Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

For

Conformational Mapping and Energetics of Saccharide-Aromatic Residue Interactions: Implications in Protein Engineering and Discrimination of Anomers and Epimers

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Table S1. Interaction energy (in kcal/mol) and some characteristics of key inter-atomic atom contacts D-H...A for the binary complexes of *p*-OHTol. These are the electron density at the H...A bond critical point (ρ_{bcp}, in a.u.), H...A (and H...centroid) distance (**BL**, in Å), CE1-CZ-OH-HH dihedral angle (**DA**, in degrees) and the type of interaction (**INT**). The non-stacking complexes are highlighted in gray.

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-1a	–16.40	OH–H···O6	3.09	1.86	28	OH···O
		O1–H···CD1	1.32	2.38		OH···π
		CE1–H···O6	0.86	2.58		CH···O
Y-1b	–14.49	OH–H···O6	3.13	1.89	-48	OH···O
		O4–H···CD1	1.03	2.50		OH···π
		C6–H···OH	1.00	2.54		CH···O
		C4–H···CE2	0.80	2.76 (2.46)		CH···π
		CB–H···O3	0.78	2.60		CH···O
Y-1c	–13.63	OH–H···O6	2.87	1.90	-158	OH···O
		O1–H···CE1	1.34	2.40		OH···π
		C5–H···CE2	0.78	2.69		CH···π
Y-1d	–12.31	OH–H···O6	1.63	2.20	51	OH···O
		OH–H···O5	1.36	2.28		OH···O
		C6–H···OH	1.15	2.48		CH···O
		C1–H···CE1	0.83	2.70		CH···π
		C2–H···CG	0.67	2.82 (2.69)		CH···π
		C4–H···CE2	0.41	3.05		CH···π
Y-1e	–11.50	OH–H···O3	2.60	1.96	-133	OH···O
		C4–H···CZ	1.40	2.42 (2.27)		CH···π
		C2–H···OH	0.73	2.66		CH···O
		CB–H···O6	0.61	2.68		CH···O
		C6–H···CD1	0.54	2.92		CH···π
Y-1f	–11.50	OH–H···O3	2.60	1.96	46	OH···O
		C4–H···CZ	1.40	2.42 (2.27)		CH···π
		C2–H···OH	0.73	2.66		CH···O
		CB–H···O6	0.61	2.68		CH···O
		C6–H···CD2	0.54	2.92		CH···π
Y-1g	–10.16	O6–H···OH	1.54	2.27	-8	OH···O
		C2–H···CG	1.24	2.47 (2.31)		CH···π
		C4–H···CE1	0.91	2.59		CH···π
		CB–H1···O2	0.41	2.87		CH···O
		CB–H2···O3	0.26	3.11		CH···O

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-1h	–9.95	OH–H···O6	1.73	2.18	-32	OH···O
		C6–H···CE1	1.02	2.57		CH···π
		C2–H···CD2	0.89	2.66		CH···π
		C4–H···CD1	0.68	2.77		CH···π
		CB–H···O3	0.30	3.06		CH···O
Y-1i	–9.66	OH–H···O5	2.30	2.02	-125	OH···O
		C6–H···OH	1.00	2.49		CH···O
		C2–H···CE2–CZ	0.96	2.57 (2.35)		CH···π
		C1–H···CE2	0.61	2.87		CH···π
		C4–H···CE1	0.47	2.97		CH···π
Y-1j	–9.23	O1–H···OH	2.19	2.03	177	OH···O
		C5–H···CE1	1.02	2.60 (2.30)		CH···π
		C6–H···CE2	0.52	3.02		CH···π
		CB–H···O4	0.49	2.80		CH···O
Y-1k	–8.73	O2–H···OH	0.99	2.47	7	OH···O
		C3–H···CG–CD1	0.98	2.54 (2.28)		CH···π
		O1–H···CE1	0.91	2.51		OH···π
		CB–H···O4	0.62	2.72		CH···O
Y-1l	–8.49	C3–H···CD1	1.00	2.61 (2.32)	177	CH···π
		O2–H···OH	1.55	2.22		OH···O
		O3–H···CE2	0.88	2.70		OH···π
		CB–H···O4	0.66	2.67		CH···O
Y-1m	–8.41	C3–H···CG–CD1	1.00	2.53 (2.27)	7	CH···π
		O2–H···OH	0.98	2.48		OH···O
		O1–H···CE1	0.89	2.53		OH···π
		CB–H···O4	0.62	2.72		CH···O
Y-1n	–8.16	OH–H···O5	2.57	1.96	-46	OH···O
		C2–H···CE2	0.74	2.69		CH···π
		C2–H···OH	0.67	2.74		CH···O
		C4–H···CE1–CZ	0.50	2.96		CH···π
Y-1o	–7.83	C2–H···OH	1.05	2.52	-17	CH···O
		C2–H···CZ	1.02	2.55		CH···π
		CB–H···O6	0.93	2.53		CH···O
		C1–H···CE2	0.89	2.64		CH···π
		C6–H···CD1	0.45	3.04		CH···π
		C4–H···CE1	0.30	3.30		CH···π
Y-1p	–7.83	C2–H···OH	1.05	2.52	166	CH···O
		C2–H···CZ	1.02	2.55		CH···π
		CB–H···O6	0.93	2.53		CH···O
		C1–H···CE1	0.89	2.64		CH···π
		C6–H···CD2	0.45	3.04		CH···π
		C4–H···CE2	0.30	3.29		CH···π

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-1q	–7.66	O4–H···OH	1.06	2.39	-169	OH···O
		C5–H···CE1	0.87	2.70 (2.38)		CH···π
		C6–H···OH	0.75	2.66		CH···O
		C6–H···CZ–CE2	0.70	2.76		CH···π
		CB–H···O1	0.67	2.64		CH···O
Y-1r	–7.66	O4–H···OH	1.06	2.39	14	OH···O
		C5–H···CE2	0.87	2.70 (2.38)		CH···π
		C6–H···OH	0.75	2.66		CH···O
		C6–H···CZ–CE1	0.70	2.76		CH···π
		CB–H···O1	0.67	2.64		CH···O
Y-1s	–6.73	CB–H···O6	0.88	2.57	-3	CH···O
		C1–H···OH	0.87	2.57		CH···O
		C6–H···CG–CD1	0.72	2.74		CH···π
		O6–H···CD2	0.63	2.71		OH···π
		C2–H···CE1	0.48	2.98		CH···π
		C2–H···OH	0.43	2.96		CH···O
		C4–H···CE1	0.26	3.37		CH···π
Y-1t	–6.34	C2–H···CD2	1.16	2.52 (2.23)	-179	CH···π
		C4–H···OH	0.72	2.68		CH···O
		C6–H···OH	0.58	2.75		CH···O
		CB–H···O2	0.33	2.99		CH···O
Y-1u	–6.17	CD1–H···O1	0.81	2.57	-4	CH···O
		C6–H···CD2–CG	0.79	2.66 (2.53)		CH···π
		CB–H1···O1	0.71	2.66		CH···O
		CB–H2···O5	0.65	2.83		CH···O
		C5–H···CD1	0.64	2.85		CH···π
Y-1v	–6.07	CD2–H···O1	0.80	2.57	-179	CH···O
		CB–H1···O1	0.80	2.58		CH···O
		C6–H···CE2	0.76	2.75 (2.56)		CH···π
		C5–H···CG	0.62	2.86		CH···π
Y-2a	–13.02	OH–H···O5	1.99	2.13	53	OH···O
		O1–H···OH	1.85	2.13		OH···O
		C6–H···CE1	0.94	2.62		CH···π
		C1–H···CE2	0.84	2.67		CH···π
		C5–H···CZ	0.73	2.82 (2.74)		CH···π
		O6–H···CD1	0.44	2.89		OH···π
Y-2b	–12.04	OH–H···O6	3.34	1.84		OH···O
		C5–H···CE2	1.06	2.55		CH···π
		CE2–H···O4	0.88	2.56		CH···O
		C3–H···CE2	0.35	3.19		CH···π

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-2c	–12.04	OH–H···O6	2.34	2.01		OH···O
		C5–H···CZ	1.24	2.49 (2.23)		CH···π
		C1–H···CE1	0.52	2.96		CH···π
		C3–H···CG	0.52	2.94		CH···π
		CB–H···O4	0.31	3.06		CH···O
Y-2d	–11.65	O1–H···OH	2.68	1.96	–162	OH···O
		OH–H···O5	2.62	1.97		OH···O
Y-2e	–11.45	OH–H···O2	2.21	2.03	44	OH···O
		C1–H···CE1	1.32	2.42		CH···π
		C3–H···CZ	1.18	2.46		CH···π
		C5–H···CD2	0.81	2.68 (2.71)		CH···π
		CB–H···O6	0.59	2.75		CH···O
Y-2f	–11.37	OH–H···O4	2.58	1.97	47	OH···O
		C3–H···CE1	1.24	2.53 (2.24)		CH···π
		C5–H···OH	0.79	2.65		CH···O
		C5–H···CE2	0.77	2.72		CH···π
		C1–H···CE2	0.34	3.27		CH···π
		CB–H···O2	0.29	3.04		CH···O
Y-2g	–11.33	OH–H···O2	2.48	1.99	–48	OH···O
		C3–H···CZ	1.38	2.44 (2.21)		CH···π
		C1–H···OH	0.62	2.75		CH···O
		C5–H···CE2	0.39	3.17		CH···π
		CB–H···O4	0.39	2.90		CH···O
Y-2h	–11.04	OH–H···O2	2.07	2.08	136	OH···O
		C3–H···CE2	1.32	2.41		CH···π
		C1–H···CZ	1.14	2.48		CH···π
		CB–H···O6	0.85	2.56		CH···O
		C5–H···CG	0.74	2.78 (2.61)		CH···π
Y-2i	–9.89	OH–H···O4	3.32	1.85	171	OH···O
		C5–H···OH	0.92	2.56		CH···O
		C6–H···CE2	0.66	2.79		CH···π
		C3–H···OH	0.61	2.69		CH···O
		CE2–H···O4	0.59	2.78		CH···O
Y-2j	–9.89	OH–H···O3	1.99	2.10	131	OH···O
		C4–H···CE2	1.25	2.51(2.32)		CH···π
		C6–H···CG	0.65	2.78		CH···π
		CB–H···O6	0.40	2.90		CH···O
Y-2k	–7.30	C4–H···CZ	1.12	2.56 (2.19)	–3	CH···π
		C6–H···CD1	0.73	2.74		CH···π
		O4–H···OH	0.61	2.65		OH···O
		C2–H···CD2	0.58	2.85		CH···π
		CB–H···O5	0.33	3.01		CH···O
		CB–H···O1	0.27	3.09		CH···O

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-2l	–6.79	C5–H···CZ	0.95	2.65 (2.36)	–177	CH···π
		C3–H···CD1	0.84	2.66		CH···π
		CB–H···O2	0.73	2.66		CH···O
		C1–H···CD2	0.66	2.85		CH···π
		C6–H···OH	0.62	2.73		CH···O
Y-2m	–6.64	C4–H···CE1	1.03	2.60 (2.32)	–3	CH···π
		C6–H···CD2	0.81	2.66		CH···π
		C2–H···CD1	0.71	2.74		CH···π
		CB–H···O1	0.68	2.67		CH···O
		CB–H···O5	0.49	2.82		CH···O
Y-2n	–6.01	C4–H···CE1	0.93	2.67 (2.28)	2	CH···π
		CB–H···O3	0.92	2.51		CH···O
		C6–H···OH	0.79	2.60		CH···O
		C2–H···CD2–CE2	0.37	3.13		CH···π
Y-2o	–5.50	CB–H···O1	0.57	2.74		CH···O
		C4–H···CE1	0.54	2.93		CH···π
		C2–H···CG	0.88	2.61		CH···π
		C6–H···OH	0.82	2.60		CH···O
Y-2p	–5.43	C2–H···CD1	0.83	2.68	–179	CH···π
		C6–H···CD2	0.79	2.69		CH···π
		CB–H···O5	0.69	2.76		CH···O
		CB–H···O6	0.56	2.81		CH···O
		C4–H···CE2	0.42	3.09 (2.81)		CH···π
		CD1–H···O1	0.40	2.95		CH···O
Y-2q	–5.07	CE2–H···O4	1.23	2.39	–5	CH···O
		C3–H···OH	0.95	2.49		CH···O
		C5–H···CE2	0.73	2.72		CH···π
		C1–H···OH	0.59	2.77		CH···O
Y-2r	–4.38	CB–H···O4	0.83	2.57	–1	CH···O
		C4–H···CE2	0.70	2.99		CH···π
		C6–H′···CG	0.61	2.88		CH···π
		C6–H···CZ	0.55	2.94		CH···π
Y-3a	–14.35	OH–H···O1	2.52	1.91	–160	OH···O
		O6–H···CE1	1.22	2.42		OH···π
		CE2–H···O1	0.68	2.74		CH···O
Y-3b	–13.02	OH–H···O6	3.16	1.88	–27	OH···O
		C5–H···OH	1.13	2.47		CH···O
		C1–H···CG	0.91	2.66 (2.41)		CH···π
Y-3c	–13.02	OH–H···O6	3.16	1.88	152	OH···O
		C5–H···OH	1.13	2.47		CH···O
		C1–H···CG	0.91	2.66 (2.41)		CH···π

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-3d	–12.66	OH–H···O3	3.09	1.89	153	OH···O
		O4–H···CE2	1.25	2.43		OH···π
		C4–H···CZ	1.07	2.51		CH···π
Y-3e	–12.20	OH–H···O5	2.71	1.96	–159	OH···O
		O1–H···OH	2.69	1.95		OH···O
Y-3f	–11.27	OH–H···O2	2.08	2.06	48	OH···O
		C1–H···CE1	1.40	2.39		CH···π
		C3–H···CZ	1.08	2.51		CH···π
		C3–H···OH	1.06	2.50		CH···O
		C5–H···CD2	0.81	2.73 (2.72)		CH···π
		CB–H···O6	0.60	2.74		CH···O
Y-3g	–11.25	OH–H···O2	1.60	2.20	135	OH···O
		C1–H···CZ	1.37	2.44 (2.15)		CH···π
		O1–H···CE1	0.71	2.74		OH···π
		CB–H···O6	0.69	2.67		CH···O
		C5–H···CD2	0.63	2.84		CH···π
		C3–H···CE2	0.54	2.91		CH···π
Y-3h	–11.04	OH–H···O5	2.76	1.94	–165	OH···O
		O1–H···OH	2.54	1.98		OH···O
Y-3i	–10.83	OH–H···O6	3.44	1.83	8	OH···O
		C5–H···OH	1.02	2.50		CH···O
		CE1–H···O6	0.74	2.63		CH···O
		C6–H···CE1	0.63	2.82		CH···π
Y-3j	–9.25	O1–H···OH	2.37	2.00	–168	OH···O
		C1–H···CE1	0.95	2.61		CH···π
		C6–H···CE2	0.71	2.75		CH···π
		C5–H···CE2	0.45	3.14 (2.89)		CH···π
Y-3k	–7.97	C5–H···CE1	1.05	2.60 (2.33)	173	CH···π
		C3–H···CD2	0.84	2.65		CH···π
		CB–H···O2	0.82	2.60		CH···O
		C1–H···CG–CD1	0.59	2.83		CH···π
		C6–H···OH	0.48	2.86		CH···O
Y-3l	–6.70	C1–H···OH	1.13	2.44	–173	CH···O
		C5–H···CE1	0.97	2.65 (2.30)		CH···π
		C6–H···CD2	0.54	2.94		CH···π
		C3–H···CE1	0.41	3.08		CH···π
Y-4a	–12.04	OH–H···O4	3.38	1.84	–167	OH···O
		O3–H···OH	2.99	1.89		OH···O
		C4–H···CE2	0.72	2.75		CH···π

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-4b	–11.47	OH–H···O4	2.45	2.00	–42	OH···O
		C5–H···CZ	1.39	2.40 (2.38)		CH···π
		C3–H···OH	0.77	2.62		CH···O
		C6–H···CE1	0.56	2.98		CH···π
		CB–H···O6	0.35	2.97		CH···O
Y-4c	–11.04	OH–H···O6	2.52	1.98	–132	OH···O
		C5–H···CZ	1.09	2.54 (2.38)		CH···π
		C6–H···CE2	0.69	2.81		CH···π
		CB–H···O4	0.39	2.95		CH···O
		C3–H···CG–CD1	0.33	3.14		CH···π
Y-4d	–10.43	OH–H···O4	2.50	2.01	–46	OH···O
		C4–H···OH	1.13	2.48		CH···O
		O3–H···CD2	0.79	2.63		OH···π
Y-4e	–10.28	OH–H···O4	3.42	1.83	–168	OH···O
		C5–H···OH	0.82	2.64		CH···O
		C6–H···OH	0.76	2.61		CH···O
		C3–H···CE2	0.69	2.77		CH···π
Y-4f	–9.18	OH–H···O1	2.08	2.05	–137	OH···O
		C5–H···CZ	1.16	2.51 (2.36)		CH···π
		C3–H···OH	0.99	2.49		CH···O
Y-4g	–8.94	O4–H···OH	1.84	2.13	–170	OH···O
		C5–H···CD1	0.95	2.64 (2.34)		CH···π
		C6–H···CE2–CD2	0.55	2.93		CH···π
		CB–H···O6	0.55	2.77		CH···O
		C3–H···CE1	0.49	2.93		CH···π
Y-4h	–6.53	CD2–H···O2	0.90	2.53	–4	CH···O
		C6–H···CG	0.87	2.72 (2.38)		CH···π
		CB–H···O5	0.80	2.59		CH···O
		C4–H···CE2	0.78	2.71		CH···π
Y-4i	–6.24	CB–H···O1	0.90	2.50	4	CH···O
		C6–H···OH	0.86	2.57		CH···O
		C5–H···CE2	0.82	2.74 (2.39)		CH···π
		C3–H···CD2	0.43	3.00		CH···π
Y-4j	–5.99	C4–H···CZ	1.05	2.56 (2.51)		CH···π
		O3–H···CD2	0.86	2.58		OH···π
		CB–H···O3	0.70	2.64		CH···O
		O4–H···CD1	0.68	2.75		OH···π
		C6–H···OH	0.59	2.76		CH···O
Y-4k	–5.73	C5–H···CD1	0.82	2.71(2.45)	5	CH···π
		CB–H···O4	0.82	2.57		CH···O
		C6–H···CE2	0.65	2.83		CH···π
		C3–H···CG	0.55	2.91		CH···π

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-4l	–4.88	CB–H···O4	0.79	2.57		CH···O
		C6–H···CE1	0.73	2.80 (2.51)		CH···π
		C5–H···CE2	0.59	2.92		CH···π
Y-5a	–10.32	OH–H···O3	2.83	1.94	–135	OH···O
		C4–H···CE2–CZ	1.15	2.47 (2.41)		CH···π
Y-5b	–10.16	OH–H···O3	2.12	2.07	–50	OH···O
		C3–H···CE1–CZ	1.42	2.36 (2.36)		CH···π
		C4–H···CE2–CZ	0.54	2.90		CH···π
		C4–H···OH	0.50	2.87		CH···O
		C5–H···CD2–CE2	0.39	3.11		CH···π
		CB–H···O1	0.36	2.90		CH···O
Y-5c	–10.14	OH–H···O5	2.41	1.98	–62	OH···O
		C2–H···CZ	0.86	2.67 (2.43)		CH···π
		C1–H···CE1	0.82	2.70		CH···π
		C6–H···OH	0.64	2.72		CH···O
Y-5d	–8.91	OH–H···O1	1.96	2.08	–144	OH···O
		C5–H···OH	1.23	2.40		CH···O
		C3–H···CE2	1.12	2.49		CH···π
Y-5e	–6.86	CB–H···O3	1.03	2.47	–3	CH···O
		C4–H···CE1	0.90	2.68 (2.40)		CH···π
		C6–H···OH	0.81	2.59		CH···O
		C3–H···CD2	0.59	2.89		CH···π
		C5–H···CE2	0.53	2.97		CH···π
Y-5f	–6.86	CB–H···O3	1.03	2.47	179	CH···O
		C4–H···CE2	0.90	2.68 (2.40)		CH···π
		C6–H···OH	0.81	2.59		CH···O
		C3–H···CD1	0.59	2.89		CH···π
		C5–H···CE1	0.53	2.97		CH···π
Y-5g	–6.68	C3–H···CD1	0.94	2.60	6	CH···π
		C5–H···CZ–CE1	0.90	2.58 (2.60)		CH···π
		CB–H···O3	0.78	2.60		CH···O
		C4–H···CD2–CG	0.58	2.87		CH···π
		C6–H···CE2	0.45	3.03		CH···π
Y-5h	–6.51	O2–H···OH	1.77	2.15	178	OH···O
		C3–H···CE1	0.90	2.67 (2.38)		CH···π
Y-5i	–5.87	CB–H···O3	0.95	2.54	178	CH···O
		C4–H···CD2–CE2	0.90	2.60 (2.39)		CH···π
		C6–H···OH	0.65	2.70		CH···O
		C5–H···CE1	0.57	2.92		CH···π
		C3–H···CD1	0.53	2.97		CH···π

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-5j	–5.70	CB–H···O1	0.88	2.52	1	CH···O
		C5–H···CD2–CE2	0.83	2.65 (2.49)		CH···π
		C4–H···CE1	0.67	2.81		CH···π
		C3–H···CD1	0.61	2.84		CH···π
		C6–H···OH	0.60	2.75		CH···O
Y-5k	–5.62	CB–H···O1	0.85	2.55	–2	CH···O
		C3–H···CD1	0.80	2.71		CH···π
		C4–H···CZ–CE1	0.77	2.68 (2.52)		CH···π
		C5–H···CD2–CG	0.65	2.80		CH···π
		C6–H···CE2	0.32	3.24		CH···π
Y-5l	–5.15	C3–H···CG	0.92	2.67 (2.32)	4	CH···π
		C4–H···OH	0.64	2.75		CH···O
		C4–H···CZ	0.63	2.82		CH···π
		C5–H···CE2	0.62	2.82		CH···π
Y-6a	–13.69	OH–H···O2	3.21	1.82	–178	OH···O
		O1–H···OH	2.74	1.93		OH···O
		CE2–H···O2	0.83	2.64		CH···O
		C1–H···CE2–CZ	0.60	2.81		CH···π
Y-6b	–9.96	OH–H···O3	2.73	1.95	42	OH···O
		C4–H···CE1–CZ	1.19	2.45 (2.37)		CH···π
Y-6c	–8.48	OH–H···O1	2.60	1.95	176	OH···O
		CE2–H···O5	0.84	2.67		CH···O
		C6–H···CD2	0.48	2.98		CH···π
Y-6d	–7.37	C5–H···CE1	1.00	2.63 (2.34)		CH···π
		CB–H···O2	0.86	2.56		CH···O
		C3–H···CD2	0.84	2.64		CH···π
		C1–H···CD1–CG	0.56	2.89		CH···π
		C6–H···OH	0.46	2.88		CH···O
Y-6e	–7.06	CB–H···O3	1.03	2.47	180	CH···O
		C4–H···CD2–CE2	0.92	2.57 (2.38)		CH···π
		C6–H···OH	0.83	2.58		CH···O
		C3–H···CD1	0.58	2.91		CH···π
		C5–H···CE1	0.48	3.03		CH···π
Y-6f	–6.49	O1–H···OH	1.18	2.38	171	OH···O
		C1–H···CZ	1.15	2.54 (2.29)		CH···π
Y-6g	–6.30	C1–H···CD2	1.00	2.58	–2	CH···π
		C5–H···CD2	0.79	2.76 (2.39)		CH···π
		CB–H···O1	0.77	2.61		CH···O
		C6–H···CD1	0.50	2.98		CH···π

Conf	E_{INT}	Atom Pair	$\rho_{bcp}*10^{-2}$	BL	DA	INT
Y-6h	–6.30	C3–H···CD1	1.14	2.55 (2.21)	–1	CH···π
		CB–H···O2	0.65	2.71		CH···O
		C5–H···CE2	0.57	2.88		CH···π
		C4–H···OH	0.40	2.95		CH···O
		C1–H···CD2	0.34	3.16		CH···π
Y-6i	–6.20	C1–H···CD1	1.22	2.51(2.23)	5	CH···π
		C5–H···CE2	0.86	2.66		CH···π
		CB–H···O2	0.55	2.77		CH···O
		C3–H···CD2	0.42	3.05		CH···π
Y-6j	–5.95	C4–H···CE2	0.81	2.75 (2.48)	8	CH···π
		C3–H···CE2	0.78	2.73		CH···π
		C3–H···OH	0.76	2.66		CH···O
		C5–H···CE1	0.61	2.92		CH···π
		C6–H···CE1	0.46	3.07		CH···π
Y-6k	–5.80	C1–H···CD2	1.00	2.62 (2.41)		CH···π
		C5–H···CD1	0.80	2.72		CH···π
		CB–H···O5	0.68	2.68		CH···O
		CB–H···O1	0.51	2.86		CH···O
Y-6l	–5.80	C3–H···OH	0.98	2.51	–177	CH···O
		C5–H···CD1	0.92	2.67 (2.36)		CH···π
		C4–H···CE2	0.49	3.01		CH···π
		C1–H···CE1	0.35	3.14		CH···π
Y-6m	–5.21	C4–H···CE1	0.78	2.78 (2.48)		CH···π
		C3–H···CE1	0.76	2.74	–176	CH···π
		C5–H···CE2–CZ	0.70	2.75		CH···π
		C3–H···OH	0.60	2.75		CH···O
		C6–H···CE2	0.37	3.21		CH···π

Table S2. Interaction energy (in kcal/mol) and some characteristics of key inter-atomic atom contacts D-H...A for the binary complexes of Tol. These are the electron density at the H...A bond critical point (ρ_{bcp}, in a.u.), H...A (and H...centroid) distance (**BL**, in Å) and the type of interaction (**INT**). The non-stacking complexes are highlighted in gray.

Conf	E_{INT}	Atom Pair	$(\rho)*10^{-2}$	BL	INT
F-1a	–8.58	O3–H···CZ	1.16	2.44	OH···π
		CB–H···O4	0.98	2.52	CH···O
		C4–H···CD2	0.96	2.64	CH···π
		C2–H···CE2	0.37	3.15	CH···π
F-1b	–8.06	O2–H···CZ–CE2	1.19	2.34	OH···π
		CB–H···O3	0.92	2.54	CH···O
		C2–H···CD2	0.89	2.66	CH···π
F-1c	–7.75	C2–H···CD2–CG	1.23	2.41(2.24)	CH···π
		O2–H···CE1	0.90	2.58	OH···π
		CB–H···O3	0.87	2.56	CH···O
F-1d	–6.76	C5–H···CG	1.05	2.55	CH···π
		CB–H···O4	0.94	2.53	CH···O
		O1–H···CE1	0.90	2.53	OH···π
		C6–H···CE2	0.45	3.02	CH···π
F-1e	–6.17	O6–H···CD2	1.21	2.37	OH···π
		CB–H···O6	0.87	2.52	CH···O
		C2–H···CE1–CD1	0.81	2.65	CH···π
		C1–H···CZ	0.54	2.91	CH···π
F-1f	–6.10	O6–H···CD2	1.32	2.33	OH···π
		CB–H···O6	0.80	2.57	CH···O
		C2–H···CE1	0.79	2.70	CH···π
		C1–H···CZ	0.44	3.04	CH···π
		C4–H···CD1–CG	0.31	3.26	CH···π
F-1g	–5.92	C4–H···CD1	0.93	2.66 (2.28)	CH···π
		C6–H···CE2	0.65	2.83	CH···π
		CB–H···O4	0.64	2.69	CH···O
		C2–H···CE1–CZ	0.36	3.10	CH···π
F-1h	–5.74	C2–H···CD1	1.06	2.58 (2.30)	CH···π
		CB–H···O3	0.72	2.66	CH···O
		C4–H···CD2	0.72	2.72	CH···π
F-1i	–5.72	C2–H···CD1	1.05	2.58 (2.30)	CH···π
		C4–H···CD2	0.73	2.71	CH···π
		CB–H···O3	0.70	2.67	CH···O
F-1j	–5.49	C2–H···CD1	1.06	2.58 (2.27)	CH···π
		CB–H···O3	0.78	2.62	CH···O
		C4–H···CD2	0.66	2.77	CH···π
F-1k	–5.39	C4–H···CD1	0.91	2.69 (2.31)	CH···π
		CB–H···O3	0.86	2.58	CH···O
		C6–H···CZ	0.55	2.93	CH···π
		C2–H···CD2–CG	0.39	3.06	CH···π
F-1l	–5.37	CB–H···O4	0.81	2.62	CH···O
		C6–H···CE2	0.70	2.81 (2.52)	CH···π
		C5–H···CG	0.54	2.92	CH···π

Conf	E_{INT}	Atom Pair	$(\rho)*10^{-2}$	BL	INT
F-1m	–5.25	C1–H···CD2	0.72	2.78	CH···π
		C2–H···CD1–CG	0.72	2.72	CH···π
		CB–H···O2	0.61	2.74	CH···O
		C6–H···CE1–CZ	0.57	2.88	CH···π
		O6–H···CZ	0.57	2.78	OH···π
		C4–H···CD1–CE1	0.20	3.50	CH···π
F-1n	–5.12	C5–H···CD1	0.80	2.78 (2.43)	CH···π
		CB–H···O1	0.72	2.64	CH···O
		C6–H···CZ	0.58	2.91	CH···π
		C3–H···CG–CD1	0.53	2.88	CH···π
F-1o	–4.96	CB–H···O4	0.91	2.52	CH···O
		C5–H···CZ–CE1	0.81	2.62 (2.47)	CH···π
		C6–H···CD2	0.65	2.95	CH···π
		C3–H···CD1	0.52	2.93	CH···π
F-1p	–4.90	C5–H···CG	0.84	2.65	CH···π
		CB–H···O1	0.83	2.56	CH···O
		C6–H···CZ	0.66	2.82 (2.80)	CH···π
F-1q	–4.86	O6–H···CD2	0.68	2.72	OH···π
		C6–H···CD2–CG	0.65	2.79	CH···π
		C1–H···CE1	0.64	2.87	CH···π
		C2–H···CD1	0.41	3.06	CH···π
F-1r	–4.32	C5–H···CE2–CZ	0.95	2.53 (2.37)	CH···π
		C6–H···CG	0.51	2.96	CH···π
		C3–H···CE1–CZ	0.43	3.02	CH···π
F-1s	–4.03	C5–H···CE2–CZ	0.83	2.61(2.46)	CH···π
		C6–H···CG	0.67	2.78	CH···π
		C3–H···CE1–CZ	0.56	2.86	CH···π
F-1t	–3.70	C6–H···CG	0.93	2.66 (2.53)	CH···π
		C4–H···CZ	0.63	2.81	CH···π
		CB–H···O6	0.28	3.07	CH···O
F-2a	–8.22	O1–H···CZ	1.19	2.39	OH···π
		CD1–H···O6	0.95	2.54	CH···O
		C1–H···CG	0.68	2.72 (2.51)	CH···π
		C5–H···CD1	0.68	2.81	CH···π
F-2b	–6.87	C3–H···CZ	1.07	2.58 (2.23)	CH···π
		CB–H···O6	0.82	2.58	CH···O
		C5–H···CD1	0.57	2.91	CH···π
		CB–H···O4	0.52	2.83	CH···O
		C1–H···CE1–CD1	0.37	3.12	CH···π
F-2c	–6.59	CB–H···O6	1.10	2.45	CH···O
		C5–H···CD1	0.98	2.62 (2.38)	CH···π
		C3–H···CZ	0.75	2.71	CH···π
		C1–H···CE2	0.62	2.85	CH···π

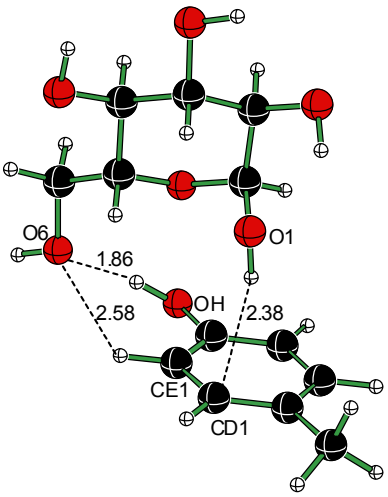
Conf	E_{INT}	Atom Pair	$(\rho)*10^{-2}$	BL	INT
F-2d	–6.31	C5–H···CZ	1.07	2.57 (2.31)	CH···π
		C1–H···CD1	0.83	2.69	CH···π
		CB–H···O2	0.73	2.66	CH···O
		C3–H···CD2	0.71	2.77	CH···π
F-2e	–5.73	C1–H···CZ	0.98	2.62 (2.40)	CH···π
		CB–H···O4	0.95	2.54	CH···O
		C3–H···CD2	0.78	2.70	CH···π
		C5–H···CD1	0.78	2.74	CH···π
F-2f	–5.59	C4–H···CG	0.97	2.65 (2.33)	CH···π
		CB–H···O3	0.95	2.52	CH···O
		C6–H···CE2	0.65	2.81	CH···π
F-2g	–5.11	C4–H···CD1	0.96	2.66 (2.31)	CH···π
		CB–H···O4	0.64	2.72	CH···O
		C6–H···CD2	0.58	2.85	CH···π
		C2–H···CZ	0.35	3.12	CH···π
F-2h	–4.76	CB–H···O4	0.98	2.52	CH···O
		C6–H···CE1	0.80	2.73 (2.24)	CH···π
		C4–H···CD1	0.66	2.78	CH···π
F-2i	–3.47	C4–H···CE1	0.79	2.69	CH···π
		C6–H···CG	0.64	2.87 (2.64)	CH···π
		C6–H′···CE2	0.56	2.99	CH···π
F-3a	–7.26	C5–H···CZ	0.90	2.67 (2.47)	CH···π
		C3–H···CD1	0.81	2.68	CH···π
		CB–H···O3	0.77	2.61	CH···O
		C4–H···CG–CD2	0.67	2.79	CH···π
F-3b	–6.81	C5–H···CZ	0.91	2.68 (2.34)	CH···π
		CB–H···O2	0.81	2.61	CH···O
		C3–H···CD2	0.74	2.76	CH···π
		C1–H···CD1	0.73	2.76	CH···π
F-3c	–6.74	C5–H···CZ	0.96	2.63 (2.45)	CH···π
		C3–H···CD2	0.80	2.70	CH···π
		CB–H···O3	0.69	2.66	CH···O
		C4–H···CD1–CG	0.67	2.79	CH···π
		C6–H···CE1	0.45	3.03	CH···π
F-3d	–6.42	O1–H···CE2	1.22	2.40	OH···π
		C1–H···CG	0.70	2.82	CH···π
F-3e	–6.35	C3–H···CZ	1.02	2.59 (2.45)	CH···π
		CB–H···O6	0.96	2.52	CH···O
		C5–H···CD2	0.70	2.79	CH···π
		C4–H···CD1–CG	0.65	2.79	CH···π
F-3f	–6.25	C5–H···CD2–CG	1.00	2.53 (2.27)	CH···π
		C3–H···CE2–CZ	0.56	2.86	CH···π
		C1–H···CD2	0.51	2.96	CH···π

Conf	E_{INT}	Atom Pair	$(\rho)*10^{-2}$	BL	INT
F-3g	–5.97	C5–H···CE1	0.97	2.63 (2.30)	CH···π
		C3–H···CE2	0.56	2.91	CH···π
F-3h	–5.87	C5–H···CE1	0.93	2.66 (2.32)	CH···π
		C3–H···CE2–CZ	0.58	2.84	CH···π
		C1–H···CE1	0.53	2.96	CH···π
F-3i	–5.73	C3–H···CD2	1.11	2.56 (2.27)	CH···π
		CB–H···O3	0.71	2.68	CH···O
		C5–H···CE1	0.53	2.91	CH···π
		C1–H···CZ	0.32	3.20	CH···π
F-3j	–5.37	C3–H···CZ–CE2	1.07	2.49 (2.27)	CH···π
		C5–H···CG–CD1	0.60	2.84	CH···π
		C1–H···CD1–CE1	0.39	3.09	CH···π
F-4a	–7.12	C5–H···CG	1.03	2.56	CH···π
		O1–H···CE1	0.97	2.50	OH···π
		CB–H···O4	0.94	2.53	CH···O
		C6–H···CE2	0.48	2.98	CH···π
F-4b	–7.12	C5–H···CG	1.03	2.56	CH···π
		O1–H···CE2	0.97	2.50	OH···π
		CB–H···O4	0.94	2.53	CH···O
		C6–H···CE1	0.48	2.98	CH···π
F-4c	–6.33	CB–H···O4	0.98	2.50	CH···O
		C5–H···CG	0.89	2.68 (2.51)	CH···π
		O1–H···CE1	0.81	2.69	OH···π
		C6–H···CD2	0.62	2.83	CH···π
F-4d	–5.58	C5–H···CD2	0.95	2.64 (2.34)	CH···π
		CB–H···O1	0.83	2.56	CH···O
		C3–H···CG–CD2	0.33	3.13	CH···π
F-4e	–5.56	C6–H···CG	0.85	2.72 (2.39)	CH···π
		CE1–H···O2	0.83	2.57	CH···O
		CB–H···O6	0.64	2.72	CH···O
		C4–H···CZ	0.55	2.87	CH···π
F-4f	–5.16	C6–H···CD1	0.76	2.77 (2.45)	CH···π
		CD2–H···O2	0.71	2.65	CH···O
		CB–H···O2	0.59	2.72	CH···O
		O6–H···CE2	0.57	2.80	OH···π
		C4–H···CG	0.46	2.97	CH···π
F-4g	–4.95	C3–H···CD1	0.99	2.61(2.28)	CH···π
		CB–H···O3	0.66	2.68	CH···O
		C5–H···CZ	0.36	3.12	CH···π
F-4h	–4.63	C2–H···CE1	0.94	2.63 (2.34)	CH···π
		CB–H···O2	0.71	2.67	CH···O
		C1–H···CD2	0.58	2.88	CH···π

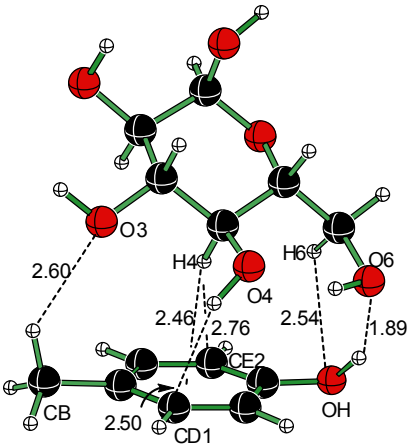
Conf	E_{INT}	Atom Pair	$(\rho)*10^{-2}$	BL	INT
F-4i	–4.26	C3–H···CG	0.93	2.65 (2.30)	CH···π
		CB–H···O1	0.87	2.54	CH···O
F-4j	–4.13	CB–H…O4	0.86	2.56	CH···O
		C4–H···CD2	0.82	2.69	CH···π
		C6–H···CE1	0.63	2.88 (2.60)	CH···π
F-5a	–6.50	C3–H···CZ	1.01	2.64 (2.27)	CH···π
		C5–H···CG	0.54	2.90	CH···π
		CB–H···O1	0.89	2.53	CH···O
		O1–H···CD2	0.64	2.75	OH···π
F-5b	–6.34	C4–H···CE2–CZ	0.87	2.61 (2.43)	CH···π
		C3–H···CD2	0.76	2.74	CH···π
		C5–H···CD1–CG	0.65	2.80	CH···π
		C6–H···CE1–CD1	0.35	3.17	CH···π
F-5c	–6.16	C3–H···CD2	0.90	2.61	CH···π
		CB–H···O3	0.87	2.56	CH···O
		C5–H···CZ–CE2	0.81	2.64 (2.64)	CH···π
		C4–H···CD1–CG	0.62	2.83	CH···π
		C6–H···CE1	0.43	3.03	CH···π
F-5d	–6.10	C3–H···CD1	0.83	2.69	CH···π
		C4–H···CZ–CE1	0.81	2.64 (2.52)	CH···π
		CB–H···O1	0.77	2.60	CH···O
		C5–H···CD2–CG	0.63	2.82	CH···π
		C6–H···CE2–CD2	0.43	3.03	CH···π
F-5e	–5.57	C5–H···CZ	0.82	2.72 (2.56)	CH···π
		CB–H···O3	0.82	2.59	CH···O
		C3–H···CD2	0.80	2.70	CH···π
		C4–H···CD1	0.65	2.86	CH···π
F-5f	–5.35	C5–H···CD2–CE2	0.82	2.64 (2.42)	CH···π
		CB–H···O1	0.82	2.57	CH···O
		C3–H···CD1–CG	0.58	2.83	CH···π
		C4–H···CD1–CE1	0.50	2.98	CH···π
F-5g	–5.26	C4–H···CE1–CZ	0.81	2.65 (2.50)	CH···π
		CB–H···O1	0.77	2.61	CH···O
		C3–H···CD1	0.76	2.75	CH···π
		C5–H···CD2	0.65	2.86	CH···π
		C6–H···CE2	0.33	3.19	CH···π
F-5h	–5.26	C4–H···CE2–CZ	0.81	2.65 (2.50)	CH···π
		CB–H···O1	0.77	2.61	CH···O
		C3–H···CD2	0.76	2.75	CH···π
		C5–H···CD1	0.65	2.86	CH···π
		C6–H···CE1	0.33	3.19	CH···π

Conf	E_{INT}	Atom Pair	$(\rho)*10^{-2}$	BL	INT
F-5i	–5.12	C4–H···CD1	0.96	2.62 (2.40)	CH···π
		C3–H···CZ	0.71	2.76	CH···π
		C6–H···CD2	0.46	2.97	CH···π
		C5–H···CE2	0.44	3.05	CH···π
F-5j	–4.70	C5–H···CE1	0.85	2.70 (2.39)	CH···π
		C3–H···CE2	0.55	2.89	CH···π
		C4–H···CD2	0.46	3.05	CH···π
F-5k	–4.61	C5–H···CD1	0.89	2.68 (2.39)	CH···π
		C3–H···CZ	0.56	2.87	CH···π
		C4–H···CE2	0.45	3.03	CH···π
F-6a	–6.70	O1–H···CE1–CZ	1.20	2.44	OH···π
		C5–H···CG	0.78	2.82	CH···π
		C1–H···CD2	0.61	2.76 (2.57)	CH···π
F-6b	–6.12	C5–H···CE1–CZ	0.92	2.59 (2.45)	CH···π
		C1–H···CD1	0.80	2.74	CH···π
		CB–H···O2	0.79	2.62	CH···O
		C3–H···CD2	0.76	2.70	CH···π
F-6c	–6.02	C1–H···CD2	0.92	2.60	CH···π
		C5–H···CD1	0.83	2.74 (2.40)	CH···π
		CB–H···O1	0.71	2.66	CH···O
		CB–H···O5	0.57	2.78	CH···O
		C6–H···CD1	0.52	2.94	CH···π
F-6d	–5.94	C3–H···CD2	0.85	2.68	CH···π
		C5–H···CZ	0.83	2.71 (2.55)	CH···π
		CB–H···O2	0.77	2.62	CH···O
		C4–H···CD1	0.62	2.89	CH···π
F-6e	–5.73	C3–H···CD1	1.09	2.57 (2.28)	CH···π
		CB–H···O2	0.84	2.59	CH···O
		C5–H···CE2	0.54	2.90	CH···π
		C1–H···CD2	0.44	3.01	CH···π
F-6f	–5.66	C5–H···CD1	0.89	2.69 (2.36)	CH···π
		C3–H···CE2	0.70	2.78	CH···π
		C1–H···CE1	0.50	3.00	CH···π
F-6g	–5.51	C3–H···CD1	1.12	2.56 (2.25)	CH···π
		CB–H···O3	0.69	2.69	CH···O
		C5–H···CE2	0.47	2.98	CH···π
		C1–H···CZ	0.36	3.13	CH···π
F-6h	–5.22	C5–H···CD1–CE1	0.92	2.58 (2.34)	CH···π
		C3–H···CD2–CE2	0.64	2.79	CH···π
		C1–H···CZ–CE2	0.41	3.06	CH···π

