
H	-0.6282850000	4.2444300000	0.2145480000
H	-1.2985720000	3.1476840000	2.3437760000
H	-5.0350830000	-2.6742360000	0.6944210000
O	-4.6636610000	-1.0462110000	-1.7978990000
H	-4.0663680000	-0.6589790000	1.3573960000
C	-4.4962220000	-0.3519810000	-0.7629210000
O	-4.8350800000	0.8365190000	-0.5715740000

Table S174. Cartesian coordinates of β -Gal-tg_Phe_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6265625			
ZPE / Hartree = 0.3932971			
BSSE / Hartree = 0.0022898123			
C	-2.8143010000	-0.5641560000	1.4088270000
C	-2.5745200000	-1.7750270000	0.5138420000
C	-1.4433620000	-1.4616140000	-0.4520310000
C	-1.7187910000	-0.1815200000	-1.2329640000
C	-2.0991040000	0.9435160000	-0.2746760000
C	-2.6228900000	2.1784420000	-1.0102440000
O	-3.1564170000	0.5472630000	0.5981310000
O	-3.8898760000	-0.8501900000	2.2410460000
O	-2.1735840000	-2.9078210000	1.2626110000
O	-1.2577920000	-2.5049950000	-1.3931490000
O	-2.7797090000	-0.3567310000	-2.1614130000
O	-1.8316070000	2.5101370000	-2.1392700000
H	-1.9092420000	-0.3277040000	1.9914830000
H	-3.5003550000	-1.9797270000	-0.0412060000
H	-0.5274960000	-1.3136550000	0.1399790000
H	-0.7988880000	0.1064580000	-1.7614040000
H	-1.2084980000	1.1959370000	0.3182930000
H	-3.6619340000	1.9918640000	-1.3033460000
H	-2.5996620000	3.0380230000	-0.3362360000
H	-3.8880140000	-0.2427090000	2.9937430000
H	-2.9296970000	-3.2266880000	1.7739710000
H	-1.2176680000	-3.3434460000	-0.9107140000
H	-2.5950120000	-1.1589980000	-2.6717260000
H	-2.0218490000	1.8634190000	-2.8339520000
H	1.9009650000	-1.5360700000	0.1706670000
H	1.4885960000	-0.8819350000	-1.4249450000
H	1.4009290000	-0.2784180000	2.1054720000
H	3.2599060000	-2.3220850000	-2.0893990000
C	2.0561540000	-0.6876230000	-0.5062290000
C	1.2755340000	0.6221400000	1.5084840000
C	1.5609100000	0.5832560000	0.1403380000
H	4.0858390000	-2.5969160000	-0.6596840000
H	0.6072670000	1.8144050000	3.1721820000

C	0.8293940000	1.8011050000	2.1093970000
N	3.9524700000	-1.9411520000	-1.4402100000
C	1.3868360000	1.7452020000	-0.6208630000
H	1.5910560000	1.7209590000	-1.6892820000
C	0.6673070000	2.9570160000	1.3448350000
C	0.9469140000	2.9257200000	-0.0235760000
C	3.5483910000	-0.6215410000	-0.8651520000
H	0.3190410000	3.8743910000	1.8092720000
H	0.8115640000	3.8181530000	-0.6272770000
H	4.8435710000	-1.8796460000	-1.9385610000
O	4.7386170000	-1.4172180000	1.0321670000
H	3.7393950000	0.1449290000	-1.6168370000
C	4.4158950000	-0.3827640000	0.3938070000
O	4.6824550000	0.8063830000	0.6734020000

Table S175. Cartesian coordinates of β -Gal-tg_Phe_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1241.6250366			
ZPE / Hartree = 0.3931627			
BSSE / Hartree = 0.0021718925			
C	-1.7907950000	-0.7734280000	1.3318120000
C	-3.0882770000	-1.3014220000	0.7298920000
C	-3.0916890000	-1.0427710000	-0.7706560000
C	-2.8281580000	0.4295740000	-1.0767320000
C	-1.5683520000	0.8757020000	-0.3387530000
C	-1.2676330000	2.3633960000	-0.4641840000
O	-1.6862370000	0.6127540000	1.0552190000
O	-1.8435180000	-0.9462440000	2.7087400000
O	-3.2187280000	-2.7004960000	0.9061200000
O	-4.3431620000	-1.3815250000	-1.3439080000
O	-3.9145170000	1.2389210000	-0.6569370000
O	-1.0222820000	2.7297790000	-1.8132110000
H	-0.9228740000	-1.2959390000	0.8965480000
H	-3.9248360000	-0.7684200000	1.2018750000
H	-2.2883610000	-1.6413260000	-1.2262210000
H	-2.6672030000	0.5380090000	-2.1583240000
H	-0.7199540000	0.3095040000	-0.7533410000
H	-2.0893440000	2.9473740000	-0.0364200000
H	-0.3544600000	2.5739440000	0.0995700000
H	-0.9520000000	-0.8594750000	3.0747720000
H	-3.4134280000	-2.8821480000	1.8354930000
H	-4.5860830000	-2.2673970000	-1.0376770000
H	-4.7286020000	0.8254530000	-0.9799810000
H	-1.8667150000	2.8493000000	-2.2671220000
H	1.1886180000	-1.3215040000	-0.5575290000
H	1.4379040000	-0.3436200000	-2.0162880000
H	1.2860520000	-0.3100580000	1.6270250000
H	2.4466570000	-2.3428520000	-2.8361690000
C	1.8497490000	-0.5838410000	-1.0288640000
C	1.6070690000	0.6276490000	1.1771360000
C	1.9180040000	0.6664540000	-0.1854410000
H	2.6912700000	-3.2030560000	-1.4224800000

H	1.4540020000	1.7333530000	3.0170900000
C	1.7037170000	1.7780580000	1.9611980000
N	3.0694590000	-2.4693360000	-2.0344080000
C	2.3222720000	1.8799670000	-0.7535580000
H	2.5558820000	1.9209340000	-1.8151140000
C	2.1162920000	2.9820850000	1.3887700000
C	2.4239860000	3.0311740000	0.0272190000
C	3.2328540000	-1.2238680000	-1.2236900000
H	2.1910340000	3.8780310000	1.9972460000
H	2.7373010000	3.9661410000	-0.4273170000
H	3.9683270000	-2.8033850000	-2.3901730000
O	3.4895270000	-2.7515580000	0.5770010000
H	3.8993030000	-0.5559250000	-1.7705010000
C	3.8581160000	-1.6351750000	0.1302380000
O	4.6374620000	-0.8144950000	0.6619200000

Table S176. Cartesian coordinates of α -Gal-gg_His_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6257430			
ZPE / Hartree = 0.3653442			
BSSE / Hartree = 0.00213556320			
C	-1.5188060000	0.5719330000	1.0942190000
C	-2.7538750000	0.8282120000	0.2302850000
C	-3.6151360000	-0.4281720000	0.1528170000
C	-2.7774360000	-1.6018620000	-0.3430340000
C	-1.5393630000	-1.7576350000	0.5376830000
C	-0.5804210000	-2.8422360000	0.0650020000
O	-0.7979020000	-0.5386740000	0.6155170000
O	-1.9752060000	0.3863320000	2.4114980000
O	-3.4980630000	1.9319610000	0.7118800000
O	-4.6856970000	-0.2511680000	-0.7607750000
O	-2.3673500000	-1.3809800000	-1.6892760000
O	0.0440300000	-2.5613670000	-1.1783570000
H	-0.8241620000	1.4163700000	1.0406310000
H	-2.4204670000	1.0916310000	-0.7778460000
H	-4.0027300000	-0.6691010000	1.1526240000
H	-3.3684780000	-2.5251940000	-0.2784610000
H	-1.8879650000	-2.0434710000	1.5395160000
H	0.2226630000	-2.9440570000	0.8000010000
H	-1.1336700000	-3.7896670000	0.0236700000
H	-1.2427360000	0.5231490000	3.0275370000
H	-3.6473000000	1.7959270000	1.6604510000
H	-5.1216230000	0.5886370000	-0.5549060000
H	-3.1556720000	-1.1754410000	-2.2131370000
H	-0.6517150000	-2.3114320000	-1.8059970000
N	4.4679710000	1.1256890000	-0.3343820000
H	4.9598860000	0.5956690000	-1.0644230000
H	5.1813690000	1.4950230000	0.2979480000
H	3.9789100000	1.9230650000	-0.7519230000
C	3.5369290000	0.1936200000	0.3723060000
H	3.3646010000	0.5953300000	1.3721800000

C	2.2269260000	0.0695130000	-0.4007060000
C	4.2187070000	-1.1919080000	0.4787910000
H	2.4354870000	-0.2961250000	-1.4141080000
H	1.6173110000	-0.6900510000	0.0983280000
C	1.4665590000	1.3564830000	-0.4711180000
O	5.2220150000	-1.3791610000	-0.2519720000
N	0.4364220000	1.5533620000	-1.3567820000
C	1.5478220000	2.5330690000	0.2379390000
H	0.0849910000	0.8736950000	-2.0206210000
C	-0.0628690000	2.7975640000	-1.1547330000
N	0.5884750000	3.4257510000	-0.1960570000
H	2.2377090000	2.7856070000	1.0321930000
H	-0.8908560000	3.1893650000	-1.7284440000
O	3.6731910000	-1.9986970000	1.2638160000

Table S177. Cartesian coordinates of α -Gal-gg_His_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6272433			
ZPE / Hartree = 0.3654630			
BSSE / Hartree = 0.00244236601			
C	-0.7243150000	-0.6146250000	1.3528950000
C	-1.6602930000	0.5862530000	1.2415840000
C	-3.0677300000	0.1274140000	0.8778840000
C	-3.0316450000	-0.7114140000	-0.3956900000
C	-2.0159200000	-1.8425830000	-0.2468530000
C	-1.8107800000	-2.6479820000	-1.5235850000
O	-0.7330650000	-1.3534660000	0.1537170000
O	-1.1510950000	-1.3741530000	2.4547990000
O	-1.6620440000	1.3559670000	2.4295340000
O	-3.9112130000	1.2408350000	0.6279110000
O	-2.6718040000	0.0976570000	-1.5101300000
O	-1.1490740000	-1.9286940000	-2.5534130000
H	0.3107290000	-0.2844600000	1.4879880000
H	-1.2837540000	1.2387610000	0.4484920000
H	-3.4768730000	-0.4858110000	1.6930190000
H	-4.0209680000	-1.1580380000	-0.5635180000
H	-2.4040560000	-2.5276730000	0.5189230000
H	-1.1837480000	-3.5139140000	-1.2984670000
H	-2.7915090000	-3.0091800000	-1.8598600000
H	-0.4413480000	-1.9725380000	2.7255790000
H	-1.8408610000	0.7574950000	3.1713810000
H	-3.7800670000	1.8841090000	1.3398480000
H	-3.2124670000	0.9015360000	-1.4839780000
H	-1.6226700000	-1.0910640000	-2.6731140000
N	4.2180870000	1.1734640000	0.0253610000
H	4.9158050000	0.7543720000	-0.6027250000
H	4.7194380000	1.4905690000	0.8588790000
H	3.7996470000	1.9953910000	-0.4190880000
C	3.2095930000	0.1207290000	0.3589090000
H	2.7780390000	0.3711530000	1.3299770000
C	2.1309240000	0.0605950000	-0.7179940000
C	3.9408360000	-1.2402000000	0.4585040000
H	2.6029260000	-0.0917300000	-1.6969110000

H	1.5120570000	-0.8209080000	-0.5184580000
C	1.2682460000	1.2837560000	-0.7495100000
O	5.0976890000	-1.2898140000	-0.0260140000
N	0.3345960000	1.4896240000	-1.7346660000
C	1.1600170000	2.3841490000	0.0700640000
H	0.1311640000	0.8596720000	-2.5011540000
C	-0.2907030000	2.6661460000	-1.4861000000
N	0.1859900000	3.2416710000	-0.3997100000
H	1.7208280000	2.6045150000	0.9688260000
H	-1.0771960000	3.0492400000	-2.1205650000
O	3.2837050000	-2.1631120000	0.9882690000

Table S178. Cartesian coordinates of α -Gal-gg_His_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6266178			
ZPE / Hartree = 0.3656858			
BSSE / Hartree = 0.00219276077			
C	1.8786610000	-1.2570430000	-1.3857870000
C	1.1796540000	-1.4105050000	-0.0328530000
C	1.3543720000	-0.1469170000	0.8025720000
C	2.8285440000	0.2195210000	0.9184580000
C	3.4416850000	0.3090560000	-0.4762870000
C	4.9385270000	0.5886750000	-0.4719010000
O	3.2313180000	-0.8995960000	-1.2103740000
O	1.1645420000	-0.2887280000	-2.1096060000
O	-0.1929320000	-1.7212260000	-0.1942590000
O	0.8549310000	-0.3331730000	2.1177760000
O	3.5311460000	-0.7630180000	1.6725180000
O	5.7223570000	-0.4835490000	0.0285530000
H	1.8962320000	-2.2098470000	-1.9217720000
H	1.6318990000	-2.2558970000	0.4934450000
H	0.8262560000	0.6833100000	0.3130700000
H	2.9202720000	1.2014370000	1.4025440000
H	2.9521890000	1.1462330000	-0.9930920000
H	5.2688950000	0.7613630000	-1.4990290000
H	5.1095240000	1.5068260000	0.1052470000
H	1.4027600000	-0.3481050000	-3.0448990000
H	-0.5836920000	-1.0331260000	-0.7574680000
H	-0.0333890000	-0.7129110000	2.0502510000
H	3.0680450000	-0.8831350000	2.5145680000
H	5.3418090000	-0.7525540000	0.8788260000
N	-4.5634030000	0.8276290000	-0.9919060000
H	-5.4097980000	0.9286540000	-0.4183660000
H	-4.8711200000	0.5745990000	-1.9336580000
H	-4.0750010000	1.7256830000	-1.0516340000
C	-3.7170420000	-0.2452070000	-0.3870690000
H	-3.0782410000	-0.6454850000	-1.1769650000
C	-2.8843650000	0.3274820000	0.7566330000
C	-4.6489220000	-1.3631480000	0.1417210000