Conf	E_{INT}	Atom Pair	$(\rho)*10^{-2}$	BL	INT
F-6i	–4.94	C3–H···CE1–CZ	1.05	2.50 (2.26)	CH···π
		C5–H···CD2–CG	0.57	2.87	CH···π
		C1–H···CE2–CD2	0.40	3.08	CH···π
F-6j	–4.94	C3–H···CE2–CZ	1.05	2.5 (2.27)	CH···π
		C5–H···CD1–CG	0.57	2.87	CH···π
		C1–H···CE1–CD1	0.40	3.08	CH···π
F-6k	–4.88	C5–H···CG	0.92	2.67 (2.37)	CH···π
		C3–H···CZ	0.61	2.87	CH···π
		C1–H···CE1–CD1	0.42	3.07	CH···π
F-6l	–4.82	C1–H···CZ	0.99	2.61 (2.32)	CH···π
		C3–H···CD2	0.69	2.76	CH···π
		C5–H···CG–CD1	0.61	2.84	CH···π



Y-1a (–16.40)



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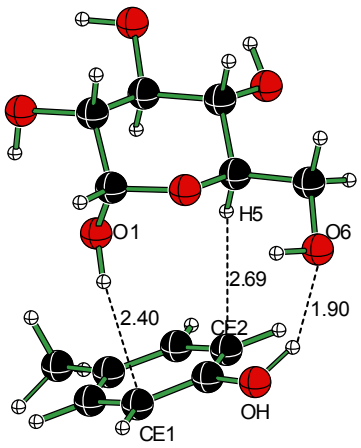
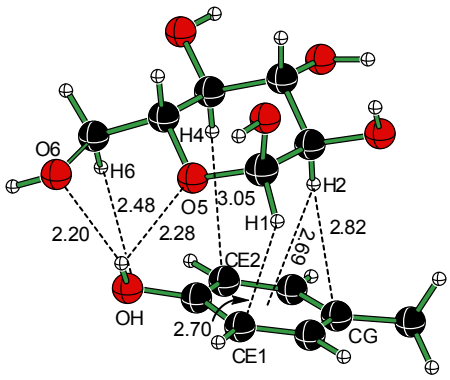


Y-1c (–13.63)



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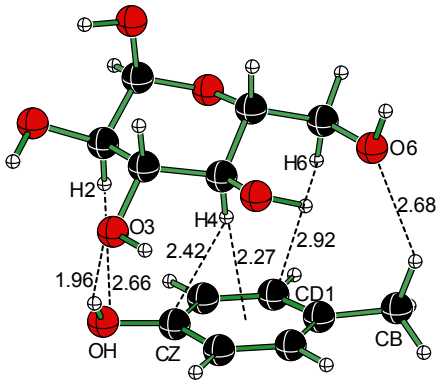
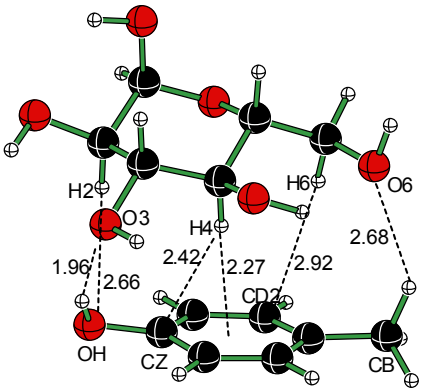


Y-1e (–11.50)



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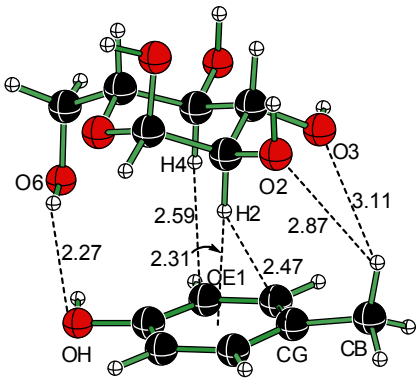

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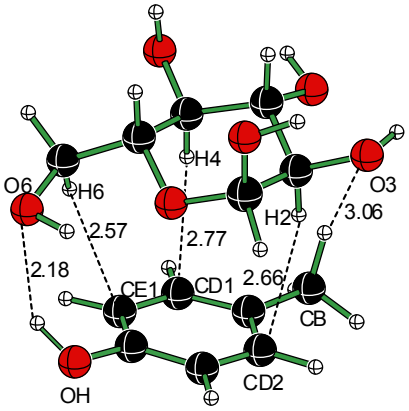
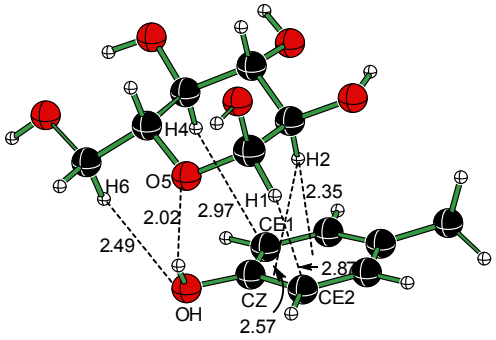


Y-1h (–9.95)



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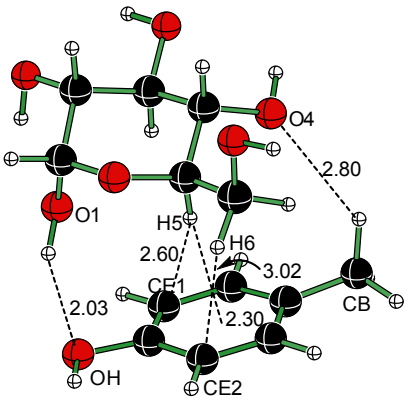

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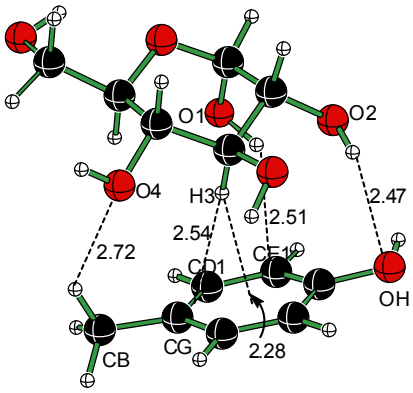
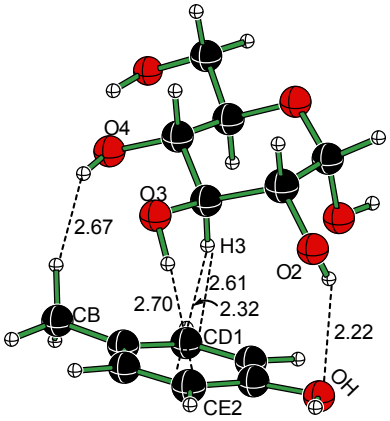
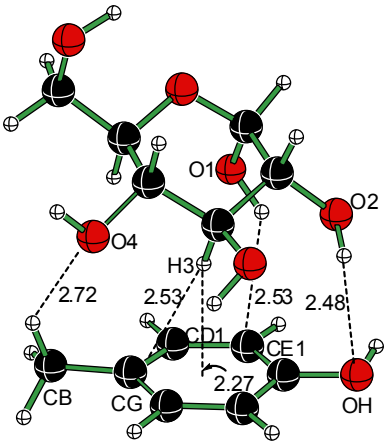


Y-1k (–8.73)



Y-1l (–8.49)



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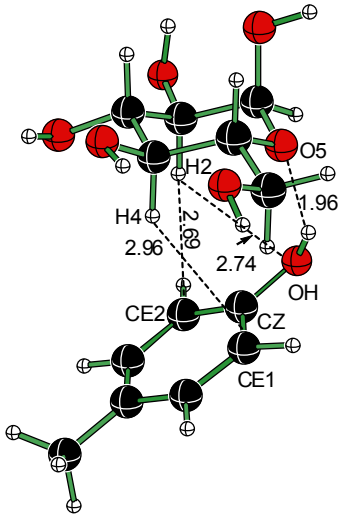

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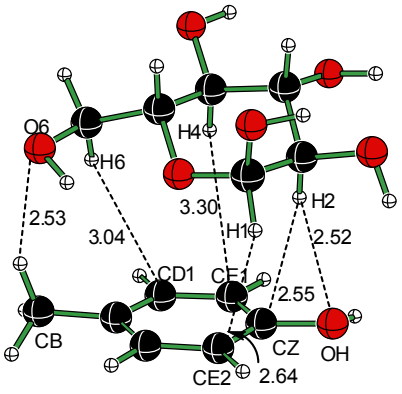

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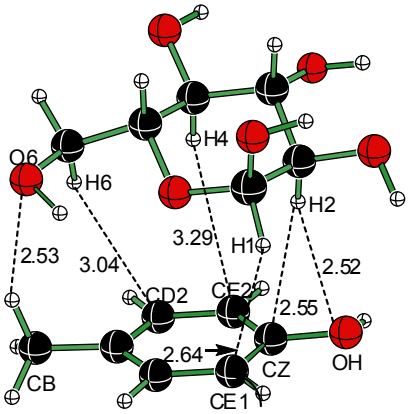

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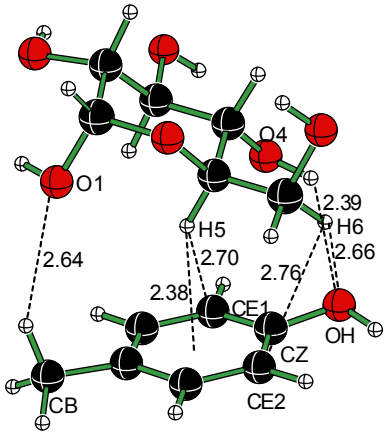

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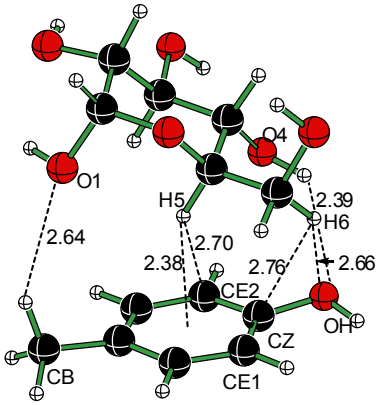
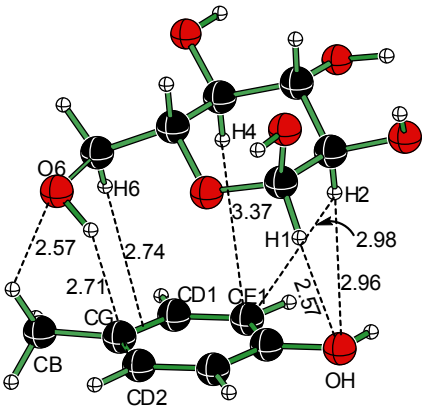
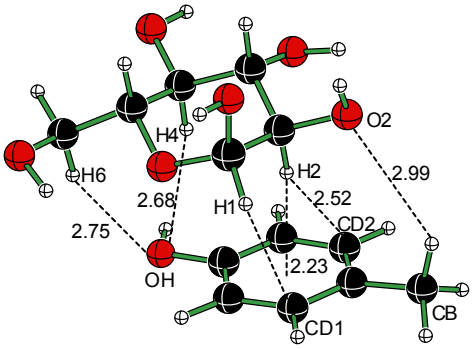


Y-1r (–7.66)



Y-1s (–6.73)



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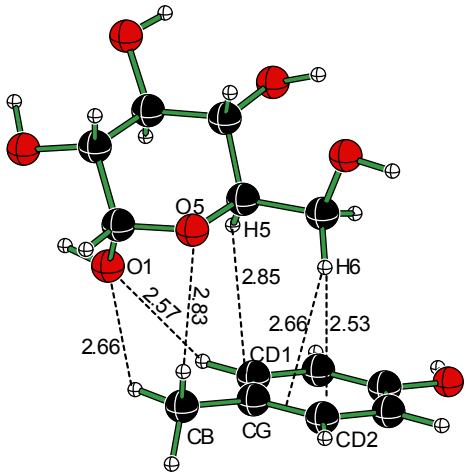

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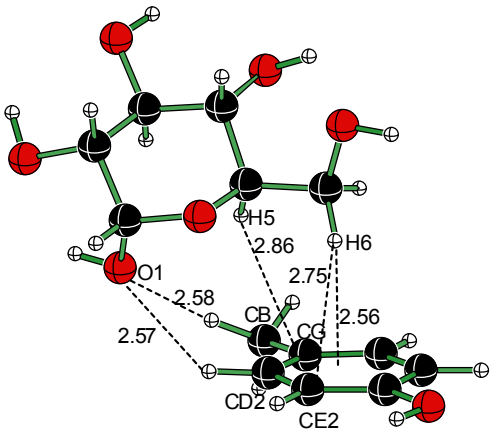


Y-1v (–6.07)

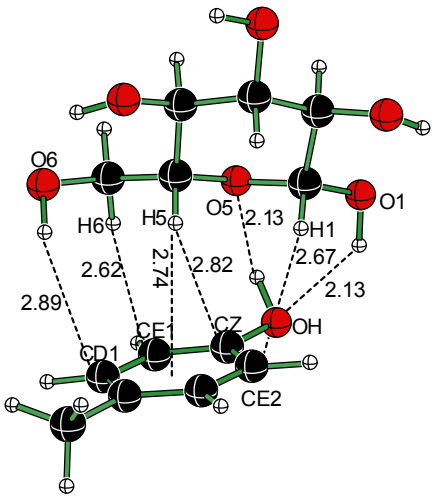
Figure S1. Optimized geometries of *p*-OHTol : α-D-glucose binary complexes. The interaction energies in kcal/mol are given in parenthesis. In this and Figures **S2** to **S12**,

(i) color code: C-black, O-red, and H-ivory,

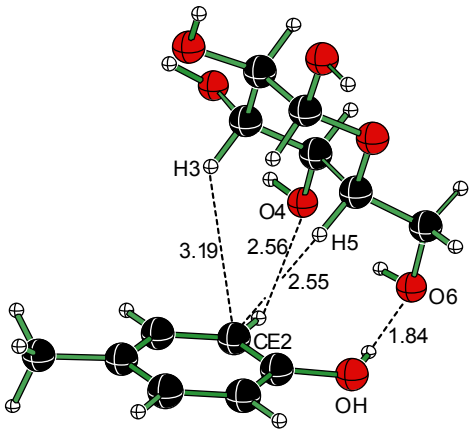
(ii) distances between key inter-atomic pairs are shown,

(iii) atoms participating in key inter-atomic interactions are labeled.

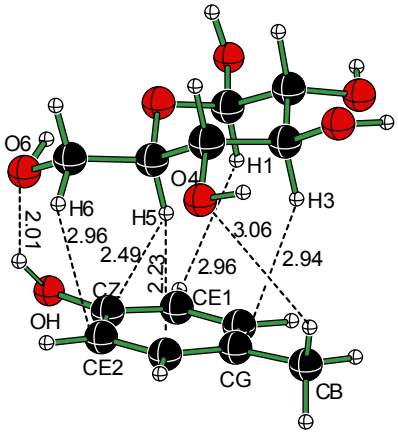
All these figures were rendered using the software Molecule.



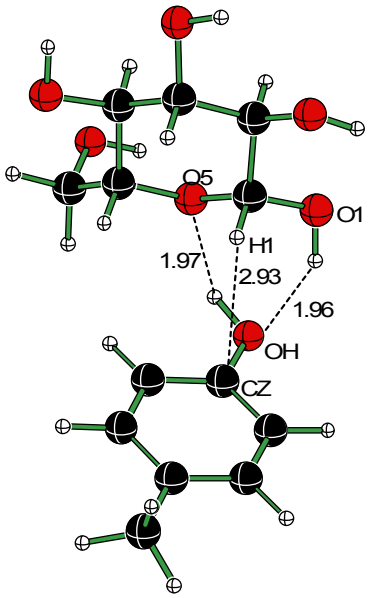
Y-2a (–13.02)



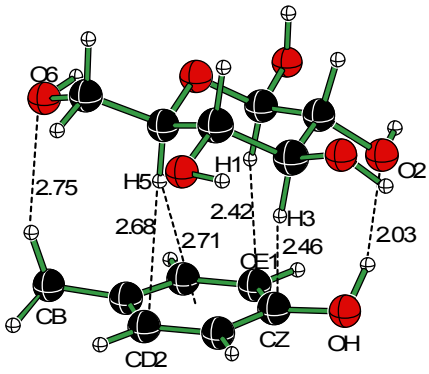
Y-2b (–12.04)



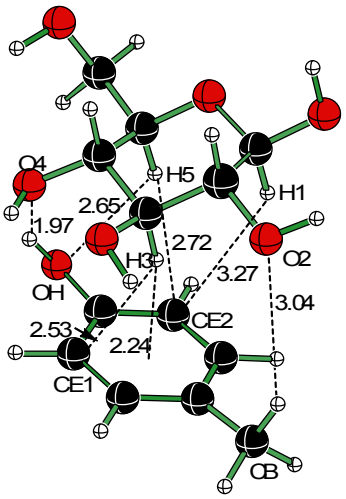
Y-2c (–12.04)



Y-2d (–11.65)



Y-2e (–11.45)



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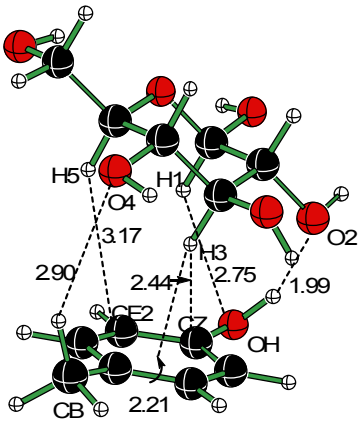
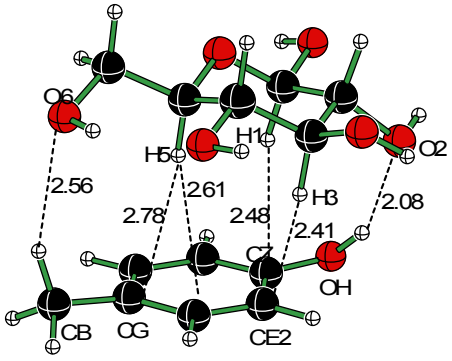
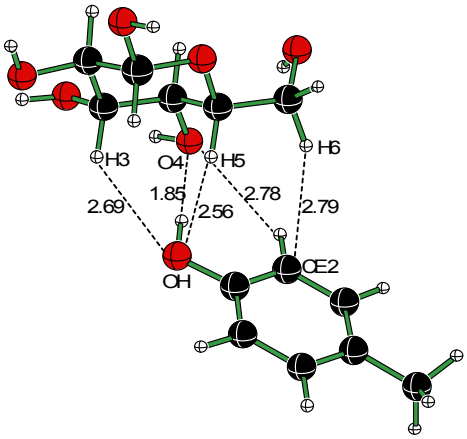
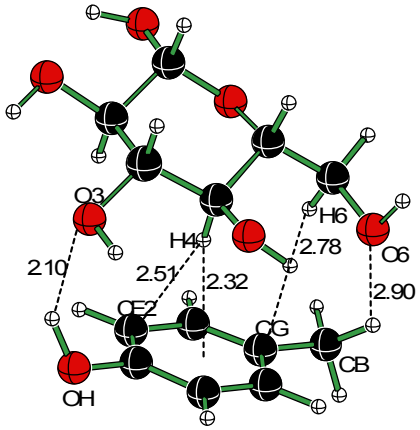




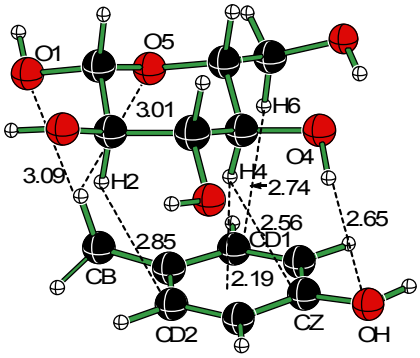
Y-2g (–11.33)



Y-2h (–11.04)



Y-2i (–9.89)



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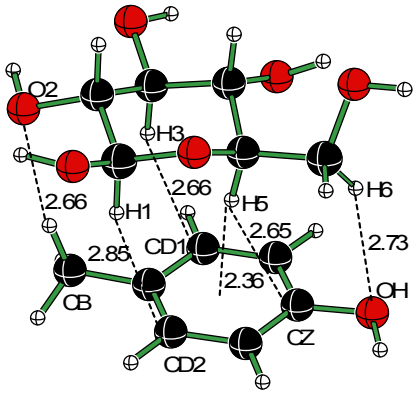
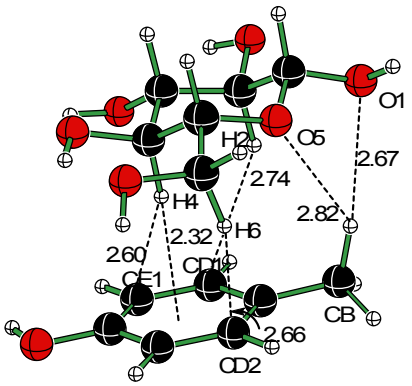


Y-2k (–7.30)



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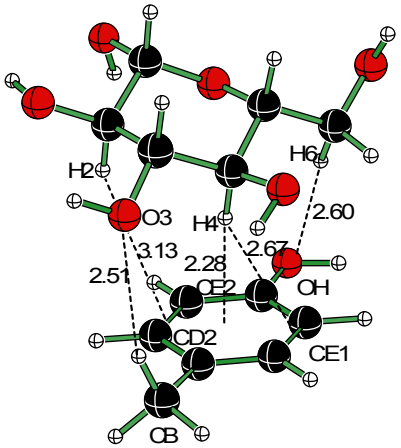
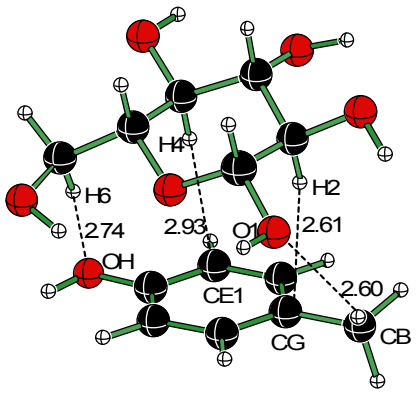
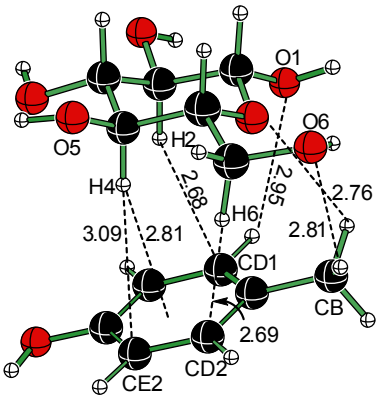


Y-2m (–6.64)

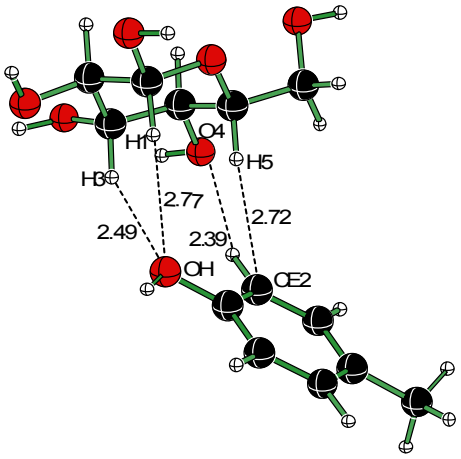
Y-2n (–6.01)



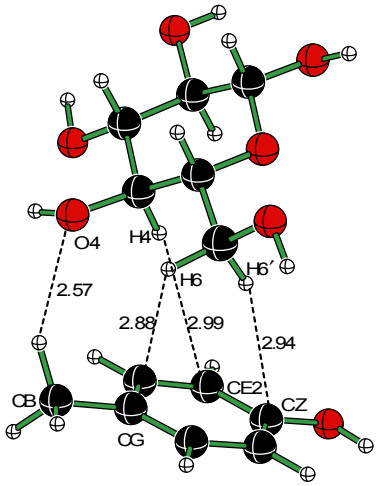
Y-2o (–5.50)



Y-2p (–5.43)

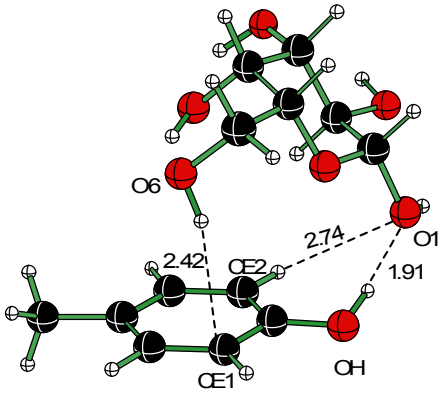


Y-2q (–5.07)

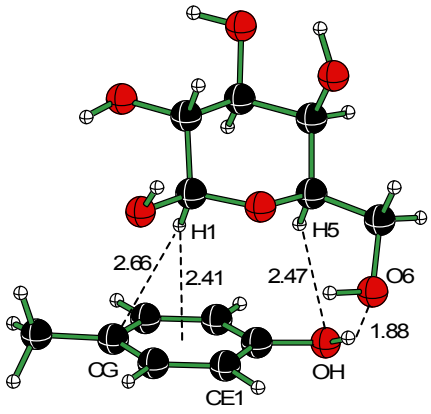


Y-2r (–4.38)

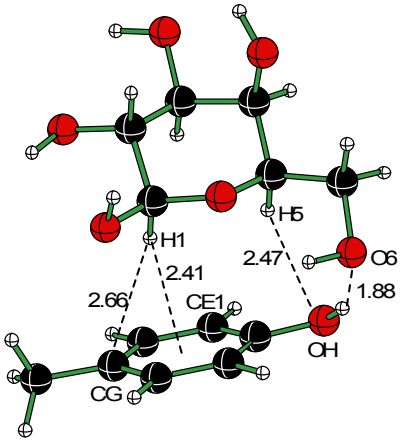
Figure S2. Optimized geometries of *p*-OHTol : β-D-glucose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



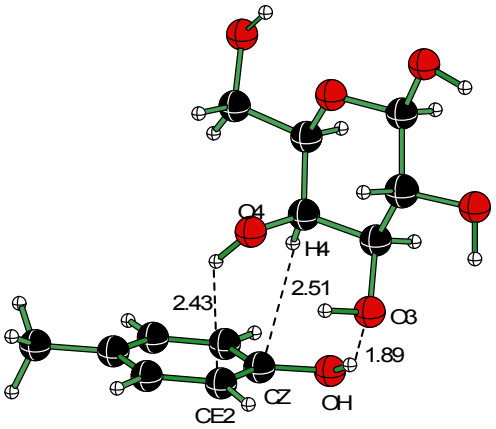
Y-3a (–14.35)



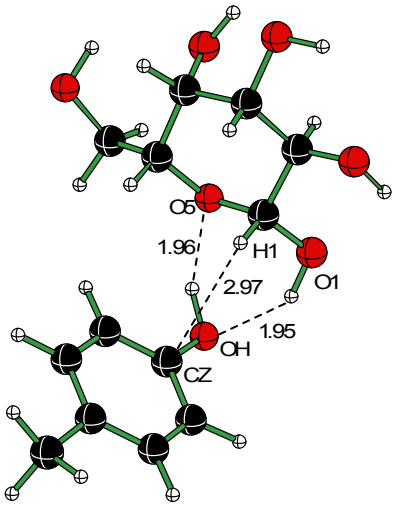
Y-3b (–13.02)



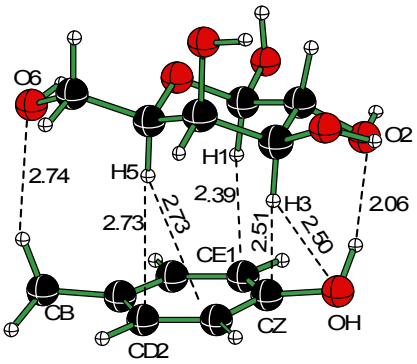
Y-3c (–13.02)



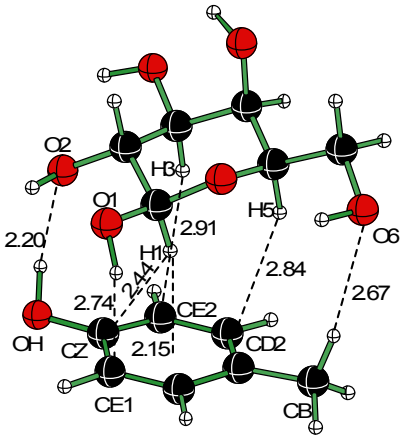
Y-3d (–12.66)



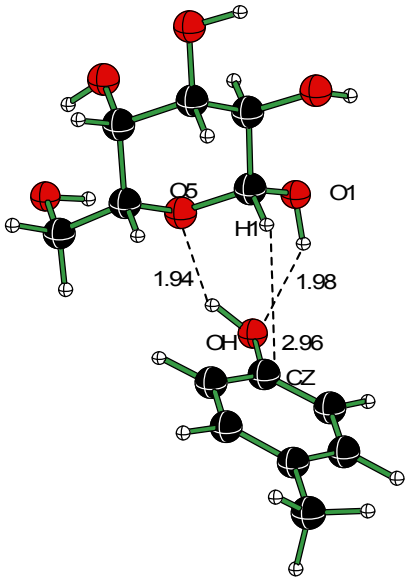
Y-3e (–12.20)



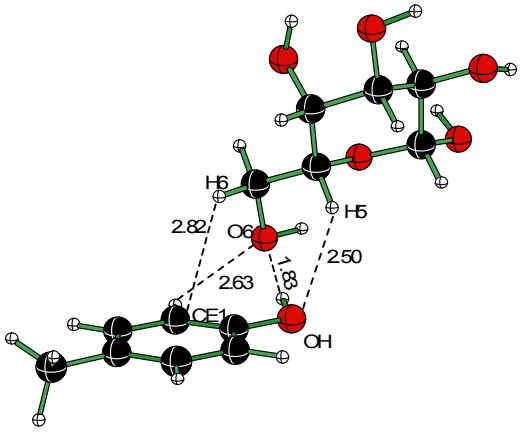
Y-3f (–11.27)



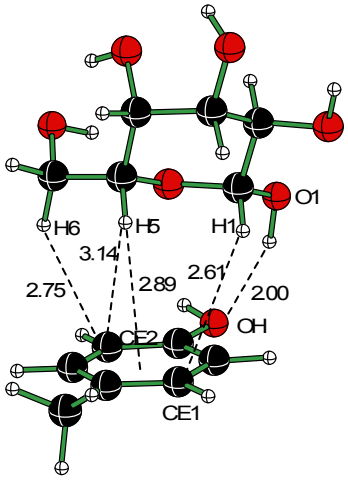
Y-3g (–11.25)



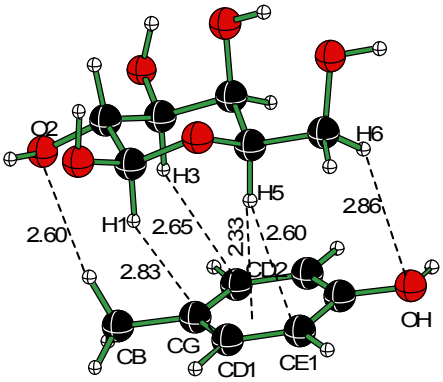
Y-3h (–11.04)



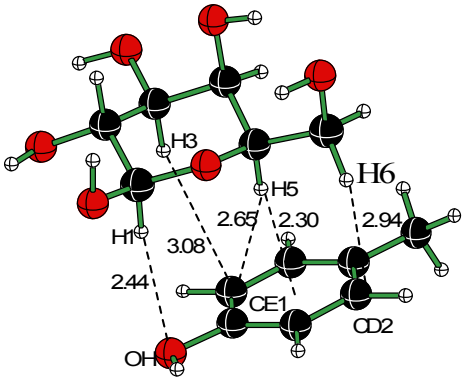
Y-3i (–10.83)



Y-3j (–9.25)

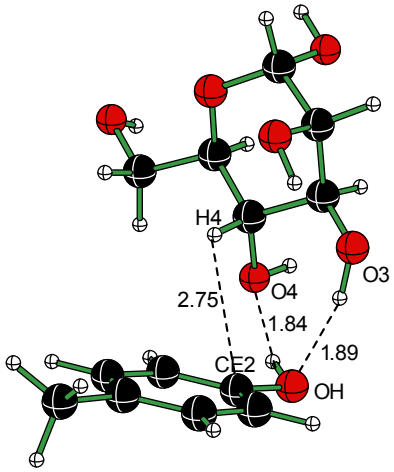


Y-3k (–7.97)

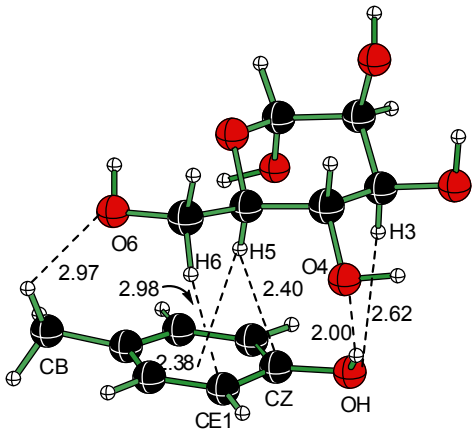


Y-3l (–6.70)

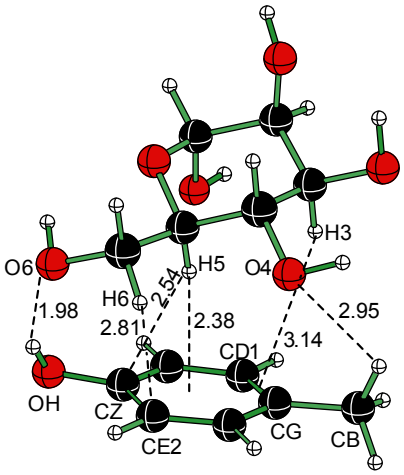
Figure S3. Optimized geometries of *p*-OHTol : β-D-galactose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



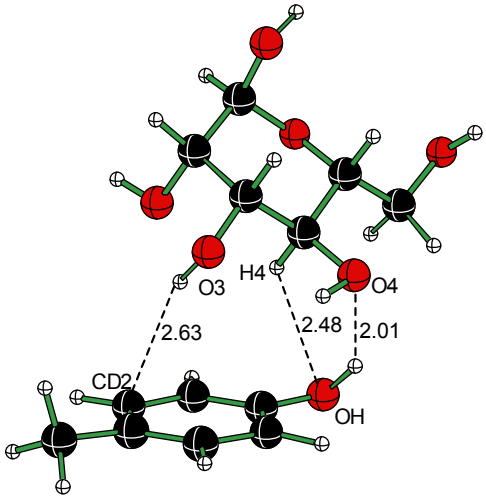
Y-4a (–12.04)



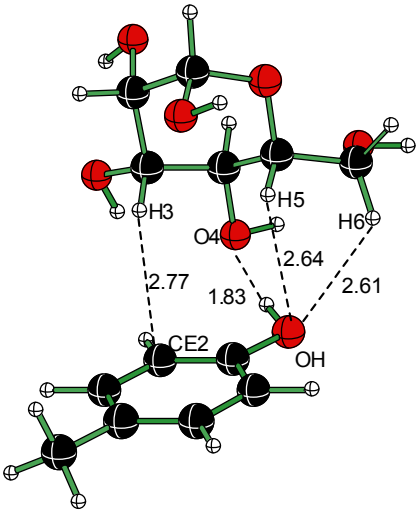
Y-4b (–11.47)



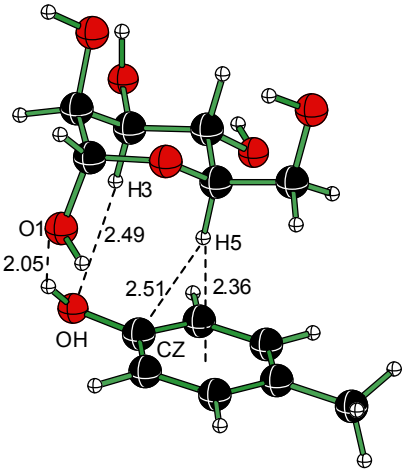
Y-4c (–11.04)



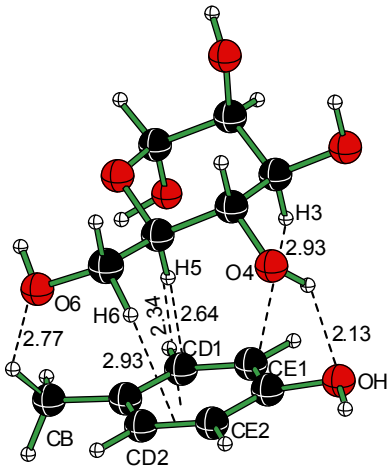
Y-4d (–10.43)



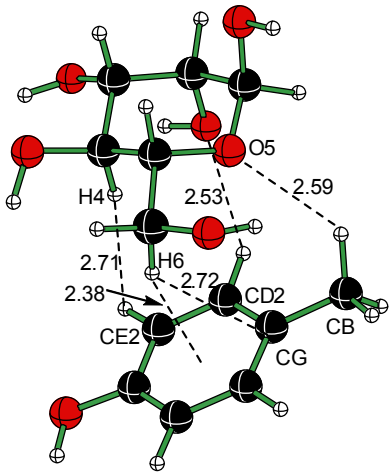
Y-4e (–10.28)



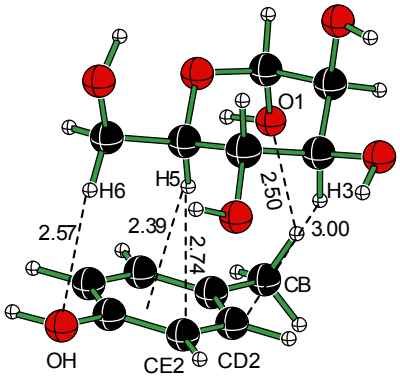
Y-4f (–9.18)



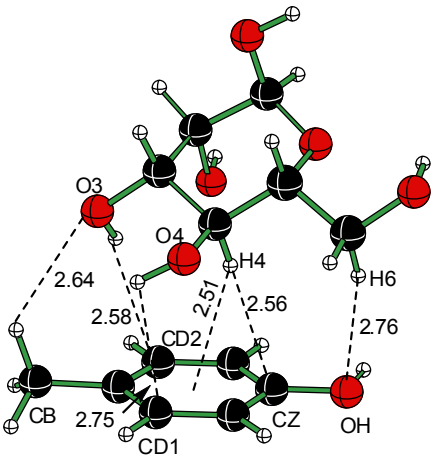
Y-4g (–8.94)



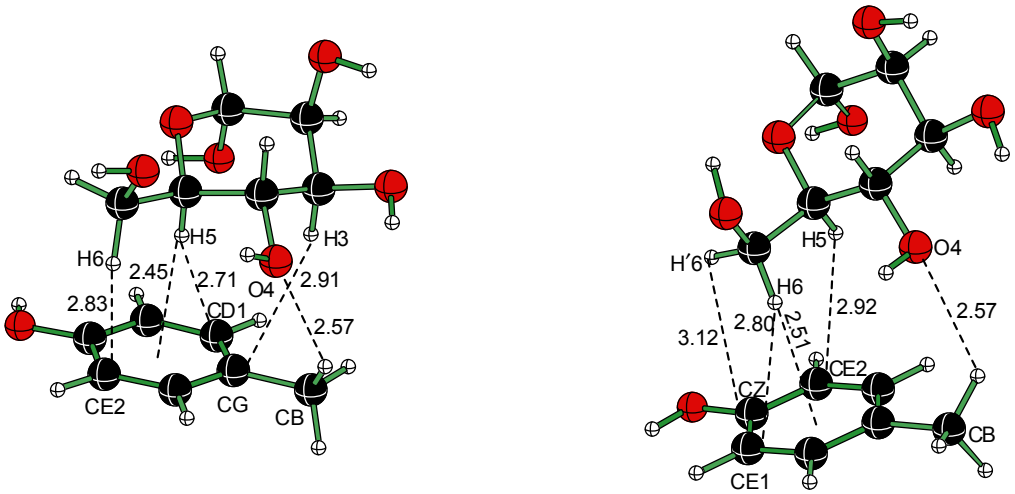
Y-4h (–6.53)



Y-4i (–6.24)

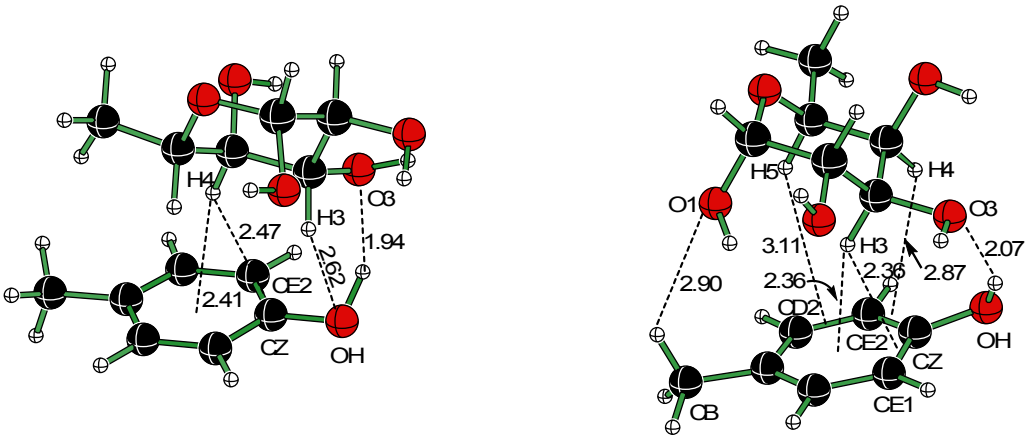


Y-4j (–5.99)

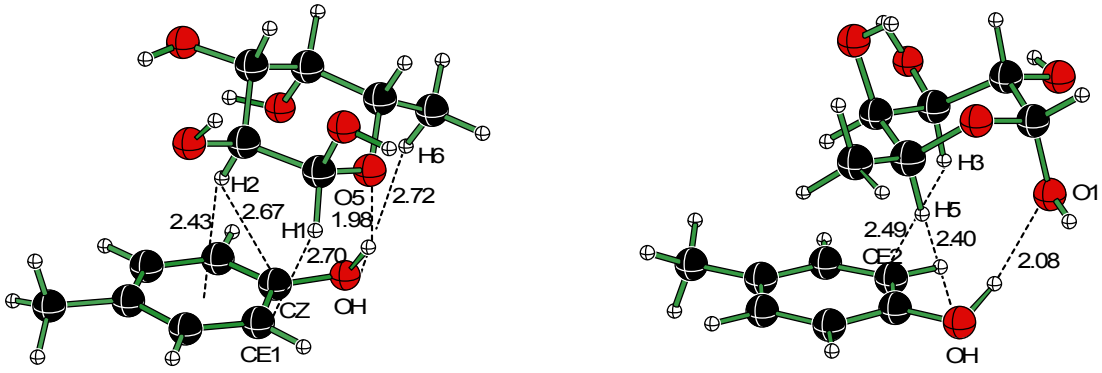


Y-4k (–5.73) **Y-4l** (–4.88)

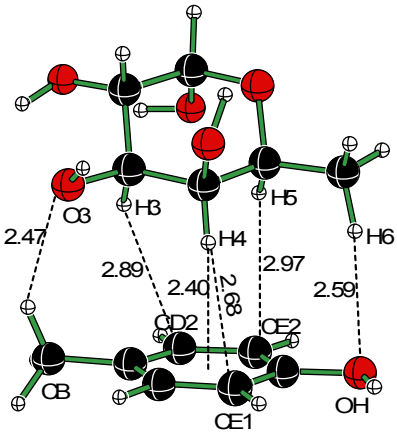
Figure S4. Optimized geometries of *p*-OHTol : α-D-mannose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



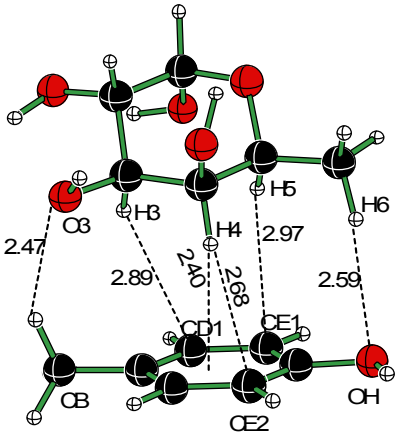
Y-5a (–10.32) **Y-5b** (–10.16)



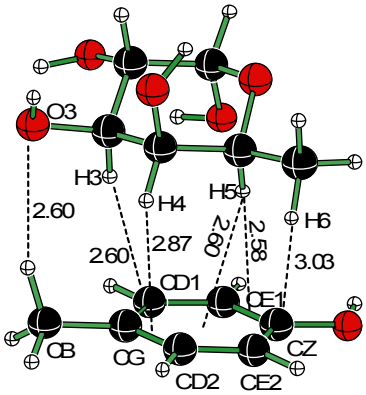
Y-5c (–10.14) **Y-5d** (–8.91)



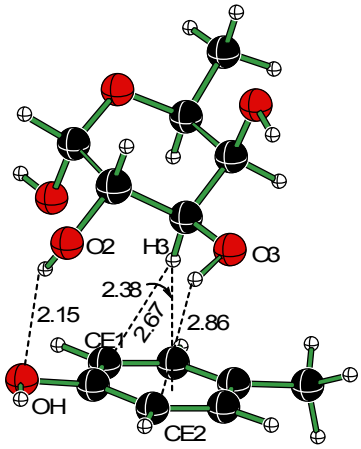
Y-5e (–6.86)



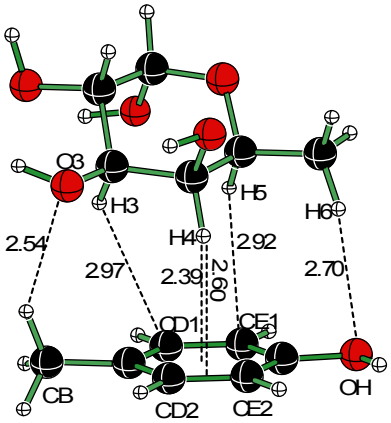
Y-5f (–6.86)



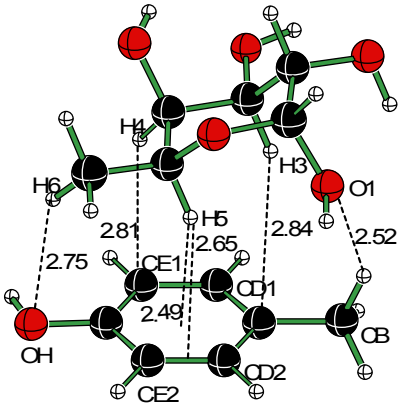
Y-5g (–6.68)



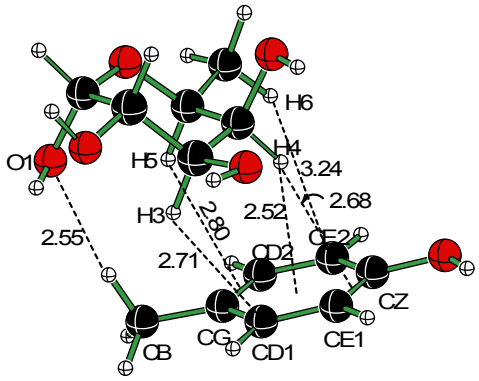
Y-5h (–6.51)



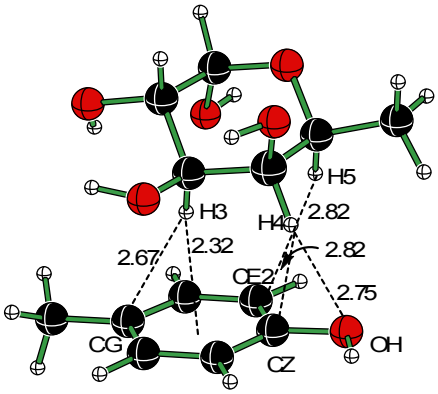
Y-5i (–5.87)



Y-5j (–5.70)

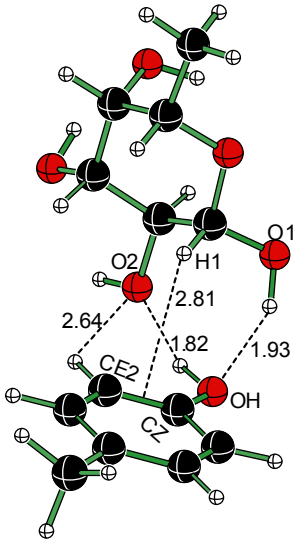


Y-5k (–5.62)

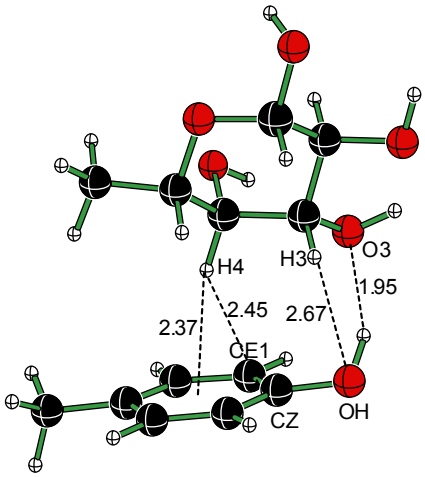


Y-5l (–5.15)

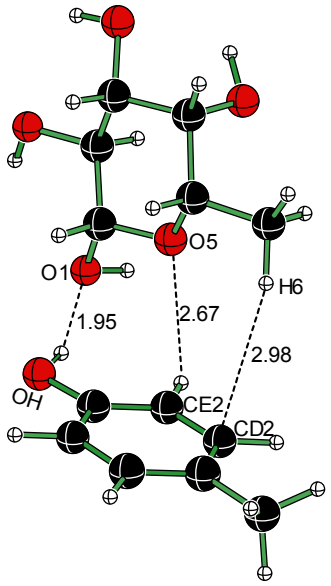
Figure S5. Optimized geometries of *p*-OHTol : α-L-fucose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



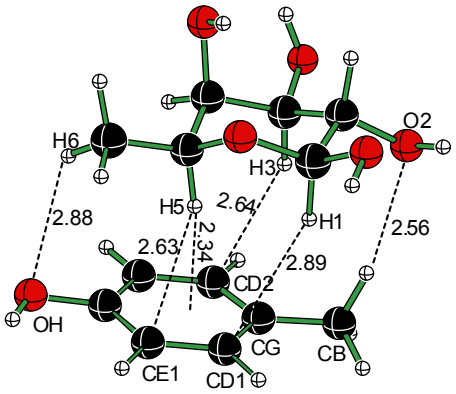
Y-6a (–13.69)



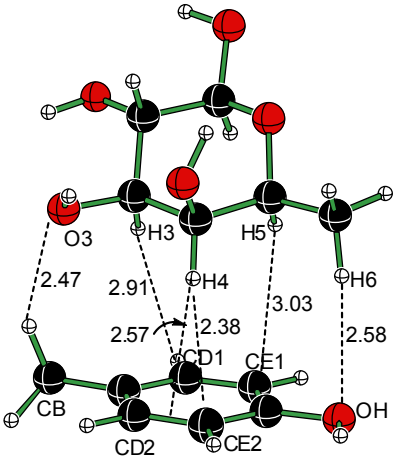
Y-6b (–9.96)



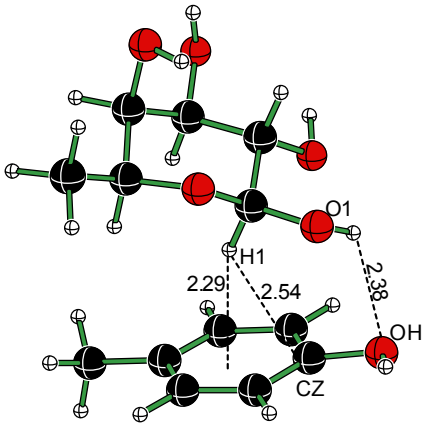
Y-6c (–8.48)



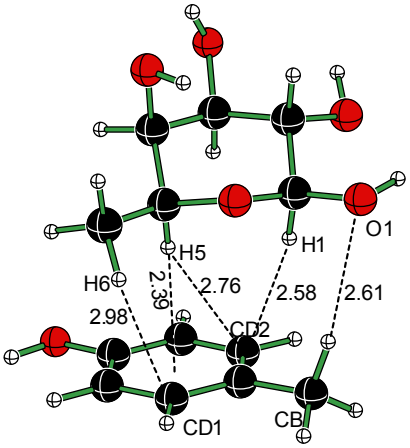
Y-6d (–7.37)



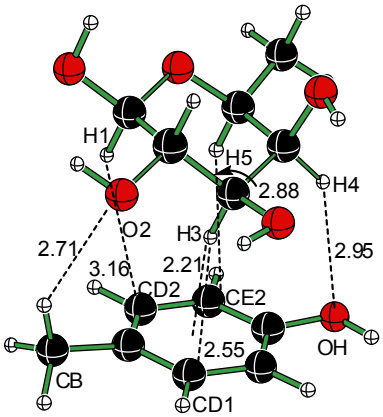
Y-6e (–7.06)



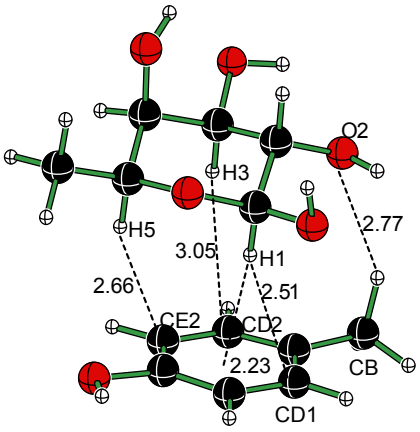
Y-6f (–6.49)



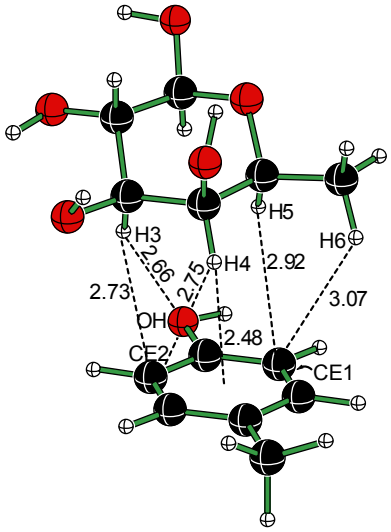
Y-6g (–6.30)



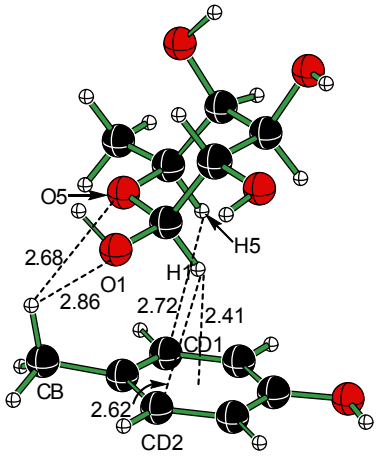
Y-6h (–6.30)



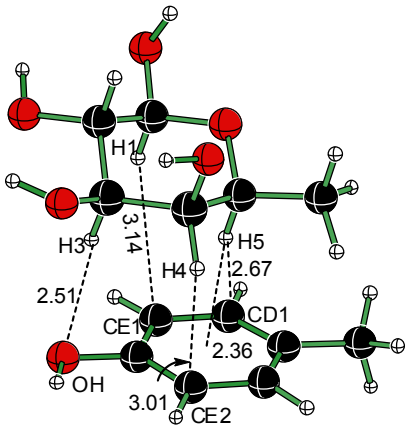
Y-6i (–6.20)



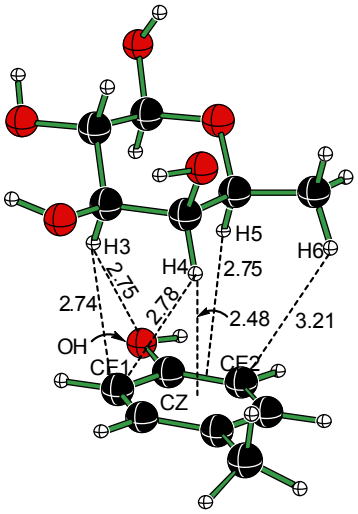
Y-6j (–5.95)



Y-6k (–5.80)

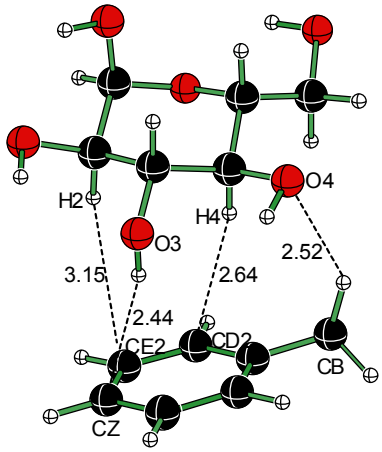


Y-6l (–5.80)

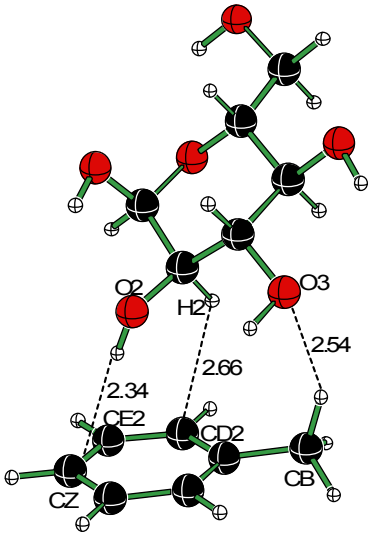


Y-6m (–5.21)

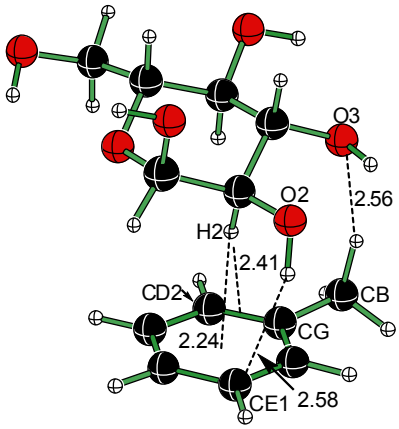
Figure S6. Optimized geometries of *p*-OHTol : β-L-fucose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



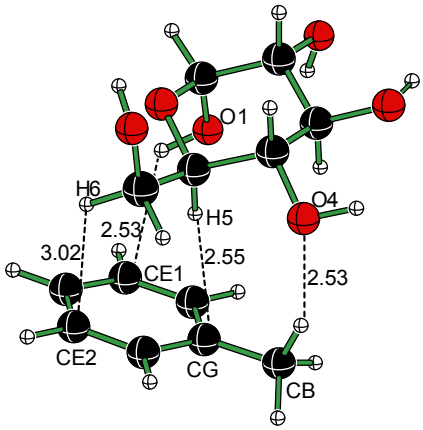
F-1a (–8.58)



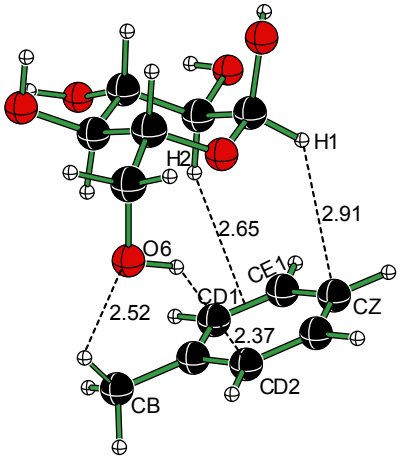
F-1b (–8.06)



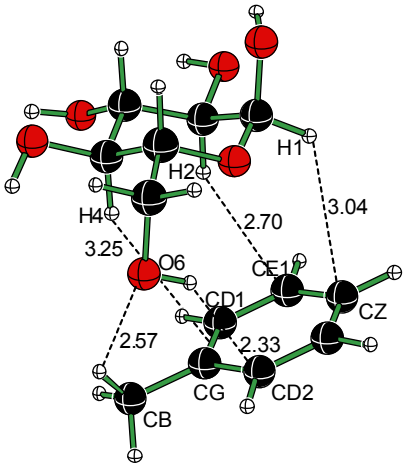
F-1c (–7.75)



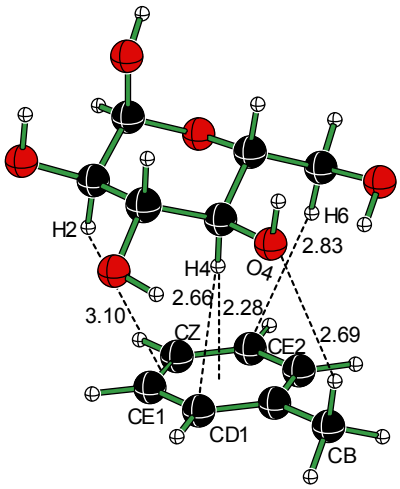
F-1d (–6.76)



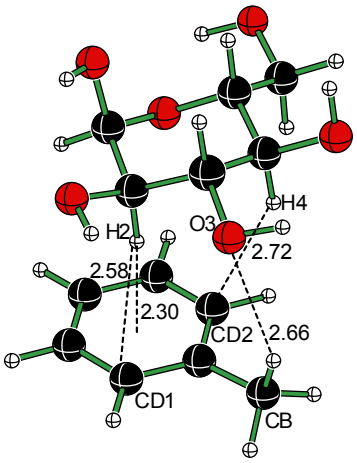
F-1e (–6.17)



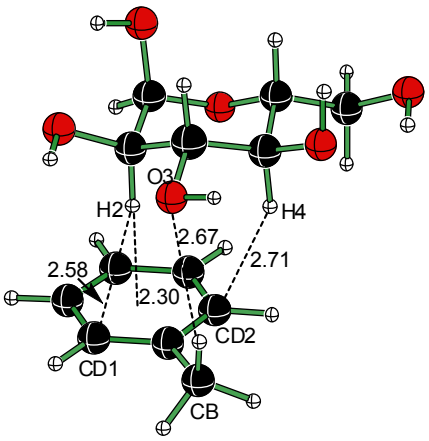
F-1f (–6.10)



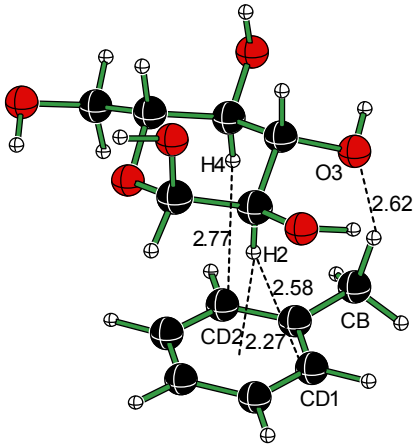
F-1g (–5.92)



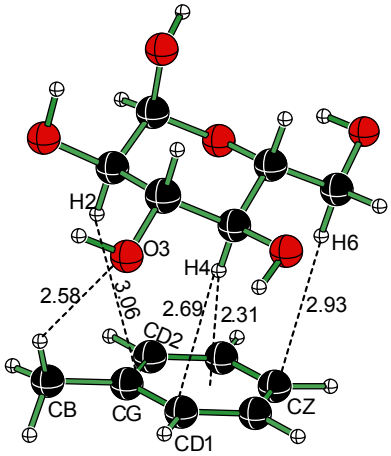
F-1h (–5.74)



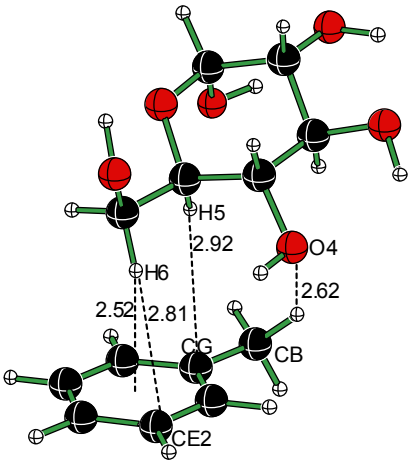
F-1i (–5.72)



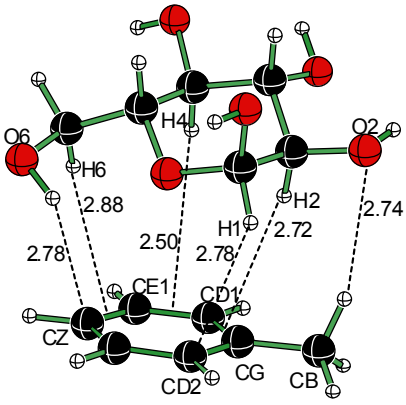
F-1j (–5.49)



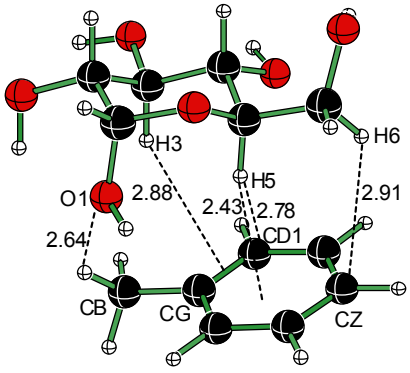
F-1k (–5.39)



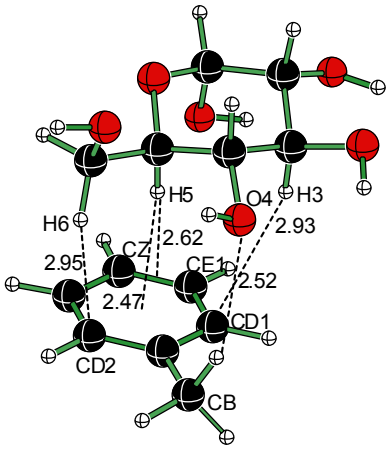
F-1l (–5.37)



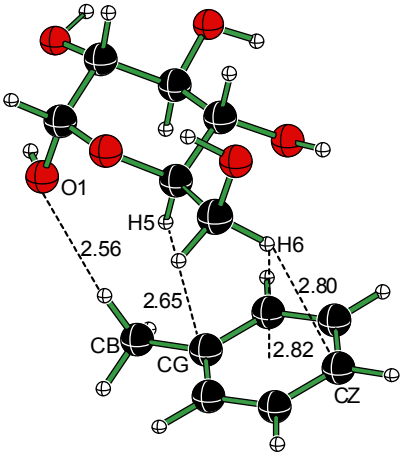
F-1m (–5.25)



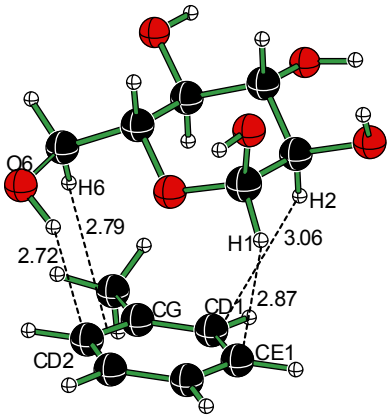
F-1n (–5.12)



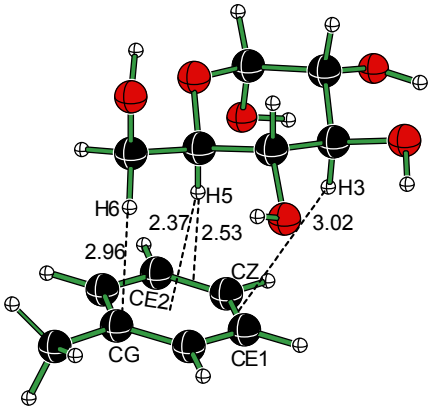
F-1o (–4.96)



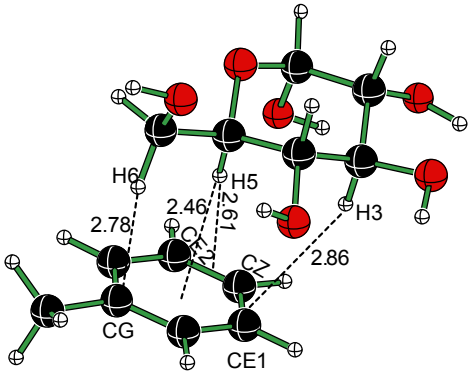
F-1p (–4.90)



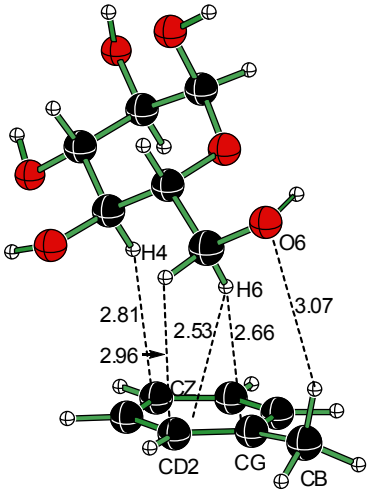
F-1q (–4.86)



F-1r (–4.32)

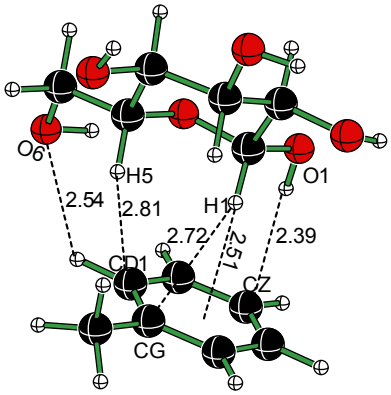


F-1s (–4.03)

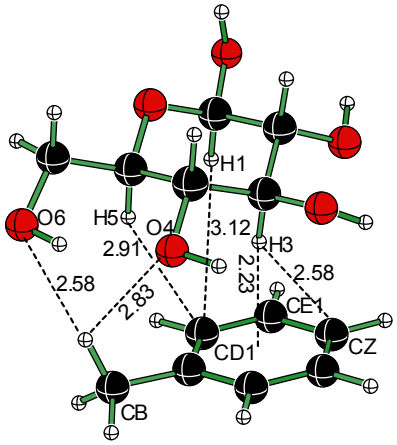


F-1t (–3.70)

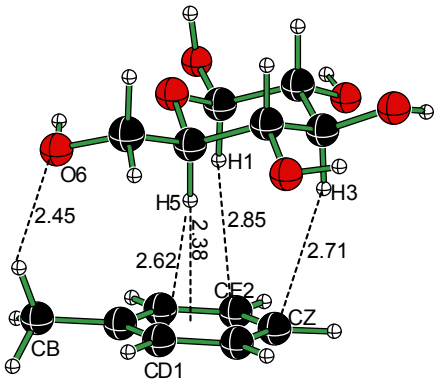
Figure S7. Optimized geometries of Tol : α-D-glucose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



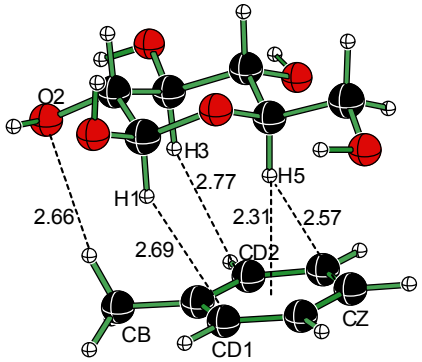
F-2a (–8.22)



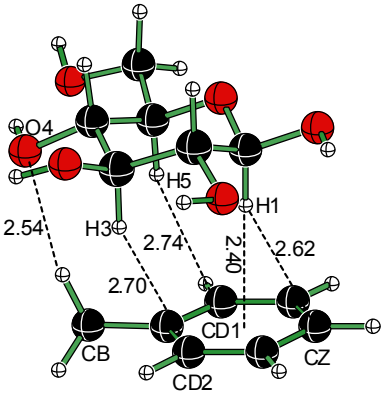
F-2b (–6.87)



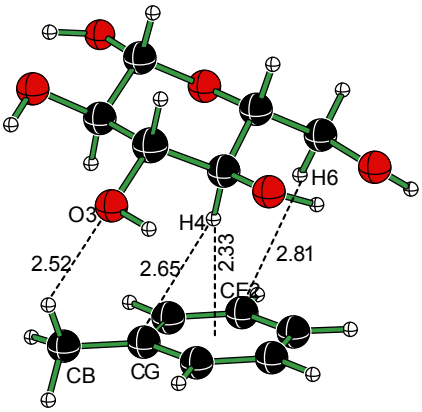
F-2c (–6.59)



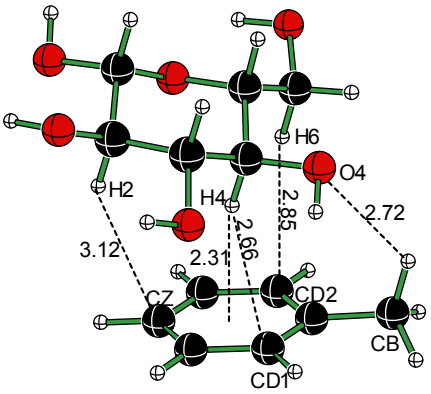
F-2d (–6.31)



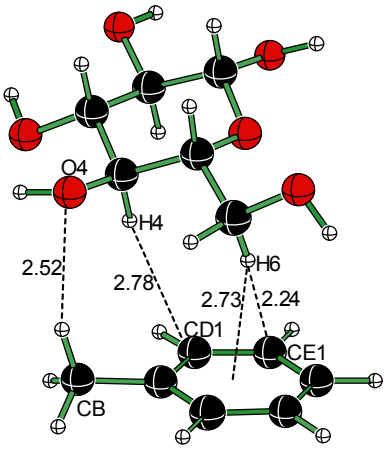
F-2e (–5.73)



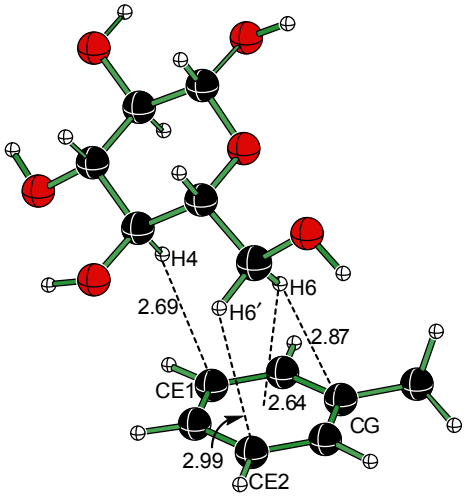
F-2f (–5.59)



F-2g (–5.11)

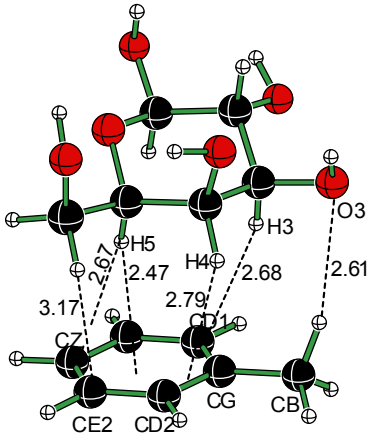


F-2h (–4.76)

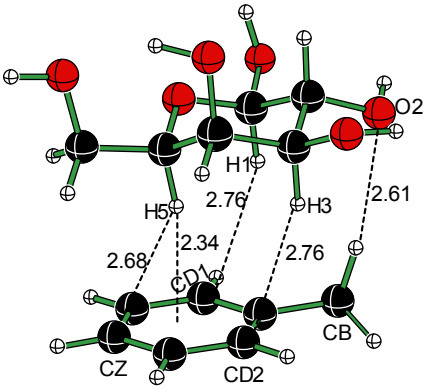


F-2i (–3.47)

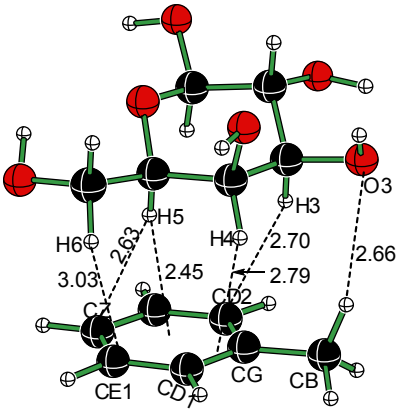
Figure S8. Optimized geometries of Tol : β-D-glucose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



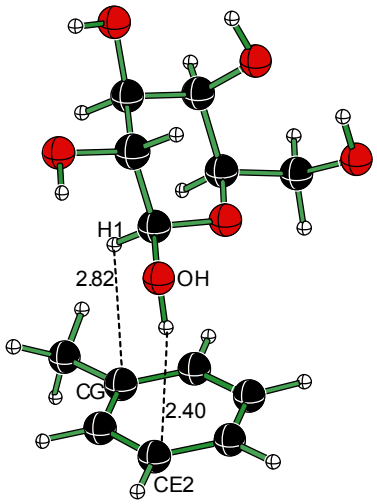
F-3a (–7.26)



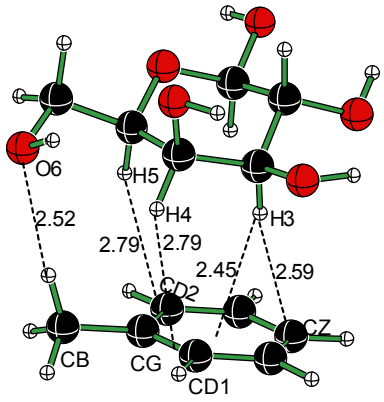
F-3b (–6.81)



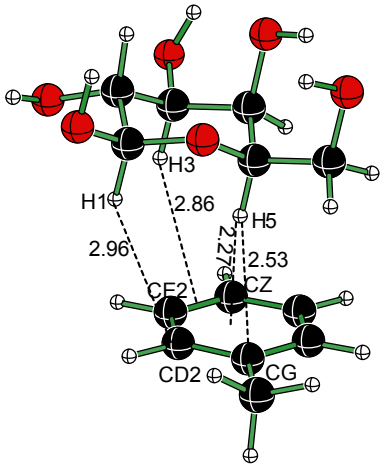
F-3c (–6.74)



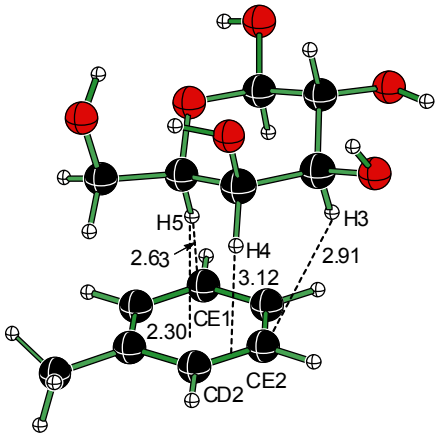
F-3d (–6.42)



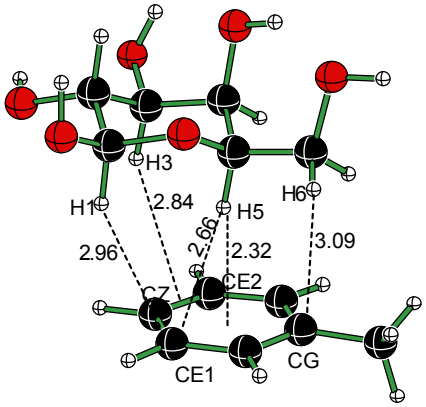
F-3e (–6.35)



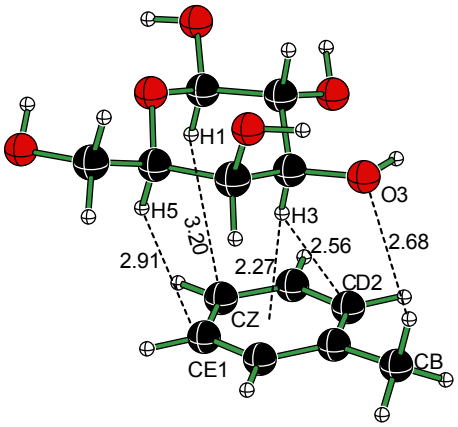
F-3f (–6.25)



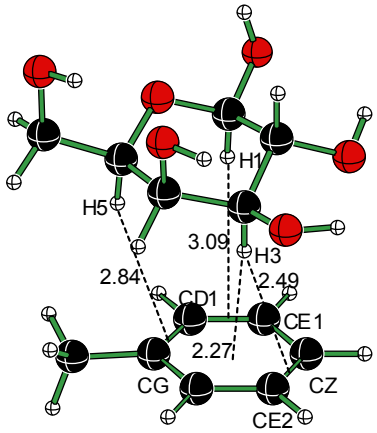
F-3g (–5.97)



F-3h (–5.87)

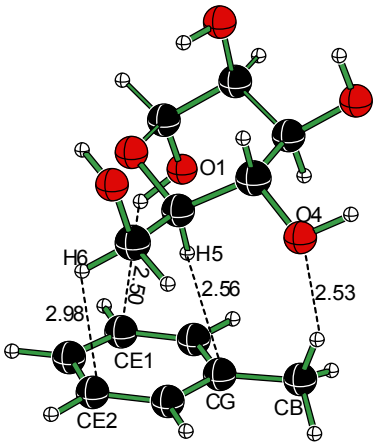


F-3i (–5.73)

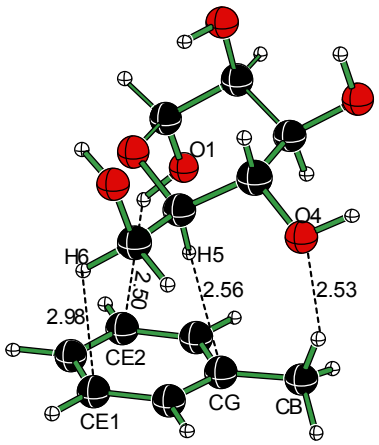


F-3j (–5.37)

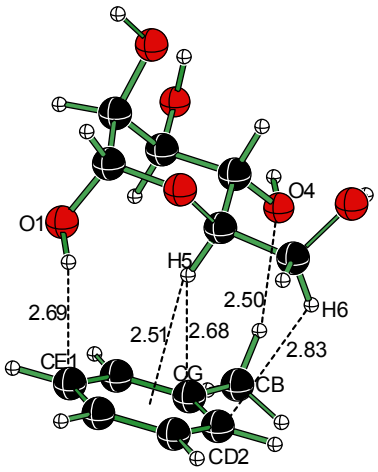
Figure S9. Optimized geometries of Tol : β-D-galactose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



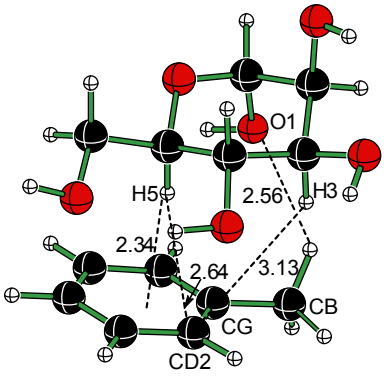
F-4a (–7.12)



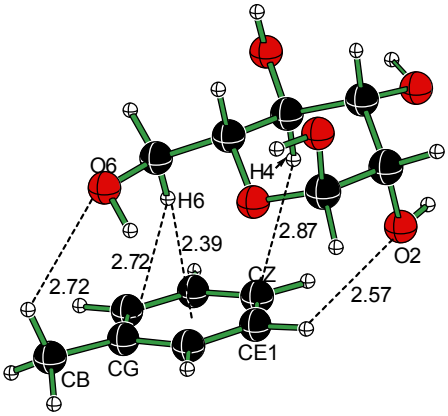
F-4b (–7.12)



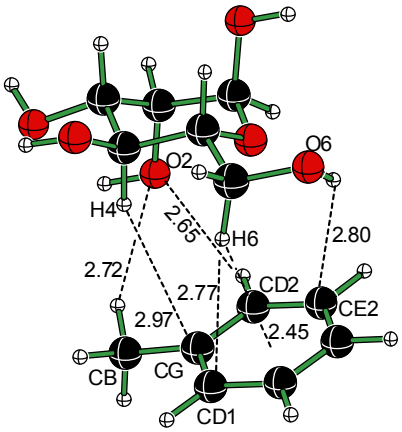
F-4c (–6.33)



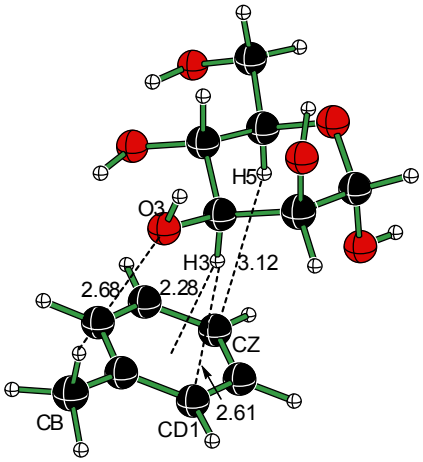
F-4d (–5.58)



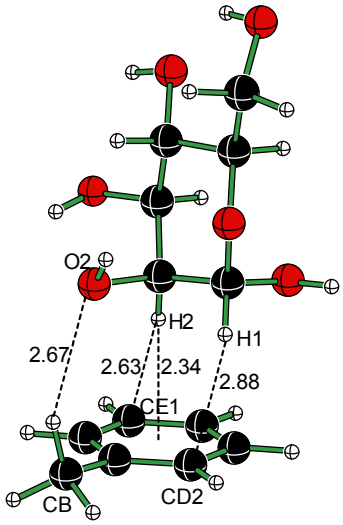
F-4e (–5.56)