H	-3.5518510000	0.7921280000	1.4929080000
H	-2.3967550000	-0.5176720000	1.2536450000
C	-1.8654270000	1.3223350000	0.2935820000
O	-5.8675540000	-1.0776380000	0.2343640000
N	-1.2080940000	2.1582950000	1.1617690000
C	-1.3664820000	1.6455460000	-0.9483950000
H	-1.3294630000	2.1874300000	2.1667430000
C	-0.3558930000	2.9289460000	0.4415410000
N	-0.4238400000	2.6485690000	-0.8456260000
H	-1.6267670000	1.2097420000	-1.9041690000
H	0.2820410000	3.6707530000	0.9003500000
O	-4.0783530000	-2.4309870000	0.4543400000

Table S179. Cartesian coordinates of α -Gal-gg_His_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6252407			
ZPE / Hartree = 0.3653226			
BSSE / Hartree = 0.00176372064			
C	4.1062120000	0.5874480000	-0.5035690000
C	3.8728780000	-0.1537070000	0.8145130000
C	2.4783600000	-0.7716250000	0.8337140000
C	1.4286440000	0.2954890000	0.5490560000
C	1.7666550000	1.0092160000	-0.7568090000
C	0.8151790000	2.1481770000	-1.0944460000
O	3.0932190000	1.5423390000	-0.7265450000
O	4.1505910000	-0.3867540000	-1.5157210000
O	4.8689770000	-1.1355790000	1.0354890000
O	2.1844340000	-1.3280820000	2.1045750000
O	1.3900500000	1.2513330000	1.6051260000
O	0.9054760000	3.2568130000	-0.2131180000
H	5.0401380000	1.1546690000	-0.4684530000
H	3.9561410000	0.5664180000	1.6334130000
H	2.4108160000	-1.5445770000	0.0544040000
H	0.4449620000	-0.1818430000	0.4448070000
H	1.6868760000	0.2669360000	-1.5629610000
H	1.0527750000	2.5247040000	-2.0924350000
H	-0.2043650000	1.7391860000	-1.1139990000
H	4.5605190000	-0.0106850000	-2.3066140000
H	4.9197200000	-1.6891250000	0.2407560000
H	2.9248050000	-1.8946370000	2.3657050000
H	1.2955800000	0.7700120000	2.4404360000
H	0.8539780000	2.9166340000	0.6935900000
N	-4.7466030000	-1.4519250000	-0.0120670000
H	-5.4566450000	-1.1684560000	-0.6990010000
H	-5.2418760000	-1.9037820000	0.7598930000
H	-4.1161280000	-2.1455720000	-0.4254350000
C	-4.0241750000	-0.2265480000	0.4454640000
H	-3.6286210000	-0.4284610000	1.4423010000
C	-2.8983150000	0.1167320000	-0.5285580000
C	-5.0395010000	0.9403520000	0.5161770000
H	-3.3201200000	0.2999810000	-1.5243590000

H	-2.4539120000	1.0570850000	-0.1864910000
C	-1.8530390000	-0.9519040000	-0.6113970000
O	-6.1366710000	0.7616130000	-0.0669210000
N	-0.9746810000	-1.0378660000	-1.6635650000
C	-1.4992880000	-1.9862610000	0.2250310000
H	-0.9471680000	-0.4249370000	-2.4693630000
C	-0.1398050000	-2.0807150000	-1.4320780000
N	-0.4290200000	-2.6832580000	-0.2959450000
H	-1.9508250000	-2.2636630000	1.1681310000
H	0.6507410000	-2.3527670000	-2.1173460000
O	-4.6445870000	1.9588530000	1.1248000000

Table S180. Cartesian coordinates of α -Gal-gg_His_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6271076			
ZPE / Hartree = 0.3655259			
BSSE / Hartree = 0.00241251172			
C	3.2481380000	-0.0790280000	-0.7467310000
C	2.6121700000	-1.4519920000	-0.9750640000
C	1.1193130000	-1.4052920000	-0.6644200000
C	0.8946420000	-0.8576340000	0.7388800000
C	1.5918350000	0.4927240000	0.8754080000
C	1.4708600000	1.1032550000	2.2634330000
O	2.9820690000	0.3866200000	0.5573590000
O	2.7288990000	0.7759900000	-1.7334720000
O	2.8430670000	-1.9123860000	-2.2941390000
O	0.5474540000	-2.7021820000	-0.7141970000
O	1.4143310000	-1.7512650000	1.7177240000
O	2.1850750000	0.3988170000	3.2672080000
H	4.3373630000	-0.1408280000	-0.8184700000
H	3.0934990000	-2.1696800000	-0.3046340000
H	0.6169360000	-0.7382580000	-1.3807750000
H	-0.1812630000	-0.7139680000	0.9029170000
H	1.1077370000	1.1821310000	0.1711080000
H	1.8783120000	2.1176530000	2.2426930000
H	0.4010440000	1.1675330000	2.5081950000
H	3.2728390000	1.5738700000	-1.7874010000
H	2.5699110000	-1.2095080000	-2.9040440000
H	0.8301780000	-3.1264360000	-1.5372390000
H	1.0341310000	-2.6272910000	1.5556320000
H	1.9443890000	-0.5378230000	3.1949230000
N	-3.8041580000	0.0930840000	-1.4624960000
H	-4.7669900000	-0.0066050000	-1.1107780000
H	-3.7292130000	-0.4919380000	-2.2979440000
H	-3.6402290000	1.0627000000	-1.7455880000
C	-2.8873300000	-0.3708000000	-0.3743750000
H	-2.0069000000	-0.8157340000	-0.8446660000
C	-2.4960840000	0.8017510000	0.5210450000
C	-3.6271930000	-1.4543190000	0.4501890000

H	-3.4023930000	1.3370280000	0.8327360000
H	-2.0454170000	0.3899430000	1.4302710000
C	-1.5341990000	1.7397600000	-0.1392460000
O	-4.8655250000	-1.5482560000	0.2669380000
N	-1.0222100000	2.8366680000	0.5089510000
C	-0.9469810000	1.7629180000	-1.3834980000
H	-1.2333120000	3.1219250000	1.4573510000
C	-0.1655780000	3.4638090000	-0.3346190000
N	-0.0964860000	2.8433030000	-1.4956290000
H	-1.0787640000	1.0631300000	-2.1984160000
H	0.3717440000	4.3584210000	-0.0543350000
O	-2.9092660000	-2.1071580000	1.2384120000

Table S181. Cartesian coordinates of α -Gal-gg_His_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6256340			
ZPE / Hartree = 0.3653638			
BSSE / Hartree = 0.00191684433			
C	3.7946560000	0.0474760000	-0.4237890000
C	3.2705670000	-1.3750570000	-0.2220170000
C	1.7569510000	-1.4117760000	-0.4062230000
C	1.0903300000	-0.3916590000	0.5086040000
C	1.7089770000	0.9849490000	0.2801400000
C	1.1722480000	2.0577720000	1.2180650000
O	3.1305070000	0.9485300000	0.4327170000
O	3.6051020000	0.3630190000	-1.7799890000
O	3.9112930000	-2.2889220000	-1.0933190000
O	1.2360350000	-2.6884800000	-0.0754650000
O	1.2537430000	-0.7575710000	1.8744150000
O	1.5627150000	1.8857310000	2.5720090000
H	4.8520050000	0.1127380000	-0.1535250000
H	3.5146440000	-1.6901470000	0.7965790000
H	1.5109990000	-1.1581410000	-1.4478210000
H	0.0221100000	-0.3331710000	0.2631200000
H	1.4544440000	1.2896100000	-0.7443660000
H	1.5594630000	3.0301180000	0.9027460000
H	0.0779490000	2.0732800000	1.1211830000
H	4.1559940000	1.1226270000	-2.0131850000
H	3.8419430000	-1.9367440000	-1.9943140000
H	1.7646780000	-3.3575470000	-0.5340860000
H	0.9436000000	-1.6693030000	1.9793420000
H	1.3552230000	0.9719730000	2.8217390000
N	-3.9687540000	-0.6409390000	-1.4367840000
H	-4.8923950000	-0.7909270000	-1.0129350000
H	-3.9016260000	-1.2725200000	-2.2380140000
H	-3.9016880000	0.3171620000	-1.7928630000
C	-2.9239900000	-0.9399200000	-0.4121110000
H	-2.0010670000	-1.1809430000	-0.9435240000
C	-2.7345770000	0.2697440000	0.5029190000
C	-3.3766480000	-2.1678320000	0.4133170000
H	-3.6954280000	0.5316730000	0.9620210000

H	-2.0641170000	-0.0364650000	1.3141990000
C	-2.1698830000	1.4585160000	-0.2112870000
O	-4.5827550000	-2.4984410000	0.3091720000
N	-2.3403440000	2.7416020000	0.2485080000
C	-1.3687710000	1.5884720000	-1.3221360000
H	-2.8808990000	3.0169800000	1.0592100000
C	-1.6510210000	3.5765610000	-0.5665690000
N	-1.0496300000	2.9131690000	-1.5345070000
H	-0.9988190000	0.8056060000	-1.9713830000
H	-1.6273820000	4.6459740000	-0.4142010000
O	-2.4905850000	-2.6853830000	1.1287180000

Table S182. Cartesian coordinates of α -Gal-gt_His_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6317111			
ZPE / Hartree = 0.3654182			
BSSE / Hartree = 0.00260600893			
C	-1.6440240000	0.5534160000	0.9886010000
C	-2.7539580000	0.6258070000	-0.0592730000
C	-3.4184430000	-0.7374810000	-0.2253230000
C	-2.3686590000	-1.8006940000	-0.5338120000
C	-1.2864680000	-1.7686650000	0.5407860000
C	-0.1472130000	-2.7251980000	0.2353680000
O	-0.7229450000	-0.4595090000	0.6598440000
O	-2.2639650000	0.3329980000	2.2320820000
O	-3.7069830000	1.6230540000	0.2619060000
O	-4.3402550000	-0.7183720000	-1.3042260000
O	-1.7653220000	-1.5560710000	-1.7969380000
O	0.7881570000	-2.7455250000	1.2973730000
H	-1.0659110000	1.4814440000	1.0067340000
H	-2.3032730000	0.9212470000	-1.0115090000
H	-3.9305770000	-1.0099050000	0.7084580000
H	-2.8450290000	-2.7909710000	-0.5267910000
H	-1.7449330000	-2.0539860000	1.4973540000
H	-0.5749410000	-3.7256330000	0.0914080000
H	0.3397110000	-2.4269320000	-0.7003470000
H	-1.6470840000	0.5617280000	2.9408760000
H	-3.9908980000	1.4775060000	1.1776290000
H	-4.8974890000	0.0680030000	-1.2101320000
H	-2.4780300000	-1.3964970000	-2.4331390000
H	1.6621930000	-2.4783450000	0.9363560000
N	4.2231400000	1.1815040000	0.1121040000
H	4.8768860000	0.9180990000	-0.6369330000
H	4.7673680000	1.2449440000	0.9753860000
H	3.8312970000	2.1079490000	-0.0805520000
C	3.1730110000	0.1198610000	0.2015590000
H	2.8166840000	0.0864810000	1.2334830000
C	2.0276430000	0.4250540000	-0.7581710000
C	3.8287840000	-1.2307700000	-0.1680590000

H	2.4182220000	0.4890710000	-1.7816810000
H	1.3349160000	-0.4213380000	-0.7194970000
C	1.2879260000	1.6789770000	-0.4133820000
O	4.9508340000	-1.1834420000	-0.7163290000
N	0.3079120000	2.1839960000	-1.2309840000
C	1.3394500000	2.5505060000	0.6506060000
H	-0.0027250000	1.7802630000	-2.1062800000
C	-0.1889940000	3.3059270000	-0.6538290000
N	0.4151380000	3.5635930000	0.4888770000
H	1.9759480000	2.5045410000	1.5247040000
H	-0.9804490000	3.8874710000	-1.1046450000
O	3.1505370000	-2.2567880000	0.0911250000