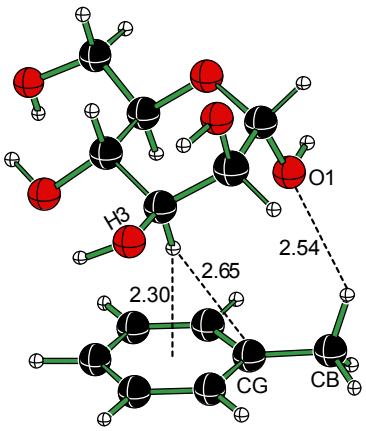
F-4f (–5.16)



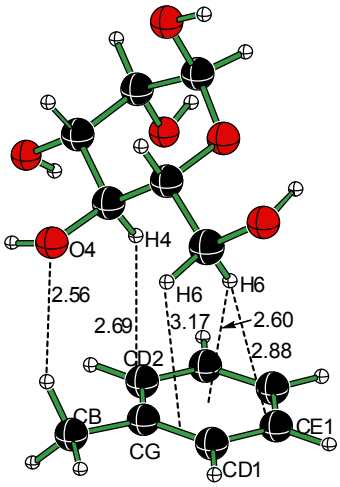
F-4g (–4.95)



F-4h (–4.63)

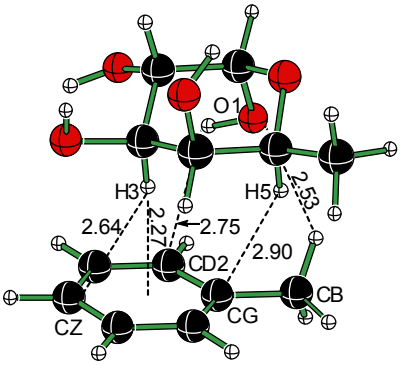


F-4i (–4.26)

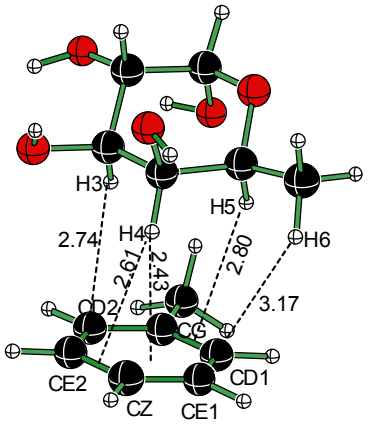


F-4j (–4.13)

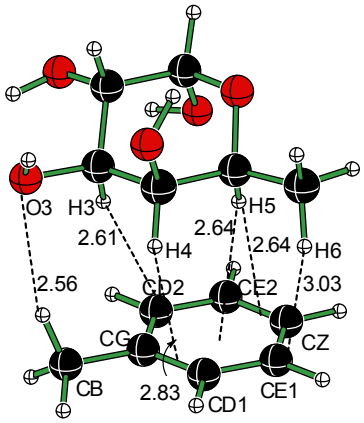
Figure S10. Optimized geometries of Tol : α-D-mannose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



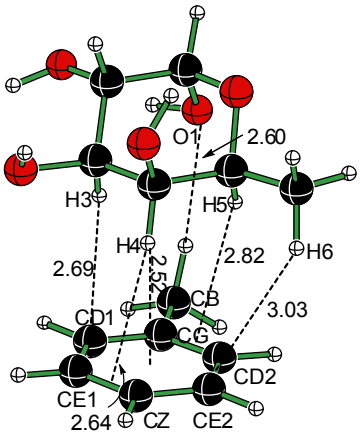
F-5a (–6.50)



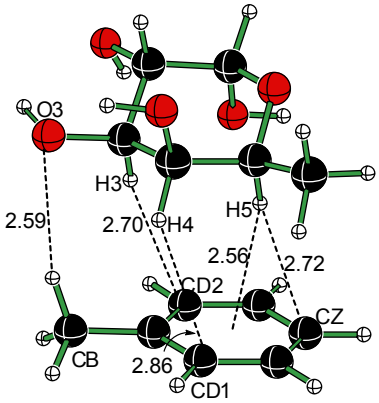
F-5b (–6.34)



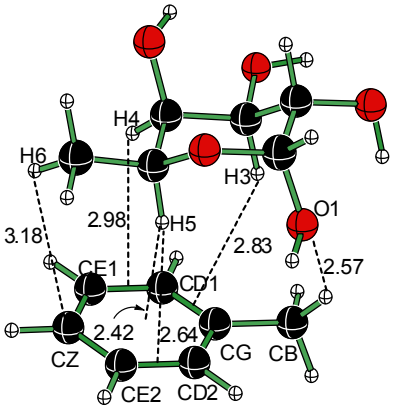
F-5c (–6.16)



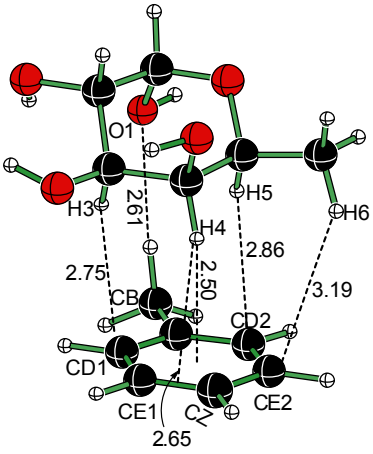
F-5d (–6.10)



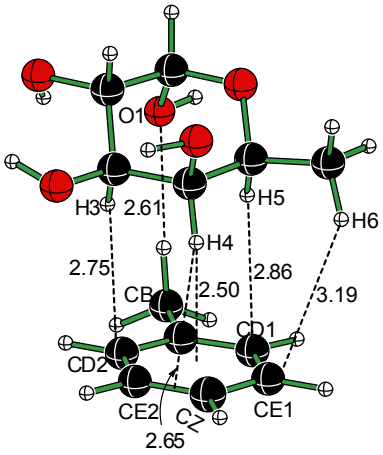
F-5e (–5.57)



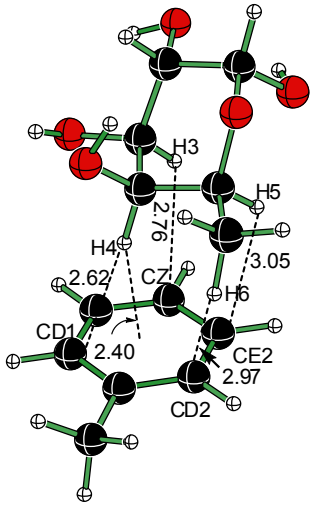
F-5f (–5.35)



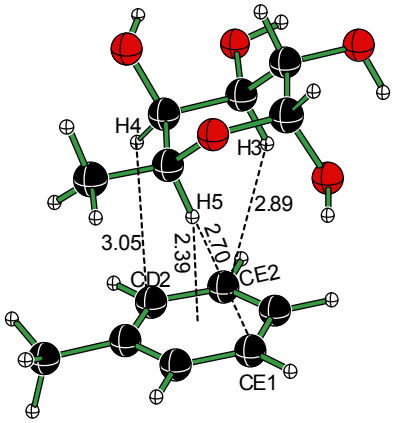
F-5g (–5.26)



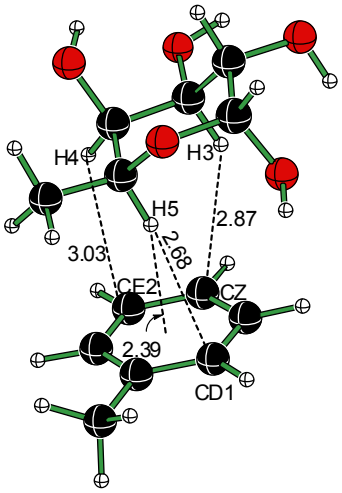
F-5h (–5.26)



F-5i ((–5.12)

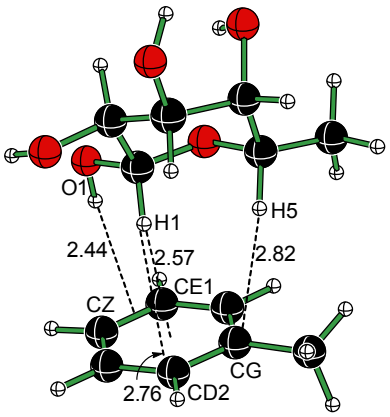


F-5j (–4.70)

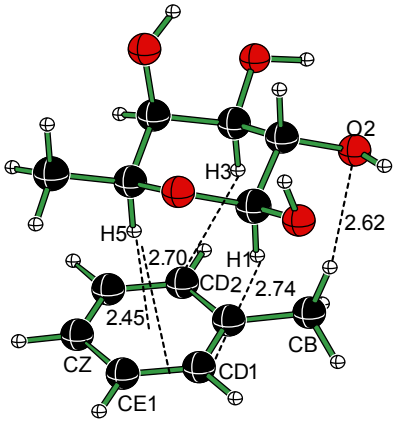


F-5k (–4.61)

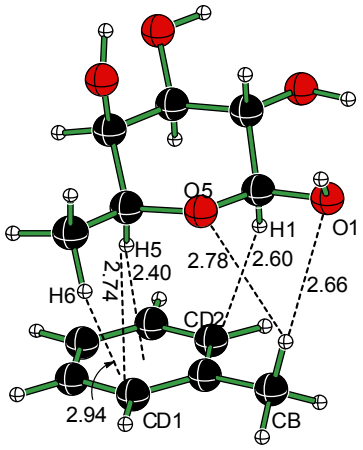
Figure S11. Optimized geometries of Tol : α-L-fucose binary complexes. The interaction energies in kcal/mol are given in parenthesis.



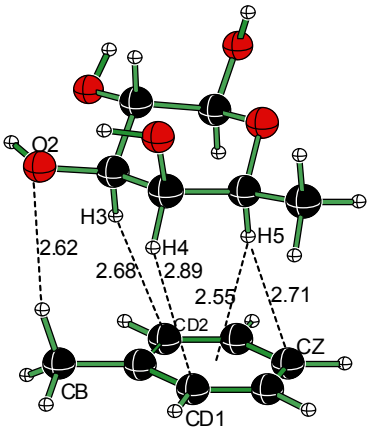
F-6a (–6.70)



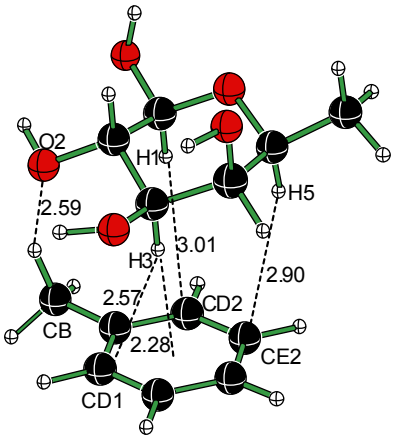
F-6b (–6.12)



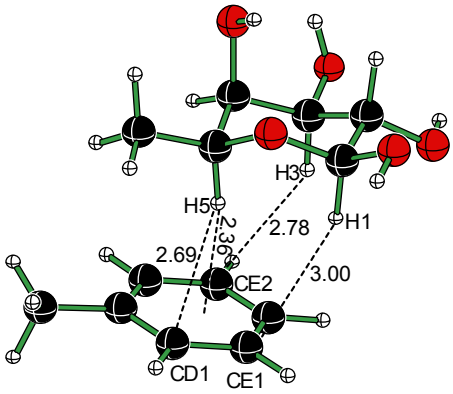
F-6c (–6.02)



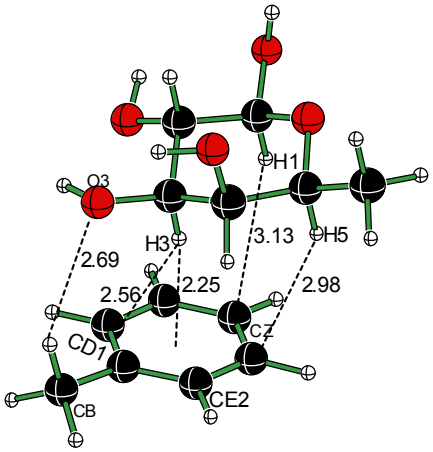
F-6d (–5.94)



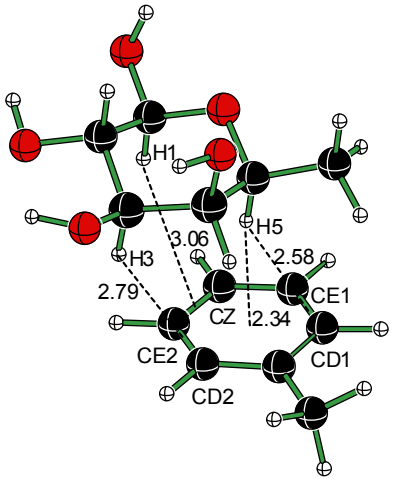
F-6e (–5.73)



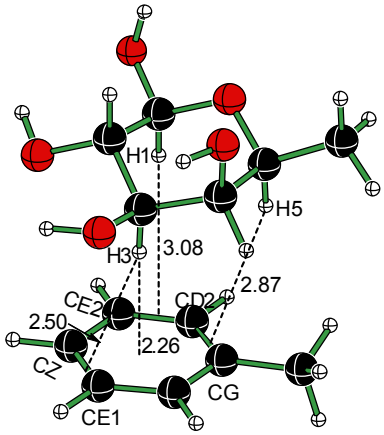
F-6f (–5.66)



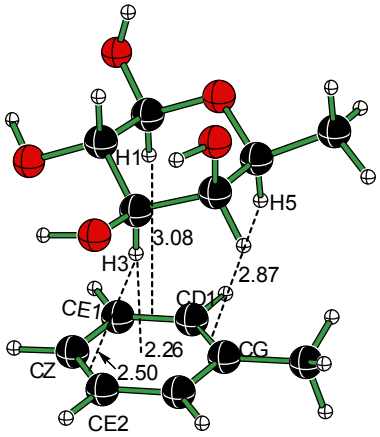
F-6g (–5.51)



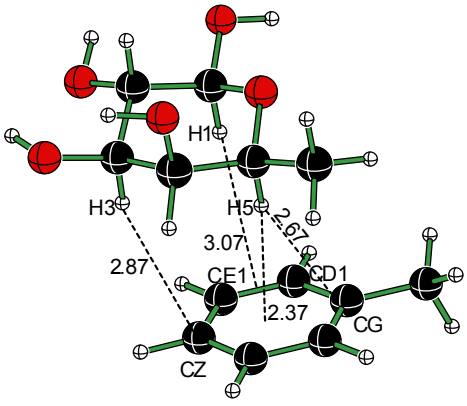
F-6h (–5.22)



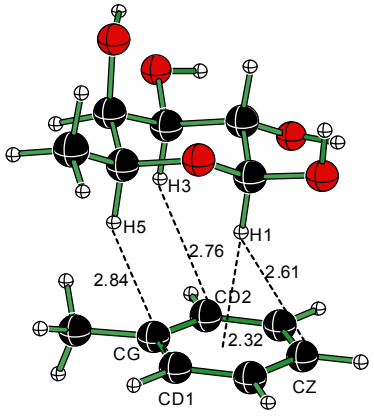
F-6i (–4.94)



F-6j (–4.94)



F-6k (–4.88)



F-6l (–4.82)

Figure S12. Optimized geometries of Tol : β-L-fucose binary complexes. The interaction energies in kcal/mol are given in parenthesis.

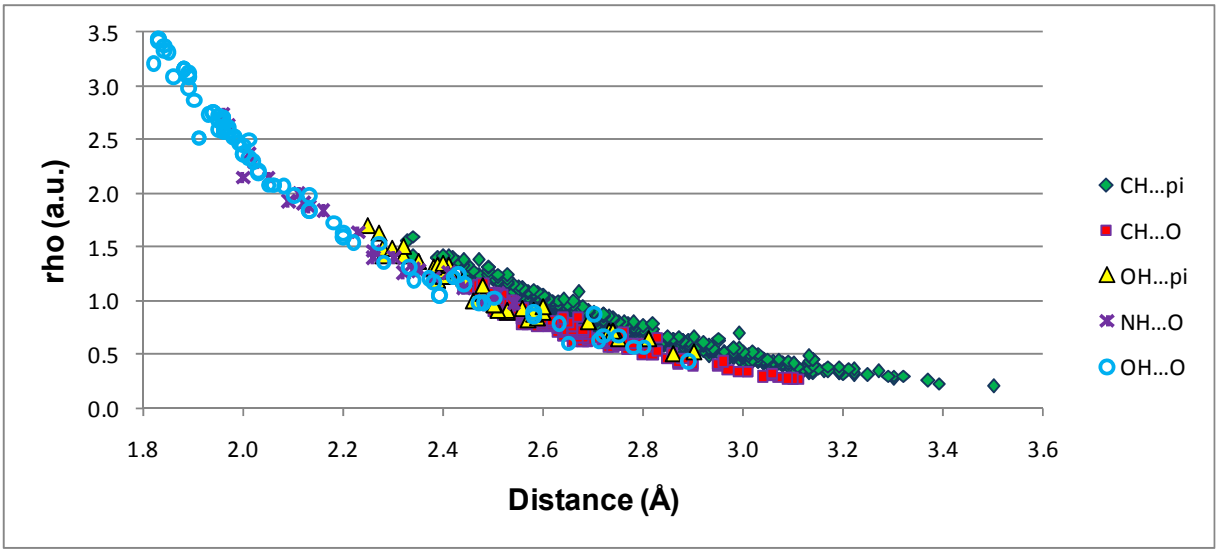
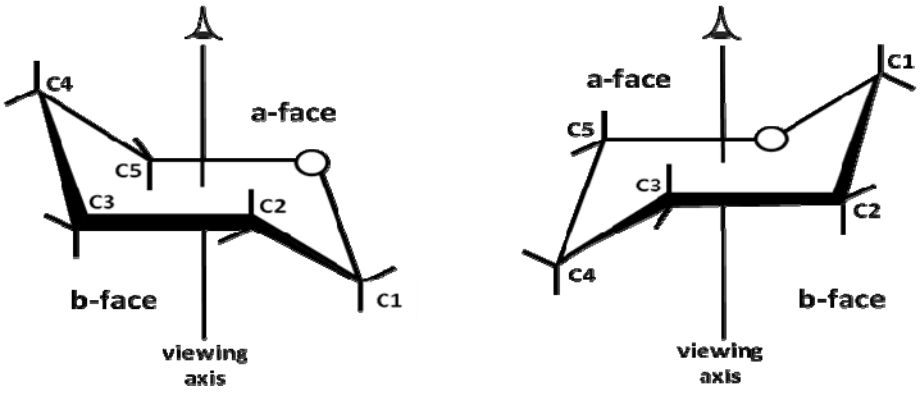
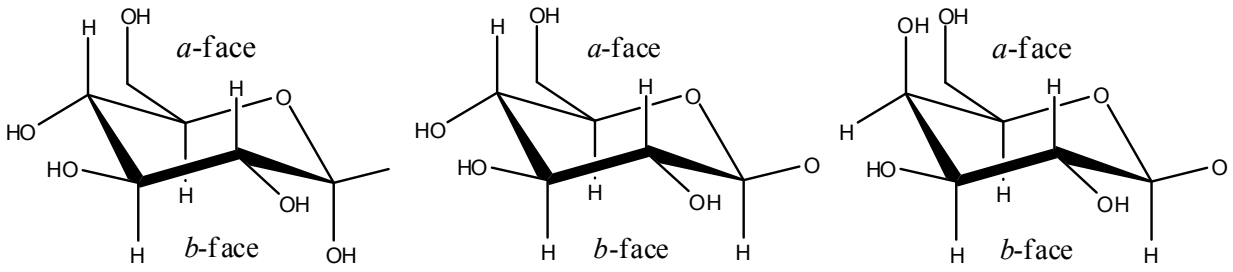


Figure S13. Correlation between the distance between the interacting atom pairs and the corresponding electron densities at bond critical points ($\rho_{bcp} \times 10^{-2}$) for the various types of interactions.

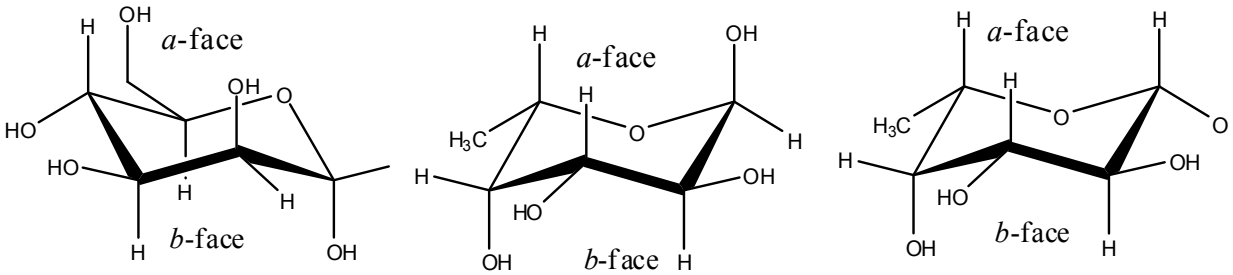
(A)



(B)



α-D-Glucose ($^4C_1$) β-D-Glucose ($^4C_1$) β-D-Galactose ($^4C_1$)



α-D-Mannose ($^4C_1$) α-L-Fucose ($^1C_4$) β-L-Fucose ($^1C_4$)

Figure S14 (A) Schematics showing the *a*-face and *b*-face of a pyranose ring in the $^4C_1$ (*left*) and $^1C_4$ (*right*) conformations. The *a*-face is towards the viewer when viewed in such a way that the atom numbering is clockwise (Sundari and Balasubramanian, 1997). **(B)** The disposition of the C-H and -OH groups in the a-face and b-face and along the periphery of the pyranose ring.

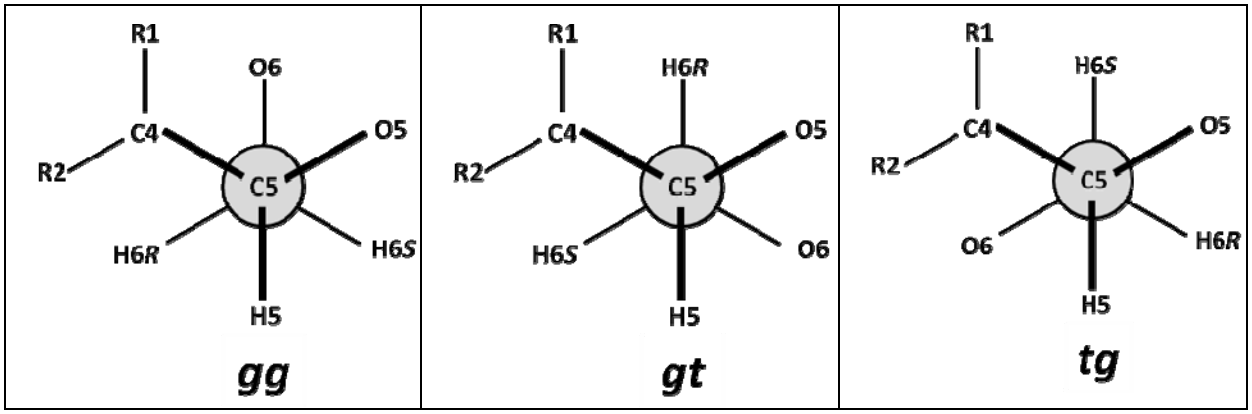
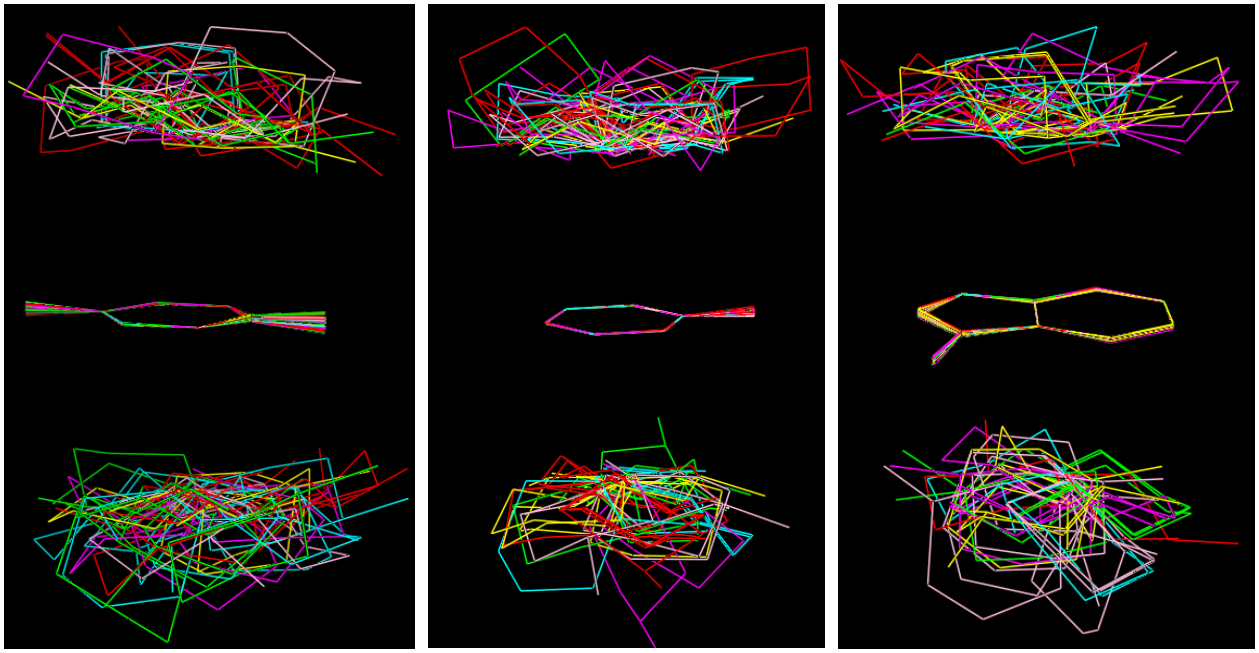


Figure S15 The nomenclature used to describe the three staggered rotamers of the exocyclic -CH_2OH group in hexopyranoses. The conformation of O6 is specified with respect to the ring oxygen atom O5 and C4 as *g* (for gauche) or *t* (for trans). R1 = OH, R2 = H for *galacto* configuration and R1 = H, R2 = OH for *gluco* configuration.



a) p-OHTol: all 6 saccharide b) Tol: all 6 saccharide c) 3-MeIn: all 6 saccharide

Figure S16 Superposition of all the stacking complexes of *p*-OHTol (Y-series; *left panel*), Tol (F-series; *middle panel*) and 3-MeIn; *right panel*). The ring atoms of the aromatic residue were used as reference for superposition. Color code used: α-D-glucose, red; β-D-glucose, green; β-D-galactose, yellow; α-D-mannose, magenta; α-L-fucose, cyan; β-L-fucose, light pink.

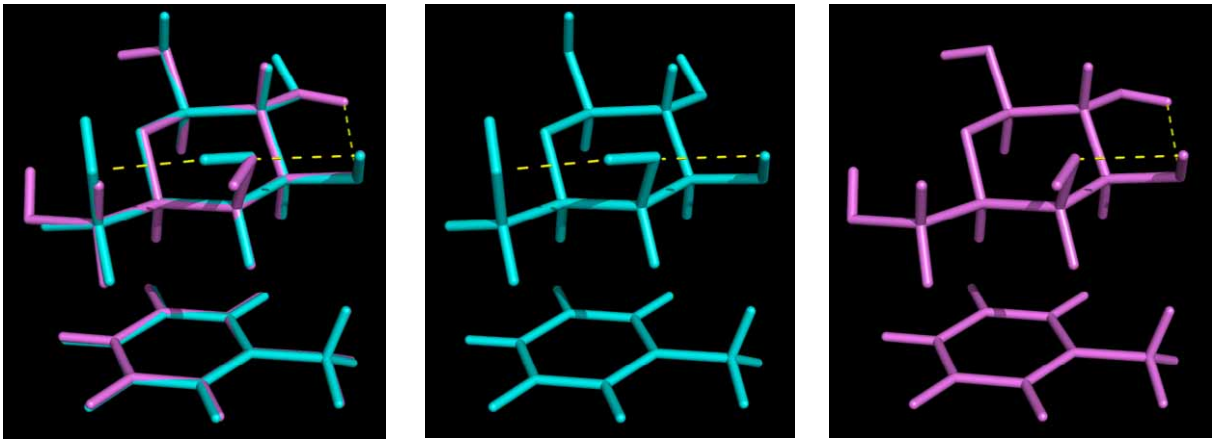


Figure S17 Superposition of **(A)** β-D-galactose - toluene complexes **F-3a** and **F-3c**. The $–CH_2OH$ group is in *gg* and *gt* conformations in **F-3a** and **F-3c**, respectively. **(B)** In **F-3a** the –O3H···O4H···O6H groups and **(C)** in **F-3c** the –O2H···O3H···O4H groups of the β-D-galactose form intramolecular hydrogen bonds. The OH···O interactions are shown in yellow dotted lines.

Legends to movies

Structural superposition of the stacking complexes of indicates saccharides with all the three aromatic residues. The six atoms of the pyranose ring were used for superposition. The carbon, oxygen and hydrogen atoms of the saccharide are rendered in green, red and white, respectively. The hydrogen atoms of the aromatic rings and the hydroxyl hydrogen atoms of the saccharide have not been shown to enhance visual clarity.

Movie S1. Complexes of α-D-glucose and β-D-glucose. The aromatic residues of the α-D-glucose complexes are rendered in blue and those of β-D-glucose are in green.

Movie S2. Complexes of α-L-fucose and β-L-fucose. The aromatic residues of the α-L-fucose complexes are rendered in light pink and those of β-L-fucose are in cyan.

Movie S3. Complexes of β-D-glucose and β-D-galactose. The aromatic residues of the β-D-glucose complexes are rendered in green and those of β-D-galactose are in magenta.

Movie S4. Complexes of α-D-glucose and α-D-mannose. The aromatic residues of the α-D-glucose complexes are rendered in blue and those of α-D-mannose are in yellow.

Movie S5. Complexes of β-D-galactose and β-L-fucose. The aromatic residues of the β-D-galactose complexes are rendered in magenta and those of β-L-fucose are in cyan.

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Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Cartesian Coordinates of optimized binary complexes

Cartesian coordinates for the optimized geometries calculated in the gas-phase are given below. All the Y-series and F-series binary complexes is optimized at MP2/6-31G(d,p) level of theory. Frequency analysis is performed on the optimized geometry. The total energy of the binary complexes in Hartree is given in parenthesis.

***p*-OHTol : Saccharide binary complexes**

(i) Optimized coordinates of *p*-OHTol:α-D-glucose complexes

Y-1a (E_t = -1031.046504)				**Y-1b** (E_t = -1031.044983)			
C	-1.156521	0.566340	-1.064859	C	-2.772906	-0.326948	1.143242
C	0.793509	-0.101367	0.198745	C	-2.681706	0.255830	-1.199617
C	1.038819	1.234990	0.513486	C	-2.410974	1.579769	-0.852825
C	0.202570	2.261817	0.051301	C	-2.297984	1.975679	0.486922
C	-0.894884	1.900251	-0.742288	C	-2.492513	1.000790	1.475124
C	-0.302959	-0.446536	-0.602018	C	-2.836335	-0.712153	-0.201482
C	0.498575	3.705648	0.360381	C	-1.922002	3.385499	0.853001
H	-2.003842	0.303063	-1.684418	H	-2.947982	-1.066585	1.915776
H	-1.562610	2.671287	-1.110921	H	-2.461266	1.292005	2.520850
H	-0.416505	4.296514	0.375442	H	-2.247549	4.089665	0.088121
H	0.979079	3.805637	1.332976	H	-2.376322	3.680361	1.798595
H	1.164375	4.145255	-0.384379	H	-0.839894	3.465164	0.957297
H	1.893932	1.483531	1.132426	H	-2.285355	2.318103	-1.637215
H	1.440446	-0.891846	0.556783	H	-2.760638	-0.051425	-2.234719
O	-0.510590	-1.764133	-0.871223	O	-3.084049	-2.009107	-0.575533
H	-0.987346	-1.818700	-1.722544	H	-2.485115	-2.569940	-0.042102
C	0.489533	-0.641960	-5.867173	C	0.666345	-0.291166	0.501261
C	-0.242684	-0.700166	-4.532843	C	1.150007	-1.541115	-0.228386
O	0.687493	-1.028942	-3.491683	O	1.716437	-1.190828	-1.504083
C	1.742849	-0.089880	-3.334941	C	2.774772	-0.258173	-1.446912
C	2.548549	0.029041	-4.622995	C	2.338775	1.035808	-0.775741

C	1.612011	0.368302	-5.771368
H	2.338884	-0.489578	-2.511855
O	1.296281	1.217069	-3.061883
H	0.876334	1.220741	-2.187378
H	3.038386	-0.923349	-4.833034
O	3.576675	1.009028	-4.516631
H	3.157985	1.748639	-4.049238
H	1.170178	1.355442	-5.587722
O	2.298186	0.351057	-7.020172
H	3.081167	0.905832	-6.892438
H	0.931946	-1.627602	-6.070907
O	-0.444588	-0.283856	-6.877246
H	0.090698	-0.057322	-7.651465
H	-0.712824	0.267363	-4.332380
C	-1.290535	-1.785345	-4.527215
H	-1.967726	-1.621019	-5.367010
H	-0.796774	-2.754586	-4.642490
O	-1.997255	-1.721251	-3.278364
H	-2.693103	-2.390379	-3.297027

C	1.771748	0.735348	0.601071
H	3.053778	-0.089854	-2.489608
O	3.878489	-0.721524	-0.690373
H	4.259426	-1.477093	-1.156830
H	1.560180	1.502755	-1.381784
O	3.406436	1.974235	-0.686367
H	4.163730	1.462755	-0.363221
H	2.566942	0.321542	1.233476
O	1.227973	1.913643	1.189203
H	1.919223	2.585859	1.096391
H	-0.180673	0.142073	-0.041574
O	0.256637	-0.707367	1.813193
H	-0.292867	0.015293	2.151769
H	1.893005	-2.046278	0.397563
C	0.009058	-2.486955	-0.579975
H	-0.645330	-1.972706	-1.288264
H	0.413744	-3.372927	-1.069710
O	-0.730031	-2.914423	0.569159
H	-0.582933	-2.236686	1.255542

Y-1c (E_t = -1031.04691)

C	3.177370	0.029322	1.047932
C	2.270142	0.748026	-1.075415
C	2.390073	-0.555086	-1.557662
C	2.910144	-1.584657	-0.763702
C	3.306517	-1.267072	0.542960
C	2.650418	1.044911	0.239982
C	2.984814	-2.997423	-1.276798
H	3.490125	0.276475	2.054382
H	3.723487	-2.041360	1.177534
H	2.052663	-3.532163	-1.086514
H	3.163220	-3.014735	-2.351282
H	3.789874	-3.548845	-0.792585
H	2.083560	-0.769974	-2.575264
H	1.889529	1.537274	-1.713009
O	2.576480	2.302166	0.764573
H	1.903488	2.798526	0.263608
C	-2.544592	0.631393	-0.616547
C	-1.189559	1.197459	-0.229581
O	-0.924467	0.900786	1.157675
C	-0.883407	-0.491136	1.448452
C	-2.216229	-1.146326	1.105238
C	-2.562674	-0.857886	-0.347840
H	-0.669149	-0.541403	2.519030
O	0.068901	-1.193280	0.689435
H	0.960600	-0.872158	0.902498
H	-2.997714	-0.733721	1.745558
O	-2.189077	-2.550464	1.341672
H	-1.336868	-2.842269	0.982589

Y-1d (E_t = -1031.036239)

C	-0.827673	0.863536	-0.410916
C	0.931786	-0.789154	-0.367910
C	1.862898	0.219559	-0.111629
C	1.474288	1.561814	-0.017006
C	0.113759	1.863753	-0.169696
C	-0.414787	-0.465977	-0.546325
C	2.487843	2.656692	0.186004
H	-1.880013	1.103189	-0.509010
H	-0.216610	2.892878	-0.076618
H	2.094403	3.440672	0.832687
H	3.397404	2.268555	0.642660
H	2.760772	3.118104	-0.764633
H	2.907181	-0.043032	0.016572
H	1.234095	-1.825819	-0.446725
O	-1.308327	-1.482661	-0.796046
H	-1.853921	-1.230178	-1.561266
C	0.903858	-1.139223	-4.343182
C	-0.617389	-1.130773	-4.268447
O	-1.051821	-0.097578	-3.364203
C	-0.615637	1.202881	-3.709747
C	0.901595	1.278096	-3.780497
C	1.411767	0.226140	-4.749357
H	-1.002754	1.845853	-2.918439
O	-1.080697	1.612535	-4.984292
H	-2.044384	1.667731	-4.938136
H	1.304195	1.081064	-2.785710
O	1.353137	2.576677	-4.159103
H	0.792302	2.828468	-4.908541

H	-1.812368	-1.332894	-0.991904
O	-3.869300	-1.326928	-0.667221
H	-3.895025	-2.248321	-0.371721
H	-3.317507	1.100624	0.008832
O	-2.756833	0.917987	-1.992189
H	-3.534962	0.401461	-2.246375
H	-0.410668	0.751571	-0.852419
C	-1.139463	2.710809	-0.322136
H	-1.146886	3.021877	-1.363985
H	-2.018246	3.133184	0.175469
O	0.054319	3.218493	0.276975
H	0.074706	2.811350	1.157060
H	1.041909	0.452522	-5.757612
O	2.835355	0.163450	-4.741781
H	3.135460	1.078524	-4.839211
H	1.298228	-1.357551	-3.340966
O	1.288146	-2.140126	-5.277183
H	2.236045	-2.006378	-5.420270
H	-1.035601	-0.947627	-5.262322
C	-1.132489	-2.441829	-3.712472
H	-0.983120	-3.215528	-4.469049
H	-0.559347	-2.701689	-2.819758
O	-2.514107	-2.267018	-3.387358
H	-2.826933	-3.110436	-3.037165

Y-1e (E_t = -1031.041254)

C	2.260631	-1.272083	-0.661676
C	2.102700	-0.817710	1.707091
C	2.685959	0.432002	1.501460
C	3.064508	0.856716	0.220659
C	2.856565	-0.023964	-0.850355
C	1.841341	-1.653236	0.614961
C	3.627631	2.236165	0.000544
H	2.074778	-1.939437	-1.493464
H	3.164526	0.269828	-1.847996
H	2.826881	2.975190	-0.057302
H	4.199554	2.281868	-0.925546
H	4.288722	2.523355	0.818056
H	2.864949	1.080151	2.352622
H	1.816236	-1.136992	2.701958
O	1.172306	-2.847659	0.764714
H	0.403554	-2.644142	1.327956
C	-0.725884	0.518026	0.513620
C	-1.233075	1.337355	-0.668067
O	-1.369252	0.488064	-1.817978
C	-2.251596	-0.593903	-1.639209
C	-1.792531	-1.495404	-0.492363
C	-1.638781	-0.661187	0.758699
H	-2.224721	-1.138656	-2.587243
O	-3.546544	-0.102710	-1.368319
H	-4.020318	-0.850096	-0.970168
H	-0.830596	-1.952370	-0.744711
O	-2.811023	-2.483474	-0.330453
H	-2.626189	-2.932751	0.505758
H	-2.622490	-0.282837	1.055623
O	-1.128568	-1.512022	1.801931
H	-0.927047	-0.906233	2.532608
H	0.271609	0.154909	0.260183
O	-0.706100	1.246155	1.740059
H	-0.076655	1.969336	1.591624
H	-2.192971	1.800403	-0.414279

Y-1f (E_t = -1031.036239)

C	-2.597792	0.681476	0.492921
C	-1.296407	2.251945	-0.804181
C	-1.608789	1.537797	-1.962178
C	-2.394267	0.377270	-1.916296
C	-2.889747	-0.029987	-0.670195
C	-1.755521	1.797860	0.434329
C	-2.656833	-0.438565	-3.154811
H	-2.988273	0.359062	1.450698
H	-3.526706	-0.905936	-0.610192
H	-3.668312	-0.844432	-3.148163
H	-2.544076	0.167154	-4.053265
H	-1.960799	-1.276430	-3.219801
H	-1.234535	1.889300	-2.917600
H	-0.666480	3.131649	-0.837234
O	-1.359566	2.463003	1.573401
H	-1.086271	1.766211	2.197443
C	0.418056	-0.769141	0.395406
C	1.569025	-1.026837	-0.570928
O	2.346825	0.170857	-0.721478
C	2.898194	0.659487	0.477839
C	1.803622	0.984140	1.495289
C	0.949792	-0.244649	1.709243
H	3.434705	1.568472	0.191206
O	3.776881	-0.304466	1.016590
H	3.882859	-0.054639	1.948221
H	1.178746	1.799328	1.117376
O	2.476512	1.359371	2.697893
H	1.804651	1.377727	3.393255
H	1.561937	-1.025440	2.172546
O	-0.120345	0.106745	2.605848
H	-0.703267	-0.668939	2.604132
H	-0.230925	-0.017085	-0.056607
O	-0.318492	-1.945519	0.724567
H	-0.700866	-2.244570	-0.115422
H	2.191591	-1.846980	-0.196763

C	-0.211781	2.380599	-1.098379
H	0.698570	1.864634	-1.398960
H	-0.590518	2.948724	-1.951158
O	0.163463	3.243511	-0.014176
H	-0.582194	3.834956	0.152807

C	1.059356	-1.315174	-1.975797
H	0.502650	-0.446308	-2.322857
H	1.899211	-1.486742	-2.653028
O	0.132641	-2.411393	-1.996105
H	0.642922	-3.220752	-1.861062

Y-1g (E_t = -1031.037171)

C	1.834340	0.784290	1.475429
C	2.894300	0.423100	-0.668360
C	3.008681	-0.934778	-0.370376
C	2.528613	-1.463439	0.836142
C	1.950137	-0.578633	1.753506
C	2.288290	1.282862	0.250984
C	2.521803	-2.945948	1.089536
H	1.384119	1.456877	2.197526
H	1.564496	-0.961250	2.690665
H	1.574872	-3.372248	0.755777
H	3.329538	-3.441146	0.551469
H	2.636162	-3.163725	2.151004
H	3.466211	-1.598022	-1.095857
H	3.262251	0.829706	-1.601646
O	2.187560	2.611327	-0.094966
H	1.661934	3.060389	0.583638
C	-1.672794	0.341830	0.715124
C	-2.003987	1.235468	-0.472884
O	-1.049111	1.041785	-1.532499
C	-0.891128	-0.305388	-1.944583
C	-0.483584	-1.220700	-0.797869
C	-1.509462	-1.116510	0.317127
H	-0.105373	-0.273766	-2.702336
O	-2.093934	-0.838270	-2.468650
H	-2.280528	-0.377555	-3.297030
H	0.476064	-0.882881	-0.415658
O	-0.286248	-2.543999	-1.266488
H	-1.116153	-2.796071	-1.696479
H	-2.477778	-1.491319	-0.053377
O	-1.071357	-1.884586	1.428318
H	-1.592013	-1.557380	2.176947
H	-0.735564	0.682276	1.153398
O	-2.651566	0.467093	1.755277
H	-3.492721	0.161417	1.384788
H	-3.015854	1.006412	-0.833903
C	-1.890025	2.711415	-0.129281
H	-2.268755	3.306108	-0.967049
H	-2.484777	2.926301	0.756709
O	-0.541791	3.049441	0.166844
H	-0.023450	2.729961	-0.587887

Y-1h (E_t = -1031.033854)

C	2.522997	0.251912	1.142539
C	2.532110	-0.607844	-1.113635
C	2.081394	-1.838141	-0.636134
C	1.817855	-2.043688	0.726175
C	2.057126	-0.980023	1.605344
C	2.702640	0.459219	-0.228498
C	1.217941	-3.333385	1.220901
H	2.731986	1.056983	1.837739
H	1.904556	-1.122451	2.670000
H	0.130849	-3.252835	1.292848
H	1.449641	-4.158429	0.548065
H	1.596832	-3.589281	2.210255
H	1.935585	-2.655251	-1.334699
H	2.712657	-0.443646	-2.168232
O	3.086224	1.671305	-0.746637
H	2.725697	2.370001	-0.177052
C	-1.449386	0.417669	1.088318
C	-1.007754	1.580004	0.209786
O	-0.263217	1.060784	-0.905122
C	-0.982548	0.175494	-1.736519
C	-1.442921	-1.038651	-0.938298
C	-2.233312	-0.592644	0.274016
H	-0.269003	-0.118471	-2.510714
O	-2.095083	0.847856	-2.283372
H	-2.695833	0.142739	-2.572896
H	-0.561622	-1.592205	-0.603032
O	-2.253990	-1.818275	-1.816382
H	-2.675950	-2.490862	-1.263202
H	-3.162214	-0.119140	-0.075573
O	-2.526336	-1.764929	1.030341
H	-2.860509	-1.452055	1.883691
H	-0.559876	-0.073479	1.488934
O	-2.203326	0.842196	2.228555
H	-2.956627	1.350781	1.894429
H	-1.875640	2.132964	-0.167663
C	-0.038312	2.507474	0.937480
H	-0.593449	3.201562	1.568174
H	0.602114	1.900669	1.580102
O	0.749523	3.262802	0.019659
H	0.751337	2.739925	-0.798848

Y-1i (E_t = -1031.033281)

C	2.162814	0.864720	1.172852
C	2.571166	0.186907	-1.111106
C	3.056949	-1.038411	-0.656684
C	3.103300	-1.336447	0.711817
C	2.662320	-0.361590	1.615459
C	2.088804	1.127179	-0.195267
C	3.568337	-2.686924	1.187438
H	1.808489	1.613346	1.869994
H	2.699765	-0.565866	2.679497
H	4.406964	-3.045840	0.591432
H	2.767094	-3.423240	1.107614
H	3.885195	-2.648837	2.228746
H	3.410812	-1.769976	-1.374478
H	2.556356	0.421278	-2.169099
O	1.554969	2.329610	-0.624217
H	0.844702	2.078877	-1.238627
C	-1.731793	0.469082	0.818356
C	-1.864399	1.243426	-0.493121
O	-0.789145	0.900529	-1.396469
C	-0.732674	-0.505465	-1.700075
C	-0.500091	-1.293243	-0.421085
C	-1.633502	-1.016887	0.540849
H	0.120768	-0.600097	-2.374681
O	-1.923185	-0.946837	-2.287401
H	-1.984259	-0.535564	-3.159366
H	0.427006	-0.925673	0.026041
O	-0.399135	-2.671087	-0.738823
H	-0.465786	-3.123385	0.114238
H	-2.577551	-1.355111	0.100527
O	-1.344208	-1.746528	1.732136
H	-2.051065	-1.519922	2.352546
H	-0.806297	0.786089	1.320028
O	-2.866871	0.633812	1.660625
H	-3.025025	1.589076	1.716961
H	-2.828681	1.001007	-0.948456
C	-1.734544	2.744873	-0.306351
H	-0.744176	2.961190	0.100822
H	-1.831578	3.239771	-1.277275
O	-2.772204	3.158473	0.591289
H	-2.609905	4.079765	0.825077

Y-1j (E_t = -1031.035845)

C	-1.660528	-0.360768	2.034390
C	-3.042659	-0.282029	0.047512
C	-2.945707	1.112847	0.048579
C	-2.196154	1.789614	1.015698
C	-1.568984	1.027709	2.012966
C	-2.363673	-1.013360	1.020045
C	-1.982052	3.276697	0.943399
H	-1.154550	-0.948261	2.787946
H	-0.995596	1.530336	2.783466
H	-2.742921	3.755906	0.328425
H	-1.003880	3.484278	0.507441
H	-2.013876	3.728740	1.934535
H	-3.461871	1.677106	-0.719887
H	-3.609746	-0.790974	-0.724905
O	-2.326457	-2.398877	1.025935
H	-2.881491	-2.721543	0.303055
C	1.606687	0.771891	-0.737386
C	0.306461	0.039825	-1.029877
O	0.560750	-1.349479	-1.323028
C	1.254857	-2.054216	-0.316040
C	2.578727	-1.382852	0.030046
C	2.327266	0.070941	0.390888
H	1.412238	-3.050629	-0.738268
O	0.558682	-2.125612	0.912901
H	-0.313869	-2.529454	0.772471
H	3.241141	-1.424164	-0.836237
O	3.249091	-2.054403	1.094738
H	2.548277	-2.250677	1.735485
H	1.691620	0.111823	1.284720
O	3.553673	0.762841	0.615718
H	4.058021	0.198802	1.219642
H	2.238543	0.758568	-1.631267
O	1.268856	2.110841	-0.372008
H	2.093102	2.494564	-0.039905
H	-0.340226	0.126234	-0.155586
C	-0.418286	0.610492	-2.225049
H	-1.310878	0.003738	-2.410763
H	-0.733253	1.625549	-1.966351
O	0.465076	0.595030	-3.341259
H	0.054955	1.116707	-4.039833

Y-1k (E_t = -1031.036154)

C	2.390257	-0.012530	1.421840
C	2.978850	0.500239	-0.867012
C	2.340393	1.731924	-0.743280

Y-1l (E_t = -1031.040603)

C	2.123273	0.405284	1.595424
C	2.987895	0.509783	-0.663419
C	2.376307	1.756463	-0.829882

C	1.696892	2.110400	0.445992
C	1.747271	1.224895	1.527358
C	2.969407	-0.391597	0.209274
C	0.926576	3.400439	0.521372
H	2.432381	-0.680667	2.276642
H	1.275294	1.494337	2.464991
H	-0.022100	3.295836	-0.006075
H	0.718190	3.674135	1.554689
H	1.480947	4.217500	0.059634
H	2.340697	2.415513	-1.585467
H	3.466130	0.202302	-1.786500
O	3.548896	-1.621717	0.005162
H	3.380671	-2.169337	0.783845
C	-1.538045	0.186558	-1.243406
C	-2.298964	0.262400	0.073848
O	-2.567268	-1.076550	0.535847
C	-1.398131	-1.814899	0.841593
C	-0.538294	-1.958995	-0.412868
C	-0.262724	-0.596335	-1.018136
H	-1.766259	-2.787716	1.178519
O	-0.674071	-1.171186	1.860872
H	0.261236	-1.325469	1.655636
H	-1.076101	-2.573824	-1.143206
O	0.687437	-2.577605	-0.022866
H	1.318707	-2.388908	-0.735722
H	0.352516	-0.023261	-0.320592
O	0.454907	-0.834318	-2.226120
H	0.817268	0.025096	-2.481591
H	-2.148151	-0.322780	-1.999255
O	-1.132738	1.484856	-1.699152
H	-1.868585	1.868374	-2.191622
H	-1.691641	0.793717	0.811675
C	-3.663843	0.910764	-0.024586
H	-3.556671	1.949437	-0.338539
H	-4.254010	0.375596	-0.780379
O	-4.312679	0.921591	1.234033
H	-4.202969	0.022642	1.574675

C	1.624173	2.339594	0.194848
C	1.522957	1.647560	1.411650
C	2.833725	-0.176219	0.542692
C	0.886902	3.634973	-0.010894
H	2.025602	-0.139303	2.524327
H	0.958093	2.086459	2.226482
H	-0.171939	3.437139	-0.181156
H	0.971445	4.280008	0.863255
H	1.278246	4.178268	-0.870234
H	2.490915	2.278605	-1.773107
H	3.577584	0.075481	-1.464819
O	3.347264	-1.436517	0.760685
H	3.763640	-1.742757	-0.056590
C	-1.760710	0.077538	-0.905024
C	-2.345788	-0.298077	0.446649
O	-2.338153	-1.735641	0.548071
C	-1.042758	-2.302747	0.494706
C	-0.304684	-1.939854	-0.792576
C	-0.342373	-0.433619	-1.001905
H	-1.208000	-3.381004	0.559356
O	-0.212578	-1.851083	1.548917
H	-0.593277	-2.174365	2.376304
H	-0.817297	-2.415326	-1.631457
O	1.026045	-2.440257	-0.789887
H	1.390278	-2.241246	0.087944
H	0.253206	0.057530	-0.229137
O	0.129432	-0.068528	-2.299430
H	1.084889	-0.214102	-2.275737
H	-2.367255	-0.398166	-1.688192
O	-1.787752	1.499637	-1.057685
H	-1.221035	1.675433	-1.824611
H	-1.739630	0.147933	1.240931
C	-3.790882	0.144706	0.616965
H	-4.376346	-0.216281	-0.237644
H	-4.195663	-0.316743	1.517060
O	-3.889799	1.549015	0.784560
H	-3.408828	1.942620	0.042249

Y-1m (E_t = -1031.039203)

C	2.566561	-0.248803	1.231179
C	2.908592	0.482940	-1.048361
C	2.361146	1.720851	-0.721201
C	1.885338	1.996089	0.570868
C	2.012267	0.997152	1.541332
C	2.974600	-0.519348	-0.076366
C	1.202022	3.302570	0.870459
H	2.670268	-1.007242	2.001123
H	1.671418	1.183932	2.553043
H	0.198412	3.300641	0.443616

Y-1n (E_t = -1031.030666)

C	-2.536032	0.583007	0.526935
C	-2.232608	-0.999819	-1.274382
C	-2.619550	-0.020096	-2.187324
C	-2.945256	1.277769	-1.771336
C	-2.907435	1.558248	-0.400581
C	-2.180213	-0.696215	0.088221
C	-3.380748	2.320619	-2.766396
H	-2.555989	0.793987	1.589824
H	-3.176136	2.549081	-0.050672
H	-3.194127	3.325056	-2.388253

H	1.121436	3.466763	1.944218
H	1.749423	4.141291	0.440264
H	2.299774	2.490706	-1.482861
H	3.262017	0.264110	-2.047649
O	3.454445	-1.744583	-0.475634
H	3.340005	-2.367795	0.254417
C	-1.633382	0.416392	-0.874631
C	-2.207801	0.382226	0.536737
O	-2.510197	-0.986009	0.872193
C	-1.363914	-1.815800	0.925445
C	-0.667611	-1.844568	-0.434759
C	-0.384281	-0.433181	-0.909794
H	-1.749974	-2.804008	1.189632
O	-0.480199	-1.341748	1.912670
H	0.410267	-1.516995	1.570288
H	-1.322868	-2.339554	-1.160293
O	0.554854	-2.564881	-0.272567
H	1.109829	-2.319556	-1.030169
H	0.348779	0.021463	-0.239489
O	0.160374	-0.557395	-2.221403
H	0.494375	0.322984	-2.442012
H	-2.373400	0.015468	-1.572436
O	-1.243666	1.743833	-1.250743
H	-2.023890	2.169388	-1.628410
H	-1.472353	0.789890	1.237207
C	-3.519809	1.125346	0.665408
H	-3.877774	1.034773	1.695463
H	-3.366169	2.182393	0.448743
O	-4.480956	0.646048	-0.267617
H	-4.546688	-0.303317	-0.094679
H	-4.447206	2.240364	-2.983142
H	-2.843268	2.210422	-3.707557
H	-2.642362	-0.262435	-3.243740
H	-1.967746	-1.998051	-1.598303
O	-1.796880	-1.685142	0.970121
H	-1.160039	-1.280727	1.583153
C	1.424171	0.786371	0.126961
C	1.407416	0.457960	1.615975
O	0.726529	-0.796358	1.835941
C	1.322620	-1.889422	1.130055
C	1.357778	-1.658832	-0.377896
C	2.052262	-0.341633	-0.676924
H	0.692443	-2.747381	1.369148
O	2.658155	-2.091483	1.533604
H	2.647273	-2.434355	2.436411
H	0.333108	-1.602125	-0.742961
O	1.954912	-2.771953	-1.018319
H	2.832537	-2.860468	-0.620794
H	3.106840	-0.413217	-0.376219
O	1.937551	-0.071883	-2.064105
H	2.272086	0.830644	-2.168281
H	0.387389	0.916107	-0.215550
O	2.214447	1.936092	-0.161144
H	1.914779	2.633657	0.441707
H	2.435697	0.395034	1.982672
C	0.619593	1.458787	2.440770
H	-0.409923	1.470278	2.074023
H	0.619116	1.145076	3.488459
O	1.241722	2.737844	2.278589
H	0.688529	3.395204	2.716431

Y-1o (E_t = -1031.032421)

C	1.627827	-1.442696	1.405156
C	2.200191	-1.793216	-0.919577
C	2.950539	-0.619290	-0.900505
C	3.051618	0.167473	0.255066
C	2.392415	-0.274044	1.407677
C	1.530680	-2.198109	0.235733
C	3.806542	1.470103	0.240012
H	1.119359	-1.765509	2.308151
H	2.468114	0.304204	2.321785
H	3.175099	2.276890	-0.134995
H	4.685262	1.404658	-0.401248
H	4.140737	1.739904	1.241234
H	3.467816	-0.310234	-1.801954
H	2.133905	-2.407516	-1.808519
O	0.729081	-3.325628	0.142829
H	0.517772	-3.613755	1.041047
C	-1.557282	1.163727	0.983313

Y-1p (E_t = -1031.032421)

C	-2.092121	2.009782	-0.818621
C	-1.550023	1.429390	1.467015
C	-2.381627	0.311571	1.370720
C	-3.061145	0.009314	0.185445
C	-2.909878	0.884476	-0.898892
C	-1.404461	2.274779	0.366214
C	-3.890883	-1.240818	0.060186
H	-1.986675	2.692710	-1.651969
H	-3.440912	0.684249	-1.822804
H	-4.243106	-1.575600	1.035263
H	-3.306606	-2.047957	-0.384104
H	-4.762461	-1.069279	-0.571134
H	-2.494464	-0.337088	2.232234
H	-1.026973	1.643684	2.393652
O	-0.537991	3.357239	0.368896
H	-0.313522	3.554798	1.288165
C	1.478740	-1.313590	0.819877

C	-0.846870	1.736880	-0.232621
O	-0.115124	0.689229	-0.904779
C	-0.904568	-0.390313	-1.336940
C	-1.616658	-1.030040	-0.147253
C	-2.447640	0.007786	0.571633
H	-0.195539	-1.091335	-1.787276
O	-1.852509	0.056334	-2.284617
H	-2.543331	-0.624189	-2.293607
H	-0.873369	-1.421142	0.545581
O	-2.500295	-2.068714	-0.592656
H	-1.946995	-2.849301	-0.739326
H	-3.227242	0.385781	-0.098875
O	-3.023085	-0.516671	1.767845
H	-3.577206	-1.259237	1.491560
H	-0.800423	0.771685	1.678112
O	-2.312487	2.206819	1.581792
H	-2.870913	1.773203	2.242659
H	-1.575614	2.176517	-0.918061
C	0.219479	2.750693	0.134759
H	-0.244332	3.641332	0.554275
H	0.872366	2.301879	0.893050
O	0.961051	3.142859	-1.013094
H	1.121580	2.315559	-1.490705

C	0.740697	-1.738252	-0.439744
O	0.074079	-0.595972	-1.019089
C	0.926969	0.468379	-1.358384
C	1.670700	0.961402	-0.119249
C	2.436765	-0.180903	0.507400
H	0.261893	1.245627	-1.746362
O	1.850788	0.049447	-2.341865
H	2.580269	0.686585	-2.293498
H	0.948928	1.334879	0.605335
O	2.615324	1.980676	-0.475373
H	2.109241	2.802037	-0.554209
H	3.195494	-0.545338	-0.193851
O	3.037298	0.204935	1.743365
H	3.635014	0.934568	1.530849
H	0.743441	-0.938603	1.546507
O	2.169337	-2.446416	1.326182
H	2.749603	-2.104268	2.021045
H	1.445100	-2.159746	-1.161088
C	-0.384553	-2.715461	-0.159073
H	0.024731	-3.664306	0.182307
H	-1.012991	-2.295491	0.635526
O	-1.143350	-2.964096	-1.335384
H	-1.253298	-2.091078	-1.740427

Y-1q (E_t = -1031.035823)

C	-2.048536	-0.794766	1.503464
C	-3.059947	0.057368	-0.523798
C	-2.683175	-1.109826	-1.192987
C	-1.975380	-2.125295	-0.541633
C	-1.677959	-1.949070	0.817891
C	-2.708883	0.224776	0.815886
C	-1.476746	-3.330092	-1.291862
H	-1.791610	-0.645304	2.542244
H	-1.150163	-2.731839	1.351412
H	-1.463148	-4.212603	-0.652628
H	-0.461705	-3.150791	-1.647841
H	-2.108195	-3.547023	-2.152709
H	-2.943449	-1.225343	-2.238931
H	-3.593850	0.841096	-1.051271
O	-2.946149	1.401125	1.505744
H	-3.556744	1.939781	0.984551
C	1.010368	1.237899	0.930875
C	0.377419	0.901659	-0.418221
O	1.432982	0.697558	-1.385895
C	2.299056	-0.371862	-1.084879
C	2.976534	-0.144954	0.263487
C	1.930485	0.104294	1.326993
H	3.033999	-0.376640	-1.895168
O	1.572227	-1.583087	-1.055832

Y-1r (E_t = -1031.035823)

C	-3.108429	0.247136	0.551170
C	-2.044469	0.158121	-1.621141
C	-1.656678	1.487368	-1.471216
C	-1.971215	2.220275	-0.317207
C	-2.713872	1.581148	0.680984
C	-2.740377	-0.470307	-0.587179
C	-1.455219	3.620415	-0.126487
H	-3.669641	-0.235978	1.344361
H	-2.987792	2.127274	1.576417
H	-1.409915	4.154668	-1.075252
H	-0.450635	3.590498	0.296707
H	-2.094738	4.187091	0.549338
H	-1.101504	1.967181	-2.269653
H	-1.774843	-0.415794	-2.495977
O	-2.995398	-1.823445	-0.728517
H	-3.627169	-2.085375	-0.045233
C	0.954333	-1.496704	-0.177039
C	0.308494	-0.617566	0.892423
O	1.353260	-0.044228	1.712183
C	2.249917	0.787839	1.013596
C	2.942935	0.007615	-0.099746
C	1.908090	-0.646925	-0.987474
H	2.971816	1.119357	1.765719
O	1.553509	1.887250	0.463598

H	2.107852	-2.177959	-0.506088
H	3.630712	0.730992	0.193927
O	3.722913	-1.324086	0.560483
H	3.942312	-1.259701	1.501565
H	1.313190	-0.796413	1.431994
O	2.635504	0.370321	2.536795
H	1.957531	0.617924	3.181437
H	1.582095	2.166988	0.829378
O	0.072705	1.326624	2.003299
H	-0.632235	1.949915	1.780805
H	-0.231614	0.001447	-0.332850
C	-0.433182	2.042364	-1.004173
H	-0.874422	1.703252	-1.947074
H	-1.246263	2.312511	-0.330937
O	0.363076	3.205160	-1.183028
H	1.126364	2.905096	-1.696247

H	2.112183	2.189462	-0.270935
H	3.574286	-0.769190	0.345270
O	3.722573	0.942888	-0.843432
H	3.955227	0.487667	-1.665966
H	1.314773	0.136980	-1.474110
O	2.625474	-1.405202	-1.957945
H	1.951945	-1.888946	-2.456813
H	1.501465	-2.307142	0.317142
O	0.031899	-2.010857	-1.137217
H	-0.691508	-2.473049	-0.692249
H	-0.276892	0.173964	0.424027
C	-0.538973	-1.396171	1.880955
H	-0.986674	-0.687178	2.584976
H	-1.347647	-1.910231	1.362192
O	0.225648	-2.390070	2.548508
H	0.987814	-1.914937	2.908218

Y-1s (E_t = -1031.036830)

C	1.649059	-1.595637	1.084581
C	2.285076	-1.670464	-1.248518
C	3.097474	-0.557000	-1.053629
C	3.199890	0.065886	0.200044
C	2.469855	-0.479082	1.261768
C	1.552241	-2.184872	-0.176323
C	4.049097	1.296686	0.375409
H	1.098597	-2.008054	1.924176
H	2.543672	-0.029851	2.245950
H	3.596017	2.142789	-0.141876
H	5.048014	1.145687	-0.034529
H	4.153672	1.552620	1.428999
H	3.673089	-0.169421	-1.887788
H	2.212579	-2.156484	-2.213083
O	0.731741	-3.258783	-0.444369
H	0.304408	-3.536011	0.376655
C	-1.387057	1.271976	0.927931
C	-0.667124	1.573902	-0.375612
O	-0.196000	0.339685	-0.959281
C	-1.206242	-0.606779	-1.240068
C	-1.984612	-0.964469	0.017921
C	-2.516714	0.298145	0.673099
H	-0.679427	-1.476677	-1.634559
O	-2.175534	-0.125612	-2.155952
H	-1.737485	-0.001340	-3.008084
H	-1.305243	-1.458383	0.714242
O	-3.040649	-1.882193	-0.249081
H	-3.460828	-1.549945	-1.056971
H	-3.242062	0.774237	0.001349
O	-3.115967	0.006153	1.933120
H	-3.754591	-0.700193	1.759973

Y-1t (E_t = -1031.036411)

C	1.985620	1.435227	-0.791449
C	2.241016	0.762334	1.519163
C	2.979054	-0.348923	1.105412
C	3.225940	-0.596245	-0.249533
C	2.723389	0.320599	-1.184874
C	1.733913	1.648896	0.566065
C	3.924612	-1.852835	-0.693874
H	1.589164	2.136820	-1.512984
H	2.915374	0.161343	-2.240519
H	4.640365	-2.190967	0.054618
H	4.462326	-1.694878	-1.628271
H	3.197346	-2.650953	-0.850662
H	3.357485	-1.037260	1.852554
H	2.052420	0.929232	2.574294
O	0.981114	2.752454	0.896096
H	0.895642	2.789601	1.857908
C	-1.662914	0.183280	1.001353
C	-2.173782	0.671262	-0.343659
O	-1.138424	0.511153	-1.343257
C	-0.683019	-0.816472	-1.508608
C	-0.164372	-1.390437	-0.199901
C	-1.220934	-1.258964	0.880838
H	0.117792	-0.748810	-2.248878
O	-1.706044	-1.700025	-1.935025
H	-1.999317	-1.411563	-2.809285
H	0.713234	-0.827146	0.101811
O	0.254976	-2.747424	-0.344054
H	-0.454249	-3.178411	-0.845486
H	-2.095293	-1.869433	0.619756
O	-0.701064	-1.648779	2.150943
H	-0.275081	-2.505408	2.003002

H	-0.674604	0.793860	1.615609
O	-1.867330	2.499834	1.457579
H	-2.457876	2.253693	2.183744
H	-1.348773	2.073474	-1.069880
C	0.583621	2.408477	-0.166576
H	0.302898	3.421591	0.114104
H	1.163288	1.964830	0.650102
O	1.354474	2.487202	-1.357499
H	1.500250	1.563323	-1.610035

H	-0.791182	0.785976	1.285565
O	-2.716121	0.323551	1.947495
H	-2.431874	-0.181465	2.722606
H	-3.056290	0.093393	-0.632836
C	-2.498740	2.150266	-0.360062
H	-3.308197	2.350019	0.339011
H	-1.607782	2.702981	-0.042386
O	-2.939375	2.557201	-1.649184
H	-2.229780	2.287857	-2.246906

Y-1u (E_t = -1031.030149)

C	2.817441	-0.159946	-1.398396
C	4.030225	-0.503052	0.665135
C	3.182174	-1.564798	0.973434
C	2.136449	-1.941649	0.117403
C	1.973579	-1.225486	-1.073310
C	3.848216	0.201138	-0.528443
C	1.220522	-3.081461	0.473104
H	2.675416	0.382724	-2.327779
H	1.160487	-1.486635	-1.738905
H	0.716893	-2.886463	1.419761
H	1.775044	-4.016065	0.570473
H	0.456566	-3.208768	-0.290881
H	3.333821	-2.108108	1.900000
H	4.839590	-0.214966	1.323412
O	4.711680	1.242758	-0.779916
H	4.503255	1.603295	-1.650962
C	-1.765456	1.544735	0.296130
C	-0.516011	0.680024	0.186383
O	-0.825163	-0.613513	0.741315
C	-1.823895	-1.294987	0.020359
C	-3.119981	-0.485028	-0.044904
C	-2.849485	0.919026	-0.547459
H	-1.982338	-2.226982	0.570197
O	-1.370026	-1.561476	-1.295193
H	-2.179822	-1.697504	-1.814289
H	-3.546385	-0.414265	0.961543
O	-3.998756	-1.183959	-0.926162
H	-4.720761	-0.568171	-1.117904
H	-2.501038	0.866174	-1.586681
O	-4.083184	1.626921	-0.471205
H	-3.858920	2.550821	-0.652428
H	-2.085425	1.554799	1.341083
O	-1.552467	2.872540	-0.181780
H	-1.078526	3.321847	0.532465
H	-0.233258	0.562126	-0.862589
C	0.658760	1.269497	0.936533
H	1.355239	0.468657	1.186301
H	1.169791	1.976140	0.275199

Y-1v (E_t = -1031.029623)

C	-4.008494	0.326570	0.621238
C	-2.927120	-0.905493	-1.157515
C	-2.087328	-1.512031	-0.221748
C	-2.189011	-1.212193	1.141991
C	-3.165868	-0.289523	1.544108
C	-3.893452	0.010628	-0.735376
C	-1.314664	-1.911524	2.149872
H	-4.763292	1.037923	0.930257
H	-3.265677	-0.043145	2.595753
H	-1.807069	-2.800790	2.547676
H	-1.087407	-1.258126	2.992788
H	-0.377794	-2.221174	1.689654
H	-1.320257	-2.197626	-0.557847
H	-2.824059	-1.140661	-2.211727
O	-4.753334	0.645168	-1.601827
H	-4.578744	0.317088	-2.492972
C	1.974831	1.297404	0.347801
C	0.617733	0.642563	0.123304
O	0.648857	-0.008355	-1.162013
C	1.589406	-1.052290	-1.224910
C	3.001710	-0.557394	-0.906991
C	3.019695	0.209353	0.400063
H	1.536898	-1.419573	-2.253855
O	1.234621	-2.077347	-0.311705
H	2.059944	-2.564316	-0.151936
H	3.330219	0.116463	-1.705604
O	3.837277	-1.712414	-0.834984
H	4.665817	-1.410876	-0.435136
H	2.773148	-0.476133	1.220856
O	4.339870	0.720433	0.557470
H	4.291859	1.322798	1.313509
H	2.183797	1.955791	-0.499200
O	2.035181	2.018167	1.577894
H	1.570031	2.848914	1.404638
H	0.431251	-0.102252	0.900165
C	-0.515126	1.645094	0.140932
H	-1.359408	1.231287	-0.411045
H	-0.824978	1.795384	1.179588

O	0.166066	1.942585	2.101887	O	-0.046277	2.875127	-0.425664
H	0.926581	2.144351	2.659103	H	-0.817846	3.432962	-0.577766

(ii) Optimized coordinates of *p*-OHTol : β-D-glucose complexes

Y-2a (E_t = -1031.033900)				**Y-2b** (E_t = -1031.041555)			
C	-2.623150	-0.694250	-1.095554	C	3.198783	0.590589	1.322200
C	-1.854789	-1.657272	0.985043	C	2.012634	0.615234	-0.783887
C	-2.601035	-0.711061	1.688225	C	2.559756	-0.632865	-1.091404
C	-3.342337	0.274972	1.022688	C	3.420789	-1.293398	-0.209134
C	-3.348977	0.260278	-0.379058	C	3.736120	-0.651924	0.996855
C	-1.845888	-1.630949	-0.410557	C	2.336281	1.237612	0.429192
C	-4.164254	1.273293	1.794450	C	4.037142	-2.619811	-0.566925
H	-2.661663	-0.723879	-2.177743	H	3.438731	1.081309	2.256561
H	-3.953314	0.981825	-0.919088	H	4.402391	-1.139271	1.700435
H	-5.130070	0.851375	2.075786	H	4.181440	-3.237095	0.319494
H	-3.655947	1.575136	2.709362	H	3.403134	-3.171781	-1.260182
H	-4.354223	2.167969	1.202820	H	5.011840	-2.491400	-1.040887
H	-2.592808	-0.730484	2.772071	H	2.300572	-1.100446	-2.035588
H	-1.273412	-2.409299	1.503268	H	1.339114	1.098227	-1.479955
O	-1.068898	-2.551540	-1.098986	O	1.828417	2.445589	0.813090
H	-0.531677	-2.024636	-1.715924	H	1.190151	2.771599	0.146449
C	1.732393	1.505097	-0.236679	C	-1.841674	0.555629	-1.042439
C	0.518036	0.736582	-0.750488	C	-1.291649	1.148313	0.251156
O	0.929842	-0.551421	-1.229625	O	-2.078143	0.634631	1.332845
C	1.503129	-1.312727	-0.149080	C	-1.864343	-0.769917	1.471985
C	2.799967	-0.678473	0.326784	C	-2.378735	-1.493753	0.238706
C	2.500491	0.722638	0.817552	C	-1.689716	-0.949464	-0.995253
H	0.780403	-1.323920	0.677962	H	-0.786906	-0.957446	1.599831
O	1.780991	-2.597986	-0.602797	O	-2.606998	-1.239200	2.555330
H	0.938002	-3.076846	-0.602838	H	-2.235797	-0.849748	3.357623
H	3.492781	-0.632201	-0.522321	H	-3.455063	-1.294693	0.171514
O	3.325563	-1.433714	1.404480	O	-2.104395	-2.887536	0.284837
H	3.425491	-2.332483	1.060840	H	-2.544131	-3.224702	1.077330
H	1.861486	0.637984	1.708163	H	-0.619042	-1.188087	-0.935803
O	3.715766	1.382928	1.126185	O	-2.252968	-1.463116	-2.197817
H	3.460079	2.290619	1.344066	H	-2.194757	-2.426484	-2.132706
H	2.410234	1.674095	-1.085370	H	-2.908492	0.804106	-1.111056
O	1.363879	2.734014	0.382192	O	-1.133990	1.101572	-2.159310
H	0.752991	3.178501	-0.226993	H	-1.392944	0.565712	-2.924161
H	-0.207897	0.617847	0.067886	H	-0.246487	0.845351	0.368877
C	-0.151203	1.443355	-1.918312	C	-1.356215	2.664847	0.298026
H	-0.877046	0.776243	-2.384525	H	-1.076182	3.002574	1.293622
H	0.594591	1.716838	-2.664119	H	-2.373456	3.006351	0.084856
O	-0.761595	2.665700	-1.491350	O	-0.415383	3.240114	-0.615070
H	-1.496677	2.412565	-0.914174	H	-0.601478	2.842927	-1.481964

Y-2c (E_t = -1031.038061)

C	-2.615523	0.175750	-0.749074
C	-2.467844	0.604449	1.624968
C	-2.135328	-0.730360	1.842725
C	-2.030805	-1.636046	0.777375
C	-2.296525	-1.165395	-0.514936
C	-2.664234	1.073321	0.319572
C	-1.626557	-3.063558	1.033499
H	-2.791786	0.547806	-1.750424
H	-2.246119	-1.852367	-1.353103
H	-0.635334	-3.100249	1.487485
H	-2.321336	-3.556873	1.714121
H	-1.599120	-3.637175	0.107656
H	-1.944966	-1.072675	2.853448
H	-2.544379	1.298276	2.453798
O	-2.910303	2.400697	0.064597
H	-2.264277	2.887316	0.605544
C	1.692437	-0.204916	0.978778
C	0.721186	0.881922	0.545949
O	1.188919	1.468427	-0.689578
C	1.145362	0.524205	-1.755005
C	2.105055	-0.616351	-1.438381
C	1.740293	-1.254232	-0.115600
H	0.129031	0.142182	-1.894829
O	1.496604	1.169602	-2.947187
H	2.331091	1.628265	-2.770395
H	3.117179	-0.192223	-1.360616
O	2.043145	-1.634115	-2.428364
H	2.156768	-1.191682	-3.281332
H	0.737080	-1.690421	-0.208788
O	2.684971	-2.240761	0.286475
H	2.725355	-2.885425	-0.433463
H	2.695366	0.228338	1.097806
O	1.228597	-0.766614	2.199396
H	1.768242	-1.559428	2.334917
H	-0.258697	0.432755	0.380370
C	0.588208	2.036761	1.513128
H	1.577350	2.464368	1.709380
H	0.162588	1.683954	2.449034
O	-0.290463	3.032397	0.981650
H	-0.004882	3.143853	0.061723

Y-2d (E_t = -1031.040797)

C	3.534160	0.213799	0.367881
C	1.876238	0.537592	-1.364942
C	2.545833	-0.389024	-2.165749
C	3.711164	-1.024964	-1.724348
C	4.192670	-0.703377	-0.448026
C	2.369724	0.831176	-0.091724
C	4.406177	-2.052390	-2.577655
H	3.910023	0.463653	1.351684
H	5.098501	-1.176057	-0.085665
H	4.053999	-3.059641	-2.349647
H	4.224234	-1.869599	-3.635893
H	5.482884	-2.033794	-2.413206
H	2.158458	-0.608072	-3.154324
H	1.001104	1.054827	-1.738405
O	1.753167	1.740172	0.746477
H	0.835761	1.866016	0.437579
C	-2.945293	-0.119812	-0.099606
C	-1.688859	0.624688	-0.530350
O	-0.974800	1.105844	0.631598
C	-0.580511	0.043837	1.532623
C	-1.813848	-0.680049	2.034074
C	-2.590685	-1.233878	0.862620
H	0.074540	-0.644141	0.978285
O	0.052307	0.600149	2.633850
H	0.904071	0.952938	2.321856
H	-2.428630	0.051187	2.572343
O	-1.460340	-1.779521	2.862383
H	-0.939685	-1.411272	3.589741
H	-1.956307	-1.961303	0.337113
O	-3.812169	-1.838900	1.269181
H	-3.575780	-2.496670	1.937963
H	-3.613362	0.586511	0.404855
O	-3.539106	-0.639788	-1.281412
H	-4.266207	-1.201861	-0.978479
H	-1.053583	-0.058783	-1.108595
C	-2.008915	1.865777	-1.342598
H	-2.604248	1.582729	-2.208274
H	-1.072460	2.317787	-1.692712
O	-2.775855	2.788566	-0.586591
H	-2.287998	2.917807	0.238405

Y-2e (E_t = -1031.035740)

C	1.474300	-1.943002	1.132321
C	1.647356	-1.658895	-1.261108
C	2.627812	-0.686041	-1.067222

Y-2f (E_t = -1031.035127)

C	2.165652	1.961042	-0.344835
C	1.873922	0.626932	1.649475
C	2.705613	-0.352265	1.106037

C	3.023498	-0.294442	0.219884
C	2.443710	-0.952900	1.311492
C	1.038457	-2.263024	-0.157337
C	3.968358	0.860138	0.419715
H	1.035704	-2.448053	1.985361
H	2.753142	-0.691903	2.317570
H	3.415043	1.801118	0.420697
H	4.497939	0.774981	1.368091
H	4.708976	0.905054	-0.378136
H	3.072499	-0.204524	-1.930959
H	1.319272	-1.935959	-2.254782
O	0.010761	-3.155042	-0.383922
H	-0.698706	-2.942218	0.247141
C	-1.339761	1.102564	-1.356639
C	-0.294377	1.621653	-0.383060
O	-0.886713	1.659256	0.935208
C	-1.127579	0.344384	1.413267
C	-2.117886	-0.371912	0.498460
C	-1.697174	-0.317208	-0.956166
H	-0.196283	-0.221668	1.469486
O	-1.624497	0.414142	2.723192
H	-2.362971	1.040583	2.700091
H	-3.094985	0.120914	0.592654
O	-2.215203	-1.751380	0.883479
H	-2.430489	-1.746859	1.828326
H	-0.803183	-0.927913	-1.093598
O	-2.734624	-0.753097	-1.833647
H	-2.813911	-1.708926	-1.715056
H	-2.236488	1.734205	-1.287327
O	-0.791951	1.124675	-2.665632
H	-1.402331	0.600172	-3.204252
H	0.565971	0.941773	-0.377234
C	0.197911	3.024283	-0.654160
H	-0.655526	3.712620	-0.641062
H	0.662139	3.063379	-1.636933
O	1.183172	3.395234	0.302611
H	0.787289	3.188969	1.161014

C	3.255184	-0.212704	-0.176264
C	2.987872	0.968297	-0.880360
C	1.564058	1.767558	0.902887
C	4.047166	-1.330615	-0.799088
H	1.963667	2.870503	-0.897921
H	3.433444	1.119307	-1.857784
H	4.711571	-0.957293	-1.577596
H	4.654239	-1.846099	-0.055577
H	3.373562	-2.062273	-1.248297
H	2.921128	-1.244911	1.683070
H	1.435031	0.512161	2.632749
O	0.660224	2.669904	1.418992
H	0.040035	2.855937	0.691034
C	-1.424854	0.757828	-0.703789
C	-1.733838	0.378308	0.736833
O	-2.169631	-0.991831	0.740281
C	-1.129268	-1.866510	0.325989
C	-0.737753	-1.569637	-1.119251
C	-0.315586	-0.123022	-1.233932
H	-0.246442	-1.765429	0.968959
O	-1.573873	-3.188686	0.466456
H	-2.460833	-3.211477	0.078068
H	-1.615835	-1.746865	-1.756437
O	0.365807	-2.372954	-1.521078
H	0.122724	-3.284723	-1.304736
H	0.582320	0.014075	-0.629342
O	-0.075122	0.288487	-2.578252
H	0.697450	-0.209640	-2.878142
H	-2.330697	0.584478	-1.293178
O	-1.069770	2.148597	-0.771639
H	-0.660641	2.249079	-1.646662
H	-0.826661	0.471844	1.345248
C	-2.822588	1.252123	1.339718
H	-2.353562	2.165335	1.716385
H	-3.263862	0.720199	2.181410
O	-3.876323	1.543886	0.431363
H	-3.532376	2.221298	-0.165374

Y-2g (E_t = -1031.036417)

C	2.756474	1.127666	0.026399
C	1.637251	0.234109	-1.922560
C	2.062642	-1.046006	-1.569410
C	2.810325	-1.270899	-0.404715
C	3.168270	-0.161820	0.371975
C	1.943816	1.318640	-1.096277
C	3.161127	-2.672499	0.015444
H	3.031818	1.982875	0.632321
H	3.782271	-0.305846	1.254610
H	3.536656	-3.255484	-0.825174

Y-2h (E_t = -1031.037458)

C	-2.645356	-0.081856	-0.938786
C	-2.058045	-0.181609	1.402056
C	-1.981355	1.212639	1.434565
C	-2.230119	1.982718	0.291857
C	-2.589435	1.310694	-0.885206
C	-2.346606	-0.835470	0.200130
C	-2.038141	3.475061	0.302603
H	-2.900542	-0.601746	-1.853671
H	-2.806943	1.884478	-1.779290
H	-2.198336	3.883694	1.299855

H	3.923029	-2.672331	0.793876
H	2.274942	-3.178050	0.401559
H	1.794083	-1.886985	-2.199209
H	1.038686	0.405182	-2.808495
O	1.416415	2.554428	-1.403071
H	1.030514	2.871376	-0.567514
C	-1.107218	-1.060508	1.152752
C	-1.838652	-1.005047	-0.179746
O	-2.577441	0.231594	-0.252244
C	-1.713266	1.364006	-0.250324
C	-0.953573	1.421091	1.063815
C	-0.177190	0.133983	1.250686
H	-1.006752	1.291621	-1.089479
O	-2.483357	2.527567	-0.320528
H	-2.855160	2.586217	-1.209750
H	-1.687701	1.528153	1.869362
O	-0.041808	2.531293	1.076652
H	-0.606079	3.318742	1.073299
H	0.554809	0.034139	0.449538
O	0.467636	0.061686	2.519107
H	1.236180	0.645086	2.460814
H	-1.843932	-1.013419	1.966803
O	-0.359942	-2.268783	1.209831
H	0.250764	-2.142816	1.951680
H	-1.103706	-1.049852	-0.993867
C	-2.864137	-2.103010	-0.363166
H	-3.566560	-2.069943	0.478257
H	-2.364933	-3.069612	-0.359862
O	-3.530855	-1.967605	-1.608780
H	-3.859321	-1.058718	-1.615753

H	-1.021964	3.719344	-0.010249
H	-2.732629	3.965497	-0.378953
H	-1.724246	1.706996	2.364521
H	-1.889552	-0.765723	2.299685
O	-2.345486	-2.210094	0.089832
H	-1.561662	-2.546743	0.557410
C	1.952860	0.335375	0.573634
C	1.242413	0.718962	-0.719391
O	1.461400	-0.355001	-1.649638
C	0.749666	-1.515719	-1.235072
C	1.288139	-2.021828	0.093737
C	1.327728	-0.924129	1.134360
H	-0.313572	-1.269851	-1.147182
O	0.963522	-2.546556	-2.155375
H	0.506071	-2.309197	-2.972310
H	2.303617	-2.392951	-0.081294
O	0.450674	-3.064772	0.619929
H	0.465525	-3.773142	-0.041230
H	0.301048	-0.676804	1.418636
O	2.092589	-1.295963	2.280259
H	1.662977	-2.075209	2.657783
H	3.007424	0.140268	0.338628
O	1.834416	1.403000	1.514596
H	2.185498	1.058940	2.348831
H	0.170666	0.851747	-0.525886
C	1.783318	1.993162	-1.348415
H	1.358404	2.096455	-2.345918
H	2.871925	1.908841	-1.451101
O	1.404758	3.145413	-0.608724
H	1.670174	2.973149	0.307160

Y-2i (E_t = -1031.035156)

C	2.927877	-1.763807	0.552339
C	2.753128	0.119392	-0.955074
C	4.008038	0.561258	-0.531699
C	4.738645	-0.135265	0.436532
C	4.179473	-1.309309	0.959849
C	2.211238	-1.052383	-0.414510
C	6.108186	0.326081	0.859688
H	2.494860	-2.667142	0.961916
H	4.724939	-1.869105	1.711648
H	6.214557	1.403003	0.733994
H	6.294639	0.090487	1.907099
H	6.889976	-0.154932	0.269421
H	4.416998	1.471063	-0.957301
H	2.203572	0.663462	-1.714155
O	0.985325	-1.540567	-0.786387
H	0.547634	-0.876937	-1.353984
C	-1.589687	0.579766	-0.972598