Table S183. Cartesian coordinates of α -Gal-gt_His_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6328617			
ZPE / Hartree = 0.3656778			
BSSE / Hartree = 0.00291138185			
C	-1.1481460000	-0.4236660000	1.4998430000
C	-2.1841250000	0.3553300000	0.6897210000
C	-2.9917330000	-0.5880560000	-0.1958700000
C	-2.0533030000	-1.4217320000	-1.0634180000
C	-1.0407440000	-2.1297930000	-0.1701030000
C	-0.0018940000	-2.9013540000	-0.9667720000
O	-0.3321240000	-1.1922870000	0.6468090000
O	-1.8591380000	-1.2150960000	2.4192940000
O	-3.0290520000	1.1218530000	1.5284740000
O	-3.8387020000	0.1482400000	-1.0652480000
O	-1.3536610000	-0.5935890000	-1.9819250000
O	0.8970450000	-3.5895460000	-0.1178390000
H	-0.4691060000	0.2598890000	2.0179870000
H	-1.6536340000	1.0669660000	0.0512280000
H	-3.5865530000	-1.2661260000	0.4327380000
H	-2.6381110000	-2.1793270000	-1.6038700000
H	-1.5846680000	-2.8314320000	0.4762750000
H	-0.5213780000	-3.6384780000	-1.5872800000
H	0.5421710000	-2.2167220000	-1.6283120000
H	-1.2606900000	-1.5116670000	3.1182040000
H	-3.3808570000	0.5328950000	2.2137740000
H	-4.2996850000	0.8183650000	-0.5396390000
H	-2.0000430000	0.0065660000	-2.3829650000
H	1.6079850000	-2.9616630000	0.1130540000
N	3.5643770000	1.6334210000	0.7223830000
H	4.4099530000	1.5551450000	0.1421320000
H	3.8685200000	1.6233080000	1.6988280000
H	3.1078980000	2.5331860000	0.5467460000
C	2.6819210000	0.4656740000	0.4083710000
H	2.0789280000	0.2518220000	1.2937280000
C	1.7895700000	0.7837790000	-0.7876190000
C	3.5924760000	-0.7447230000	0.0922140000
H	2.4130150000	1.0452480000	-1.6517290000

H	1.2430240000	-0.1312130000	-1.0348220000
C	0.8152500000	1.8835690000	-0.5033760000
O	4.7942140000	-0.4949880000	-0.1515470000
N	0.0078820000	2.4141600000	-1.4793140000
C	0.4733110000	2.5671700000	0.6412950000
H	-0.0099070000	2.1361920000	-2.4528040000
C	-0.7764580000	3.3624490000	-0.9102790000
N	-0.5203270000	3.4865760000	0.3769480000
H	0.8723140000	2.4409920000	1.6392970000
H	-1.5045130000	3.9268190000	-1.4750470000
O	3.0295520000	-1.8660560000	0.0805230000

Table S184. Cartesian coordinates of α -Gal-gt_His_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6260225			
ZPE / Hartree = 0.3647418			
BSSE / Hartree = 0.00216154789			
C	-3.4597270000	0.6815100000	0.8200340000
C	-2.3289560000	0.4254780000	1.8187620000
C	-1.0640920000	-0.0170140000	1.0884950000
C	-1.3521410000	-1.2172860000	0.1936050000
C	-2.5101320000	-0.8733490000	-0.7340760000
C	-2.9635170000	-2.0460120000	-1.5824560000
O	-3.6622020000	-0.4526960000	0.0063170000
O	-3.0993250000	1.8150700000	0.0728800000
O	-2.0771280000	1.5701990000	2.6140310000
O	-0.0553570000	-0.4027530000	2.0088940000
O	-1.6987110000	-2.3545160000	0.9695670000
O	-3.9702570000	-1.6514150000	-2.5036600000
H	-4.4077580000	0.8427850000	1.3397100000
H	-2.6475860000	-0.3663710000	2.5025900000
H	-0.7092090000	0.8107900000	0.4598480000
H	-0.4650740000	-1.4312900000	-0.4204260000
H	-2.1871890000	-0.0570760000	-1.3942870000
H	-2.1185100000	-2.4153680000	-2.1688430000
H	-3.3256960000	-2.8525870000	-0.9351370000
H	-3.8851250000	2.1825630000	-0.3542720000
H	-1.9433600000	2.3220220000	2.0156020000
H	0.0399040000	0.3016450000	2.6664410000
H	-1.0381670000	-2.4386970000	1.6731810000
H	-4.7200200000	-1.3152500000	-1.9930370000
N	4.5978980000	1.0186740000	-0.6063730000
H	5.1375680000	0.4977950000	-1.3077310000
H	5.2742330000	1.4914050000	-0.0028480000
H	4.0341410000	1.7391300000	-1.0675150000
C	3.7628220000	0.0512270000	0.1671820000
H	3.5036050000	0.5253770000	1.1155310000
C	2.5075550000	-0.3075890000	-0.6254090000
C	4.6044280000	-1.2200820000	0.4339730000

H	2.7979180000	-0.7442790000	-1.5887830000
H	1.9824380000	-1.0852280000	-0.0609960000
C	1.6058450000	0.8657810000	-0.8501410000
O	5.6514200000	-1.3501880000	-0.2454850000
N	0.6233800000	0.8652660000	-1.8097550000
C	1.4903330000	2.0891490000	-0.2314540000
H	0.4185690000	0.1100100000	-2.4527720000
C	-0.0392660000	2.0458840000	-1.7355850000
N	0.4607700000	2.8176720000	-0.7908770000
H	2.0826870000	2.4797860000	0.5851990000
H	-0.8670270000	2.2870990000	-2.3872860000
O	4.1303610000	-2.0064160000	1.2833680000

Table S185. Cartesian coordinates of α -Gal-gt_His_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6249693			
ZPE / Hartree = 0.3648726			
BSSE / Hartree = 0.00206002406			
C	-3.4062210000	-1.7025050000	0.2411770000
C	-1.9717530000	-2.1626720000	-0.0225700000
C	-0.9786160000	-1.0557430000	0.3220480000
C	-1.3397120000	0.2298590000	-0.4163310000
C	-2.7913360000	0.5827330000	-0.1239920000
C	-3.2800710000	1.7764200000	-0.9219590000
O	-3.6710870000	-0.5006930000	-0.4479830000
O	-3.5425370000	-1.5621940000	1.6318940000
O	-1.6727090000	-3.3515890000	0.6861130000
O	0.3342390000	-1.4217770000	-0.0725140000
O	-1.1643390000	0.0731910000	-1.8169630000
O	-4.5944640000	2.1502260000	-0.5344870000
H	-4.1238980000	-2.4287240000	-0.1495110000
H	-1.8804040000	-2.4025230000	-1.0859080000
H	-1.0102990000	-0.8575730000	1.4036430000
H	-0.7080190000	1.0465320000	-0.0448040000
H	-2.8769760000	0.8098280000	0.9471720000
H	-2.6300320000	2.6324820000	-0.7215720000
H	-3.2427550000	1.5451590000	-1.9924460000
H	-4.4812740000	-1.5394600000	1.8628200000
H	-1.9103030000	-3.2102410000	1.6157160000
H	0.5000140000	-2.3270370000	0.2296500000
H	-0.3039020000	-0.3518370000	-1.9520950000
H	-5.1772220000	1.3976260000	-0.7067610000
N	4.4086410000	0.3746210000	1.1552420000
H	5.2964240000	0.4480080000	0.6418070000
H	4.6000440000	-0.1581470000	2.0066040000
H	4.0887800000	1.3060020000	1.4353510000
C	3.4291830000	-0.3328380000	0.2737510000
H	2.7036840000	-0.8391420000	0.9125950000
C	2.7292400000	0.6640640000	-0.6438050000
C	4.2028390000	-1.3775030000	-0.5676040000

H	3.4784190000	1.2141470000	-1.2271520000
H	2.1278740000	0.0796700000	-1.3471140000
C	1.8495530000	1.6201080000	0.0990750000
O	5.4524740000	-1.2572940000	-0.5975310000
N	1.2542110000	2.6944350000	-0.5156630000
C	1.4051470000	1.6711730000	1.4002970000
H	1.3591690000	2.9594030000	-1.4873830000
C	0.4882270000	3.3349590000	0.4021920000
N	0.5569160000	2.7447090000	1.5790880000
H	1.6361250000	0.9930420000	2.2113130000
H	-0.0869450000	4.2175190000	0.1616700000
O	3.4939530000	-2.2197980000	-1.1607740000

Table S186. Cartesian coordinates of α -Gal-gt_His_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6265184			
ZPE / Hartree = 0.3651487			
BSSE / Hartree = 0.00213407034			
C	3.6681040000	0.2880380000	0.0321060000
C	3.4437290000	-1.1384550000	-0.4728460000
C	1.9554850000	-1.4071130000	-0.6828080000
C	1.1735450000	-1.0933220000	0.5889910000
C	1.4873040000	0.3359400000	1.0107030000
C	0.8400150000	0.7387950000	2.3212230000
O	2.8971360000	0.5243170000	1.1890450000
O	3.3286980000	1.1530990000	-1.0207520000
O	4.1748910000	-1.3864240000	-1.6600200000
O	1.7325690000	-2.7720060000	-0.9979340000
O	1.5322570000	-1.9801410000	1.6374690000
O	1.0668200000	2.1133310000	2.6001030000
H	4.7080070000	0.4327790000	0.3368690000
H	3.8273250000	-1.8320050000	0.2808760000
H	1.5790260000	-0.7615270000	-1.4903700000
H	0.0978020000	-1.1699720000	0.3750000000
H	1.1368370000	1.0077190000	0.2171770000
H	-0.2423590000	0.6021350000	2.2477770000
H	1.2212160000	0.1100200000	3.1340910000
H	3.6920550000	2.0319970000	-0.8457360000
H	3.9720330000	-0.6740690000	-2.2862160000
H	2.3584490000	-3.0265190000	-1.6915190000
H	1.5011680000	-2.8798400000	1.2796880000
H	2.0232640000	2.2485630000	2.6525410000
N	-4.3700110000	0.4761670000	-1.3253540000
H	-5.1087360000	0.8570710000	-0.7232570000
H	-4.8369980000	-0.0129850000	-2.0928140000
H	-3.8249970000	1.2429260000	-1.7310620000
C	-3.5222000000	-0.4575160000	-0.5244760000
H	-2.9739030000	-1.0846400000	-1.2294360000
C	-2.5608810000	0.3367120000	0.3613510000
C	-4.4472950000	-1.3386330000	0.3475170000
H	-3.1366140000	0.9963820000	1.0218670000

H	-2.0452140000	-0.3882700000	0.9998110000
C	-1.5765140000	1.1448850000	-0.4276080000
O	-5.6333730000	-0.9492060000	0.4759070000
N	-1.1298650000	2.3782710000	-0.0190870000
C	-0.9210690000	0.9120810000	-1.6153210000
H	-1.4048250000	2.8609190000	0.8278700000
C	-0.2442540000	2.8326500000	-0.9384630000
N	-0.0936940000	1.9699100000	-1.9254880000
H	-0.9995360000	0.0443430000	-2.2564920000
H	0.2533170000	3.7869070000	-0.8412740000
O	-3.9012670000	-2.3388140000	0.8639190000

Table S187. Cartesian coordinates of α -Gal-gt_His_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6314759			
ZPE / Hartree = 0.3654979			
BSSE / Hartree = 0.00231380792			
C	-3.8431580000	0.2609720000	-0.2894120000
C	-3.3286160000	-1.1583570000	-0.0364240000
C	-2.0338570000	-1.1270550000	0.7720500000
C	-1.0069930000	-0.2395770000	0.0708830000
C	-1.6254000000	1.1423390000	-0.1161950000
C	-0.7225980000	2.1074140000	-0.8603450000
O	-2.8380150000	1.0569480000	-0.8769530000
O	-4.2663130000	0.7690350000	0.9505940000
O	-4.3129250000	-1.9503840000	0.6053670000
O	-1.4900600000	-2.4296940000	0.8993020000
O	-0.6471930000	-0.7691180000	-1.1886820000
O	-1.3190610000	3.3930850000	-0.9645370000
H	-4.6673440000	0.2525560000	-1.0075440000
H	-3.1291080000	-1.6291360000	-1.0029300000
H	-2.2396120000	-0.7053000000	1.7671200000
H	-0.1233800000	-0.1317520000	0.7173020000
H	-1.8521060000	1.5608790000	0.8733480000
H	0.2062950000	2.2309710000	-0.2964390000
H	-0.4848900000	1.7071420000	-1.8528230000
H	-4.8363070000	1.5364840000	0.8060710000
H	-4.6303590000	-1.4573950000	1.3778500000
H	-2.1865800000	-3.0098950000	1.2387330000
H	-0.0203490000	-1.5172520000	-1.0572870000
H	-2.1566520000	3.2907970000	-1.4377610000
N	3.9214150000	-1.4594380000	0.9713760000
H	4.5784580000	-1.9662200000	0.3656550000
H	3.8258610000	-2.0091550000	1.8284230000
H	4.3215070000	-0.5525400000	1.2282400000
C	2.6181320000	-1.3311320000	0.2511060000
H	1.8340620000	-1.2451450000	1.0063990000
C	2.6363350000	-0.1120650000	-0.6683260000
C	2.3830870000	-2.6198450000	-0.5688310000

H	3.5128830000	-0.1663250000	-1.3256340000
H	1.7479860000	-0.1701830000	-1.3065340000
C	2.6251880000	1.1860710000	0.0760360000
O	3.3530050000	-3.3963010000	-0.6994610000
N	2.8830860000	2.3816470000	-0.5480820000
C	2.3120160000	1.5265660000	1.3712830000
H	3.1411770000	2.5023150000	-1.5197080000
C	2.7142460000	3.3755170000	0.3585270000
N	2.3710010000	2.8953520000	1.5371310000
H	2.0432100000	0.8695570000	2.1875660000
H	2.8597600000	4.4169470000	0.1101790000
O	1.2276460000	-2.7479930000	-1.0487930000