Y-2j (E_t = -1031.032136)

C	-2.624745	1.369327	0.615531
C	-1.472721	1.490128	-1.507381
C	-1.980099	0.233083	-1.846496
C	-2.807316	-0.476484	-0.966818
C	-3.129185	0.119346	0.261879
C	-1.771767	2.046192	-0.259996
C	-3.375300	-1.823389	-1.329722
H	-2.850092	1.820103	1.573277
H	-3.774763	-0.409913	0.954157
H	-4.435483	-1.750466	-1.576668
H	-2.861310	-2.246000	-2.192398
H	-3.273125	-2.518955	-0.496644
H	-1.729240	-0.197888	-2.809380
H	-0.835712	2.033354	-2.195670
O	-1.261157	3.265443	0.134751
H	-0.306315	3.224740	-0.030728
C	0.475712	-0.179990	0.948179

C	-0.965554	0.908942	0.377046
O	-2.045741	1.081360	1.307293
C	-2.748949	-0.141111	1.502049
C	-3.426283	-0.567721	0.210609
C	-2.384167	-0.702908	-0.878711
H	-2.039984	-0.919769	1.827294
O	-3.762165	0.060953	2.440833
H	-3.342654	0.302688	3.276721
H	-4.136474	0.222205	-0.060557
O	-4.065377	-1.831355	0.333073
H	-4.723908	-1.735065	1.034578
H	-1.707818	-1.527005	-0.616715
O	-2.964283	-0.919137	-2.161926
H	-3.505701	-1.716831	-2.083771
H	-2.263578	1.399829	-1.233784
O	-0.558461	0.468364	-1.971158
H	-1.012567	0.122032	-2.757183
H	-0.325797	0.077237	0.700980
C	-0.139046	2.186735	0.335009
H	0.869867	1.934670	-0.000426
H	-0.075135	2.582327	1.347880
O	-0.718703	3.203081	-0.472951
H	-0.525581	2.958160	-1.387045
C	0.951977	-1.611750	0.694745
O	1.698653	-1.682316	-0.523941
C	2.846574	-0.855894	-0.494879
C	2.413798	0.598350	-0.388970
C	1.641840	0.784884	0.893233
H	3.467563	-1.115293	0.379823
O	3.523201	-1.104703	-1.691010
H	4.101615	-0.339183	-1.822970
H	1.759239	0.810642	-1.243480
O	3.599921	1.384308	-0.430945
H	3.336465	2.291394	-0.224844
H	2.307392	0.577984	1.741763
O	1.202982	2.147049	0.953509
H	0.601446	2.187395	1.714030
H	-0.234989	0.083104	0.161631
O	-0.106122	-0.011264	2.238732
H	-0.931673	-0.519064	2.206791
H	1.567387	-1.936731	1.548093
C	-0.216212	-2.561981	0.468865
H	0.153812	-3.579164	0.319716
H	-0.730847	-2.244109	-0.435229
O	-1.187501	-2.500650	1.520298
H	-0.806510	-2.945815	2.288564

Y-2k (E_t = -1031.034013)

C	-2.845159	-0.024956	0.664895
C	-2.102378	-1.274112	-1.269908
C	-1.389548	-2.128127	-0.430517
C	-1.368839	-1.945216	0.959813
C	-2.123037	-0.891122	1.489392
C	-2.797095	-0.194449	-0.720481
C	-0.487188	-2.788798	1.841350
H	-3.402193	0.800196	1.096327
H	-2.148657	-0.739272	2.562671
H	-0.895195	-2.863359	2.848938
H	-0.382474	-3.797865	1.443415
H	0.508853	-2.347187	1.913315
H	-0.836120	-2.952143	-0.867407
H	-2.083582	-1.394721	-2.344083
O	-3.399899	0.675222	-1.602956
H	-3.868379	1.348844	-1.092653
C	0.312081	1.027165	-0.418088
C	1.078346	1.489946	0.817537
O	1.742382	0.338822	1.367663
C	2.716741	-0.185684	0.475266
C	2.069798	-0.650384	-0.816739
C	1.286847	0.484421	-1.443339
H	3.469269	0.589740	0.260091
O	3.294675	-1.315415	1.064604

Y-2l (E_t = -1031.025307)

C	2.555254	-0.289066	-1.245119
C	2.768102	-0.826364	1.104676
C	1.916986	-1.919321	0.923680
C	1.376249	-2.222695	-0.331801
C	1.714053	-1.387623	-1.407650
C	3.081356	-0.006899	0.017762
C	0.425370	-3.376820	-0.512932
H	2.803377	0.357710	-2.075801
H	1.316766	-1.602281	-2.393498
H	0.621177	-4.159463	0.219527
H	-0.613222	-3.061066	-0.394166
H	0.530616	-3.812930	-1.506201
H	1.680736	-2.549105	1.774061
H	3.177892	-0.612149	2.086290
O	3.889632	1.103196	0.126347
H	4.222592	1.147736	1.032021
C	-1.066686	1.318358	-0.825292
C	-0.236944	1.207555	0.451900
O	-1.131003	0.903392	1.534457
C	-1.637693	-0.408104	1.364578
C	-2.481520	-0.474076	0.098638
C	-1.680330	-0.034593	-1.107333
H	-0.795248	-1.113636	1.276906
O	-2.408727	-0.676105	2.501832

H	3.747472	-1.025234	1.867353
H	1.372702	-1.457707	-0.564483
O	3.040683	-1.071813	-1.768515
H	3.514949	-1.810310	-1.362919
H	1.984167	1.283041	-1.732987
O	0.541667	0.042061	-2.571777
H	1.182592	-0.381586	-3.160027
H	-0.346999	0.218945	-0.102094
O	-0.449845	2.114099	-0.947314
H	-0.977845	1.741352	-1.669772
H	1.810008	2.262105	0.541572
C	0.173853	2.039616	1.910462
H	0.767859	2.190964	2.811559
H	-0.593574	1.289612	2.128711
O	-0.380413	3.294328	1.552377
H	-0.755492	3.168140	0.667594

H	-2.983551	-1.413792	2.251136
H	-3.325342	0.213420	0.231867
O	-2.937274	-1.822265	-0.022258
H	-3.399583	-1.869638	-0.871108
H	-0.866232	-0.749042	-1.279603
O	-2.569995	-0.010726	-2.220037
H	-2.071119	0.408790	-2.935365
H	-1.865449	2.043815	-0.649201
O	-0.285634	1.685724	-1.961749
H	-0.118763	2.632806	-1.847044
H	0.485685	0.392915	0.342371
C	0.525004	2.480397	0.762460
H	1.509408	2.425413	0.289342
H	0.658340	2.541490	1.845691
O	-0.215886	3.597961	0.256509
H	0.226821	4.400047	0.557337

Y-2m (E_t = -1031.028397)

C	2.117392	-1.405663	1.189839
C	2.886613	-0.341161	-0.839623
C	1.958148	-1.083178	-1.568386
C	1.089586	-1.991277	-0.945264
C	1.192186	-2.138279	0.443229
C	2.952876	-0.488147	0.548714
C	0.043038	-2.731984	-1.733650
H	2.162829	-1.527601	2.266444
H	0.547360	-2.843472	0.955267
H	-0.883635	-2.158335	-1.782255
H	0.382817	-2.914722	-2.753095
H	-0.181784	-3.695121	-1.276264
H	1.920503	-0.969511	-2.646647
H	3.563679	0.351614	-1.323163
O	3.880305	0.276718	1.213682
H	3.798164	0.098701	2.159110
C	-0.261975	1.170728	0.543566
C	-0.939400	1.629720	-0.745196
O	-1.639135	0.522634	-1.326818
C	-2.681978	-0.001693	-0.497584
C	-2.101963	-0.516929	0.805802
C	-1.313853	0.595248	1.465462
H	-3.413658	0.795242	-0.290971
O	-3.253524	-1.069788	-1.182904
H	-3.632225	-0.712195	-1.996783
H	-1.421921	-1.340786	0.564012
O	-3.167309	-0.937180	1.643308
H	-2.768620	-1.042912	2.518824
H	-2.012202	1.404991	1.723489
O	-0.736534	0.053600	2.651717
H	-0.182965	0.765122	3.004696

Y-2n (E_t = -1031.025341)

C	-2.619054	1.425625	-0.058545
C	-1.796567	0.249148	1.888376
C	-2.222011	-0.953388	1.329133
C	-2.853598	-0.997515	0.076661
C	-3.042929	0.210219	-0.602236
C	-1.995380	1.444592	1.190395
C	-3.271372	-2.311202	-0.526402
H	-2.778813	2.350983	-0.601710
H	-3.531027	0.210089	-1.570311
H	-3.742412	-2.951794	0.219159
H	-3.983936	-2.160862	-1.336789
H	-2.401407	-2.835591	-0.921164
H	-2.066727	-1.875642	1.877942
H	-1.322740	0.285828	2.860944
O	-1.543808	2.597576	1.787667
H	-1.758750	3.345947	1.215500
C	0.411331	-0.143496	-1.108809
C	1.431385	0.979401	-0.933173
O	2.037190	0.900792	0.364417
C	2.716031	-0.321205	0.587715
C	1.726924	-1.475040	0.504471
C	1.080106	-1.480027	-0.859794
H	3.526855	-0.471034	-0.136473
O	3.320735	-0.265283	1.852944
H	2.664687	0.146591	2.434417
H	0.950549	-1.311813	1.264893
O	2.376129	-2.728304	0.677566
H	2.889131	-2.651880	1.494628
H	1.861730	-1.628386	-1.618252
O	0.084761	-2.494961	-0.978236
H	0.521816	-3.321975	-0.729624

H	0.462738	0.393141	0.290318
O	0.342867	2.231891	1.276952
H	0.938848	2.674403	0.652552
H	-1.626929	2.456307	-0.515923
C	0.048675	2.044724	-1.819902
H	-0.492807	2.416023	-2.694394
H	0.615278	1.155537	-2.102333
O	0.904234	3.054822	-1.270392
H	1.641231	3.179356	-1.879297

Y-2o (E_t = -1031.030716)

C	-2.351344	-0.609940	-1.699497
C	-2.545513	-0.185897	0.674619
C	-1.915858	-1.401430	0.936133
C	-1.483572	-2.234843	-0.101469
C	-1.723424	-1.822929	-1.419824
C	-2.774787	0.204661	-0.646648
C	-0.816306	-3.550448	0.202163
H	-2.532381	-0.287919	-2.716615
H	-1.395756	-2.448755	-2.242456
H	-0.243016	-3.903831	-0.654928
H	-0.137690	-3.444358	1.048212
H	-1.547360	-4.321441	0.451237
H	-1.716977	-1.683982	1.962822
H	-2.851975	0.459857	1.491128
O	-3.370196	1.399616	-0.977759
H	-3.614785	1.854930	-0.161239
C	1.070279	1.323184	-0.869492
C	0.847093	1.757116	0.571882
O	0.559112	0.598137	1.378380
C	1.643084	-0.323946	1.395740
C	1.885100	-0.857699	-0.003467
C	2.185981	0.298986	-0.931012
H	2.546773	0.183623	1.768988
O	1.299753	-1.413730	2.203552
H	1.262729	-1.104663	3.118082
H	0.965180	-1.354714	-0.328180
O	3.009109	-1.730586	-0.048359
H	2.795452	-2.478237	0.525892
H	3.118169	0.779042	-0.600756
O	2.296968	-0.122055	-2.285760
H	2.965207	-0.821437	-2.292730
H	0.150095	0.850841	-1.237890
O	1.397883	2.483649	-1.621424
H	1.654033	2.159875	-2.496634
H	1.749977	2.254043	0.952068
C	-0.354368	2.672935	0.725668
H	-1.190935	2.248233	0.163599
H	-0.120134	3.648599	0.304709

H	-0.388114	-0.012335	-0.375628
O	-0.095135	-0.068748	-2.437254
H	-0.664424	-0.845233	-2.534032
H	2.202580	0.869441	-1.711465
C	0.790968	2.350501	-1.038226
H	0.204315	2.513194	-0.135743
H	0.122534	2.353288	-1.903941
O	1.739352	3.408132	-1.087262
H	2.205364	3.331882	-1.928488

Y-2p (E_t = -1031.030998)

C	2.203177	-1.078455	-1.165184
C	3.176761	0.050572	0.738214
C	2.641999	1.258073	0.282989
C	1.874416	1.321387	-0.885365
C	1.672821	0.134031	-1.601925
C	2.959784	-1.121372	0.009338
C	1.316901	2.627685	-1.383611
H	2.046799	-1.996563	-1.716943
H	1.066431	0.155732	-2.500186
H	0.441689	2.447853	-2.005400
H	1.016327	3.267743	-0.554182
H	2.052889	3.173562	-1.976590
H	2.821766	2.162019	0.854794
H	3.763493	0.023955	1.650459
O	3.461491	-2.342763	0.386446
H	3.941842	-2.231406	1.216479
C	-0.909266	-0.435974	1.412665
C	-1.479951	0.922227	1.034202
O	-1.341634	1.106193	-0.389064
C	-2.086274	0.146949	-1.131415
C	-1.586673	-1.255218	-0.833511
C	-1.655483	-1.516368	0.654861
H	-3.152542	0.229153	-0.867869
O	-1.874939	0.377018	-2.495780
H	-2.314089	1.205524	-2.728074
H	-0.543474	-1.311795	-1.157200
O	-2.394635	-2.242061	-1.467541
H	-2.305446	-2.096133	-2.418902
H	-2.709449	-1.492664	0.966931
O	-1.062663	-2.761883	1.003043
H	-1.501896	-3.429449	0.457968
H	0.148002	-0.467854	1.118012
O	-1.065086	-0.600735	2.815933
H	-0.857040	-1.530261	2.988016
H	-2.542444	0.966656	1.310034
C	-0.737358	2.081582	1.667429
H	0.331223	1.950017	1.473428
H	-0.901836	2.073630	2.742888

O	-0.683947	2.856493	2.095943
H	-0.638264	1.967864	2.475093

O	-1.211425	3.324628	1.165474
H	-1.236252	3.206393	0.206132

Y-2q (E_t = -1031.024233)

C	-3.138854	-1.865705	-0.574560
C	-2.220025	-0.080845	0.783697
C	-3.430481	0.600620	0.676108
C	-4.509173	0.078665	-0.051384
C	-4.344403	-1.167421	-0.664421
C	-2.082689	-1.323095	0.158288
C	-5.822640	0.811692	-0.121436
H	-3.026888	-2.827426	-1.064166
H	-5.160582	-1.595881	-1.235074
H	-6.379728	0.533110	-1.015206
H	-6.448938	0.586557	0.743314
H	-5.668061	1.889968	-0.144107
H	-3.532574	1.564893	1.161674
H	-1.389293	0.330616	1.342837
O	-0.861352	-1.955332	0.280889
H	-0.918683	-2.823073	-0.140103
C	1.622689	1.068135	0.852258
C	0.989743	1.066716	-0.535201
O	1.954272	0.594011	-1.487829
C	2.309459	-0.756070	-1.223443
C	3.015956	-0.852805	0.115774
C	2.094972	-0.330283	1.195742
H	1.399388	-1.376314	-1.210660
O	3.217000	-1.183149	-2.198870
H	2.780056	-1.091681	-3.055424
H	3.913707	-0.226402	0.058675
O	3.336172	-2.199899	0.451575
H	3.927231	-2.515245	-0.245458
H	1.221811	-0.990793	1.253315
O	2.746960	-0.248127	2.462647
H	3.069407	-1.139922	2.651771
H	2.480820	1.746853	0.841392
O	0.641598	1.507284	1.791615
H	1.023916	1.313254	2.660158
H	0.118507	0.399734	-0.525281
C	0.531157	2.437474	-0.970027
H	-0.291873	2.733598	-0.312951
H	0.154992	2.366937	-1.996375
O	1.633151	3.331924	-0.878076
H	1.290093	4.225057	-0.992306

Y-2r (E_t = -1031.022637)

C	3.807216	-1.136855	0.075762
C	2.308404	-0.177260	1.713133
C	2.339862	1.029555	1.019835
C	3.099436	1.185482	-0.149647
C	3.829548	0.084035	-0.605023
C	3.044318	-1.267863	1.237898
C	3.099254	2.497155	-0.887678
H	4.387211	-1.977223	-0.291565
H	4.430242	0.175655	-1.503186
H	2.081313	2.767529	-1.167086
H	3.503445	3.298234	-0.267211
H	3.704098	2.438177	-1.791846
H	1.763098	1.868330	1.392522
H	1.726878	-0.294987	2.618323
O	2.981217	-2.429124	1.968303
H	3.523101	-3.096222	1.528540
C	-0.957523	0.986111	-0.183834
C	-0.946593	-0.113947	-1.242289
O	-1.560175	-1.284637	-0.684202
C	-2.928678	-1.064365	-0.383956
C	-3.050271	-0.025501	0.715009
C	-2.384639	1.251145	0.253476
H	-3.452332	-0.717535	-1.289854
O	-3.482060	-2.249647	0.107815
H	-3.390936	-2.916474	-0.585521
H	-2.526178	-0.418455	1.593934
O	-4.405146	0.295180	1.009716
H	-4.824200	-0.531652	1.284677
H	-2.943341	1.637641	-0.610404
O	-2.328378	2.233296	1.284380
H	-3.238761	2.351133	1.589631
H	-0.382696	0.636139	0.681824
O	-0.384002	2.170670	-0.730192
H	-0.625931	2.874784	-0.110180
H	-1.508367	0.225775	-2.123521
C	0.449558	-0.489172	-1.668528
H	0.963755	-0.945804	-0.817874
H	0.980921	0.425911	-1.941594
O	0.337638	-1.386551	-2.769995
H	1.232307	-1.671726	-2.987816

(iii) Optimized coordinates of *p*-OHTol : β-D-galactose complexes

Y-3a (E_t = -1031.047091)

C	3.429243	-0.777384	-0.346500
C	1.569231	-0.653982	1.191308
C	2.027804	0.586684	1.632674
C	3.185309	1.171063	1.101606
C	3.882108	0.460110	0.115737
C	2.267843	-1.346582	0.192148
C	3.692478	2.493797	1.610903
H	3.961387	-1.319457	-1.117667
H	4.779525	0.888199	-0.316788
H	2.870467	3.122935	1.950714
H	4.376259	2.359468	2.450736
H	4.227842	3.033545	0.830612
H	1.464486	1.114025	2.394662
H	0.674410	-1.093281	1.610677
O	1.882053	-2.566210	-0.275265
H	0.938811	-2.692709	-0.070536
C	-1.719659	1.226847	-0.935561
C	-0.959205	0.243049	-1.832596
O	-0.502087	-0.897559	-1.097629
C	-1.571070	-1.605509	-0.509127
C	-2.291511	-0.718745	0.483288
C	-2.855098	0.505009	-0.218691
H	-1.555944	-0.385062	1.222371
O	-3.311696	-1.511155	1.079842
H	-3.856752	-0.891624	1.586608
H	-3.621891	0.187655	-0.931173
O	-3.500820	1.346807	0.729963
H	-2.775488	1.845573	1.139704
H	-1.648903	-0.081797	-2.628356
C	0.275194	0.839733	-2.489197
H	0.763928	0.066622	-3.086806
H	-0.028632	1.652726	-3.149550
O	1.182275	1.404653	-1.543189
H	1.646869	0.673625	-1.103346
O	-0.969447	-2.709095	0.130446
H	-1.584159	-2.987346	0.826765
H	-2.270388	-1.950101	-1.288295
O	-0.923053	1.773737	0.108412
H	-0.023038	1.886262	-0.253503
H	-2.131915	2.022777	-1.572158

Y-3b (E_t = -1031.043487)

C	2.160354	1.467385	0.833511
C	2.326144	0.717421	-1.457912
C	2.968742	-0.442721	-1.022211
C	3.194432	-0.683166	0.339163
C	2.791385	0.298107	1.254101
C	1.916501	1.680122	-0.529681
C	3.820087	-1.965062	0.820267
H	1.886739	2.230764	1.552118
H	2.959998	0.140454	2.313251
H	4.237776	-2.533722	-0.009507
H	4.622338	-1.769921	1.532101
H	3.080140	-2.590892	1.321746
H	3.280952	-1.180611	-1.753036
H	2.146368	0.901082	-2.509636
O	1.279097	2.798256	-0.999703
H	0.686515	3.122624	-0.292052
C	-2.419358	0.170439	-0.968377
C	-1.368292	0.994463	-0.243330
O	-0.964228	0.368421	0.989130
C	-0.351937	-0.895537	0.757944
C	-1.379429	-1.812261	0.113499
C	-1.870284	-1.232265	-1.196839
H	-2.233805	-1.887353	0.798739
O	-0.830006	-3.091266	-0.181233
H	-0.408021	-3.398212	0.633434
H	-1.022490	-1.186243	-1.893088
O	-2.931216	-2.015943	-1.735305
H	-2.642623	-2.937222	-1.664270
H	-0.495135	1.084898	-0.898752
C	-1.824625	2.378850	0.169873
H	-2.045878	2.985322	-0.706926
H	-2.720376	2.297893	0.787215
O	-0.772874	3.041830	0.885754
H	-0.502451	2.395567	1.557158
O	0.082360	-1.414098	1.986419
H	-0.681901	-1.365121	2.580614
H	0.540827	-0.791434	0.135644
O	-3.595421	0.114899	-0.175372
H	-4.119142	-0.604204	-0.560736
H	-2.622164	0.636592	-1.942694

Y-3c (E_t = -1031.043487)

C	2.407429	0.460233	-1.515165
C	2.445026	0.967011	0.847528
C	2.873271	-0.332604	1.111944
C	3.069972	-1.260074	0.080653
C	2.849115	-0.834108	-1.235350

Y-3d (E_t = -1031.034412)

C	3.005433	-0.326017	1.531628
C	2.565992	-1.416632	-0.580191
C	3.401143	-0.493817	-1.219073
C	4.035789	0.530516	-0.506635
C	3.839406	0.580321	0.881196

C	2.201378	1.369171	-0.472289
C	3.474961	-2.675763	0.393654
H	2.231106	0.788190	-2.531791
H	3.004721	-1.528327	-2.053829
H	3.761127	-3.211344	-0.510573
H	4.320065	-2.701622	1.081786
H	2.652033	-3.217595	0.862561
H	3.043397	-0.634021	2.139217
H	2.331497	1.680931	1.654644
O	1.756393	2.625332	-0.790843
H	1.251576	2.965372	-0.024899
C	-2.343403	0.683014	-0.853216
C	-1.142611	1.228677	-0.098370
O	-0.817830	0.409087	1.040465
C	-0.444261	-0.907243	0.648472
C	-1.635708	-1.556685	-0.037172
C	-2.056328	-0.758609	-1.253919
H	-2.468959	-1.560341	0.677551
O	-1.328555	-2.869883	-0.490773
H	-0.942684	-3.333549	0.265590
H	-1.234992	-0.781057	-1.982300
O	-3.254128	-1.283917	-1.818722
H	-3.129801	-2.243097	-1.858762
H	-0.287283	1.240804	-0.782787
C	-1.336082	2.615868	0.479360
H	-1.473705	3.345287	-0.317223
H	-2.213119	2.621145	1.128062
O	-0.163166	3.004799	1.208201
H	0.009663	2.250931	1.794188
O	-0.070972	-1.626359	1.793110
H	-0.796501	-1.513835	2.425967
H	0.433753	-0.888789	-0.002582
O	-3.486518	0.741576	-0.013619
H	-4.139743	0.170366	-0.445955
H	-2.490445	1.282807	-1.762254

C	2.363621	-1.335666	0.804282
C	4.960644	1.499493	-1.193809
H	2.841931	-0.274970	2.600319
H	4.324391	1.359265	1.458802
H	5.995888	1.159008	-1.143149
H	4.699637	1.612256	-2.245247
H	4.913373	2.483053	-0.727781
H	3.553303	-0.574106	-2.289942
H	2.116582	-2.227057	-1.141996
O	1.535379	-2.185383	1.484095
H	0.858646	-2.513759	0.860532
C	-0.564988	0.088942	0.207668
C	-1.437399	1.287222	0.564361
O	-2.653920	1.301030	-0.193029
C	-3.441011	0.158770	0.080296
C	-2.694266	-1.060861	-0.430241
C	-1.370660	-1.207909	0.297094
H	-2.503752	-0.886368	-1.496146
O	-3.537733	-2.188283	-0.225830
H	-3.021103	-2.964273	-0.483106
H	-1.558676	-1.473845	1.339472
O	-0.631176	-2.299843	-0.277940
H	-0.277707	-1.902230	-1.094993
H	-1.677788	1.229389	1.636624
C	-0.784785	2.625424	0.277731
H	0.146169	2.712438	0.839895
H	-0.555935	2.671504	-0.790238
O	-1.625432	3.689525	0.690063
H	-2.475695	3.515096	0.262858
O	-4.646559	0.346752	-0.597840
H	-5.020971	-0.539018	-0.711910
H	-3.601636	0.071911	1.169114
O	-0.088247	0.170636	-1.145370
H	0.876964	0.243381	-1.107309
H	0.274368	0.044136	0.905171

Y-3e (E_t = -1031.042518)

C	2.968687	-1.922703	-0.455577
C	2.449742	0.237928	0.501786
C	3.337096	0.837349	-0.393549
C	4.045593	0.080624	-1.333126
C	3.855535	-1.307914	-1.336662
C	2.266915	-1.146588	0.468673
C	5.030270	0.729144	-2.269603
H	2.817927	-2.994535	-0.465545
H	4.394576	-1.917442	-2.053112
H	4.756733	1.764318	-2.469627
H	6.036640	0.727515	-1.848048
H	5.070361	0.201590	-3.221931

Y-3f (E_t = -1031.036854)

C	-1.914605	1.883184	0.435173
C	-1.929118	0.983249	-1.806974
C	-2.748777	-0.059999	-1.374690
C	-3.133831	-0.177469	-0.031274
C	-2.718176	0.821630	0.857866
C	-1.474260	1.936695	-0.891208
C	-3.889129	-1.384878	0.455925
H	-1.604215	2.653444	1.131815
H	-3.027643	0.773604	1.896047
H	-4.501067	-1.141550	1.323916
H	-4.544940	-1.778311	-0.320083
H	-3.190460	-2.173375	0.741965

H	3.471817	1.912641	-0.360947
H	1.935049	0.833503	1.245427
O	1.404947	-1.796487	1.329746
H	0.762849	-1.141423	1.666003
C	-2.308174	1.611942	0.369254
C	-0.981857	1.167682	0.973975
O	-0.908323	-0.258215	1.164292
C	-1.139914	-0.996096	-0.050960
C	-2.541087	-0.693102	-0.537077
C	-2.664666	0.779702	-0.851507
H	-3.225687	-0.952653	0.277042
O	-2.849543	-1.394355	-1.734968
H	-2.715798	-2.331856	-1.537020
H	-1.972192	1.015941	-1.670086
O	-4.002202	1.117145	-1.209051
H	-4.295542	0.419472	-1.813168
H	-0.178967	1.489909	0.297677
C	-0.800708	1.762228	2.370897
H	-1.390846	1.151678	3.056588
H	0.245424	1.705042	2.671835
O	-1.173924	3.130130	2.414813
H	-2.141710	3.122748	2.405829
O	-1.086947	-2.355732	0.222685
H	-0.166140	-2.561928	0.460928
H	-0.386103	-0.692931	-0.794192
O	-3.319649	1.481835	1.365282
H	-4.155469	1.509994	0.872925
H	-2.202078	2.660537	0.068821

H	-3.079923	-0.805100	-2.089847
H	-1.612593	1.061919	-2.839506
O	-0.599220	2.905600	-1.335876
H	0.135726	2.953362	-0.699885
C	1.427753	-1.220129	-1.156960
C	0.467894	-1.591736	-0.038594
O	0.971148	-1.134991	1.233198
C	1.026777	0.278059	1.280294
C	1.949598	0.805599	0.188411
C	1.589469	0.292945	-1.192153
H	2.970238	0.477112	0.416278
O	1.875092	2.240569	0.147806
H	2.079873	2.539867	1.046583
H	0.648981	0.748509	-1.508837
O	2.628687	0.576536	-2.128600
H	2.783172	1.530160	-2.088565
H	-0.498466	-1.109038	-0.236092
C	0.241176	-3.077222	0.142236
H	-0.147289	-3.508816	-0.779917
H	1.195004	-3.555198	0.379620
O	-0.734735	-3.306156	1.153135
H	-0.426761	-2.793658	1.913721
O	1.490794	0.674691	2.544756
H	2.285002	0.145664	2.712989
H	0.030698	0.710757	1.170445
O	2.679146	-1.844982	-0.911345
H	3.297670	-1.412949	-1.519447
H	1.000732	-1.548710	-2.114717

Y-3g (E_t = -1031.038550)

C	-1.946540	2.043954	1.515105
C	-1.691958	1.951460	-0.886642
C	-2.432710	0.768155	-0.913419
C	-2.927398	0.188986	0.263982
C	-2.691178	0.862752	1.471889
C	-1.395404	2.558722	0.338496
C	-3.638070	-1.138351	0.233646
H	-1.749577	2.556196	2.448698
H	-3.103297	0.461424	2.391741
H	-4.298545	-1.247104	1.093188
H	-4.241753	-1.236431	-0.668221
H	-2.923498	-1.963990	0.248427
H	-2.641303	0.294731	-1.866891
H	-1.318475	2.391693	-1.803927
O	-0.593426	3.674946	0.419277
H	0.180564	3.488313	-0.134475
C	1.500829	-1.334458	-1.549627
C	0.404328	-1.811105	-0.606627
O	0.678036	-1.404307	0.744361

Y-3h (E_t = -1031.037665)

C	-3.257314	1.709674	-0.002779
C	-2.407810	-0.515246	0.421642
C	-3.374920	-1.038856	-0.438139
C	-4.286069	-0.209209	-1.099851
C	-4.217127	1.169229	-0.854983
C	-2.353562	0.862955	0.641702
C	-5.349344	-0.782751	-1.998443
H	-3.201732	2.775044	0.179537
H	-4.913285	1.834021	-1.353655
H	-5.031850	-1.734420	-2.422548
H	-6.277601	-0.955836	-1.451798
H	-5.572521	-0.105357	-2.821892
H	-3.409870	-2.109864	-0.602946
H	-1.729660	-1.173981	0.950070
O	-1.423423	1.441534	1.481340
H	-0.722737	0.786813	1.665750
C	2.596730	-1.485844	0.125953
C	1.230452	-1.274372	0.791137
O	1.008670	0.120276	1.085805

C	0.655176	0.016009	0.833367
C	1.801455	0.581523	0.019366
C	1.649172	0.179752	-1.432521
H	2.734612	0.171782	0.417557
O	1.811126	2.015985	0.061004
H	1.832565	2.241628	1.003723
H	0.745545	0.664718	-1.824628
O	2.795626	0.548205	-2.195616
H	3.025204	1.447122	-1.921160
H	-0.545670	-1.361171	-0.929787
C	0.233317	-3.314066	-0.536405
H	-0.025501	-3.710146	-1.518003
H	1.174466	-3.763118	-0.211476
O	-0.840193	-3.637548	0.342666
H	-0.617883	-3.185280	1.168691
O	0.847649	0.414793	2.157712
H	-0.020388	0.407632	2.582702
H	-0.297639	0.377442	0.446478
O	2.716895	-1.972690	-1.196954
H	3.406311	-1.460644	-1.646372
H	1.211467	-1.579196	-2.581854
C	1.071251	0.960126	-0.097235
C	2.400920	0.788475	-0.802519
C	2.627369	-0.667748	-1.155334
H	3.195030	1.123540	-0.131226
O	2.397444	1.512282	-2.029912
H	2.298400	2.444363	-1.793201
H	1.790921	-0.994894	-1.793145
O	3.861488	-0.855540	-1.815926
H	3.907833	-0.145639	-2.472265
H	0.451756	-1.639430	0.105822
C	1.078333	-1.974186	2.131908
H	0.047471	-1.866577	2.485797
H	1.294617	-3.037233	2.028469
O	1.995296	-1.459411	3.097089
H	1.867047	-0.498548	3.084790
O	0.967990	2.285280	0.295370
H	0.055027	2.421133	0.601497
H	0.247055	0.657917	-0.760436
O	3.672109	-1.053958	0.937056
H	3.473252	-1.341603	1.842163
H	2.686613	-2.551913	-0.129790

Y-3i (E_t = -1031.039447)

C	3.305628	-0.967498	0.440952
C	3.326388	0.221497	-1.665620
C	4.484288	0.885837	-1.269800
C	5.069641	0.653132	-0.017631
C	4.465053	-0.289043	0.820879
C	2.734356	-0.714871	-0.811995
C	6.342419	1.350435	0.384276
H	2.857822	-1.706004	1.095304
H	4.898254	-0.492818	1.794049
H	6.424541	1.421047	1.468389
H	7.221460	0.815782	0.020218
H	6.380714	2.361056	-0.021540
H	4.932547	1.610779	-1.940468
H	2.871819	0.406863	-2.630195
O	1.597452	-1.342438	-1.248168
H	1.221920	-1.854127	-0.503444
C	-1.561567	1.088198	0.716528
C	-1.076612	-0.314300	0.384245
O	-2.164462	-1.259404	0.330076
C	-3.126264	-0.920979	-0.658215
C	-3.721573	0.436790	-0.319712
C	-2.642439	1.498208	-0.274526
H	-4.173687	0.360191	0.677058
O	-4.667293	0.850806	-1.297559
H	-5.297396	0.123155	-1.394468
H	-2.206838	1.594734	-1.277636

Y-3j (E_t = -1031.037906)

C	-2.490516	1.368878	-0.478259
C	-2.626114	0.028809	1.532291
C	-3.212947	-1.002009	0.795238
C	-3.439657	-0.875567	-0.580211
C	-3.081570	0.331453	-1.197206
C	-2.256201	1.209360	0.888412
C	-4.109525	-1.974776	-1.361410
H	-2.212775	2.299152	-0.957113
H	-3.255096	0.459768	-2.259559
H	-3.928832	-2.946734	-0.904118
H	-5.189217	-1.824727	-1.405958
H	-3.738516	-2.009502	-2.385022
H	-3.494800	-1.917970	1.302505
H	-2.465866	-0.082873	2.599243
O	-1.657549	2.261632	1.555303
H	-1.389560	1.949783	2.430739
C	1.843950	-1.417806	-0.452180
C	0.635726	-1.014463	0.394833
O	0.798618	0.292610	0.955172
C	0.971584	1.319363	-0.049789
C	2.238443	1.035699	-0.826708
C	2.134920	-0.338478	-1.481559
H	3.073070	1.039502	-0.116391
O	2.389627	2.025936	-1.830722
H	3.061450	1.662064	-2.426424
H	1.330852	-0.298606	-2.222584

O	-3.170513	2.742927	0.172133
H	-3.988931	2.879084	-0.326605
H	-0.571048	-0.292770	-0.589256
C	-0.131777	-0.889760	1.417844
H	0.772607	-0.287306	1.485576
H	-0.627283	-0.910704	2.388767
O	0.277829	-2.208232	1.027218
H	-0.546851	-2.676394	0.824410
O	-4.112884	-1.915381	-0.678608
H	-4.389042	-2.033814	0.242312
H	-2.681123	-0.909297	-1.660034
O	-2.087002	1.089361	2.036021
H	-2.576630	1.923142	2.106604
H	-0.713124	1.780412	0.628717

Y-3k (E_t = -1031.028407)

C	-2.796096	0.023761	-1.508796
C	-2.867513	-0.219707	0.897096
C	-2.220047	-1.451476	0.783522
C	-1.837358	-1.964904	-0.463188
C	-2.139183	-1.203641	-1.602249
C	-3.152878	0.521188	-0.253228
C	-1.102319	-3.276116	-0.563367
H	-3.037841	0.603038	-2.390479
H	-1.868526	-1.582015	-2.581661
H	-1.177712	-3.685344	-1.570324
H	-1.520406	-4.007066	0.128543
H	-0.043595	-3.160608	-0.322670
H	-2.014911	-2.023217	1.681879
H	-3.154301	0.156364	1.873815
O	-3.766404	1.753256	-0.213812
H	-4.057420	1.918150	0.692377
C	0.851749	0.880340	1.228303
C	0.339962	1.152014	-0.184122
O	1.365139	0.883240	-1.146638
C	1.667677	-0.501469	-1.137406
C	2.205209	-0.946919	0.221075
C	1.257581	-0.584808	1.358007
H	3.157890	-0.426675	0.389153
O	2.374160	-2.359782	0.206131
H	2.879022	-2.548021	-0.598570
H	0.371511	-1.217394	1.281098
O	1.828756	-0.831281	2.631753
H	2.438559	-0.091069	2.771241
H	-0.506988	0.479430	-0.361300
C	-0.164774	2.556625	-0.420021
H	-0.391692	2.666555	-1.483640
H	-1.089964	2.694970	0.148263

O	3.330768	-0.618131	-2.204531
H	3.961108	-0.902939	-1.523803
H	-0.260819	-1.044642	-0.242758
C	0.424090	-1.915184	1.601977
H	-0.535261	-1.676964	2.064842
H	0.421590	-2.964474	1.307124
O	1.494416	-1.748879	2.539983
H	1.563386	-0.787088	2.653827
O	1.064436	2.534794	0.599089
H	0.164140	2.750867	0.888703
H	0.105451	1.273109	-0.725032
O	3.049253	-1.559597	0.295355
H	2.806347	-1.811946	1.203149
H	1.603493	-2.359607	-0.965752

Y-3l (E_t = -1031.029883)

C	-1.946002	-1.591965	1.078452
C	-2.557125	-0.984245	-1.183044
C	-3.180606	0.166229	-0.694118
C	-3.187307	0.468313	0.672766
C	-2.570491	-0.437952	1.548099
C	-1.944480	-1.868765	-0.292445
C	-3.892260	1.691912	1.195983
H	-1.468754	-2.290971	1.753201
H	-2.564803	-0.231994	2.612699
H	-4.915654	1.459993	1.494787
H	-3.378293	2.097290	2.066969
H	-3.937878	2.472478	0.437313
H	-3.660462	0.842216	-1.393274
H	-2.557848	-1.196044	-2.246832
O	-1.307267	-3.017882	-0.692771
H	-1.285582	-3.041651	-1.658714
C	1.196093	1.391561	0.749100
C	0.272082	0.975728	-0.399558
O	0.980720	0.181413	-1.372324
C	1.522049	-1.014231	-0.814247
C	2.443278	-0.693953	0.352401
C	1.713184	0.120165	1.401612
H	3.292022	-0.104265	-0.012482
O	2.870189	-1.897880	0.985378
H	3.263548	-2.446421	0.293120
H	0.843763	-0.466327	1.736754
O	2.556262	0.438225	2.492344
H	3.005850	-0.389170	2.715337
H	-0.560067	0.398941	0.014134
C	-0.291846	2.134309	-1.200209
H	-1.022452	1.747987	-1.915387
H	-0.791532	2.843206	-0.540043

O	0.840771	3.490690	-0.010039	O	0.744173	2.856218	-1.875312
H	0.500022	4.382299	-0.143580	H	1.219123	2.179966	-2.381341
O	2.605068	-0.762223	-2.149849	O	2.204572	-1.698823	-1.832145
H	3.330137	-0.137270	-2.001800	H	2.863036	-1.076925	-2.175240
H	0.777186	-1.088573	-1.391091	H	0.723808	-1.685734	-0.487415
O	2.028693	1.616545	1.547612	O	2.313044	2.144618	0.306348
H	1.891641	2.516139	1.210869	H	1.979232	2.745957	-0.378964
H	0.045217	1.091564	1.944898	H	0.599975	1.951731	1.484497

(iv) Optimized coordinates of *p*-OHTol : α-D-mannose: complexes

Y-4a (E_t = -1031.034160)				**Y-4b** (E_t = -1031.038479)			
C	3.359357	-1.227918	0.544376	C	-2.634234	-0.499101	-0.578935
C	2.321744	0.943441	0.810924	C	-2.029719	0.169341	1.666131
C	3.137916	1.446376	-0.203982	C	-1.977412	-1.176939	2.037578
C	4.065303	0.633044	-0.863594	C	-2.224205	-2.200302	1.113836
C	4.167348	-0.706367	-0.463106	C	-2.562501	-1.836277	-0.196117
C	2.439305	-0.397314	1.185951	C	-2.309624	0.505750	0.340816
C	4.966294	1.191469	-1.932913	C	-2.074417	-3.651784	1.480312
H	3.431184	-2.264769	0.845869	H	-2.881599	-0.226053	-1.597713
H	4.877250	-1.357920	-0.960105	H	-2.771590	-2.610612	-0.925501
H	4.501610	2.041333	-2.431152	H	-2.960660	-4.224033	1.205191
H	5.188593	0.439242	-2.688956	H	-1.223843	-4.082357	0.950658
H	5.915378	1.530120	-1.514230	H	-1.914425	-3.774879	2.550970
H	3.038586	2.486617	-0.492919	H	-1.747077	-1.433308	3.066820
H	1.614537	1.586876	1.321388	H	-1.794150	0.958583	2.367728
O	1.658057	-0.955395	2.178703	O	-2.251570	1.829632	-0.034889
H	0.938063	-0.327280	2.384964	H	-1.805687	1.830263	-0.900774
C	-1.110733	0.041818	0.644084	C	0.906763	1.005940	-1.410199
C	-2.304470	0.913213	0.251350	C	0.740086	-0.353337	-0.754330
O	-2.721644	0.631947	-1.083167	O	1.955171	-0.649819	-0.024792
C	-3.078117	-0.720309	-1.291452	C	2.232629	0.276075	1.006805
C	-1.936092	-1.668270	-0.973607	C	2.409616	1.693803	0.465726
C	-1.405413	-1.438136	0.438420	C	1.201172	2.080273	-0.372375
H	-3.321350	-0.771468	-2.354885	H	3.164820	-0.093837	1.449621
O	-4.162450	-1.113194	-0.475034	O	1.195908	0.367190	1.955050
H	-4.903278	-0.537881	-0.708587	H	0.878959	-0.529748	2.134535
H	-2.171645	-1.744563	1.165518	H	0.325016	2.194563	0.266159
O	-0.248696	-2.258689	0.531313	O	1.403596	3.328722	-1.033115
H	0.346215	-1.928470	1.228527	H	2.325020	3.296182	-1.335066
H	-0.240519	0.318141	0.047885	H	1.749751	0.950602	-2.109765
O	-0.742061	0.320017	2.016119	O	-0.292169	1.356382	-2.120629
H	-1.462640	-0.004479	2.576446	H	-0.115962	2.259587	-2.431796
H	-3.126915	0.705802	0.953077	H	-0.103120	-0.346329	-0.066262
C	-1.963442	2.392780	0.293625	C	0.580644	-1.499763	-1.730117
H	-1.441781	2.611121	1.229724	H	-0.354019	-1.384241	-2.274257
H	-1.293474	2.607932	-0.538282	H	1.411392	-1.477911	-2.445988

O	-3.101252	3.224514	0.111585
H	-3.627930	3.168072	0.917490
O	-0.905710	-1.404138	-1.909220
H	-0.126216	-1.842647	-1.532863
H	-2.299619	-2.699250	-1.051759

Y-4c (E_t = -1031.030798)

C	-2.357500	-0.027321	1.580050
C	-2.875491	0.004719	-0.779899
C	-2.450687	1.328719	-0.853480
C	-1.973420	2.000667	0.280217
C	-1.947110	1.305179	1.494849
C	-2.782024	-0.694313	0.430396
C	-1.451947	3.407908	0.165648
H	-2.293247	-0.579849	2.507727
H	-1.599183	1.810727	2.389562
H	-1.292936	3.851986	1.147865
H	-0.501826	3.417709	-0.370620
H	-2.146745	4.044543	-0.382707
H	-2.490290	1.848813	-1.803679
H	-3.249097	-0.507754	-1.658618
O	-3.115705	-2.026530	0.512923
H	-2.652725	-2.447422	-0.233163
C	1.395094	0.275342	-1.163643
C	0.476401	-0.825557	-0.668120
O	1.271405	-1.769234	0.094533
C	1.846426	-1.219510	1.245660
C	2.740212	-0.016072	0.915877
C	1.992245	0.981806	0.045375
H	2.449431	-2.029683	1.675546
O	0.797698	-0.836713	2.117781
H	1.185754	-0.435772	2.906852
H	1.172523	1.428391	0.611643
O	2.840811	2.049678	-0.368317
H	3.667344	1.618249	-0.635326
H	2.205361	-0.174506	-1.752512
O	0.643002	1.194568	-1.944435
H	1.213254	1.974470	-2.022308
H	-0.302131	-0.401842	-0.033520
C	-0.150451	-1.656496	-1.764081
H	-0.799988	-1.031263	-2.370419
H	0.638500	-2.076838	-2.396684
O	-0.951846	-2.703296	-1.206185
H	-0.403153	-3.084563	-0.504048
O	3.876581	-0.405521	0.143475
H	4.475143	-0.911899	0.706174
H	3.057970	0.472449	1.846939

O	0.521800	-2.742723	-1.042319
H	1.299425	-2.741537	-0.467544
O	3.527033	1.772367	-0.422923
H	4.335385	1.792093	0.103244
H	2.518164	2.389029	1.303647

Y-4d (E_t = -1031.031510)

C	-3.114969	-0.186798	0.804968
C	-2.221608	0.402437	-1.363063
C	-2.600340	1.728977	-1.146945
C	-3.221382	2.125302	0.045728
C	-3.474963	1.144123	1.012776
C	-2.471951	-0.559222	-0.380973
C	-3.570778	3.567876	0.299263
H	-3.340888	-0.943688	1.547335
H	-3.965469	1.422610	1.938712
H	-2.776212	4.075206	0.848836
H	-4.483781	3.651153	0.887824
H	-3.723785	4.103926	-0.636562
H	-2.401678	2.467594	-1.915655
H	-1.726142	0.099003	-2.275981
O	-2.069451	-1.856256	-0.609515
H	-1.618835	-2.140816	0.205834
C	0.641020	-0.848151	0.550541
C	1.876438	-1.709484	0.349230
O	2.726440	-1.062833	-0.613507
C	3.148606	0.228132	-0.233159
C	1.982820	1.175815	0.056159
C	1.042932	0.528133	1.057453
H	3.722804	0.580944	-1.097202
O	3.933451	0.213208	0.940674
H	4.652498	-0.412977	0.779145
H	1.557394	0.417884	2.013857
O	-0.114280	1.313527	1.318098
H	-0.523523	1.489490	0.454024
H	0.137503	-0.738623	-0.414022
O	-0.235004	-1.470950	1.500440
H	-0.752174	-0.727425	1.857501
H	2.399656	-1.814015	1.307879
C	1.549599	-3.080694	-0.208007
H	0.757639	-3.526084	0.401270
H	1.178089	-2.962455	-1.225283
O	2.691612	-3.924754	-0.290833
H	2.916192	-4.182754	0.610963
O	1.200217	1.401755	-1.115454
H	1.692333	1.992698	-1.698302
H	2.374516	2.112806	0.463870

Y-4e (E_t = -1031.037207)

C	-3.150662	0.710023	0.979560
C	-1.961913	0.932844	-1.114123
C	-2.297042	2.287384	-1.148597
C	-3.062722	2.875381	-0.136449
C	-3.481858	2.061554	0.924793
C	-2.380896	0.140775	-0.038975
C	-3.385839	4.345833	-0.160387
H	-3.477288	0.082073	1.798345
H	-4.082228	2.490612	1.719537
H	-2.638635	4.925826	0.383976
H	-4.354285	4.541722	0.299042
H	-3.416600	4.723201	-1.181960
H	-1.966195	2.890190	-1.987119
H	-1.391912	0.487669	-1.920936
O	-2.085860	-1.194946	0.054427
H	-1.397928	-1.407014	-0.607197
C	1.297807	-1.419958	-0.642317
C	1.039850	-1.503319	0.855739
O	2.283998	-1.200680	1.508896
C	2.714985	0.127567	1.245849
C	2.863046	0.434683	-0.241425
C	1.614867	0.010143	-1.011556
H	3.692477	0.188788	1.729775
O	1.805279	1.082007	1.747733
H	1.709927	0.905621	2.693173
H	0.772414	0.658089	-0.748503
O	1.931246	0.121076	-2.399794
H	1.289195	-0.439496	-2.858395
H	2.165119	-2.040073	-0.867680
O	0.174122	-1.860285	-1.432000
H	0.202225	-2.829075	-1.353484
H	0.283052	-0.771325	1.151275
C	0.571391	-2.882102	1.282915
H	0.928778	-3.069780	2.297921
H	-0.521011	-2.893243	1.281047
O	1.085164	-3.851727	0.356823
H	0.867928	-4.726461	0.700062
O	3.988579	-0.292875	-0.706490
H	3.904109	-0.278108	-1.672000
H	3.011503	1.514160	-0.354596

Y-4f (E_t = -1031.036295)

C	-1.946570	-1.627356	0.821505
C	-2.105805	-1.258986	-1.562623
C	-3.049198	-0.254557	-1.339591
C	-3.452919	0.084665	-0.041834
C	-2.901267	-0.632988	1.028113
C	-1.528956	-1.926860	-0.476454
C	-4.495332	1.145623	0.194288
H	-1.485662	-2.143627	1.652297
H	-3.195433	-0.388296	2.042330
H	-4.490489	1.885198	-0.605673
H	-5.496179	0.713272	0.240357
H	-4.316469	1.665895	1.134640
H	-3.480864	0.266858	-2.187096
H	-1.826009	-1.540975	-2.571922
O	-0.544621	-2.877260	-0.646748
H	0.061146	-2.521995	-1.317381
C	1.145270	0.566251	1.191817
C	0.266459	1.073351	0.063116
O	1.091703	1.306393	-1.109898
C	1.807468	0.187454	-1.567306
C	2.670101	-0.465333	-0.490223
C	1.858447	-0.709817	0.772368
H	2.434896	0.578720	-2.375073
O	0.937939	-0.826028	-2.061142
H	0.241847	-0.360871	-2.547896
H	1.116510	-1.488007	0.590378
O	2.689361	-1.178077	1.832557
H	3.463628	-0.594488	1.808914
H	1.888204	1.338529	1.421136
O	0.309218	0.308745	2.313337
H	0.868558	-0.192904	2.924951
H	-0.509057	0.339583	-0.158581
C	-0.368918	2.415230	0.360359
H	-0.966055	2.329932	1.266269
H	-1.028645	2.681604	-0.473699
O	0.612438	3.416134	0.589653
H	1.211979	3.359149	-0.166946
O	3.726902	0.418443	-0.104030
H	4.439997	0.340267	-0.749033
H	3.065420	-1.412323	-0.870829

Y-4g (E_t = -1031.032704)

C	-1.785595	-1.277001	-1.415949
C	-2.536753	-1.189898	0.884452
C	-3.036289	0.091644	0.666119

Y-4h (E_t = -1031.033535)

C	3.633553	0.360500	0.985633
C	2.319169	-1.117955	-0.404745
C	1.884822	-0.024610	-1.150572

C	-2.910964	0.718887	-0.581066
C	-2.295115	0.007669	-1.617453
C	-1.896111	-1.865074	-0.157328
C	-3.395417	2.131802	-0.762882
H	-1.301819	-1.824271	-2.214504
H	-2.201704	0.460391	-2.598317
H	-2.866843	2.790151	-0.073237
H	-3.225501	2.479386	-1.781737
H	-4.462286	2.217495	-0.554844
H	-3.500973	0.626279	1.486111
H	-2.610441	-1.647550	1.864833
O	-1.305237	-3.104046	0.015471
H	-1.587284	-3.456149	0.871027
C	1.395992	-0.539445	0.972809
C	0.480083	0.666186	0.784268
O	1.223824	1.763566	0.198368
C	1.756196	1.461129	-1.072006
C	2.659549	0.232551	-1.037433
C	1.951340	-0.950801	-0.388016
H	2.329051	2.355903	-1.342845
O	0.754948	1.175359	-2.025642
H	0.071216	1.851511	-1.921406
H	1.113628	-1.250647	-1.023308
O	2.817624	-2.070340	-0.307478
H	3.621455	-1.731819	0.113545
H	2.225800	-0.252830	1.626605
O	0.694377	-1.599499	1.612648
H	0.412223	-2.223363	0.927400
H	-0.348118	0.397123	0.127046
C	-0.073550	1.225288	2.075592
H	-0.700824	0.477212	2.552915
H	0.757729	1.470988	2.747031
O	-0.885406	2.369753	1.822356
H	-0.321053	2.951292	1.294510
O	3.812396	0.473967	-0.227158
H	4.438159	0.998975	-0.740227
H	2.941963	-0.035343	-2.060130

Y-4i (E_t = -1031.037336)

C	3.072808	0.133431	0.810237
C	2.331380	-0.276038	-1.456609
C	1.944150	-1.560505	-1.085369
C	2.111457	-2.031135	0.226379
C	2.678183	-1.160853	1.163343
C	2.896521	0.574173	-0.502574
C	1.664922	-3.417200	0.607887
H	3.520625	0.788638	1.550389
H	2.834957	-1.498783	2.182039
H	1.943175	-4.140678	-0.158184
C	2.315003	1.276282	-0.847465
C	3.198346	1.447363	0.222492
C	3.197841	-0.926575	0.666378
C	1.845226	2.444135	-1.672842
H	4.310336	0.516335	1.819183
H	3.540143	2.442623	0.482545
H	2.276909	2.421425	-2.674336
H	0.760817	2.419716	-1.775640
H	2.128071	3.389878	-1.210499
H	1.168806	-0.183815	-1.947384
H	1.998562	-2.124426	-0.643599
O	3.580166	-2.045117	1.371208
H	4.222667	-1.775856	2.039865
C	-1.247998	-0.953659	0.680847
C	-1.202932	0.548487	0.912888
O	-1.039775	1.193587	-0.369561
C	-2.109039	0.941940	-1.268776
C	-2.320696	-0.543911	-1.525981
C	-2.423199	-1.300533	-0.209415
H	-1.801227	1.438285	-2.193254
O	-3.336159	1.431359	-0.779731
H	-3.208541	2.371347	-0.593821
H	-3.350463	-1.024989	0.304914
O	-2.410619	-2.689491	-0.534839
H	-2.248592	-3.140577	0.306695
H	-0.326029	-1.253057	0.176370
O	-1.434463	-1.693298	1.895447
H	-0.564020	-1.824744	2.291476
H	-2.133178	0.886851	1.379285
C	-0.016824	0.993377	1.747839
H	-0.160231	0.660131	2.775946
H	0.894220	0.539200	1.349917
O	0.083531	2.409122	1.784606
H	0.125501	2.672211	0.855345
O	-1.202897	-1.009530	-2.270556
H	-1.237890	-1.974534	-2.180312
H	-3.249204	-0.667044	-2.093907

Y-4j (E_t = -1031.032275)

C	-2.344451	1.724258	-0.485924
C	-2.180891	0.610624	1.655902
C	-2.769831	-0.526508	1.098318
C	-3.166257	-0.560501	-0.244409
C	-2.935336	0.583445	-1.022924
C	-1.949424	1.730948	0.854880
C	-3.765366	-1.802878	-0.849427
H	-2.160168	2.602087	-1.090777
H	-3.241495	0.590922	-2.063375
H	-2.989322	-2.435897	-1.281752

H	0.582323	-3.450814	0.728874
H	2.124000	-3.730954	1.545144
H	1.512967	-2.216451	-1.833695
H	2.185480	0.088530	-2.463576
O	3.239375	1.841061	-0.920447
H	3.663594	2.300535	-0.184002
C	-1.265466	0.893034	-0.865479
C	-0.450378	0.879046	0.419258
O	-1.360692	0.602085	1.508142
C	-1.992082	-0.662033	1.399829
C	-2.737375	-0.854984	0.085561
C	-1.848976	-0.483774	-1.095469
H	-2.699084	-0.681467	2.233125
O	-1.051362	-1.714126	1.474299
H	-0.496829	-1.531036	2.245272
H	-1.030102	-1.205046	-1.194142
O	-2.683566	-0.490902	-2.253281
H	-2.190101	0.013955	-2.916484
H	-2.085770	1.603666	-0.747101
O	-0.482983	1.207834	-2.021522
H	-0.366035	2.167103	-2.027900
H	0.325395	0.113127	0.367064
C	0.166315	2.221771	0.741956
H	0.661492	2.151750	1.717020
H	0.918825	2.470937	-0.004756
O	-0.807878	3.259177	0.720614
H	-1.516787	2.953542	1.304453
O	-3.872534	-0.003392	0.123596
H	-4.162008	0.051463	-0.800095
H	-3.032305	-1.907626	0.008218
H	-4.296018	-2.386604	-0.097799
H	-4.472899	-1.549667	-1.638238
H	-2.951177	-1.388347	1.731816
H	-1.875544	0.611733	2.696395
O	-1.353890	2.877547	1.323642
H	-1.071823	2.725260	2.234764
C	0.600115	-0.151481	-0.827941
C	1.906984	0.606842	-0.699139
O	2.471974	0.367350	0.611392
C	2.742317	-0.994254	0.873200
C	1.488513	-1.859277	0.764584
C	0.810888	-1.637780	-0.580180
H	3.122293	-0.996485	1.901303
O	3.673836	-1.546695	-0.028980
H	4.451179	-0.971779	-0.017828
H	1.439395	-2.041144	-1.375185
O	-0.433265	-2.331056	-0.650496
H	-0.918772	-2.038563	0.137872
H	-0.100023	0.228140	-0.076348
O	0.105211	0.071010	-2.142582
H	-0.688167	-0.480658	-2.201979
H	2.607273	0.271411	-1.469544
C	1.738294	2.109724	-0.783734
H	1.374565	2.375688	-1.773887
H	0.995522	2.426553	-0.042677
O	2.985042	2.768457	-0.595450
H	3.318797	2.424710	0.243490
O	0.533363	-1.475034	1.758672
H	0.778488	-1.906737	2.585895
H	1.766401	-2.912232	0.869038

Y-4k (E_t = -1031.030351)

C	2.623257	0.118971	-1.485197
C	3.112573	-0.141795	0.868435
C	2.445648	1.051702	1.129549
C	1.857005	1.803889	0.100803
C	1.963341	1.319804	-1.206347
C	3.205121	-0.609611	-0.446867
C	1.157920	3.099994	0.412072
H	2.697392	-0.234038	-2.508900
H	1.510802	1.870871	-2.022165
H	0.383359	2.937679	1.160611
H	0.691610	3.516887	-0.479952
H	1.858649	3.840229	0.801001
H	2.374875	1.405800	2.151870
H	3.580294	-0.714316	1.659191
O	3.877550	-1.793337	-0.642123
H	3.931670	-1.959176	-1.591752
C	-1.505237	0.092776	0.932589

Y-4l (E_t = -1031.033778)

C	3.895739	-0.436123	0.649275
C	2.569184	-0.660664	-1.360438
C	2.319349	0.708445	-1.339176
C	2.842622	1.532776	-0.331233
C	3.638715	0.937743	0.652905
C	3.358700	-1.236676	-0.360049
C	2.587957	3.016576	-0.349536
H	4.507174	-0.878177	1.428693
H	4.062568	1.549897	1.441108
H	3.177470	3.507753	-1.124980
H	1.536249	3.219851	-0.546273
H	2.853946	3.471080	0.604615
H	1.695646	1.144761	-2.110959
H	2.167218	-1.296443	-2.138829
O	3.548197	-2.596092	-0.421585
H	4.110276	-2.859607	0.318114
C	-1.370821	0.755488	0.465808

C	-0.522401	-0.968633	0.462836
O	-1.212063	-1.799323	-0.491616
C	-1.626593	-1.079953	-1.639327
C	-2.491355	0.137635	-1.329165
C	-1.853244	0.986867	-0.234726
H	-2.208430	-1.806266	-2.212499
O	-0.519729	-0.587028	-2.371880
H	0.094117	-1.329033	-2.456571
H	-0.941425	1.459799	-0.612908
O	-2.819868	1.966090	0.148067
H	-2.542337	2.256355	1.029503
H	-2.412610	-0.414966	1.263366
O	-0.977905	0.916869	1.977423
H	-1.028572	0.366181	2.772664
H	0.342899	-0.498390	-0.011238
C	-0.031832	-1.837311	1.601397
H	0.272733	-2.804952	1.194258
H	0.842458	-1.355887	2.047246
O	-1.080685	-1.972429	2.567363
H	-0.807415	-2.645328	3.201521
O	-3.754942	-0.341703	-0.897652
H	-4.159471	0.418435	-0.452120
H	-2.584677	0.731002	-2.246090

C	-0.732874	-0.606620	0.232919
O	-1.756956	-1.612501	0.382078
C	-2.825928	-1.471759	-0.539993
C	-3.495720	-0.106340	-0.469675
C	-2.454539	1.000220	-0.560788
H	-3.536285	-2.248211	-0.245524
O	-2.385516	-1.624813	-1.871075
H	-1.964547	-2.493249	-1.924110
H	-2.006680	1.011521	-1.560739
O	-3.134221	2.225939	-0.290706
H	-2.432546	2.861077	-0.086042
H	-1.823220	0.759931	1.459104
O	-0.435888	1.832395	0.327570
H	0.114397	1.835317	1.122098
H	-0.293766	-0.648090	-0.767775
C	0.315880	-0.950080	1.269370
H	0.688212	-1.960720	1.070843
H	1.156800	-0.263384	1.190464
O	-0.207950	-0.829113	2.587319
H	-1.017035	-1.360532	2.587841
O	-4.169108	-0.037639	0.778084
H	-4.356427	0.905663	0.899256
H	-4.197515	-0.021774	-1.306723

(v) Optimized coordinates of *p*-OHTol : α-L-fucose complexes

Y-5a (E_t = -956.012262)

C	2.093359	-0.948216	-1.438094
C	2.368522	-1.479240	0.904802
C	3.205616	-0.372669	1.050057
C	3.496909	0.466540	-0.033220
C	2.940193	0.148859	-1.279842
C	1.791728	-1.756903	-0.339278
C	4.433131	1.635925	0.122639
H	1.643369	-1.181001	-2.394800
H	3.159288	0.777571	-2.136118
H	4.193137	2.427012	-0.587168
H	5.468838	1.339206	-0.050996
H	4.373029	2.054701	1.126589
H	3.634277	-0.156415	2.022473
H	2.141386	-2.117151	1.750431
O	0.914644	-2.802959	-0.513106
H	0.303826	-2.764081	0.245799
C	-0.463494	0.548260	0.691777
C	-0.790277	1.700013	-0.248580
O	-2.210411	1.964038	-0.296473
C	-2.997634	0.851547	-0.637432
C	-2.744578	-0.328289	0.288265

Y-5b (E_t = -956.005517)

C	2.524914	0.287022	1.317867
C	2.099450	1.409327	-0.780278
C	2.395982	0.229820	-1.462342
C	2.727076	-0.946376	-0.774882
C	2.802046	-0.891924	0.622957
C	2.115286	1.425097	0.616778
C	2.934553	-2.237841	-1.520081
H	2.579578	0.320154	2.399443
H	3.093200	-1.778103	1.176563
H	1.974163	-2.691454	-1.770581
H	3.502120	-2.950303	-0.922382
H	3.476025	-2.072469	-2.451049
H	2.356439	0.218794	-2.546050
H	1.813783	2.310400	-1.308116
O	1.694927	2.564183	1.271165
H	1.033226	2.259992	1.915748
C	-1.415586	1.206190	0.014418
C	-1.698860	0.470140	-1.290251
O	-2.471977	-0.725031	-1.052378
C	-1.878926	-1.629580	-0.163343
C	-1.632245	-0.963161	1.192471

C	-1.267163	-0.672993	0.277479
H	-4.031431	1.196258	-0.555842
O	-2.732301	0.357967	-1.944335
H	-2.977686	1.051648	-2.570405
H	-3.030999	-0.044674	1.299943
O	-3.527821	-1.468233	-0.059785
H	-3.424253	-1.562712	-1.019184
H	-0.967419	-0.992617	-0.725008
O	-1.024346	-1.740308	1.216248
H	-1.823418	-2.291674	1.162078
H	0.606139	0.339601	0.608132
O	-0.805326	0.924694	2.022067
H	-0.702448	0.115234	2.543212
H	-0.448778	1.406354	-1.247569
C	-0.133921	2.995532	0.173921
H	-0.386056	3.788139	-0.527762
H	0.948180	2.866861	0.192586
H	-0.477026	3.269946	1.167625
C	-0.754695	0.247705	0.983245
H	-2.604354	-2.446383	-0.070549
O	-0.655241	-2.114004	-0.688763
H	-0.102950	-2.334629	0.077329
H	-2.585466	-0.662989	1.632325
O	-0.891237	-1.827487	2.072270
H	-1.500713	-2.491192	2.421624
H	0.194771	-0.086309	0.567291
O	-0.531840	0.940249	2.224302
H	-0.329767	0.242567	2.866683
H	-0.721742	2.032373	-0.188816
O	-2.640840	1.689429	0.554016
H	-2.417397	2.016610	1.437119
H	-0.733418	0.188285	-1.722035
C	-2.505989	1.296653	-2.266599
H	-2.676927	0.726607	-3.177180
H	-1.967992	2.210740	-2.516233
H	-3.460976	1.559145	-1.819900

Y-5c (E_t = -956.012005)

C	-1.766153	1.174842	-1.389512
C	-1.715919	1.584392	0.990568
C	-2.710701	0.621278	1.165490
C	-3.236461	-0.091869	0.079309
C	-2.751704	0.205448	-1.200687
C	-1.213410	1.836149	-0.287352
C	-4.257347	-1.179941	0.281676
H	-1.416088	1.426507	-2.383928
H	-3.162198	-0.313198	-2.060168
H	-4.982434	-1.193876	-0.531702
H	-4.801221	-1.039080	1.214970
H	-3.780939	-2.161179	0.315648
H	-3.087683	0.422473	2.162993
H	-1.286443	2.117746	1.827514
O	-0.206327	2.765097	-0.450380
H	0.535511	2.268393	-0.836104
C	2.076848	-0.183474	1.223777
C	2.643561	0.520973	-0.002558
O	1.648649	0.641525	-1.053801
C	1.066050	-0.591348	-1.446253
C	0.418564	-1.298048	-0.268912
C	1.441981	-1.510000	0.833211
H	0.321765	-0.327955	-2.198733
O	2.024250	-1.497906	-1.964111
H	2.349660	-1.136206	-2.798759
H	-0.391571	-0.677357	0.108283
O	-0.166478	-2.540802	-0.654520
H	0.515611	-2.993807	-1.173319
H	2.220007	-2.196650	0.477467

Y-5d (E_t = -956.006918)

C	-2.369469	-1.628907	-0.011664
C	-1.813766	0.070563	-1.640001
C	-2.737719	0.931178	-1.044964
C	-3.488938	0.535201	0.068118
C	-3.303291	-0.764800	0.558631
C	-1.617691	-1.209069	-1.112454
C	-4.512646	1.455307	0.678605
H	-2.212487	-2.627137	0.376713
H	-3.878846	-1.098179	1.415164
H	-4.632318	1.256255	1.743005
H	-5.488496	1.329848	0.206696
H	-4.219777	2.497967	0.561920
H	-2.866840	1.928049	-1.450783
H	-1.254921	0.382427	-2.515076
O	-0.693850	-2.089504	-1.631884
H	0.078174	-1.582457	-1.931803
C	0.692267	0.546527	1.168071
C	1.025230	-0.939784	1.156689
O	2.444604	-1.089548	0.882872
C	2.803589	-0.616057	-0.411284
C	2.547376	0.878716	-0.487485
C	1.096750	1.192246	-0.152553
H	3.868674	-0.838309	-0.507786
O	2.071241	-1.255284	-1.439978
H	2.284888	-2.197684	-1.382474
H	3.182121	1.335012	0.285326
O	2.894402	1.366786	-1.768793
H	2.537439	2.267145	-1.789045
H	0.463998	0.820905	-0.956249

O	0.800367	-2.031885	1.995648
H	0.161120	-2.679860	1.663100
H	2.907015	-0.375225	1.919162
O	1.102419	0.656439	1.820299
H	0.562688	0.062469	2.365391
H	3.469937	-0.085501	-0.386820
C	3.103351	1.931502	0.296561
H	3.506556	2.391286	-0.603910
H	3.880143	1.915214	1.060057
H	2.263557	2.516638	0.661863

Y-5e (E_t = -956.008442)

C	3.242963	-0.011470	0.891741
C	2.450063	0.142162	-1.388756
C	1.945344	-1.154129	-1.288393
C	2.072240	-1.902556	-0.109749
C	2.729152	-1.306887	0.973901
C	3.100214	0.715239	-0.293278
C	1.483378	-3.282406	0.011477
H	3.751886	0.428715	1.742838
H	2.844996	-1.861782	1.898096
H	0.543051	-3.242957	0.561714
H	2.160456	-3.950338	0.543924
H	1.293127	-3.712575	-0.971320
H	1.452775	-1.594184	-2.148641
H	2.362686	0.713362	-2.304007
O	3.570281	1.999172	-0.445758
H	3.984626	2.273491	0.382583
C	-0.467807	0.549093	0.671426
C	-0.670218	1.573504	-0.437435
O	-2.089010	1.862837	-0.515645
C	-2.860024	0.748578	-0.915257
C	-2.722943	-0.376974	0.104707
C	-1.258308	-0.710441	0.349248
H	-3.889714	1.116696	-0.955819
O	-2.432871	0.297566	-2.182199
H	-2.741912	-0.620768	-2.235182
H	-3.174197	-0.050634	1.049181
O	-3.415055	-1.509846	-0.415899
H	-3.129158	-2.255896	0.131842
H	-0.849295	-1.181424	-0.546200
O	-1.168499	-1.676243	1.399035
H	-1.214812	-1.145937	2.211443
H	0.586670	0.302156	0.787339
O	-0.914116	1.056582	1.939482
H	-1.686055	1.606400	1.732177
H	-0.342042	1.140162	-1.383682
C	0.025253	2.893677	-0.190486
H	-0.250155	3.600629	-0.970193

O	0.919622	2.606647	-0.113134
H	1.207774	2.855268	0.780265
H	-0.376982	0.696874	1.335188
O	1.372851	1.223817	2.236761
H	2.245655	0.805415	2.290883
H	0.459866	-1.425021	0.362549
C	0.757785	-1.633315	2.473658
H	-0.309400	-1.595293	2.689761
H	1.294050	-1.147379	3.285232
H	1.069611	-2.673855	2.413553

Y-5f (E_t = -956.008442)

C	2.598009	-0.210415	0.688493
C	2.956861	0.720638	-1.515441
C	2.355471	1.910424	-1.101200
C	1.867498	2.067519	0.201818
C	2.002223	0.986793	1.084614
C	3.075786	-0.343342	-0.617357
C	1.180054	3.340248	0.617778
H	2.712948	-1.038895	1.375514
H	1.645321	1.083856	2.104172
H	1.706649	4.212689	0.230981
H	1.142584	3.426019	1.703305
H	0.160592	3.360391	0.232002
H	2.267906	2.729531	-1.806084
H	3.331475	0.622582	-2.528941
O	3.646138	-1.548754	-0.955551
H	3.921463	-1.507951	-1.880543
C	-0.610731	-0.309694	-0.929505
C	-0.545135	-1.638965	-0.188764
O	-1.905500	-2.101994	0.005690
C	-2.661300	-1.259972	0.851556
C	-2.781474	0.130277	0.236128
C	-1.408796	0.690945	-0.106750
H	-3.641459	-1.740608	0.927028
O	-2.042925	-1.168756	2.116588
H	-2.395073	-0.352666	2.505999
H	-3.373464	0.056110	-0.683766
O	-3.439258	0.962333	1.189254
H	-3.304380	1.867604	0.872015
H	-0.876264	0.911833	0.819836
O	-1.570585	1.933701	-0.793974
H	-1.728389	1.673837	-1.716441
H	0.387910	0.082166	-1.117907
O	-1.244524	-0.456208	-2.210733
H	-1.930161	-1.129217	-2.076106
H	-0.080442	-1.478540	0.785500
C	0.177019	-2.730901	-0.946184
H	-0.255112	-2.857512	-1.936688

H	1.104805	2.752521	-0.205202
H	-0.264568	3.302305	0.775378
H	0.091648	-3.668490	-0.401014
H	1.230467	-2.475833	-1.049920

Y-5g (E_t = -956.008082)

C	-2.386624	-0.868633	-0.892297
C	-2.916217	-0.046311	1.320044
C	-2.567052	1.241344	0.915084
C	-2.134114	1.507303	-0.392065
C	-2.046736	0.428086	-1.280947
C	-2.802987	-1.109762	0.420122
C	-1.718333	2.892504	-0.813608
H	-2.297521	-1.689956	-1.594515
H	-1.732755	0.605031	-2.304263
H	-0.635406	3.019115	-0.756748
H	-2.179539	3.646389	-0.176407
H	-2.020997	3.092874	-1.841407
H	-2.659220	2.059196	1.621381
H	-3.259953	-0.248820	2.326104
O	-3.139399	-2.357789	0.880819
H	-2.952331	-3.000412	0.184542
C	1.106282	0.810181	1.025705
C	0.685144	-0.630157	1.281305
O	1.788778	-1.486256	0.889893
C	2.061222	-1.439131	-0.495003
C	2.460671	-0.024056	-0.904401
C	1.414839	0.984783	-0.452875
H	2.890096	-2.137795	-0.643852
O	0.922852	-1.843872	-1.226407
H	1.039585	-1.443571	-2.102997
H	3.419933	0.219175	-0.432368
O	2.582665	-0.010321	-2.325393
H	2.607523	0.927238	-2.568549
H	0.505953	0.826512	-1.033391
O	1.869045	2.306437	-0.750715
H	2.463446	2.525327	-0.014468
H	0.312185	1.498778	1.321118
O	2.269158	1.167275	1.787076
H	2.801342	0.357288	1.826819
H	-0.182762	-0.855899	0.661520
C	0.393715	-0.938120	2.732024
H	0.153424	-1.993252	2.842213
H	-0.458021	-0.346298	3.063737
H	1.251705	-0.699694	3.357077

Y-5h (E_t = -956.010135)

C	2.204849	-0.473733	-1.468754
C	2.787972	-0.439112	0.880769
C	2.810884	0.956038	0.847295
C	2.519502	1.658315	-0.326798
C	2.233754	0.918749	-1.483869
C	2.476121	-1.150360	-0.278526
C	2.567533	3.162834	-0.360153
H	1.957022	-1.045963	-2.351877
H	2.013519	1.440576	-2.408566
H	3.568088	3.522407	-0.605935
H	2.291306	3.582641	0.606283
H	1.881267	3.558911	-1.107874
H	3.032310	1.501986	1.756783
H	3.002791	-0.968771	1.803247
O	2.371033	-2.526981	-0.304294
H	2.618802	-2.867030	0.566488
C	-1.731280	1.134936	0.505932
C	-2.386519	0.770105	-0.819654
O	-2.875297	-0.587584	-0.809559
C	-1.893500	-1.552734	-0.516572
C	-1.215667	-1.282367	0.817198
C	-0.645953	0.127020	0.841370
H	-2.429271	-2.505250	-0.494105
O	-0.848716	-1.585846	-1.478826
H	-1.239228	-1.877245	-2.313239
H	-1.968230	-1.360366	1.601806
O	-0.207802	-2.246598	1.111405
H	0.315899	-2.350761	0.299371
H	0.167266	0.206916	0.115756
O	-0.178153	0.436775	2.156559
H	0.344389	-0.335334	2.418643
H	-1.272645	2.129424	0.401881
O	-2.720553	1.140534	1.526258
H	-2.213766	1.112321	2.352198
H	-1.620614	0.864956	-1.598393
C	-3.584706	1.637104	-1.139489
H	-4.329110	1.525647	-0.356118
H	-4.015964	1.338507	-2.092855
H	-3.285878	2.683252	-1.198317

Y-5i (E_t = -956.002482)

C	2.522929	0.224446	-1.306384

Y-5j (E_t = 956.007864)

C	-2.419337	-0.154987	1.422056

C	3.220854	0.065320	1.004433
C	2.731826	-1.240856	1.053478
C	2.132980	-1.838158	-0.062326
C	2.041264	-1.082552	-1.239179
C	3.108168	0.802537	-0.177605
C	1.559336	-3.226882	0.026463
H	2.457053	0.804847	-2.217500
H	1.591456	-1.522869	-2.122319
H	1.379238	-3.640017	-0.965461
H	0.615155	-3.205933	0.570915
H	2.237203	-3.899215	0.552482
H	2.818686	-1.802045	1.977091
H	3.682423	0.508582	1.880583
O	3.552878	2.098188	-0.296814
H	3.904803	2.380308	0.557245
C	-0.518046	0.515295	0.671132
C	-0.717112	1.516369	-0.459555
O	-2.120827	1.743771	-0.710795
C	-2.835325	0.586185	-1.028900
C	-2.724683	-0.446852	0.092131
C	-1.270606	-0.767483	0.360504
H	-3.874409	0.917692	-1.147686
O	-2.352389	0.025582	-2.237834
H	-2.632632	-0.902353	-2.218419
H	-3.170531	-0.043233	1.003524
O	-3.342997	-1.689998	-0.290635
H	-4.298504	-1.588904	-0.188515
H	-0.836655	-1.237336	-0.527870
O	-1.150147	-1.630347	1.495670
H	-1.815209	-2.321616	1.362966
H	0.549135	0.289437	0.753650
O	-1.015661	1.076810	1.883192
H	-1.012430	0.340086	2.511799
H	-0.262317	1.091705	-1.358672
C	-0.121060	2.873266	-0.156085
H	-0.327013	3.553013	-0.980501
H	0.957770	2.786510	-0.033266
H	-0.560030	3.270015	0.755619

C	-3.094975	0.123146	-0.883635
C	-2.499244	1.382597	-0.894926
C	-1.854942	1.900926	0.238217
C	-1.826115	1.109465	1.391695
C	-3.048907	-0.651859	0.278587
C	-1.178320	3.244864	0.200285
H	-2.396151	-0.745539	2.332090
H	-1.347561	1.486950	2.288561
H	-1.120485	3.681550	1.196813
H	-1.724107	3.939400	-0.438206
H	-0.164984	3.150477	-0.190808
H	-2.549950	1.980507	-1.798533
H	-3.598058	-0.273136	-1.755954
O	-3.641455	-1.890728	0.228426
H	-3.549232	-2.309730	1.093839
C	0.918207	-1.293156	0.619532
C	0.337801	-1.152667	-0.780495
O	1.369225	-0.827690	-1.744115
C	2.102807	0.327583	-1.440450
C	2.736696	0.256254	-0.060855
C	1.675102	-0.028078	0.987318
H	2.866634	0.397558	-2.219307
O	1.301033	1.507343	-1.423028
H	0.895022	1.587184	-2.296586
H	3.456272	-0.561537	-0.054378
O	3.458696	1.444447	0.261101
H	2.867590	2.172136	0.016413
H	0.972485	0.812217	1.031074
O	2.290270	-0.244215	2.257775
H	2.985919	0.427444	2.319255
H	0.084867	-1.427799	1.321698
O	1.799457	-2.408458	0.657305
H	2.295200	-2.296269	1.482668
H	-0.389055	-0.336875	-0.752175
C	-0.312234	-2.421607	-1.284751
H	-1.158091	-2.686027	-0.651863
H	0.412771	-3.231382	-1.280799
H	-0.676126	-2.267618	-2.298989

Y-5k (E_t = -956.001862)

C	2.706226	0.271146	-1.387104
C	3.122229	-0.082904	0.969172
C	2.330920	1.025361	1.265090
C	1.720916	1.783072	0.254138
C	1.918952	1.380170	-1.071577
C	3.304883	-0.466762	-0.362799
C	0.838214	2.957040	0.588117
H	2.841845	-0.022632	-2.422346
H	1.466369	1.948274	-1.876842

Y-5l (E_t = -956.007369)

C	-2.304042	-1.081742	1.064549
C	-1.928381	-0.967799	-1.322735
C	-2.394590	0.344966	-1.323992
C	-2.809456	0.973804	-0.141512
C	-2.770894	0.232890	1.045432
C	-1.883709	-1.683181	-0.123734
C	-3.339676	2.383406	-0.158032
H	-2.259623	-1.629815	1.999497
H	-3.081233	0.693707	1.976135

H	0.840060	3.685998	-0.222391
H	1.185537	3.460014	1.490331
H	-0.193696	2.643867	0.758657
H	2.200887	1.318385	2.301158
H	3.602749	-0.658970	1.749234
O	4.100925	-1.561216	-0.594679
H	4.124995	-1.724014	-1.546081
C	-0.459622	-1.100350	0.031621
C	-0.872572	-0.614195	1.414056
O	-2.309240	-0.549749	1.540805
C	-2.932355	0.254835	0.585208
C	-2.605711	-0.218960	-0.831023
C	-1.107401	-0.238835	-1.038703
H	-4.005827	0.157675	0.788253
O	-2.526288	1.608035	0.736064
H	-2.709325	2.024557	-0.120724
H	-2.997241	-1.227948	-0.975684
O	-3.132871	0.696511	-1.809959
H	-4.077345	0.516330	-1.905681
H	-0.723194	0.782172	-0.962900
O	-0.777337	-0.807936	-2.306496
H	-1.361061	-0.373409	-2.944364
H	0.628871	-1.012817	-0.054951
O	-0.881126	-2.451895	-0.128561
H	-0.743866	-2.640325	-1.068560
H	-0.459366	0.389122	1.545722
C	-0.395107	-1.529866	2.519068
H	-0.711226	-1.139298	3.484235
H	0.692437	-1.592201	2.497371
H	-0.811534	-2.523304	2.376597
H	-4.419760	2.399258	-0.312602
H	-2.884202	2.963504	-0.960267
H	-3.133268	2.890795	0.783827
H	-2.414183	0.896349	-2.257062
H	-1.604124	-1.453193	-2.234041
O	-1.374752	-2.961368	-0.176875
H	-1.432149	-3.348659	0.706440
C	1.362794	-0.875081	0.815564
C	1.782277	-1.225578	-0.605182
O	2.630292	-0.199889	-1.169983
C	2.062052	1.085205	-1.171871
C	1.639420	1.523381	0.221810
C	0.706933	0.493332	0.831870
H	2.841332	1.741388	-1.568296
O	0.883849	1.169623	-1.966390
H	1.141766	0.972248	-2.876436
H	2.530171	1.607300	0.843437
O	1.019046	2.809362	0.210736
H	0.364396	2.758865	-0.502523
H	-0.219751	0.463095	0.254525
O	0.440291	0.825410	2.196774
H	0.284064	1.781707	2.193822
H	0.634170	-1.626224	1.147745
O	2.508401	-0.873023	1.658321
H	2.217975	-0.403676	2.455260
H	0.867833	-1.299317	-1.202078
C	2.572336	-2.512561	-0.683612
H	1.958562	-3.340356	-0.330203
H	3.461945	-2.434028	-0.064559
H	2.864725	-2.706544	-1.713697

(vi) Optimized coordinates of *p*-OHTol : β-L-fucose complexes

Y-6a (E_t = -956.011636)

C	3.433303	-0.603782	-1.221412
C	2.258045	-0.512025	0.893334
C	3.146046	0.472690	1.329839
C	4.176356	0.943621	0.509202
C	4.306599	0.381768	-0.768232
C	2.412047	-1.058363	-0.384379
C	5.151912	1.979310	1.002144
H	3.533752	-1.035889	-2.208521
H	5.095930	0.729569	-1.425179
H	5.481434	2.625361	0.189056
H	4.701245	2.607878	1.769289
H	6.039300	1.514017	1.434347
H	3.021906	0.889935	2.323054
H	1.460717	-0.865884	1.534348

Y-6b (E_t = -956.007072)

C	2.508561	-1.378063	0.781113
C	2.294267	-0.821396	-1.562440
C	3.046814	0.333248	-1.347717
C	3.523182	0.666921	-0.072227
C	3.251112	-0.214351	0.982275
C	2.006496	-1.671645	-0.491651
C	4.359264	1.900549	0.145363
H	2.294719	-2.048105	1.605071
H	3.620540	0.013334	1.976149
H	4.219654	2.295984	1.150864
H	5.421561	1.685483	0.018478
H	4.094116	2.683567	-0.564398
H	3.254524	0.993511	-2.182779
H	1.904690	-1.067736	-2.541969

O	1.573820	-2.034177	-0.879857
H	0.892391	-2.241270	-0.209541
C	-3.053396	0.869639	0.745788
C	-2.305952	1.622739	-0.351857
O	-2.006288	0.681561	-1.396787
C	-1.041592	-0.282840	-0.981973
C	-1.669796	-1.117425	0.129563
C	-2.165209	-0.247875	1.275972
H	-0.144470	0.230913	-0.601510
O	-0.766608	-1.041828	-2.114623
H	0.131921	-1.396350	-1.999950
H	-2.513045	-1.653490	-0.319900
O	-0.713564	-2.058248	0.632226
H	-1.118870	-2.438815	1.426654
H	-1.297348	0.177419	1.789263
O	-2.840889	-1.063358	2.230211
H	-3.732829	-1.169997	1.861391
H	-3.340648	1.537130	1.561206
O	-4.263241	0.296826	0.239459
H	-4.052927	0.027602	-0.669438
H	-1.367758	2.015527	0.064791
C	-3.106105	2.743051	-0.979238
H	-3.324099	3.508331	-0.235311
H	-4.046460	2.360461	-1.368163
H	-2.539540	3.188309	-1.793418

O	1.215814	-2.772813	-0.723076
H	0.599272	-2.819110	0.029687
C	-0.427638	0.422317	0.536305
C	-0.906633	1.570768	-0.346099
O	-2.337834	1.719664	-0.304054
C	-3.021468	0.550574	-0.706883
C	-2.648389	-0.599805	0.215287
C	-1.161626	-0.852326	0.144435
H	-2.798040	0.286235	-1.748776
O	-4.401823	0.802692	-0.650183
H	-4.537618	1.294615	0.173126
H	-2.906377	-0.301296	1.238127
O	-3.297620	-1.810498	-0.157218
H	-4.241983	-1.604928	-0.206877
H	-0.890779	-1.143138	-0.876860
O	-0.794584	-1.908077	1.054313
H	-1.541981	-2.527858	1.027587
H	0.645421	0.300886	0.372823
O	-0.702115	0.742511	1.895528
H	-0.501172	-0.067129	2.387026
H	-0.607161	1.329453	-1.376689
C	-0.318190	2.900773	0.069189
H	0.769441	2.848586	0.026578
H	-0.622431	3.128241	1.087146
H	-0.665622	3.686193	-0.598487