Table S188. Cartesian coordinates of α -Gal-tg_His_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6236263			
ZPE / Hartree = 0.3648449			
BSSE / Hartree = 0.00194395416			
C	1.4857780000	-0.6610370000	1.0998150000
C	2.6642590000	-0.9853630000	0.1815990000
C	3.5583060000	0.2386890000	0.0126220000
C	2.7339160000	1.4235640000	-0.4804020000
C	1.5611280000	1.6518430000	0.4669850000
C	0.5765980000	2.7020750000	-0.0387560000
O	0.7826880000	0.4639400000	0.6270460000
O	2.0140990000	-0.4591850000	2.3865200000
O	3.3982360000	-2.0965970000	0.6617220000
O	4.5716800000	-0.0087000000	-0.9493270000
O	2.2262100000	1.1782370000	-1.7838840000
O	1.2009890000	3.9632990000	-0.2161340000
H	0.7578160000	-1.4788640000	1.1030350000
H	2.2694520000	-1.2711730000	-0.7975990000
H	4.0075480000	0.5009250000	0.9809320000
H	3.3675270000	2.3212590000	-0.4821480000
H	1.9658640000	1.9682270000	1.4373770000
H	0.1168960000	2.3521750000	-0.9694430000
H	-0.2096800000	2.8309100000	0.7096670000
H	1.3098950000	-0.5563170000	3.0419410000
H	3.6027090000	-1.9332240000	1.5955340000
H	4.9958410000	-0.8509940000	-0.7296360000
H	2.9670240000	0.8860810000	-2.3351310000
H	1.6437410000	3.9789380000	-1.0746650000
N	-4.5464620000	-1.0191930000	-0.3975480000
H	-5.0053510000	-0.4823120000	-1.1446210000
H	-5.2842630000	-1.3534130000	0.2264220000
H	-4.0789100000	-1.8399250000	-0.7935890000
C	-3.5963300000	-0.1068430000	0.3100180000
H	-3.4813310000	-0.4753680000	1.3306900000
C	-2.2534750000	-0.0790950000	-0.4160430000
C	-4.2113380000	1.3139650000	0.3360740000
H	-2.4054690000	0.2577830000	-1.4490500000

H	-1.6261830000	0.6669180000	0.0811790000
C	-1.5563870000	-1.4036030000	-0.4130810000
O	-5.1785220000	1.5182560000	-0.4377590000
N	-0.5455410000	-1.7017000000	-1.2932690000
C	-1.6830750000	-2.5293250000	0.3681530000
H	-0.1741240000	-1.0829320000	-2.0041240000
C	-0.1006250000	-2.9524510000	-1.0180160000
N	-0.7693560000	-3.4896220000	-0.0169150000
H	-2.3759140000	-2.7005920000	1.1810030000
H	0.7027210000	-3.4165330000	-1.5725140000
O	-3.6539820000	2.1254400000	1.1074490000

Table S189. Cartesian coordinates of α -Gal-tg_His_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6249122			
ZPE / Hartree = 0.3651213			
BSSE / Hartree = 0.00237405510			
C	-0.6096850000	-0.4660650000	1.3786960000
C	-1.4521030000	0.7991360000	1.2387580000
C	-2.9049920000	0.4346360000	0.9572630000
C	-2.9971810000	-0.4651210000	-0.2708270000
C	-2.0642570000	-1.6616430000	-0.1094760000
C	-1.9199130000	-2.4627570000	-1.4016850000
O	-0.7315730000	-1.2595690000	0.2207970000
O	-1.0460260000	-1.1313620000	2.5355470000
O	-1.3417800000	1.6260640000	2.3824600000
O	-3.6730210000	1.5978730000	0.6908100000
O	-2.6314480000	0.2380000000	-1.4491730000
O	-3.1804830000	-2.8262090000	-1.9394120000
H	0.4534140000	-0.2153890000	1.4534270000
H	-1.0607820000	1.3779230000	0.3971760000
H	-3.3198710000	-0.1072770000	1.8188290000
H	-4.0276720000	-0.8356970000	-0.3582770000
H	-2.4670320000	-2.2997860000	0.6872420000
H	-1.3394180000	-1.8735550000	-2.1202010000
H	-1.3787220000	-3.3877380000	-1.1915140000
H	-0.3754820000	-1.7719460000	2.8096560000
H	-1.5291870000	1.0811220000	3.1624440000
H	-3.4730940000	2.2533590000	1.3750080000
H	-3.0968120000	1.0876960000	-1.4400450000
H	-3.5668840000	-2.0472740000	-2.3629920000
N	4.4110540000	0.8418810000	-0.2246560000
H	5.0443320000	0.2904660000	-0.8176720000
H	4.9605230000	1.1708490000	0.5726400000
H	4.0845880000	1.6646130000	-0.7391090000
C	3.2954530000	-0.0543570000	0.2107430000
H	2.9270600000	0.3186170000	1.1687250000
C	2.1851510000	-0.0669260000	-0.8357020000
C	3.8650240000	-1.4810970000	0.4033670000

H	2.6167670000	-0.2918760000	-1.8193690000
H	1.5051270000	-0.8887190000	-0.5876300000
C	1.4177720000	1.2177330000	-0.8900210000
O	4.9992730000	-1.7029740000	-0.0864540000
N	0.4509790000	1.4488980000	-1.8372870000
C	1.4336240000	2.3590700000	-0.1211140000
H	0.1582540000	0.8027240000	-2.5601470000
C	-0.0719910000	2.6798060000	-1.6160460000
N	0.5024080000	3.2660350000	-0.5841400000
H	2.0569330000	2.5773540000	0.7358220000
H	-0.8605210000	3.0922290000	-2.2292910000
O	3.1145550000	-2.2780610000	1.0084380000

Table S190. Cartesian coordinates of α -Gal-tg_His_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6248757			
ZPE / Hartree = 0.3659582			
BSSE / Hartree = 0.00214735711			
C	1.7801680000	-1.6224020000	-1.2313350000
C	1.0950510000	-1.5497960000	0.1346130000
C	1.3838280000	-0.2096210000	0.8033830000
C	2.8845120000	0.0499030000	0.8665140000
C	3.4765220000	-0.0850790000	-0.5322000000
C	4.9994680000	-0.0031250000	-0.5535770000
O	3.1591810000	-1.3548210000	-1.1078010000
O	1.1324090000	-0.6973990000	-2.0661860000
O	-0.3000880000	-1.7676910000	0.0208830000
O	0.8919720000	-0.1908530000	2.1343090000
O	3.5254790000	-0.8786920000	1.7282280000
O	5.4617450000	1.2365250000	-0.0408970000
H	1.7147900000	-2.6322300000	-1.6449200000
H	1.4883610000	-2.3570690000	0.7589260000
H	0.9184650000	0.5923370000	0.2133400000
H	3.0486120000	1.0767840000	1.2228650000
H	3.0610810000	0.7199250000	-1.1529400000
H	5.4204720000	-0.8449690000	0.0055470000
H	5.3368640000	-0.0699150000	-1.5905180000
H	1.3393750000	-0.8969910000	-2.9894610000
H	-0.6396530000	-1.1326490000	-0.6308390000
H	-0.0363330000	-0.4661230000	2.1163810000
H	3.0246440000	-0.9015080000	2.5568710000
H	5.4802870000	1.1921650000	0.9239160000
N	-4.4952040000	0.9413870000	-1.0495980000
H	-5.3489210000	1.1038900000	-0.5006710000
H	-4.7915130000	0.6701720000	-1.9899630000
H	-3.9607540000	1.8115480000	-1.1278700000
C	-3.7195360000	-0.1490970000	-0.3835100000
H	-3.1112500000	-0.6367000000	-1.1478700000
C	-2.8444200000	0.4307820000	0.7253910000
C	-4.7213530000	-1.1709410000	0.2077460000
H	-3.4765480000	0.9643310000	1.4459140000

H	-2.3939660000	-0.4164530000	1.2525210000
C	-1.7813760000	1.3483660000	0.2041310000
O	-5.9160870000	-0.7957990000	0.2948900000
N	-1.0769220000	2.1977360000	1.0211440000
C	-1.2823290000	1.5837790000	-1.0575920000
H	-1.1827020000	2.2843150000	2.0245050000
C	-0.1985490000	2.8893600000	0.2545990000
N	-0.2955550000	2.5464070000	-1.0149980000
H	-1.5755920000	1.1147230000	-1.9877670000
H	0.4782970000	3.6228080000	0.6688570000
O	-4.2236310000	-2.2600040000	0.5676210000

Table S191. Cartesian coordinates of α -Gal-tg_His_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6241079			
ZPE / Hartree = 0.3650887			
BSSE / Hartree = 0.00233742695			
C	-3.6003640000	-1.4392160000	0.3314130000
C	-2.2316870000	-2.0929390000	0.1386240000
C	-1.1191060000	-1.0617180000	0.3006330000
C	-1.3546410000	0.1232170000	-0.6296010000
C	-2.7561160000	0.6768110000	-0.4028640000
C	-3.1364900000	1.7563230000	-1.4111430000
O	-3.7503220000	-0.3413090000	-0.5407740000
O	-3.6894320000	-1.0636590000	1.6818040000
O	-2.0500620000	-3.1808830000	1.0267630000
O	0.1388730000	-1.6269150000	-0.0335400000
O	-1.2236880000	-0.2642670000	-1.9896200000
O	-2.2362380000	2.8523540000	-1.3631130000
H	-4.4022550000	-2.1336720000	0.0672090000
H	-2.1894570000	-2.5059840000	-0.8733600000
H	-1.1073740000	-0.6923810000	1.3368060000
H	-0.6274020000	0.9100130000	-0.3891100000
H	-2.7907490000	1.0976180000	0.6110810000
H	-3.1769450000	1.3209760000	-2.4149990000
H	-4.1263030000	2.1421560000	-1.1571100000
H	-4.6163350000	-0.9135850000	1.9127000000
H	-2.2445590000	-2.8662910000	1.9232670000
H	0.2191040000	-2.4765730000	0.4242510000
H	-0.3945920000	-0.7594370000	-2.0697910000
H	-1.4293820000	2.6177370000	-1.8409060000
N	4.2484680000	0.0308090000	1.2593190000
H	5.1418710000	0.2579550000	0.8047640000
H	4.4438130000	-0.6882640000	1.9601210000
H	3.8873500000	0.8541590000	1.7494580000
C	3.3088500000	-0.4748460000	0.2120720000
H	2.5726400000	-1.1134090000	0.7030510000
C	2.6185010000	0.6911510000	-0.4896260000
C	4.1206210000	-1.3078200000	-0.8084780000

H	3.3715630000	1.3515050000	−0.9368360000
H	2.0291810000	0.2669520000	−1.3103560000
C	1.7225570000	1.4700860000	0.4210280000
O	5.3686840000	−1.1762060000	−0.7723690000
N	1.1958000000	2.6875200000	0.0638030000
C	1.1689590000	1.1954130000	1.6492400000
H	1.3891970000	3.1935200000	−0.7917080000
C	0.3580440000	3.0897540000	1.0513250000
N	0.3177560000	2.2112050000	2.0334460000
H	1.3206620000	0.3196230000	2.2665720000
H	−0.1839930000	4.0234010000	1.0056790000
O	3.4403130000	−2.0078690000	−1.5907150000

Table S192. Cartesian coordinates of α -Gal-tg_His_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6261206			
ZPE / Hartree = 0.3654018			
BSSE / Hartree = 0.00239759438			
C	-2.3620280000	-1.3336450000	1.5418760000
C	-1.6326410000	-2.2783390000	0.5850350000
C	-0.7528440000	-1.4786960000	-0.3696830000
C	-1.5692690000	-0.4133790000	-1.0918990000
C	-2.3173430000	0.4367870000	-0.0738260000
C	-3.3251310000	1.3813560000	-0.7277780000
O	-3.0926280000	-0.3689380000	0.8195700000
O	-1.3849660000	-0.7553050000	2.3692410000
O	-0.8712200000	-3.2405680000	1.2915270000
O	-0.1789690000	-2.3140550000	-1.3607340000
O	-2.5153230000	-0.9973210000	-1.9759590000
O	-2.7529310000	2.1121690000	-1.8004430000
H	-3.1023790000	-1.8773610000	2.1348830000
H	-2.3806760000	-2.8309580000	0.0094050000
H	0.0341380000	-0.9763600000	0.2136480000
H	-0.8820560000	0.2375170000	-1.6516890000
H	-1.5740060000	1.0069840000	0.4972080000
H	-4.1869150000	0.7973010000	-1.0682260000
H	-3.6671120000	2.1092870000	0.0117230000
H	-1.8097230000	-0.3659360000	3.1458560000
H	-0.3119180000	-2.7671360000	1.9268030000
H	0.2785270000	-3.0426420000	-0.9168100000
H	-2.0466840000	-1.6398990000	-2.5283840000
H	-2.6709500000	1.5192170000	-2.5603850000
N	3.9717580000	0.9267730000	0.9346770000
H	4.7786410000	1.0630560000	0.3114260000
H	4.3304790000	0.5261130000	1.8046800000
H	3.5468320000	1.8312410000	1.1584700000
C	3.0217360000	-0.0056920000	0.2535640000
H	2.4510730000	-0.5236170000	1.0271330000
C	2.0973620000	0.7718390000	-0.6809900000
C	3.8496250000	-1.0341510000	-0.5548500000
H	2.7023250000	1.3463760000	-1.3939690000

H	1.5322920000	0.0347460000	−1.2631730000
C	1.1674700000	1.6883630000	0.0540260000
O	5.0494840000	−0.7363840000	−0.7737690000
N	0.4185690000	2.6455720000	−0.5862450000
C	0.8481090000	1.8286690000	1.3854290000
H	0.3976570000	2.8184090000	−1.5837670000
C	−0.3073090000	3.3080900000	0.3467680000
N	−0.0710590000	2.8430710000	1.5576360000
H	1.2232520000	1.2582360000	2.2249450000
H	−0.9863750000	4.1086810000	0.0901070000
O	3.2218370000	−2.0456440000	−0.9367330000

Table S193. Cartesian coordinates of α -Gal-tg_His_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6210469			
ZPE / Hartree = 0.3646152			
BSSE / Hartree = 0.00137448808			
C	-3.6330630000	0.7930900000	1.2849290000
C	-4.6739360000	0.0770220000	0.4240190000
C	-4.0802390000	-1.1934040000	-0.1759950000
C	-2.7975650000	-0.8732770000	-0.9362480000
C	-1.8416160000	-0.1127900000	-0.0233840000
C	-0.6087530000	0.4118280000	-0.7529340000
O	-2.4651410000	1.0457670000	0.5368920000
O	-3.3873340000	-0.0274270000	2.3980210000
O	-5.8470660000	-0.2098090000	1.1633800000
O	-4.9846390000	-1.7859590000	-1.0949920000
O	-3.0704250000	-0.0744260000	-2.0778950000
O	0.1153200000	-0.6360260000	-1.3772300000
H	-3.9972520000	1.7751500000	1.5982300000
H	-4.9716820000	0.7498390000	-0.3851710000
H	-3.8410240000	-1.8990750000	0.6322840000
H	-2.3223060000	-1.8169270000	-1.2377750000
H	-1.5289550000	-0.7923790000	0.7798730000
H	-0.9110190000	1.1725720000	-1.4809050000
H	0.0600490000	0.8747400000	-0.0216510000
H	-2.9623190000	0.4925220000	3.0936210000
H	-5.5804320000	-0.6690110000	1.9748270000
H	-5.8529190000	-1.8400010000	-0.6699300000
H	-3.7984350000	-0.4939960000	-2.5595390000
H	-0.3205400000	-0.8647730000	-2.2090360000
N	5.4514360000	0.3593500000	0.7570870000
H	6.1586130000	0.1020110000	0.0584260000
H	5.9065600000	0.3070830000	1.6717910000
H	5.1556410000	1.3290320000	0.6100180000
C	4.3121630000	-0.6024330000	0.6582770000
H	3.7764470000	-0.5727890000	1.6085450000
C	3.3947120000	-0.2167040000	-0.4999680000
C	4.8887780000	-2.0202710000	0.4295320000

H	3.9664290000	-0.2246500000	-1.4360170000
H	2.6282480000	-0.9933580000	-0.5815390000
C	2.7481030000	1.1208970000	-0.3152510000
O	6.0918630000	-2.0838230000	0.0768650000
N	2.2479560000	1.8461700000	-1.3680540000
C	2.4783440000	1.8858070000	0.7961890000
H	2.2629970000	1.5682710000	-2.3414500000
C	1.6982970000	2.9822290000	-0.8750980000
N	1.8225320000	3.0453460000	0.4359060000
H	2.7168660000	1.6670330000	1.8282790000
H	1.2298850000	3.7212570000	-1.5090890000
O	4.0799660000	-2.9608670000	0.5896110000

Table S194. Cartesian coordinates of β -Gal-gg_His_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6255706			
ZPE / Hartree = 0.3654623			
BSSE / Hartree = 0.00250127161			
C	1.6317820000	0.6424830000	0.9382120000
C	3.0719790000	0.4968490000	0.4624370000
C	3.0758810000	-0.1005210000	-0.9357450000
C	2.2939670000	-1.4096100000	-0.9630890000
C	0.9063790000	-1.2073320000	-0.3524610000
C	0.1012970000	-2.4962250000	-0.2413850000
O	0.9984900000	-0.6268620000	0.9461240000
O	1.6537820000	1.1300650000	2.2396750000
O	3.7163350000	1.7550410000	0.3766240000
O	4.3937360000	-0.3833520000	-1.3738200000
O	2.9806420000	-2.4132160000	-0.2231510000
O	0.6013910000	-3.4028710000	0.7300890000
H	1.0821460000	1.3204790000	0.2677570000
H	3.6028640000	-0.1685950000	1.1566500000
H	2.5900370000	0.6127010000	-1.6190720000
H	2.1707210000	-1.7314380000	-2.0055980000
H	0.3502760000	-0.5285350000	-1.0195430000
H	-0.9236760000	-2.2589290000	0.0554000000
H	0.0715960000	-2.9601210000	-1.2367370000
H	0.7881410000	1.5031530000	2.4570490000
H	3.8641270000	2.0901930000	1.2715010000
H	4.9362130000	0.4064530000	-1.2354130000
H	3.8978250000	-2.4410450000	-0.5334450000
H	1.5472740000	-3.5253860000	0.5566320000
N	-4.1299080000	0.7118450000	-1.1533000000
H	-4.9860450000	0.7461080000	-0.5845480000
H	-4.4003540000	0.3806610000	-2.0822150000
H	-3.7398840000	1.6533000000	-1.2583000000
C	-3.1796620000	-0.2321170000	-0.4893630000
H	-2.5305970000	-0.6506410000	-1.2615570000
C	-2.3603560000	0.5022690000	0.5709820000
C	-4.0081730000	-1.3618350000	0.1731550000

H	-3.0322790000	0.8926460000	1.3444770000
H	-1.7082900000	-0.2370520000	1.0487810000
C	-1.5411870000	1.6217250000	0.0080500000
O	-5.2398740000	-1.1498790000	0.2949390000
N	-1.1068750000	2.6693570000	0.7834490000
C	-1.0331520000	1.8800110000	-1.2447130000
H	-1.3264520000	2.8148070000	1.7615040000
C	-0.3653260000	3.4938320000	0.0026820000
N	-0.2995290000	3.0480200000	-1.2364920000
H	-1.1496870000	1.2897240000	-2.1441050000
H	0.0914600000	4.3961180000	0.3830770000
O	-3.3547270000	-2.3572180000	0.5532100000

Table S195. Cartesian coordinates of β -Gal-gg_His_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6267365			
ZPE / Hartree = 0.3656107			
BSSE / Hartree = 0.00290338028			
C	-2.3113100000	1.1148330000	1.4165110000
C	-1.3253990000	1.4391330000	0.3002870000
C	-2.0712350000	1.6336970000	-1.0144540000
C	-3.0116690000	0.4653280000	-1.3199840000
C	-3.8870870000	0.2036050000	-0.0876270000
C	-4.8365530000	-0.9752830000	-0.2470850000
O	-3.0708980000	-0.0291900000	1.0596230000
O	-1.5823420000	0.8233040000	2.5637480000
O	-0.6275600000	2.6448870000	0.5598840000
O	-1.1686400000	1.7990100000	-2.0919220000
O	-2.3380570000	-0.6999230000	-1.7717560000
O	-4.1827570000	-2.2307520000	-0.3508030000
H	-2.9926780000	1.9638400000	1.5853950000
H	-0.6186950000	0.6037650000	0.2131780000
H	-2.6980130000	2.5326360000	-0.9072740000
H	-3.6667180000	0.7617820000	-2.1460460000
H	-4.5070930000	1.0991230000	0.0800240000
H	-5.4816390000	-1.0311190000	0.6330910000
H	-5.4671630000	-0.7853020000	-1.1257860000
H	-2.1581570000	0.8936760000	3.3375430000
H	0.0065510000	2.4888490000	1.2730470000
H	-0.5951610000	2.5503150000	-1.8838180000
H	-1.6360680000	-1.0000360000	-1.1539250000
H	-3.5317710000	-2.1506760000	-1.0654710000
N	4.4079060000	-1.6819480000	-0.5836460000
H	5.1329570000	-1.8543140000	0.1232160000
H	4.8225260000	-1.8981390000	-1.4931090000
H	3.6216620000	-2.3227570000	-0.4394140000
C	3.9950300000	-0.2490170000	-0.4986470000
H	3.5444940000	0.0203120000	-1.4551520000
C	3.0028890000	-0.0590430000	0.6485650000
C	5.2574030000	0.6130460000	-0.2551390000
H	3.4709030000	-0.3735940000	1.5885080000

H	2.8036740000	1.0140350000	0.7289420000
C	1.7223330000	-0.8096550000	0.4470630000
O	6.2880730000	0.0019080000	0.1183520000
N	0.9630030000	-1.2677380000	1.4984190000
C	1.0174230000	-1.1681240000	-0.6768390000
H	1.1893600000	-1.1743300000	2.4811970000
C	-0.1444930000	-1.8585830000	0.9978010000
N	-0.1471370000	-1.8195250000	-0.3220370000
H	1.2704600000	-0.9852380000	-1.7120410000
H	-0.9134370000	-2.2864750000	1.6246170000
O	5.1063820000	1.8430700000	-0.4244500000

Table S196. Cartesian coordinates of β -Gal-gg_His_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6247804			
ZPE / Hartree = 0.3648586			
BSSE / Hartree = 0.00211658677			
C	-3.2851750000	-0.9523430000	-0.5899880000
C	-2.1977790000	-0.5489960000	-1.5801050000
C	-0.9738420000	-0.0724220000	-0.8142240000
C	-1.3425830000	1.0354270000	0.1640260000
C	-2.5096070000	0.5794960000	1.0392890000
C	-3.0077200000	1.6500380000	2.0007400000
O	-3.6085940000	0.1528740000	0.2386140000
O	-4.4167770000	-1.3027390000	-1.3161190000
O	-1.7858320000	-1.6498480000	-2.3701390000
O	0.0200160000	0.4391830000	-1.6853270000
O	-1.7192400000	2.2182950000	-0.5319150000
O	-3.6441390000	2.7447930000	1.3610010000
H	-2.9386700000	-1.7888850000	0.0383110000
H	-2.5887270000	0.2613910000	-2.2102530000
H	-0.5779220000	-0.9235620000	-0.2421490000
H	-0.4812300000	1.2414770000	0.8139760000
H	-2.1444520000	-0.2645920000	1.6465130000
H	-3.7491430000	1.2068870000	2.6697800000
H	-2.1536280000	1.9853070000	2.6040100000
H	-5.0132420000	-1.8170450000	-0.7550700000
H	-2.4983820000	-1.8769350000	-2.9828380000
H	0.2070340000	-0.2298620000	-2.3595600000
H	-1.0146980000	2.4362910000	-1.1598390000
H	-3.0537450000	3.0565510000	0.6577530000
N	4.6726580000	-0.9336520000	0.1959920000
H	5.3985630000	-0.3795330000	0.6698960000
H	5.1340360000	-1.4512520000	-0.5551530000
H	4.2778740000	-1.6190110000	0.8461010000
C	3.6492800000	0.0206260000	-0.3343850000
H	3.2214120000	-0.4177300000	-1.2382140000
C	2.5672840000	0.2706670000	0.7121310000
C	4.3618610000	1.3488950000	-0.6919310000

H	3.0300180000	0.6396810000	1.6360310000
H	1.9267780000	1.0705260000	0.3263240000
C	1.7430580000	-0.9454700000	0.9961200000
O	5.5259080000	1.4974320000	-0.2455580000
N	0.8264250000	-0.9876330000	2.0178830000
C	1.6358810000	-2.1698600000	0.3782440000
H	0.6354010000	-0.2441950000	2.6787610000
C	0.2078160000	-2.1939680000	1.9798300000
N	0.6750640000	-2.9412970000	0.9994580000
H	2.1858440000	-2.5345170000	-0.4791090000
H	-0.5624680000	-2.4722560000	2.6849060000
O	3.6848430000	2.1533600000	-1.3683050000

Table S197. Cartesian coordinates of β -Gal-gg_His_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6239143			
ZPE / Hartree = 0.3642500			
BSSE / Hartree = 0.00173375040			
C	4.0401480000	0.3527170000	-0.6164840000
C	3.8145690000	-0.4320100000	0.6722190000
C	2.3947880000	-0.9767480000	0.6955170000
C	1.3860110000	0.1449200000	0.4799100000
C	1.7512640000	0.9329190000	-0.7775410000
C	0.8380700000	2.1235930000	-1.0363410000
O	3.0938210000	1.4059290000	-0.7058000000
O	5.3123370000	0.9091190000	-0.5573350000
O	4.6874740000	-1.5434010000	0.7615770000
O	2.0939920000	-1.5853150000	1.9394050000
O	1.3772930000	1.0326290000	1.5933340000
O	0.9777260000	3.1706360000	-0.0893810000
H	3.9330170000	-0.3078010000	-1.4916080000
H	3.9647430000	0.2515100000	1.5189120000
H	2.2857180000	-1.7050480000	-0.1222320000
H	0.3877110000	-0.2917730000	0.3458200000
H	1.6456760000	0.2468570000	-1.6336320000
H	1.0818190000	2.5518430000	-2.0116090000
H	-0.1957850000	1.7532610000	-1.0701360000
H	5.5898460000	1.1795850000	-1.4433400000
H	5.5844730000	-1.2224760000	0.9263090000
H	2.7988910000	-2.2152000000	2.1476630000
H	1.2621100000	0.5042590000	2.3968800000
H	0.9177810000	2.7769790000	0.7949310000
N	-4.8430760000	-1.3426600000	-0.0261130000
H	-5.5809900000	-1.0037820000	-0.6567080000
H	-5.3074660000	-1.8266060000	0.7457340000
H	-4.2533220000	-2.0253410000	-0.5114120000
C	-4.0690820000	-0.1590710000	0.4568280000
H	-3.6478120000	-0.4127650000	1.4310150000
C	-2.9641290000	0.1922300000	-0.5376510000
C	-5.0466170000	1.0324480000	0.6083560000
H	-3.4109720000	0.4288420000	-1.5109590000

H	-2.4809140000	1.1040980000	-0.1720050000
C	-1.9557770000	-0.9029090000	-0.6967980000
O	-6.1673430000	0.9090400000	0.0561520000
N	-1.0959940000	-0.9593670000	-1.7663000000
C	-1.6268450000	-1.9942490000	0.0748150000
H	-1.0567080000	-0.3022960000	-2.5361730000
C	-0.2959210000	-2.0424430000	-1.6072220000
N	-0.5899620000	-2.6977900000	-0.5020640000
H	-2.0735380000	-2.3078870000	1.0088470000
H	0.4740200000	-2.3031960000	-2.3196730000
O	-4.6020440000	2.0135230000	1.2434320000

Table S198. Cartesian coordinates of β -Gal-gg_His_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6245529			
ZPE / Hartree = 0.3649475			
BSSE / Hartree = 0.00207071535			
C	2.2351200000	-0.1460630000	1.5420460000
C	3.5518370000	-0.0084720000	0.7848620000
C	3.2761770000	0.4424780000	-0.6416260000
C	2.2763440000	-0.4876900000	-1.3202760000
C	1.0415320000	-0.6439380000	-0.4347040000
C	0.0011250000	-1.6044580000	-0.9918880000
O	1.4015590000	-1.0798360000	0.8741710000
O	2.5190090000	-0.6371760000	2.8103590000
O	4.3890830000	0.9712060000	1.3718800000
O	4.4608120000	0.4385520000	-1.4190670000
O	2.8526690000	-1.7690700000	-1.5448220000
O	0.4225000000	-2.9591980000	-1.0140950000
H	1.7192640000	0.8264530000	1.5963640000
H	4.0450500000	-0.9900470000	0.7761270000
H	2.8422360000	1.4538670000	-0.6102570000
H	1.9642370000	-0.0419010000	-2.2745100000
H	0.5689490000	0.3462970000	-0.3742030000
H	-0.8902960000	-1.5656680000	-0.3591170000
H	-0.2758040000	-1.2566020000	-1.9967580000
H	1.7664570000	-0.4737990000	3.3953730000
H	4.7339500000	0.6264410000	2.2066260000
H	5.1452500000	0.9172410000	-0.9295690000
H	3.6915450000	-1.6446400000	-2.0126650000
H	1.2946990000	-2.9879320000	-1.4370660000
N	-4.6196280000	0.9659900000	-0.8064420000
H	-5.4478610000	1.0173080000	-0.1967390000
H	-4.9493030000	0.7056940000	-1.7385500000
H	-4.1814890000	1.8880870000	-0.8780380000
C	-3.7083670000	-0.0729480000	-0.2335000000
H	-3.1783690000	-0.5487020000	-1.0612820000
C	-2.7257720000	0.5635410000	0.7448030000
C	-4.5786200000	-1.1291100000	0.4935940000

H	-3.2804610000	1.1192260000	1.5114730000
H	-2.2022420000	-0.2512180000	1.2560860000
C	-1.7314380000	1.4582430000	0.0721420000
O	-5.7745410000	-0.8140300000	0.7110860000
N	-0.8115250000	2.1905850000	0.7820610000
C	-1.4513260000	1.7296330000	-1.2475530000
H	-0.7251730000	2.2241630000	1.7906550000
C	-0.0264770000	2.8540870000	-0.1025790000
N	-0.3861920000	2.6014050000	-1.3454360000
H	-1.9450550000	1.3412320000	-2.1284460000
H	0.7810740000	3.5000880000	0.2112660000
O	-3.9855950000	-2.1808560000	0.8167430000

Table S199. Cartesian coordinates of β -Gal-gg_His_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6226131			
ZPE / Hartree = 0.3644441			
BSSE / Hartree = 0.00141093236			
C	4.2853700000	0.6954610000	0.2644820000
C	4.3268680000	-0.6979320000	-0.3541640000
C	3.0239180000	-0.9668590000	-1.0915000000
C	1.8286290000	-0.7449770000	-0.1717720000
C	1.9292900000	0.6287700000	0.4897330000
C	0.8216860000	0.8921510000	1.5016350000
O	3.1822350000	0.7873600000	1.1508760000
O	5.4534480000	0.8726030000	0.9967660000
O	5.3718250000	-0.8133020000	-1.3029130000
O	2.9603860000	-2.3050370000	-1.5545250000
O	1.7862170000	-1.7433960000	0.8422120000
O	0.9308660000	0.1149800000	2.6842730000
H	4.1880020000	1.4618230000	-0.5204800000
H	4.4528970000	-1.4280370000	0.4569290000
H	2.9495800000	-0.2652830000	-1.9358770000
H	0.9064770000	-0.7754030000	-0.7670570000
H	1.8316450000	1.3812010000	-0.3082000000
H	0.8632380000	1.9396100000	1.8113950000
H	-0.1403270000	0.7149590000	1.0012970000
H	5.5892980000	1.8153350000	1.1638460000
H	6.2177840000	-0.8189650000	-0.8348270000
H	3.7786210000	-2.5008290000	-2.0330880000
H	1.8553890000	-2.6090050000	0.4129920000
H	1.0250630000	-0.8119890000	2.4157400000
N	-5.0225980000	0.0359380000	-1.5033310000
H	-5.8419480000	0.5755580000	-1.2006890000
H	-5.3618260000	-0.6832510000	-2.1469960000
H	-4.3826400000	0.6434250000	-2.0235200000
C	-4.3731120000	-0.5707400000	-0.3019560000
H	-3.7351580000	-1.3837090000	-0.6521600000
C	-3.5553520000	0.4853350000	0.4415510000
C	-5.4774970000	-1.1369520000	0.6215550000
H	-4.2135780000	1.3073090000	0.7462450000

H	-3.1799980000	0.0154980000	1.3560320000
C	-2.4193510000	1.0269510000	-0.3700480000
O	-6.6519930000	-0.7642560000	0.3831460000
N	-1.9393800000	2.3026790000	-0.2020230000
C	-1.6194040000	0.4774020000	-1.3452590000
H	-2.2983680000	2.9922700000	0.4466410000
C	-0.8923250000	2.4740680000	-1.0451110000
N	-0.6701790000	1.3882250000	-1.7595190000
H	-1.6721430000	-0.5177020000	-1.7659690000
H	-0.3376890000	3.3999120000	-1.1001070000
O	-5.0756760000	-1.8885370000	1.5373000000

Table S200. Cartesian coordinates of β -Gal-gt_His_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6252924			
ZPE / Hartree = 0.3641248			
BSSE / Hartree = 0.00230770794			
C	-1.5451260000	0.2153340000	1.2519830000
C	-1.0423170000	-1.2117230000	1.0700300000
C	-1.1359690000	-1.5890020000	-0.4020670000
C	-2.5536260000	-1.3821770000	-0.9277590000
C	-3.0068470000	0.0372260000	-0.5965950000
C	-4.4537780000	0.3043800000	-0.9659020000
O	-2.8897810000	0.2947190000	0.8028370000
O	-1.5071360000	0.5272470000	2.6048890000
O	0.3179330000	-1.3380680000	1.4439270000
O	-0.7944790000	-2.9485210000	-0.6074130000
O	-3.4525950000	-2.3048440000	-0.3336130000
O	-4.7937950000	1.6648220000	-0.7410750000
H	-0.9290210000	0.9137050000	0.6686950000
H	-1.6752990000	-1.8812660000	1.6685370000
H	-0.4608260000	-0.9335790000	-0.9735270000
H	-2.5488840000	-1.5039110000	-2.0198040000
H	-2.3608310000	0.7402450000	-1.1468610000
H	-4.5983480000	0.1086670000	-2.0310900000
H	-5.1090520000	-0.3592450000	-0.3907380000
H	-1.5072330000	1.4890370000	2.7119500000
H	0.3844300000	-1.2544230000	2.4049290000
H	0.0453190000	-3.1215060000	-0.1570410000
H	-3.0422550000	-3.1812400000	-0.3795980000
H	-4.6713430000	1.8475820000	0.2010440000
N	4.4608940000	1.2739970000	-0.0237480000
H	5.0314150000	1.1367700000	-0.8660150000
H	5.1094410000	1.3742560000	0.7604150000
H	3.9310370000	2.1472200000	-0.1014420000
C	3.5722660000	0.0859050000	0.1545230000
H	3.2660190000	0.0602660000	1.2022730000
C	2.3566840000	0.1916610000	-0.7637170000
C	4.3819710000	-1.1894230000	-0.1812520000

H	2.6889010000	0.2486920000	-1.8075330000
H	1.7946450000	-0.7404380000	-0.6467470000
C	1.4822700000	1.3643960000	-0.4447670000
O	5.4747360000	-1.0188570000	-0.7740930000
N	0.5356710000	1.8336100000	-1.3226010000
C	1.3742910000	2.1838780000	0.6558260000
H	0.3386770000	1.4593720000	-2.2428060000
C	-0.0966560000	2.8832440000	-0.7416800000
N	0.3877410000	3.1282580000	0.4599570000
H	1.9442000000	2.1434820000	1.5748270000
H	-0.8906880000	3.4259040000	-1.2345090000
O	3.8414410000	-2.2681010000	0.1492970000

Table S201. Cartesian coordinates of β -Gal-gt_His_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6251847			
ZPE / Hartree = 0.3647390			
BSSE / Hartree = 0.00247037016			
C	-1.4074670000	-1.4211090000	0.5449970000
C	-1.1096450000	-0.0526180000	1.1469060000
C	-2.3870830000	0.5602710000	1.7019040000
C	-3.4773950000	0.6000990000	0.6337640000
C	-3.6324350000	-0.7897500000	0.0218360000
C	-4.5993640000	-0.8175730000	-1.1472330000
O	-2.3834630000	-1.2709340000	-0.4750240000
O	-0.2394560000	-1.9012020000	-0.0340300000
O	-0.1889110000	-0.1345260000	2.2202050000
O	-2.1599080000	1.8930270000	2.1294580000
O	-3.1421610000	1.5212770000	-0.3920710000
O	-4.7880090000	-2.1419730000	-1.6234680000
H	-1.7869230000	-2.1126690000	1.3134220000
H	-0.7168340000	0.5880480000	0.3478270000
H	-2.7401670000	-0.0565040000	2.5414490000
H	-4.4283380000	0.8848900000	1.1049370000
H	-3.9968780000	-1.4717980000	0.8056140000
H	-5.5751220000	-0.4515370000	-0.8189380000
H	-4.2267800000	-0.1677310000	-1.9469060000
H	-0.3171620000	-2.8550290000	-0.1736570000
H	0.7037460000	-0.2350390000	1.8608260000
H	-1.3441070000	1.9061260000	2.6515390000
H	-2.7681420000	2.3080630000	0.0333090000
H	-3.9292430000	-2.4717180000	-1.9226990000
N	4.6833160000	1.0288050000	-0.6047080000
H	5.2056280000	0.5496180000	-1.3472970000
H	5.3736070000	1.4763390000	0.0020870000
H	4.1007880000	1.7665470000	-1.0121220000
C	3.8769520000	0.0171580000	0.1427350000
H	3.6202830000	0.4527640000	1.1102280000
C	2.6209180000	-0.3379780000	-0.6500460000
C	4.7463360000	-1.2451940000	0.3552590000
H	2.9103910000	-0.7149090000	-1.6386770000

H	2.1190650000	-1.1580520000	-0.1270040000
C	1.6839750000	0.8196630000	-0.8053790000
O	5.7807330000	-1.3369250000	-0.3492820000
N	0.7366330000	0.8721110000	-1.7983570000
C	1.5083570000	1.9840120000	-0.0928230000
H	0.5767030000	0.1664550000	-2.5065470000
C	0.0385090000	2.0251710000	-1.6558820000
N	0.4790450000	2.7286970000	-0.6313380000
H	2.0619610000	2.3246410000	0.7719090000
H	-0.7702980000	2.2981470000	-2.3182720000
O	4.3042900000	-2.0646010000	1.1909090000

Table S202. Cartesian coordinates of β -Gal-gt_His_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6250026			
ZPE / Hartree = 0.3644757			
BSSE / Hartree = 0.00230427874			
C	1.6510420000	-1.1808520000	-1.1468730000
C	1.0233640000	-1.5011350000	0.2055440000
C	1.1926660000	-0.3050040000	1.1315250000
C	2.6574800000	0.1037090000	1.2394940000
C	3.2225730000	0.2960080000	-0.1646360000
C	4.7140240000	0.5732690000	-0.1726400000
O	3.0240900000	-0.8738910000	-0.9589310000
O	1.5582280000	-2.3111510000	-1.9485650000
O	-0.3689150000	-1.7386400000	0.0933770000
O	0.7244630000	-0.5955610000	2.4375860000
O	3.4140860000	-0.8893130000	1.9132930000
O	5.1767210000	0.8442300000	-1.4875130000
H	1.1453560000	-0.3178330000	-1.6096840000
H	1.5363710000	-2.3776940000	0.6241920000
H	0.6329070000	0.5376210000	0.7040790000
H	2.7201930000	1.0614240000	1.7757180000
H	2.6953700000	1.1432990000	-0.6312510000
H	4.9201870000	1.4606220000	0.4305500000
H	5.2484260000	-0.2808330000	0.2581330000
H	1.6840240000	-2.0610280000	-2.8742780000
H	-0.5084160000	-2.6107620000	-0.2997210000
H	-0.1360480000	-1.0331050000	2.3574730000
H	2.9211410000	-1.1390680000	2.7089880000
H	4.9900250000	0.0660350000	-2.0310820000
N	-4.3356290000	0.9975140000	-1.2121320000
H	-5.2067590000	1.1437290000	-0.6875870000
H	-4.6017390000	0.7111280000	-2.1568740000
H	-3.8219270000	1.8803450000	-1.2851560000
C	-3.5482980000	-0.0682010000	-0.5194760000
H	-2.8820290000	-0.5196860000	-1.2568900000
C	-2.7531530000	0.5336680000	0.6359980000
C	-4.5323400000	-1.1375570000	0.0123810000

H	-3.4383640000	1.0392820000	1.3271880000
H	-2.2948500000	-0.3011690000	1.1760990000
C	-1.6897520000	1.4822800000	0.1798240000
O	-5.7448000000	-0.8143870000	0.0486230000
N	-1.0849350000	2.3697080000	1.0354620000
C	-1.0465970000	1.6615880000	-1.0231980000
H	-1.3101030000	2.4999900000	2.0140940000
C	-0.1189860000	3.0278530000	0.3476170000
N	-0.0685920000	2.6274980000	-0.9078330000
H	-1.2257590000	1.1458910000	-1.9572210000
H	0.5036580000	3.7845140000	0.8029110000
O	-4.0063370000	-2.2099720000	0.3831890000

Table S203. Cartesian coordinates of β -Gal-gt_His_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6239666			
ZPE / Hartree = 0.3642916			
BSSE / Hartree = 0.00178849826			
C	4.0221390000	0.5294630000	-0.4184210000
C	3.8569980000	-0.5687320000	0.6275330000
C	2.4506710000	-1.1456210000	0.5513000000
C	1.4050010000	-0.0410170000	0.6667600000
C	1.7113150000	1.0453530000	-0.3589230000
C	0.7912810000	2.2457840000	-0.2462160000
O	3.0438800000	1.5340580000	-0.2012020000
O	5.2798500000	1.0951270000	-0.2499750000
O	4.7555300000	-1.6396920000	0.4022790000
O	2.2171890000	-2.0661860000	1.6035350000
O	1.4166450000	0.5348170000	1.9644610000
O	1.0056760000	3.1583670000	-1.3129110000
H	3.9024330000	0.1181500000	-1.4329150000
H	4.0218200000	-0.1223640000	1.6176300000
H	2.3269020000	-1.6413690000	-0.4235020000
H	0.4146750000	-0.4654750000	0.4506410000
H	1.6045810000	0.6071450000	-1.3637500000
H	-0.2479560000	1.9131680000	-0.3128630000
H	0.9431670000	2.7362980000	0.7217070000
H	5.5245660000	1.5821790000	-1.0487330000
H	5.6499870000	-1.3486780000	0.6256530000
H	2.9564080000	-2.6908230000	1.6288210000
H	1.4063000000	-0.1926700000	2.6039450000
H	1.9177820000	3.4746110000	-1.2540150000
N	-4.9238300000	-0.9615500000	-0.8039330000
H	-5.3810550000	-0.2240050000	-1.3511140000
H	-5.6618460000	-1.5931620000	-0.4848480000
H	-4.2941750000	-1.4989090000	-1.4073150000
C	-4.2034850000	-0.3396780000	0.3461260000
H	-4.0111320000	-1.1289040000	1.0746650000
C	-2.8947970000	0.2852840000	-0.1397470000
C	-5.1131980000	0.7408850000	0.9760690000

H	-3.1160020000	1.0429550000	-0.9011020000
H	-2.4486120000	0.8048620000	0.7142520000
C	-1.9369880000	-0.7246250000	-0.6937220000
O	-6.1016020000	1.1087450000	0.2956290000
N	-1.1065580000	-0.4551080000	-1.7544920000
C	-1.6216120000	-2.0113200000	-0.3206570000
H	-1.0708120000	0.4113270000	-2.2783330000
C	-0.3345880000	-1.5471300000	-1.9740020000
N	-0.6203220000	-2.5143450000	-1.1239060000
H	-2.0544970000	-2.5949700000	0.4801870000
H	0.4084520000	-1.5834920000	-2.7579990000
O	-4.7462230000	1.1621720000	2.0955220000

Table S204. Cartesian coordinates of β -Gal-gt_His_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6258578			
ZPE / Hartree = 0.3648716			
BSSE / Hartree = 0.00215032855			
C	-3.2052810000	-0.5159490000	-1.1085830000
C	-3.8576930000	-0.0565620000	0.1916470000
C	-2.8207100000	0.6215440000	1.0766060000
C	-1.6116720000	-0.2841890000	1.2922430000
C	-1.0981100000	-0.7608240000	-0.0619830000
C	0.0351210000	-1.7626940000	0.0459780000
O	-2.1373030000	-1.3993120000	-0.8050670000
O	-4.1558100000	-1.2100190000	-1.8464570000
O	-4.8814600000	0.8928040000	-0.0456710000
O	-3.3591260000	0.9243790000	2.3526340000
O	-1.9589450000	-1.4143300000	2.0771490000
O	0.5503470000	-2.0855190000	-1.2375180000
H	-2.8143370000	0.3470110000	-1.6713440000
H	-4.2584380000	-0.9430140000	0.7019620000
H	-2.4808360000	1.5404340000	0.5760310000
H	-0.8174160000	0.2941270000	1.7847370000
H	-0.7455960000	0.1187440000	-0.6220300000
H	0.8547520000	-1.3213450000	0.6218510000
H	-0.3133440000	-2.6641800000	0.5622760000
H	-3.8646410000	-1.2753490000	-2.7663750000
H	-5.6448130000	0.4401120000	-0.4290500000
H	-4.1990340000	1.3883240000	2.2246400000
H	-2.4663900000	-1.0946970000	2.8377800000
H	-0.1689190000	-2.4763530000	-1.7534340000
N	4.4665060000	1.3636360000	0.7165230000
H	5.3319100000	1.3040560000	0.1651550000
H	4.7430480000	1.4498090000	1.6973770000
H	3.9526140000	2.2117430000	0.4608780000
C	3.6788010000	0.1155760000	0.4762890000
H	3.0258950000	-0.0356280000	1.3383010000
C	2.8659610000	0.2475660000	-0.8084810000
C	4.6664390000	-1.0711670000	0.3658260000
H	3.5328540000	0.5320700000	-1.6319960000

H	2.460200000	-0.740866000	-1.048403000
C	1.747499000	1.235867000	-0.688284000
O	5.874688000	-0.779007000	0.191278000
N	1.037110000	1.676716000	-1.778049000
C	1.164442000	1.866332000	0.386917000
H	1.196300000	1.409985000	-2.741863000
C	0.075586000	2.527037000	-1.339844000
N	0.123294000	2.669579000	-0.030112000
H	1.431982000	1.784812000	1.432134000
H	-0.620767000	3.009207000	-2.010966000
O	4.146900000	-2.206965000	0.431630000

Table S205. Cartesian coordinates of β -Gal-gt_His_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6220208			
ZPE / Hartree = 0.3641650			
BSSE / Hartree = 0.00135090999			
C	4.1019620000	1.4545710000	-0.0167910000
C	4.6015030000	0.0666580000	-0.4051480000
C	3.5053550000	-0.6911100000	-1.1411140000
C	2.2201060000	-0.7185970000	-0.3185120000
C	1.8571460000	0.7056660000	0.0903710000
C	0.6539760000	0.7665010000	1.0114650000
O	2.9390860000	1.3249890000	0.7859800000
O	5.0922190000	2.0701170000	0.7386940000
O	5.7114910000	0.1393110000	-1.2816720000
O	3.8882640000	-2.0352450000	-1.3788500000
O	2.3897760000	-1.5033460000	0.8504720000
O	0.2893390000	2.1098430000	1.2922040000
H	3.8607740000	2.0440310000	-0.9151560000
H	4.8667290000	-0.4688250000	0.5164670000
H	3.3033430000	-0.1770260000	-2.0922880000
H	1.4065060000	-1.1246540000	-0.9370270000
H	1.6378260000	1.2801260000	-0.8230630000
H	-0.2013250000	0.2998380000	0.5153800000
H	0.8672210000	0.2189900000	1.9368400000
H	4.9339760000	3.0238370000	0.7640170000
H	6.4842000000	0.4382000000	-0.7833560000
H	4.7774350000	-2.0337520000	-1.7619700000
H	2.8045990000	-2.3368830000	0.5826470000
H	1.0401790000	2.5339170000	1.7304370000
N	-5.4958550000	-0.8114660000	0.4136480000
H	-6.0422900000	-1.0741390000	-0.4149110000
H	-6.1666420000	-0.5945610000	1.1547650000
H	-4.9336860000	-1.6097110000	0.7242920000
C	-4.6579060000	0.3783150000	0.0747830000
H	-4.3826400000	0.8626330000	1.0131480000
C	-3.4157610000	-0.0557370000	-0.7006450000
C	-5.5081630000	1.3460490000	-0.7832870000

H	-3.7220180000	-0.5688210000	-1.6203560000
H	-2.8877750000	0.8558040000	-0.9984550000
C	-2.5074170000	-0.9422520000	0.0935700000
O	-6.5569450000	0.8728320000	-1.2847410000
N	-1.5490970000	-1.7244500000	-0.5030780000
C	-2.3616140000	-1.1775810000	1.4414620000
H	-1.3735180000	-1.7947100000	-1.4977450000
C	-0.8724720000	-2.3801870000	0.4718510000
N	-1.3399080000	-2.0771580000	1.6660910000
H	-2.9293700000	-0.7504020000	2.2573280000
H	-0.0591840000	-3.0585150000	0.2563500000
O	-5.0395560000	2.4980460000	-0.9160880000

Table S206. Cartesian coordinates of β -Gal-tg_His_H1 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6244189			
ZPE / Hartree = 0.3644458			
BSSE / Hartree = 0.00256505572			
C	1.7755130000	0.6775700000	0.9717680000
C	3.1324950000	0.3553020000	0.3592640000
C	2.9220000000	-0.4365160000	-0.9229520000
C	2.0670920000	-1.6734820000	-0.6650800000
C	0.7839710000	-1.2695190000	0.0583830000
C	-0.0540500000	-2.4613120000	0.5071160000
O	1.0767930000	-0.5280030000	1.2405810000
O	1.9829110000	1.3440320000	2.1730990000
O	3.8312020000	1.5351330000	0.0042260000
O	4.1562790000	-0.8760650000	-1.4642890000
O	2.7660230000	-2.6127650000	0.1368320000
O	-0.4607310000	-3.2533440000	-0.5989440000
H	1.1872550000	1.2892640000	0.2729440000
H	3.7096520000	-0.2404840000	1.0793780000
H	2.3961980000	0.2082930000	-1.6442540000
H	1.8020300000	-2.1216270000	-1.6325600000
H	0.1897390000	-0.6473450000	-0.6298860000
H	0.5106230000	-3.0547810000	1.2336400000
H	-0.9651170000	-2.0910620000	0.9832290000
H	1.1722800000	1.8087670000	2.4252920000
H	4.1096230000	1.9871750000	0.8122460000
H	4.7577290000	-0.1182600000	-1.5000320000
H	3.6525050000	-2.7150260000	-0.2398330000
H	0.2598390000	-3.8487100000	-0.8431790000
N	-3.8567650000	0.6926400000	-1.3448690000
H	-4.8212610000	0.6905460000	-0.9808230000
H	-3.8836530000	0.2915020000	-2.2847670000
H	-3.5154740000	1.6542870000	-1.4290020000
C	-3.0353080000	-0.1356620000	-0.4071490000
H	-2.3149100000	-0.7034860000	-1.0004520000
C	-2.3198800000	0.7547310000	0.6066840000
C	-3.9901540000	-1.1139200000	0.3268980000
H	-3.0625120000	1.2847420000	1.2159710000

H	-1.7616370000	0.0937940000	1.2787400000
C	-1.3929720000	1.7432790000	-0.0298700000
O	-5.2201520000	-0.8906430000	0.2011560000
N	-0.8656540000	2.8025180000	0.6677790000
C	-0.8628150000	1.8596870000	-1.2947310000
H	-1.0511690000	3.0281180000	1.6376870000
C	-0.0536130000	3.4967410000	-0.1677920000
N	-0.0282400000	2.9553940000	-1.3696170000
H	-1.0277840000	1.2143040000	-2.1478180000
H	0.4846600000	4.3787810000	0.1480730000
O	-3.4332840000	-2.0088520000	0.9969780000

Table S207. Cartesian coordinates of β -Gal-tg_His_H2 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6244208			
ZPE / Hartree = 0.3639138			
BSSE / Hartree = 0.00268967884			
C	-0.9522920000	-0.6489820000	1.5592990000
C	-1.3119750000	0.7775920000	1.1615800000
C	-2.7968590000	0.8635840000	0.8499120000
C	-3.1770510000	-0.1593450000	-0.2167100000
C	-2.6794270000	-1.5420720000	0.1998360000
C	-2.8585230000	-2.5916680000	-0.8931220000
O	-1.2838350000	-1.5192500000	0.4869810000
O	0.4200960000	-0.7091110000	1.7639080000
O	-1.0401560000	1.7026950000	2.1975760000
O	-3.1328370000	2.1485290000	0.3523410000
O	-2.5950150000	0.1733650000	-1.4679020000
O	-4.2136670000	-2.6991570000	-1.2978040000
H	-1.5060700000	-0.9564970000	2.4602900000
H	-0.7402440000	1.0274020000	0.2603300000
H	-3.3671170000	0.6470390000	1.7653260000
H	-4.2718300000	-0.1871690000	-0.3031090000
H	-3.2392990000	-1.8466430000	1.0971030000
H	-2.2102510000	-2.3455920000	-1.7404420000
H	-2.5608290000	-3.5650210000	-0.4969150000
H	0.6421480000	-1.5275070000	2.2294300000
H	-0.0932900000	1.9022280000	2.1893070000
H	-2.7051330000	2.8084660000	0.9181390000
H	-2.7329230000	1.1219720000	-1.6103880000
H	-4.4122470000	-1.9861810000	-1.9191300000
N	4.4633990000	0.5673510000	-0.2234890000
H	5.0670650000	0.0646490000	-0.8868920000
H	5.0359160000	0.7814780000	0.5960990000
H	4.1610910000	1.4556220000	-0.6334510000
C	3.3186140000	-0.3311670000	0.1236230000
H	2.9726810000	-0.0634520000	1.1237020000
C	2.1973510000	-0.1683470000	-0.8976950000
C	3.8332680000	-1.7919930000	0.1268050000

H	2.5891580000	-0.3562970000	-1.9052220000
H	1.4505480000	-0.9391010000	-0.6823800000
C	1.5518870000	1.1801160000	-0.8362820000
O	4.9454210000	-1.9945600000	-0.4200010000
N	0.6410470000	1.5964170000	-1.7749700000
C	1.6147230000	2.2120740000	0.0724560000
H	0.3391520000	1.0704050000	-2.5860840000
C	0.1846140000	2.8199610000	-1.4077330000
N	0.7571020000	3.2296600000	-0.2932570000
H	2.2184630000	2.2775090000	0.9685980000
H	-0.5509810000	3.3610870000	-1.9855930000
O	3.0671410000	-2.6296270000	0.6513350000

Table S208. Cartesian coordinates of β -Gal-tg_His_H3 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6316706			
ZPE / Hartree = 0.3654192			
BSSE / Hartree = 0.00298679981			
C	-0.4818390000	-1.1108440000	-0.8004490000
C	-1.2320060000	-0.1039650000	-1.6666820000
C	-1.9798000000	0.8624550000	-0.7647530000
C	-2.8952900000	0.1069020000	0.1948690000
C	-2.1174470000	-1.0024870000	0.9024530000
C	-3.0299380000	-1.9380040000	1.6927530000
O	-1.4278360000	-1.8356700000	-0.0254870000
O	0.2149140000	-1.9903010000	-1.6057370000
O	-0.3354180000	0.6603330000	-2.4531790000
O	-2.7906110000	1.7577040000	-1.5091360000
O	-3.9872800000	-0.4825080000	-0.4952220000
O	-3.8955830000	-1.2238370000	2.5596560000
H	0.1897150000	-0.5749690000	-0.1128020000
H	-1.9387690000	-0.6539480000	-2.3041440000
H	-1.2398500000	1.4213850000	-0.1705040000
H	-3.2639320000	0.8133500000	0.9510700000
H	-1.3915530000	-0.5234980000	1.5784430000
H	-3.5987480000	-2.5546700000	0.9890620000
H	-2.4169380000	-2.5938550000	2.3146780000
H	1.1261220000	-2.1333580000	-1.2430270000
H	0.1158170000	0.0600110000	-3.0638390000
H	-2.2505600000	2.1414000000	-2.2149070000
H	-4.3675130000	0.1950050000	-1.0735510000
H	-4.6152690000	-0.8522840000	2.0311300000
N	3.8726500000	0.0157240000	1.6342210000
H	4.8182750000	-0.0664910000	1.2394100000
H	3.8493380000	-0.5609110000	2.4790810000
H	3.7026540000	0.9853320000	1.9157230000
C	2.8953200000	-0.4701450000	0.6128580000
H	2.0179820000	-0.8369550000	1.1497230000
C	2.5254470000	0.6611120000	-0.3451460000
C	3.5366750000	-1.6495990000	-0.1513200000
H	3.4424730000	1.1345430000	-0.7179050000

H	2.0225890000	0.2194500000	-1.2133980000
C	1.6284840000	1.6798490000	0.2876480000
O	4.7695340000	-1.8012560000	-0.0328670000
N	1.2452630000	2.8251430000	-0.3651820000
C	0.9882530000	1.7391980000	1.5041450000
H	1.5245070000	3.1010630000	-1.2984860000
C	0.4100980000	3.5154660000	0.4492740000
N	0.2320010000	2.8894050000	1.5957100000
H	1.0259360000	1.0218200000	2.3134100000
H	-0.0325340000	4.4578230000	0.1601540000
O	2.7451680000	-2.3409370000	-0.8450850000

Table S209. Cartesian coordinates of β -Gal-tg_His_H4 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6235494			
ZPE / Hartree = 0.3646352			
BSSE / Hartree = 0.00194754418			
C	4.1037940000	0.2012380000	0.2756420000
C	3.6407520000	-0.3129060000	-1.0833650000
C	2.1435030000	-0.0881380000	-1.2317220000
C	1.3843970000	-0.7007820000	-0.0588570000
C	1.9884010000	-0.2025570000	1.2521380000
C	1.3872690000	-0.8718390000	2.4837640000
O	3.3862000000	-0.4699520000	1.3004530000
O	5.4522980000	-0.1018600000	0.4119530000
O	4.2726070000	0.3802720000	-2.1439010000
O	1.6505790000	-0.6871630000	-2.4178310000
O	1.4589370000	-2.1170380000	-0.0833300000
O	-0.0181070000	-0.6581350000	2.5528950000
H	3.9266710000	1.2849700000	0.3594860000
H	3.8604620000	-1.3881110000	-1.1332540000
H	1.9508920000	0.9958450000	-1.2425250000
H	0.3378090000	-0.3740850000	-0.1165090000
H	1.8188240000	0.8840470000	1.3111670000
H	1.6196930000	-1.9406740000	2.4738340000
H	1.8274870000	-0.4240630000	3.3772960000
H	5.8356530000	0.4393080000	1.1158480000
H	5.2008060000	0.1121430000	-2.1817010000
H	2.2109340000	-0.4054100000	-3.1551980000
H	1.2190120000	-2.4063660000	-0.9760220000
H	-0.4683320000	-1.3379950000	2.0324340000
N	-4.9061940000	0.8860730000	0.0130410000
H	-5.3443730000	0.4557170000	0.8365400000
H	-5.6600850000	1.1225950000	-0.6361550000
H	-4.4378430000	1.7575960000	0.2799360000
C	-3.9594480000	-0.1034580000	-0.5845970000
H	-3.8189620000	0.1652600000	-1.6327560000
C	-2.6317870000	-0.0741150000	0.1714590000
C	-4.5953480000	-1.5111140000	-0.4855800000

H	-2.8104490000	-0.3166360000	1.2266060000
H	-2.0082680000	-0.8745890000	-0.2417130000
C	-1.9298000000	1.2455690000	0.0704860000
O	-5.5681160000	-1.6295760000	0.2989750000
N	-0.9986560000	1.6448040000	0.9973470000
C	-1.9855280000	2.2738070000	-0.8421670000
H	-0.6714600000	1.0742410000	1.7775750000
C	-0.5227240000	2.8538190000	0.6165450000
N	-1.1024290000	3.2743390000	-0.4916550000
H	-2.6079200000	2.3503420000	-1.7236300000
H	0.2354280000	3.3812570000	1.1780330000
O	-4.0476380000	-2.3976790000	-1.1770790000

Table S210. Cartesian coordinates of β -Gal-tg_His_H5 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6247037			
ZPE / Hartree = 0.3645652			
BSSE / Hartree = 0.00255747008			
C	3.2177030000	0.0588140000	-0.5852470000
C	2.7042390000	-1.3695780000	-0.7340060000
C	1.2055000000	-1.3975180000	-0.4782540000
C	0.8686000000	-0.7647070000	0.8668880000
C	1.5207900000	0.6113530000	0.9681050000
C	1.3748480000	1.2325160000	2.3546930000
O	2.9223840000	0.5297940000	0.7201830000
O	4.5980400000	0.0347410000	-0.7426470000
O	2.9100370000	-1.8612890000	-2.0458850000
O	0.7069110000	-2.7246360000	-0.4598350000
O	1.3312490000	-1.5637630000	1.9441990000
O	0.0206660000	1.2585110000	2.7775690000
H	2.7422070000	0.7200080000	-1.3271020000
H	3.2215610000	-1.9969350000	0.0048060000
H	0.7081220000	-0.8142350000	-1.2680770000
H	-0.2214070000	-0.6461180000	0.9283940000
H	1.0516440000	1.2637990000	0.2170330000
H	1.9992910000	0.6794790000	3.0641800000
H	1.7209410000	2.2682210000	2.3172370000
H	4.9188620000	0.9294840000	-0.9211800000
H	3.8565180000	-2.0072980000	-2.1787760000
H	1.0107030000	-3.1750800000	-1.2608830000
H	1.0268860000	-2.4697840000	1.7875640000
H	-0.2218880000	0.3783470000	3.0965250000
N	-3.6581510000	-0.1839510000	-1.7229270000
H	-4.6444690000	-0.3235900000	-1.4596600000
H	-3.4569970000	-0.8299380000	-2.4892180000
H	-3.5246700000	0.7676350000	-2.0753460000
C	-2.8327720000	-0.4920010000	-0.5122340000
H	-1.9098660000	-0.9707680000	-0.8493340000
C	-2.5295930000	0.7846520000	0.2660600000
C	-3.6230390000	-1.4900610000	0.3713060000
H	-3.4661670000	1.3232010000	0.4596430000

H	-2.1253810000	0.4922950000	1.2410500000
C	-1.5502090000	1.6697490000	-0.4391740000
O	-4.8309100000	-1.6652120000	0.0770830000
N	-1.1121060000	2.8541540000	0.0998170000
C	-0.8783110000	1.5600100000	-1.6350140000
H	-1.3938020000	3.2424900000	0.9916230000
C	-0.2123520000	3.3999890000	-0.7547400000
N	-0.0459180000	2.6441330000	-1.8223600000
H	-0.9398200000	0.7652560000	-2.3669390000
H	0.2827280000	4.3387790000	-0.5521600000
O	-2.9726530000	-2.0025080000	1.3079080000

Table S211. Cartesian coordinates of β -Gal-tg_His_H6 optimized at the M06-2X/6-31++G(d,p) level in water (IEF-PCM/Bondi)

Energy / Hartree = -1235.6205547			
ZPE / Hartree = 0.3640431			
BSSE / Hartree = 0.00136086664			
C	-3.5302840000	1.1921590000	-0.0676690000
C	-4.3133310000	0.0008780000	-0.6084330000
C	-4.1196800000	-1.1952800000	0.3119170000
C	-2.6375970000	-1.4889690000	0.5243660000
C	-1.9190490000	-0.2126540000	0.9551130000
C	-0.4035830000	-0.3712360000	1.0106280000
O	-2.1588080000	0.8441010000	0.0293700000
O	-3.6537190000	2.2369010000	-0.9757090000
O	-5.7036170000	0.2671640000	-0.6513900000
O	-4.7109210000	-2.3622610000	-0.2345780000
O	-2.0362240000	-1.9650620000	-0.6693530000
O	-0.0138670000	-1.4094550000	1.8950440000
H	-3.9044120000	1.4805600000	0.9271280000
H	-3.9288990000	-0.2337860000	-1.6103270000
H	-4.5714620000	-0.9593280000	1.2867450000
H	-2.5414890000	-2.2372830000	1.3226860000
H	-2.2969080000	0.0706110000	1.9494610000
H	-0.0221860000	-0.5494510000	-0.0004100000
H	0.0329930000	0.5579450000	1.3866690000
H	-3.4055380000	3.0681450000	-0.5479750000
H	-5.8820080000	0.8855940000	-1.3726830000
H	-5.6170420000	-2.1480210000	-0.4995400000
H	-2.5975170000	-2.6739200000	-1.0164630000
H	-0.1078370000	-2.2577180000	1.4415940000
N	5.3666450000	0.8122320000	-0.0995600000
H	5.8831430000	0.6370440000	-0.9710300000
H	6.0558640000	0.8573590000	0.6545840000
H	4.9017160000	1.7234950000	-0.1459950000
C	4.4037410000	-0.3138550000	0.1014700000
H	4.2221330000	-0.4079300000	1.1732670000
C	3.1020010000	-0.0348400000	-0.6465390000
C	5.0571700000	-1.6131170000	-0.4299940000

H	3.3158880000	0.1000300000	−1.7138960000
H	2.4771780000	−0.9293800000	−0.5518130000
C	2.3708010000	1.1597300000	−0.1169000000
O	6.0651030000	−1.4715850000	−1.1650310000
N	1.3665990000	1.7752770000	−0.8225400000
C	2.4413560000	1.8533560000	1.0690930000
H	1.0363700000	1.5119000000	−1.7429440000
C	0.8699060000	2.7797270000	−0.0604280000
N	1.5010870000	2.8629830000	1.0941570000
H	3.1103810000	1.6824190000	1.9018890000
H	0.0622840000	3.4149040000	−0.3950640000
O	4.4880930000	−2.6750560000	−0.0953570000