Y-6c (E_t = -956.007948)

C	3.221441	-1.349269	1.128588
C	2.329392	-0.476051	-0.941845
C	3.307333	0.519976	-0.928415
C	4.251817	0.605360	0.100550
C	4.191190	-0.349630	1.124233
C	2.284324	-1.415630	0.092975
C	5.329794	1.656670	0.082229
H	3.172153	-2.083668	1.921984
H	4.909748	-0.307565	1.935432
H	5.000655	2.545701	-0.454913
H	5.601303	1.957313	1.093840
H	6.234514	1.291229	-0.406776
H	3.331383	1.243339	-1.736502
H	1.590878	-0.509099	-1.731672
O	1.355544	-2.421583	0.152678
H	0.727103	-2.329900	-0.583827
C	-2.396929	1.568596	0.509831
C	-0.918105	1.272120	0.274208
O	-0.759100	0.218290	-0.695423
C	-1.370030	-0.984928	-0.288100
C	-2.867759	-0.777803	-0.167236
C	-3.140226	0.289606	0.873087

Y-6d (E_t = -956.003238)

C	2.828558	0.475818	-1.245185
C	2.754634	-0.121019	1.097750
C	2.142788	-1.326674	0.761593
C	1.850180	-1.657388	-0.571414
C	2.205087	-0.734580	-1.562704
C	3.091424	0.788602	0.090416
C	1.150806	-2.947650	-0.910955
H	3.101166	1.171726	-2.031779
H	2.011152	-0.968972	-2.603673
H	1.534938	-3.766728	-0.303271
H	0.075933	-2.878828	-0.732193
H	1.304753	-3.207008	-1.958162
H	1.898531	-2.030767	1.549521
H	2.985181	0.127940	2.125572
O	3.678609	1.966141	0.485966
H	3.868535	2.493923	-0.300308
C	-0.932297	0.821840	1.473245
C	-0.372186	1.366626	0.167132
O	-1.447243	1.299898	-0.799551
C	-1.705605	-0.068227	-1.107652
C	-2.252507	-0.814167	0.099532
C	-1.353178	-0.641658	1.320239

H	-0.949770	-1.361477	0.651057
O	-1.059026	-1.961745	-1.264728
H	-1.199215	-1.526361	-2.120104
H	-3.241629	-0.426730	-1.136433
O	-3.538574	-1.955229	0.265322
H	-3.297446	-2.656917	-0.354790
H	-2.788136	-0.081449	1.844807
O	-4.527733	0.607517	0.926597
H	-4.993859	-0.240736	0.941411
H	-2.480566	2.276932	1.345702
O	-2.944910	2.118233	-0.678797
H	-3.904639	2.076777	-0.549430
H	-0.486611	0.933433	1.226993
C	-0.147031	2.459693	-0.256673
H	0.896311	2.183289	-0.391461
H	-0.209979	3.289961	0.445880
H	-0.573071	2.769822	-1.206972

H	-0.764946	-0.534570	-1.437269
O	-2.691284	-0.133369	-2.098430
H	-2.327100	0.268243	-2.897820
H	-3.239247	-0.386396	0.320837
O	-2.348854	-2.201829	-0.193686
H	-2.926831	-2.267098	-0.966948
H	-0.465720	-1.260554	1.175254
O	-1.987847	-1.091621	2.504975
H	-2.554396	-0.348719	2.765760
H	-0.198064	0.899302	2.277782
O	-2.072078	1.589857	1.883405
H	-2.535405	1.798160	1.055980
H	0.445633	0.722017	-0.165592
C	0.094012	2.802514	0.238193
H	-0.690213	3.437636	0.643921
H	0.355056	3.150999	-0.759649
H	0.974423	2.872240	0.875984

Y-6e (E_t = -956.003122)

C	2.778957	0.414517	-0.961005
C	3.258104	-0.751537	1.103784
C	2.739273	-1.924118	0.551553
C	2.234238	-1.956415	-0.754033
C	2.267400	-0.767458	-1.496398
C	3.275532	0.421498	0.344766
C	1.632753	-3.216201	-1.316535
H	2.819386	1.327619	-1.541012
H	1.898509	-0.767021	-2.516396
H	0.617521	-3.347658	-0.941555
H	1.598619	-3.179703	-2.404890
H	2.217445	-4.089752	-1.028550
H	2.730269	-2.828475	1.149418
H	3.647586	-0.751158	2.116383
O	3.760484	1.616668	0.823271
H	4.067335	1.481773	1.729265
C	-0.383327	0.041870	0.722346
C	-0.460759	1.486274	0.233637
O	-1.854424	1.855419	0.171007
C	-2.515641	1.125729	-0.850107
C	-2.546416	-0.341094	-0.462614
C	-1.140810	-0.871806	-0.236938
H	-1.965716	1.247591	-1.798682
O	-3.804031	1.662480	-0.935662
H	-4.336067	0.982494	-1.374258
H	-3.108627	-0.407329	0.477965
O	-3.222529	-1.045212	-1.498276
H	-3.134143	-1.982740	-1.274827
H	-0.620033	-0.919128	-1.196806
O	-1.211320	-2.208757	0.260034

Y-6f (E_t = -956.002293)

C	2.598369	-0.780648	0.974005
C	2.774304	0.301812	-1.184047
C	2.499497	1.530005	-0.580816
C	2.268733	1.629772	0.796996
C	2.334046	0.455249	1.560549
C	2.802022	-0.856933	-0.405372
C	2.019738	2.965011	1.448181
H	2.604661	-1.691787	1.556143
H	2.164795	0.504723	2.630583
H	1.550114	3.659547	0.752110
H	1.367349	2.862912	2.315052
H	2.951784	3.418775	1.789000
H	2.463900	2.422558	-1.195598
H	2.921609	0.240359	-2.256443
O	2.994375	-2.110712	-0.941541
H	2.975048	-2.028055	-1.904586
C	-2.610111	0.721571	0.324320
C	-1.683145	1.225573	-0.781125
O	-1.261828	0.081374	-1.547298
C	-0.417050	-0.742099	-0.752660
C	-1.247984	-1.372944	0.348623
C	-1.873299	-0.282865	1.207238
H	0.369090	-0.121698	-0.307010
O	0.117484	-1.695255	-1.628345
H	0.622577	-2.305044	-1.067616
H	-2.040376	-1.961938	-0.131688
O	-0.396067	-2.212858	1.117669
H	-0.917872	-2.466154	1.893045
H	-1.070440	0.216036	1.758715
O	-2.741038	-0.861521	2.178217

H	-1.336129	-2.094237	1.216788
H	0.650670	-0.287900	0.809349
O	-0.968467	-0.084222	2.027043
H	-1.722611	0.527203	2.023943
H	-0.025579	1.536839	-0.773216
C	0.224229	2.480753	1.144649
H	1.297054	2.296095	1.157768
H	-0.163493	2.391354	2.156942
H	0.041203	3.490498	0.783734

Y-6g (E_t = -956.001794)

C	3.115002	1.000357	-0.232187
C	2.312399	0.022038	1.829038
C	2.080528	-1.176155	1.155776
C	2.350450	-1.316139	-0.214916
C	2.871596	-0.207537	-0.890801
C	2.825291	1.118884	1.129520
C	2.047884	-2.601943	-0.937803
H	3.528379	1.843478	-0.776036
H	3.103943	-0.287809	-1.946804
H	2.255881	-3.462325	-0.301821
H	0.999892	-2.652256	-1.236994
H	2.657689	-2.693326	-1.835910
H	1.697290	-2.025430	1.711230
H	2.114623	0.123305	2.888318
O	3.038656	2.272037	1.844367
H	3.430865	2.928937	1.255283
C	-1.590159	1.499626	0.118678
C	-0.473687	0.869386	-0.710372
O	-0.993456	-0.346734	-1.292291
C	-1.253782	-1.304311	-0.278226
C	-2.391513	-0.812102	0.593265
C	-2.039407	0.532338	1.210783
H	-0.352180	-1.431435	0.337289
O	-1.584282	-2.488482	-0.951660
H	-2.037286	-3.038282	-0.294971
H	-3.271517	-0.693477	-0.052229
O	-2.628642	-1.805075	1.584558
H	-3.253385	-1.405917	2.207143
H	-1.232261	0.383462	1.934046
O	-3.157199	1.037325	1.935907
H	-3.716375	1.441389	1.252842
H	-1.259236	2.438045	0.569431
O	-2.721400	1.817718	-0.703030
H	-2.762043	1.103126	-1.358649
H	0.367276	0.624620	-0.053745
C	-0.003152	1.737539	-1.855194
H	0.740984	1.198937	-2.436397
H	0.445071	2.651119	-1.465599

H	-3.564377	-1.023526	1.690121
H	-2.983927	1.547896	0.933291
O	-3.761132	0.079110	-0.238015
H	-3.426596	-0.390439	-1.019079
H	-0.801441	1.692625	-0.320221
C	-2.344632	2.189462	-1.741226
H	-2.645805	3.093965	-1.213940
H	-3.229021	1.736040	-2.181794
H	-1.648352	2.454304	-2.533574

Y-6h (E_t = -956.004616)

C	2.736853	0.669194	1.033896
C	2.236150	0.662833	-1.333094
C	2.227157	-0.731811	-1.317428
C	2.462529	-1.452534	-0.137859
C	2.726317	-0.726188	1.029835
C	2.465300	1.365248	-0.146804
C	2.348594	-2.952447	-0.103793
H	2.924999	1.210643	1.954539
H	2.924837	-1.257003	1.954305
H	3.065197	-3.386171	0.593217
H	1.346822	-3.238905	0.218478
H	2.530232	-3.383598	-1.087612
H	2.042231	-1.268382	-2.241638
H	2.062435	1.219415	-2.245194
O	2.416241	2.737500	-0.213172
H	2.579774	3.090855	0.670788
C	-1.202604	1.376587	0.235355
C	-1.549808	1.112465	-1.227487
O	-2.392657	-0.046349	-1.373441
C	-1.798956	-1.217365	-0.851091
C	-1.561730	-1.042149	0.639243
C	-0.625843	0.120832	0.867886
H	-0.851943	-1.452862	-1.354648
O	-2.660939	-2.300044	-1.098493
H	-3.547508	-1.971611	-0.887688
H	-2.528141	-0.829475	1.112204
O	-0.949998	-2.201124	1.204971
H	-1.507921	-2.946555	0.939420
H	0.332934	-0.114684	0.404279
O	-0.457799	0.386742	2.261932
H	-0.284451	-0.473911	2.669522
H	-0.440875	2.168489	0.266035
O	-2.380524	1.772489	0.926296
H	-2.155952	1.673256	1.863908
H	-0.602667	0.924257	-1.751622
C	-2.292684	2.262864	-1.869839
H	-3.225911	2.429719	-1.339026
H	-2.503857	2.031503	-2.911641

H	-0.838045	2.006724	-2.498092

Y-6i (E_t = -956.004250)

C	-2.723767	1.082619	0.754311
C	-1.901997	0.964705	-1.517449
C	-2.192373	-0.397806	-1.542668
C	-2.736109	-1.051133	-0.426643
C	-3.006236	-0.284823	0.712379
C	-2.145452	1.703044	-0.354706
C	-2.933326	-2.542890	-0.432719
H	-2.924386	1.652352	1.655029
H	-3.430822	-0.760163	1.588960
H	-1.981901	-3.042894	-0.245652
H	-3.639794	-2.849805	0.337550
H	-3.310998	-2.887779	-1.395044
H	-1.991995	-0.963747	-2.445971
H	-1.487658	1.470802	-2.380190
O	-1.795301	3.031521	-0.377133
H	-1.942745	3.399283	0.503803
C	2.382073	0.373347	-0.827186
C	1.489418	1.401629	-0.137405
O	1.098357	0.964105	1.177554
C	0.405500	-0.270714	1.149369
C	1.310481	-1.351482	0.586950
C	1.708924	-0.992795	-0.826123
H	-0.509052	-0.204442	0.560239
O	0.007432	-0.583119	2.461985
H	0.786233	-0.408949	3.011904
H	2.213406	-1.404275	1.207252
O	0.641182	-2.611479	0.536530
H	0.267610	-2.741677	1.420271
H	0.799957	-0.960169	-1.440984
O	2.647369	-1.929716	-1.353609
H	2.307744	-2.804121	-1.115263
H	2.533633	0.693479	-1.867875
O	3.621628	0.297835	-0.137276
H	4.034428	-0.514905	-0.466961
H	0.585497	1.513916	-0.748622
C	2.165696	2.742098	0.044437
H	1.468998	3.441789	0.500964
H	2.480999	3.138061	-0.920192
H	3.038520	2.625273	0.681095

Y-6k (E_t = -956.003498)

C	2.467759	0.077325	-1.488083
C	2.952417	1.201019	0.597674

H	-1.690899	3.169613	-1.821549

Y-6j (E_t = -956.000996)

C	-2.317453	0.445930	1.644374
C	-2.040324	-1.656397	0.477728
C	-2.929090	-1.218300	-0.500817
C	-3.519024	0.052861	-0.439705
C	-3.211363	0.866392	0.656512
C	-1.735795	-0.820493	1.555062
C	-4.502665	0.499861	-1.488221
H	-2.085626	1.094970	2.482649
H	-3.660000	1.850388	0.735815
H	-5.508068	0.139180	-1.265452
H	-4.544754	1.586653	-1.547067
H	-4.224991	0.120132	-2.470739
H	-3.149131	-1.869369	-1.339080
H	-1.575711	-2.631581	0.418665
O	-0.806219	-1.281857	2.460666
H	-0.741397	-0.646982	3.186263
C	0.384346	0.469522	-0.798004
C	0.822376	1.413118	0.319722
O	2.257655	1.536213	0.260936
C	2.875369	0.302587	0.598051
C	2.548646	-0.720082	-0.474091
C	1.044519	-0.892567	-0.603225
H	2.484570	-0.045571	1.569221
O	4.247221	0.564682	0.663808
H	4.677302	-0.296535	0.557997
H	2.953177	-0.333473	-1.418916
O	3.194648	-1.936541	-0.117929
H	2.840997	-2.602957	-0.724549
H	0.670925	-1.363319	0.308286
O	0.749754	-1.780061	-1.680152
H	0.798676	-1.215248	-2.468391
H	-0.700155	0.360236	-0.815847
O	0.765959	0.990479	-2.079281
H	1.629557	1.408965	-1.933816
H	0.536642	0.963944	1.279929
C	0.248661	2.807015	0.198936
H	0.642993	3.441110	0.990079
H	0.510211	3.238033	-0.764449
H	-0.836583	2.761428	0.277086

Y-6l (E_t = -956.003054)

C	1.913369	1.276283	1.386927
C	2.239510	1.390294	-1.007907

C	2.833434	-0.016171	1.271890
C	2.534496	-1.200633	0.590094
C	2.357572	-1.129202	-0.798716
C	2.755116	1.250752	-0.784675
C	2.312390	-2.490291	1.330358
H	2.340977	0.130015	-2.561848
H	2.137938	-2.035224	-1.353198
H	1.250511	-2.612365	1.542061
H	2.644622	-3.344547	0.740522
H	2.854309	-2.499150	2.275322
H	2.968347	-0.039875	2.346626
H	3.186533	2.107398	1.146292
O	2.852162	2.410382	-1.515633
H	3.048456	3.135929	-0.909620
C	-2.313983	-0.331244	-1.247277
C	-1.132354	-1.259187	-0.980369
O	-0.840813	-1.352316	0.426610
C	-0.537046	-0.093061	1.000087
C	-1.738629	0.825501	0.864532
C	-2.070034	1.023497	-0.597298
H	0.347500	0.356094	0.539519
O	-0.214782	-0.298442	2.353997
H	-0.906484	-0.886729	2.693538
H	-2.592360	0.342389	1.355486
O	-1.475943	2.112017	1.416306
H	-1.133199	1.951509	2.306852
H	-1.218323	1.519931	-1.081234
O	-3.261408	1.791643	-0.755481
H	-3.179065	2.533586	-0.139324
H	-2.403948	-0.193405	-2.334050
O	-3.492807	-0.915984	-0.712971
H	-4.138588	-0.193133	-0.699061
H	-0.257253	-0.829431	-1.485390
C	-1.375737	-2.674107	-1.456327
H	-0.496950	-3.284795	-1.258408
H	-1.580406	-2.682097	-2.526382
H	-2.231203	-3.089691	-0.930719
C	3.012352	0.228059	-0.948448
C	3.236954	-0.436515	0.262322
C	2.684948	0.116673	1.427005
C	1.697839	1.920956	0.165302
C	4.094091	-1.672841	0.323710
H	1.487455	1.703530	2.285603
H	2.844359	-0.377200	2.378983
H	3.741140	-2.353988	1.097266
H	4.079145	-2.205900	-0.626098
H	5.132085	-1.423584	0.549804
H	3.431426	-0.172989	-1.864598
H	2.078687	1.890998	-1.956980
O	0.923951	3.056709	0.188415
H	0.816482	3.375942	-0.717326
C	-0.988114	-0.329983	-1.426687
C	-0.221888	-1.238947	-0.470130
O	-1.075317	-1.745574	0.575333
C	-1.650772	-0.708848	1.343684
C	-2.529546	0.149401	0.448397
C	-1.694199	0.770641	-0.647299
H	-0.884160	-0.091311	1.829170
O	-2.407887	-1.288931	2.376785
H	-2.891318	-2.016447	1.958071
H	-3.278952	-0.508992	-0.008130
O	-3.137790	1.214306	1.171054
H	-3.557738	0.805333	1.940978
H	-0.958234	1.438846	-0.186795
O	-2.512481	1.491118	-1.572396
H	-3.135531	1.994058	-1.028095
H	-0.261858	0.127840	-2.112986
O	-1.943197	-1.101753	-2.141648
H	-2.549364	-0.446579	-2.520027
H	0.569348	-0.636859	-0.012734
C	0.372636	-2.446971	-1.158184
H	0.920490	-3.048475	-0.435333
H	1.056862	-2.127226	-1.943421
H	-0.421633	-3.043209	-1.599837

Y-6m (E_t = -956.001998)

C	-2.047400	-1.487299	0.904974
C	-2.350676	0.841899	1.485839
C	-3.228867	0.986985	0.409262
C	-3.522665	-0.086052	-0.439299
C	-2.921211	-1.323388	-0.166860
C	-1.756461	-0.397962	1.729719
C	-4.428851	0.087993	-1.629118
H	-1.585526	-2.443181	1.113851
H	-3.134537	-2.172891	-0.805450
H	-5.022140	-0.809050	-1.803053

H	-5.114378	0.921262	-1.480124
H	-3.855532	0.286637	-2.535914
H	-3.689239	1.952398	0.231243
H	-2.136923	1.686098	2.133310
O	-0.841887	-0.603897	2.738724
H	-0.781506	0.203021	3.266855
C	0.389549	0.321814	-0.893450
C	0.836415	1.447732	0.034419
O	2.270721	1.530676	0.120981
C	2.853150	0.330569	0.589816
C	2.529801	-0.801217	-0.371544
C	1.032254	-0.986330	-0.458704
H	2.502923	0.077619	1.599304
O	4.241781	0.522532	0.690023
H	4.494709	0.977928	-0.126564
H	2.910766	-0.517996	-1.360255
O	3.083865	-2.036123	0.070321
H	4.020703	-1.862012	0.238431
H	0.659397	-1.268459	0.532663
O	0.691224	-1.975869	-1.429587
H	1.307569	-2.707634	-1.280900
H	-0.699870	0.227491	-0.823258
O	0.788270	0.636473	-2.223209
H	0.690520	-0.198291	-2.705954
H	0.440947	1.213481	1.032270
C	0.351876	2.805770	-0.421650
H	0.686850	3.573820	0.272728
H	-0.736571	2.810984	-0.466241
H	0.748561	3.015371	-1.411374

Tol : Saccharide binary complexes

(i) Optimized coordinates of Tol : α-D-glucose complexes

F-1a (E_t = -955.997388)				**F-1b** (E_t = -955.996248)			
C	3.878788	-0.581842	0.553548	C	-4.268115	-0.382013	-0.841233
C	2.766817	-0.763429	-1.583172	C	-3.267379	-1.573849	1.006455
C	2.327826	0.558401	-1.461024	C	-2.814668	-0.361507	1.536365
C	2.656087	1.329367	-0.336618	C	-3.076165	0.853641	0.888045
C	3.432863	0.736596	0.668920	C	-3.806488	0.822738	-0.308065
C	3.543574	-1.339058	-0.573232	C	-3.994244	-1.587637	-0.188596
C	2.146986	2.737639	-0.181982	C	-2.531409	2.150684	1.422790
H	4.481942	-1.018069	1.339662	H	-4.836088	-0.382087	-1.762921
H	3.701917	1.318187	1.543703	H	-4.026368	1.753512	-0.819138
H	2.921563	3.388230	0.223284	H	-2.334200	2.081682	2.491752
H	1.829082	3.146331	-1.140172	H	-1.598598	2.404145	0.916845
H	1.296796	2.759309	0.501160	H	-3.235896	2.965839	1.260366

H	1.735749	1.001850	-2.253958
H	2.512759	-1.336653	-2.466354
H	3.892015	-2.359608	-0.667539
C	-0.632949	0.524951	0.635401
C	-2.070344	0.843132	0.261379
O	-2.410894	0.083989	-0.920553
C	-2.359376	-1.314120	-0.748952
C	-0.949995	-1.745126	-0.339670
C	-0.516896	-0.964893	0.887101
H	-2.624014	-1.729014	-1.726346
O	-3.282275	-1.707821	0.239631
H	-2.981984	-2.584108	0.528973
H	-0.260229	-1.531558	-1.166751
O	-0.994541	-3.140997	-0.055957
H	-0.222642	-3.313286	0.504046
H	-1.170518	-1.227733	1.721056
O	0.795543	-1.347570	1.314107
H	1.420228	-1.112629	0.608276
H	0.010458	0.791878	-0.213572
O	-0.269186	1.265302	1.794051
H	0.489822	0.790793	2.167094
H	-2.741812	0.575318	1.080449
C	-2.289526	2.288426	-0.131662
H	-1.591380	2.538386	-0.941413
H	-2.076427	2.932896	0.719380
O	-3.636556	2.511175	-0.512608
H	-3.843191	1.796595	-1.130558

F-1c (E_t = -955.994982)

C	-2.274586	-2.511378	0.655721
C	-2.527701	-0.208785	1.338820
C	-2.754610	0.155041	0.009485
C	-2.732672	-0.799370	-1.017143
C	-2.494452	-2.137801	-0.673495
C	-2.279181	-1.543788	1.665245
C	-2.880528	-0.386148	-2.455952
H	-2.121771	-3.555182	0.905751
H	-2.497210	-2.893869	-1.451387
H	-3.306115	-1.190783	-3.054615
H	-3.526910	0.485631	-2.549682
H	-1.901359	-0.133045	-2.864578
H	-2.949445	1.193113	-0.236304
H	-2.542067	0.546394	2.114419
H	-2.116017	-1.831788	2.696227
C	1.019860	1.486405	-0.903338
C	1.596353	1.768025	0.474664
O	1.026882	0.851843	1.438187
C	1.296936	-0.518507	1.144466
C	0.680518	-0.858856	-0.205547

H	-2.264484	-0.357688	2.470800
H	-3.063443	-2.500612	1.528532
H	-4.354053	-2.523440	-0.596739
C	2.055461	1.183207	-0.088514
C	2.919030	-0.061212	0.036710
O	2.135243	-1.118776	0.634384
C	1.015633	-1.507641	-0.126949
C	0.082236	-0.315589	-0.343554
C	0.844911	0.851170	-0.933189
H	0.524243	-2.281411	0.474364
O	1.431972	-2.022663	-1.370937
H	0.660687	-1.930232	-1.952483
H	-0.346114	-0.013642	0.614991
O	-0.944197	-0.643975	-1.286472
H	-1.712658	-0.973329	-0.795995
H	1.192666	0.576369	-1.935618
O	0.024702	2.019317	-0.998889
H	-0.757217	1.753140	-1.504755
H	1.711744	1.481870	0.912394
O	2.835010	2.206747	-0.689881
H	2.209702	2.907536	-0.922580
H	3.264682	-0.373586	-0.951337
C	4.105230	0.110089	0.961429
H	3.738791	0.433527	1.943895
H	4.764666	0.880598	0.567315
O	4.852503	-1.092237	1.050793
H	4.195889	-1.781976	1.218168

F-1d (E_t = -955.999704)

C	-2.740006	-1.695454	-0.830875
C	-3.459225	0.601729	-0.667138
C	-3.058343	0.627319	0.669166
C	-2.481477	-0.499209	1.274239
C	-2.329556	-1.659581	0.505549
C	-3.297457	-0.561256	-1.425054
C	-1.977423	-0.429027	2.690725
H	-2.643665	-2.614545	-1.398371
H	-1.889886	-2.542356	0.955362
H	-2.682873	0.101203	3.330341
H	-1.829707	-1.426281	3.103590
H	-1.026562	0.105003	2.722312
H	-3.189419	1.532406	1.252076
H	-3.904108	1.482505	-1.113485
H	-3.618488	-0.587500	-2.458792
C	1.482473	1.036184	0.648406
C	0.358310	0.993386	-0.373025
O	0.866831	0.483450	-1.630012
C	1.428737	-0.810451	-1.549655
C	2.576101	-0.860448	-0.549102

C	1.269544	0.039329	-1.272409
H	0.804233	-1.070255	1.951095
O	2.670926	-0.794371	1.083514
H	3.039858	-0.601337	1.955791
H	-0.383494	-0.642698	-0.129893
O	0.888972	-2.210953	-0.607044
H	0.106371	-2.696819	-0.314963
H	2.348217	-0.134795	-1.347438
O	0.640622	-0.190208	-2.535338
H	0.709998	-1.146505	-2.673533
H	-0.069151	1.639398	-0.871005
O	1.635769	2.376205	-1.824248
H	1.395303	2.046364	-2.701597
H	2.682068	1.644674	0.444297
C	1.255052	3.146387	1.000467
H	0.164855	3.268879	0.979649
H	1.700940	3.902661	0.358044
O	1.775706	3.331111	2.308791
H	1.467322	2.560509	2.804108

F-1e (E_t = -955.995676)

C	2.689220	-1.317305	0.393706
C	3.250597	0.633427	-0.910604
C	2.904550	1.449471	0.167500
C	2.431555	0.899166	1.369395
C	2.329095	-0.493745	1.464302
C	3.143016	-0.755097	-0.800490
C	2.021561	1.795662	2.507418
H	2.610853	-2.393477	0.491753
H	1.978387	-0.938397	2.389250
H	1.840438	1.219032	3.413499
H	2.797407	2.530356	2.723538
H	1.110694	2.336465	2.250856
H	3.002838	2.526346	0.081168
H	3.609181	1.079000	-1.830176
H	3.423628	-1.391101	-1.630738
C	-1.934033	0.395133	0.458529
C	-1.539492	0.960531	-0.901172
O	-0.356863	0.293567	-1.376862
C	-0.475607	-1.103941	-1.512367
C	-0.838083	-1.747741	-0.178371
C	-2.093715	-1.108880	0.370633
H	0.511003	-1.435811	-1.845126
O	-1.470999	-1.395442	-2.471592
H	-1.716263	-2.318813	-2.301137
H	-0.018939	-1.586259	0.527233
O	-1.041471	-3.137895	-0.433702
H	-1.467291	-3.491327	0.360448
H	-2.920697	-1.329698	-0.320086

F-1f (E_t = -955.998168)

C	2.257129	-1.731246	0.627490
C	3.247149	-0.377339	-1.106391
C	3.199724	0.732793	-0.261590
C	2.664514	0.634432	1.032982
C	2.193694	-0.611978	1.462446
C	2.774705	-1.614743	-0.663150
C	2.582271	1.851230	1.916455
H	1.901775	-2.690262	0.985077
H	1.789001	-0.711112	2.463754
H	1.850532	2.556106	1.521356
H	2.289369	1.579387	2.929686
H	3.543817	2.362245	1.968132
H	3.584442	1.687383	-0.604908
H	3.658255	-0.278318	-2.103266
H	2.822141	-2.480134	-1.312040
C	-1.535919	0.951632	0.405129
C	-1.266263	1.012350	-1.093620
O	-0.379999	-0.072538	-1.428919
C	-0.932127	-1.348375	-1.186968
C	-1.327679	-1.507341	0.280467
C	-2.214717	-0.361240	0.718305
H	-0.134187	-2.049522	-1.446536
O	-2.064634	-1.530136	-2.008572
H	-2.583433	-2.222525	-1.568995
H	-0.422246	-1.497413	0.893145
O	-2.014178	-2.754535	0.390924
H	-2.440594	-2.740179	1.259923
H	-3.160297	-0.406410	0.163560

O	-2.342624	-1.695982	1.644309
H	-3.020021	-1.142016	2.058505
H	-1.154921	0.641859	1.180763
O	-3.134124	0.986452	0.970188
H	-3.819761	0.849509	0.300126
H	-2.361142	0.817135	-1.614587
C	-1.151297	2.425318	-0.834087
H	-1.976290	3.003509	-0.420202
H	-0.942970	2.778511	-1.849496
O	-0.034048	2.614429	0.020354
H	0.636939	1.982419	-0.281232

O	-2.447365	-0.534262	2.113803
H	-2.929690	0.257366	2.391752
H	-0.579915	0.994588	0.935060
O	-2.414182	1.990695	0.844981
H	-1.869038	2.775564	0.984261
H	-2.206558	0.918127	-1.645341
C	-0.547258	2.275242	-1.514568
H	-1.203377	3.134086	-1.372180
H	-0.303599	2.201671	-2.578756
O	0.614111	2.504067	-0.725168
H	1.143016	1.693383	-0.789269

F-1g (E_t = -955.992524)

C	-1.733685	-2.150611	0.860844
C	-2.160926	-0.088473	2.041836
C	-2.874404	0.391263	0.940368
C	-3.034653	-0.391943	-0.210652
C	-2.452806	-1.665953	-0.233515
C	-1.583470	-1.360413	2.002793
C	-3.763528	0.140947	-1.415079
H	-1.285742	-3.134997	0.814974
H	-2.568441	-2.289147	-1.113425
H	-3.055321	0.564806	-2.127656
H	-4.316972	-0.650548	-1.919681
H	-4.470175	0.920656	-1.133299
H	-3.320415	1.379272	0.979011
H	-2.060090	0.526633	2.927815
H	-1.033913	-1.735368	2.857238
C	0.362040	0.392300	-0.638602
C	1.095089	1.535075	0.053598
O	1.805647	1.006617	1.185868
C	2.735973	-0.005086	0.854071
C	2.089315	-1.201787	0.160788
C	1.310829	-0.721461	-1.055264
H	3.173440	-0.307222	1.808201
O	3.732752	0.458567	-0.040863
H	4.257185	1.122128	0.426140
H	1.379636	-1.665340	0.848252
O	3.065368	-2.181037	-0.142314
H	3.758820	-1.711077	-0.626968
H	2.023739	-0.318540	-1.792517
O	0.588314	-1.813237	-1.601191
H	-0.109888	-1.408008	-2.136298
H	-0.378509	-0.017649	0.045863
O	-0.400325	0.832804	-1.783757
H	0.223684	1.273954	-2.381349
H	1.794690	2.008089	-0.647169
C	0.155351	2.591146	0.619003
H	0.742655	3.335767	1.155122

F-1h (E_t = -955.994611)

C	2.787937	1.956937	0.682125
C	2.347082	-0.330383	1.318255
C	2.469513	-0.718804	-0.017828
C	2.740736	0.219319	-1.022903
C	2.900304	1.561472	-0.652049
C	2.501388	1.011830	1.670575
C	2.780193	-0.188575	-2.470782
H	2.919007	2.998394	0.948609
H	3.118375	2.300500	-1.415112
H	3.071571	-1.232884	-2.578289
H	1.792551	-0.059781	-2.915233
H	3.486992	0.421181	-3.032704
H	2.366823	-1.765788	-0.283370
H	2.128836	-1.070148	2.077718
H	2.416134	1.315895	2.706342
C	-1.099158	-1.145789	-0.821708
C	-1.621593	-1.421927	0.580800
O	-0.975991	-0.539593	1.517838
C	-1.175994	0.833957	1.265112
C	-0.657914	1.205580	-0.120177
C	-1.300641	0.317185	-1.163095
H	-0.597558	1.348518	2.037460
O	-2.551924	1.132466	1.365848
H	-2.659241	1.972451	0.891741
H	0.422820	1.065752	-0.146536
O	-1.011812	2.573636	-0.330297
H	-0.819691	2.756154	-1.260844
H	-2.380401	0.524606	-1.175109
O	-0.723092	0.649376	-2.425012
H	-1.027723	-0.037555	-3.036300
H	-0.032297	-1.372449	-0.865526
O	-1.713207	-1.976725	-1.814000
H	-2.670627	-1.871483	-1.712691
H	-2.705509	-1.258625	0.616885
C	-1.303615	-2.813447	1.086986
H	-0.214843	-2.948175	1.059991

H	-0.515400	2.103439	1.332847
O	-0.552675	3.274364	-0.404930
H	-1.022378	2.588489	-0.900751

H	-1.757431	-3.558135	0.435200
O	-1.826896	-3.007816	2.389494
H	-1.542436	-2.231327	2.891185

F-1i (E_t = -955.994288)

C	-3.382625	0.667490	-0.861501
C	-1.750156	-0.716243	-1.980350
C	-1.752546	-1.588862	-0.889682
C	-2.555656	-1.344345	0.232355
C	-3.371613	-0.204832	0.228443
C	-2.563433	0.418529	-1.965727
C	-2.485090	-2.235720	1.442684
H	-4.023585	1.540299	-0.847009
H	-4.005841	-0.003342	1.084689
H	-3.448271	-2.289576	1.949141
H	-2.187586	-3.247822	1.170108
H	-1.752962	-1.840196	2.147841
H	-1.133237	-2.479509	-0.914489
H	-1.112858	-0.917082	-2.831771
H	-2.570629	1.093381	-2.812457
C	1.420112	-0.569045	0.658612
C	2.125688	-0.037317	-0.586589
O	1.184499	0.706005	-1.371640
C	0.619294	1.813210	-0.707627
C	-0.126315	1.373155	0.547944
C	0.800235	0.572355	1.437029
H	-0.077426	2.247161	-1.429973
O	1.642050	2.725618	-0.365079
H	1.254261	3.286176	0.325567
H	-0.973583	0.750040	0.261256
O	-0.556029	2.566340	1.205332
H	-0.898239	2.286121	2.065745
H	1.604540	1.235211	1.786142
O	0.032036	0.103563	2.544706
H	0.604114	-0.521803	3.013102
H	0.628595	-1.257438	0.355910
O	2.287311	-1.336773	1.516576
H	3.069463	-0.787828	1.680829
H	2.964443	0.603864	-0.290529
C	2.640117	-1.144889	-1.494474
H	3.050979	-0.695939	-2.397113
H	1.794137	-1.778842	-1.786716
O	3.684511	-1.888098	-0.883133
H	3.310577	-2.257034	-0.071094

F-1j (E_t = -955.991683)

C	-2.636930	2.136255	-0.614288
C	-2.468231	-0.206942	-1.172872
C	-2.557243	-0.530572	0.182943
C	-2.678894	0.467906	1.158724
C	-2.719465	1.804478	0.739089
C	-2.502670	1.129941	-1.574145
C	-2.686770	0.121738	2.622979
H	-2.671287	3.175164	-0.917760
H	-2.820358	2.590263	1.479635
H	-1.671787	0.179158	3.017505
H	-3.310352	0.814099	3.187791
H	-3.063896	-0.887109	2.787513
H	-2.545278	-1.571715	0.488116
H	-2.369795	-0.993580	-1.910186
H	-2.442529	1.384728	-2.624952
C	1.057365	-1.171046	0.835944
C	1.465149	-1.531651	-0.586297
O	0.856678	-0.620477	-1.521936
C	1.209963	0.746145	-1.297467
C	0.723112	1.169702	0.077272
C	1.362264	0.286140	1.128547
H	0.680556	1.298235	-2.077420
O	2.598103	0.944574	-1.358963
H	2.870793	0.776912	-2.270647
H	-0.354181	0.995651	0.097068
O	1.026326	2.539328	0.277534
H	0.760705	2.724679	1.188899
H	2.448893	0.444618	1.111316
O	0.824910	0.675580	2.393651
H	1.120756	-0.000758	3.020143
H	-0.017925	-1.322488	0.952221
O	1.672610	-2.023293	1.809792
H	2.629306	-1.946046	1.681079
H	2.556586	-1.476083	-0.682858
C	0.991707	-2.903964	-1.019083
H	-0.098364	-2.945690	-0.903208
H	1.434753	-3.667065	-0.381882
O	1.388430	-3.176816	-2.353727
H	1.081054	-2.413164	-2.860775

F-1k (E_t = -955.997955)

F-1l (E_t = -955.996334)

C	2.946639	1.253561	0.822171
C	2.208170	1.454137	-1.467657
C	2.323900	0.069330	-1.621781
C	2.753688	-0.739468	-0.563197
C	3.060062	-0.127109	0.661151
C	2.519126	2.049813	-0.244331
C	2.861279	-2.232782	-0.711672
H	3.191225	1.709497	1.773563
H	3.391391	-0.741838	1.490701
H	2.744969	-2.535681	-1.751608
H	3.828634	-2.592851	-0.360834
H	2.086750	-2.718477	-0.119512
H	2.090844	-0.385824	-2.578304
H	1.881532	2.064117	-2.301068
H	2.435369	3.122507	-0.123514
C	-0.425329	0.292464	0.954828
C	-1.573122	1.096410	0.369016
O	-1.859873	0.611336	-0.966655
C	-2.230930	-0.750158	-1.022174
C	-1.158693	-1.645076	-0.412911
C	-0.822670	-1.168119	0.990088
H	-2.367133	-0.962937	-2.085591
O	-3.411658	-1.030860	-0.291573
H	-4.137757	-0.545532	-0.704836
H	-0.257075	-1.577889	-1.024726
O	-1.553722	-3.014068	-0.405996
H	-2.469400	-3.008285	-0.088008
H	-1.706442	-1.274291	1.632097
O	0.268358	-1.914909	1.527942
H	0.012561	-2.844115	1.431247
H	0.449655	0.403325	0.308339
O	-0.163439	0.792848	2.260010
H	0.517485	0.208510	2.621959
H	-2.463891	0.988913	0.994679
C	-1.253911	2.565019	0.188198
H	-0.340591	2.651250	-0.410080
H	-1.075975	3.017766	1.161194
O	-2.345447	3.250665	-0.411041
H	-2.535160	2.753605	-1.217569

C	-3.825028	0.615525	-1.147867
C	-3.896103	-0.253264	1.102272
C	-2.986824	-1.249222	0.742677
C	-2.478451	-1.326223	-0.562512
C	-2.913830	-0.383462	-1.501336
C	-4.318281	0.684544	0.155417
C	-1.512053	-2.417721	-0.937178
H	-4.147383	1.336711	-1.888699
H	-2.532765	-0.429019	-2.515531
H	-1.012548	-2.192378	-1.879084
H	-0.754380	-2.524915	-0.162653
H	-2.024452	-3.374474	-1.049854
H	-2.665502	-1.978867	1.477869
H	-4.280232	-0.211919	2.114351
H	-5.022311	1.458876	0.432107
C	0.973131	0.081518	1.089108
C	0.416770	0.789244	-0.142656
O	1.463767	1.610236	-0.704007
C	2.589978	0.883916	-1.141757
C	3.214227	0.110452	0.017100
C	2.165999	-0.753750	0.684611
H	3.284116	1.639348	-1.521539
O	2.204530	-0.011095	-2.161600
H	2.902936	-0.684819	-2.179009
H	3.607548	0.820273	0.753157
O	4.256242	-0.692983	-0.532617
H	4.488039	-1.328916	0.159682
H	1.824881	-1.508658	-0.034569
O	2.798838	-1.376525	1.799007
H	2.094650	-1.846016	2.267912
H	1.283096	0.835964	1.818612
O	0.042534	-0.835778	1.670939
H	-0.678469	-0.321318	2.057634
H	0.079241	0.052392	-0.875153
C	-0.703818	1.757324	0.177086
H	-1.564315	1.223562	0.577050
H	-1.016352	2.244303	-0.751553
O	-0.299343	2.706133	1.158055
H	0.488914	3.128283	0.789371

F-1m (E_t = -955.990747)

C	2.348959	0.713837	1.593622
C	3.205666	0.761846	-0.660353
C	3.020308	-0.618965	-0.755884
C	2.497851	-1.353753	0.316564
C	2.165116	-0.665939	1.491811
C	2.866402	1.435011	0.514898
C	2.266017	-2.838096	0.199004

F-1n (E_t = -955.995796)

C	-2.785158	-0.661618	-1.108730
C	-3.196203	-0.128163	1.209582
C	-2.652896	1.140813	1.010042
C	-2.167845	1.529410	-0.247658
C	-2.238495	0.610136	-1.300002
C	-3.268509	-1.033182	0.145926
C	-1.599575	2.908936	-0.447703

H	2.103420	1.223349	2.517871
H	1.777924	-1.221063	2.339754
H	2.959774	-3.284905	-0.512571
H	2.407868	-3.330427	1.160874
H	1.252019	-3.061249	-0.139712
H	3.301587	-1.137087	-1.666596
H	3.625728	1.308128	-1.496619
H	3.010581	2.505410	0.592091
C	-1.860567	0.674449	0.823682
C	-1.157317	1.422898	-0.304094
O	-0.072572	0.624367	-0.814152
C	-0.482790	-0.642714	-1.320411
C	-1.088970	-1.447147	-0.183763
C	-2.290397	-0.703487	0.362354
H	0.440691	-1.102144	-1.678147
O	-1.442591	-0.525582	-2.337301
H	-1.013450	-0.084873	-3.082556
H	-0.332176	-1.489307	0.608330
O	-1.421410	-2.745068	-0.641738
H	-1.975177	-3.123893	0.056182
H	-3.045833	-0.602033	-0.423664
O	-2.790250	-1.480740	1.449082
H	-3.540101	-0.982083	1.801584
H	-1.159246	0.544096	1.657777
O	-3.050050	1.345903	1.254997
H	-2.792264	2.044983	1.867644
H	-1.874369	1.634703	-1.102251
C	-0.487628	2.705468	0.161635
H	0.093366	2.483122	1.065491
H	-1.243647	3.452826	0.404973
O	0.334029	3.255350	-0.852143
H	0.897270	2.515885	-1.124710

F-1o (E_t = -955.992259)

C	1.432890	-2.431325	-0.018650
C	2.702610	-1.259029	1.662866
C	3.257935	-0.445676	0.670060
C	2.905182	-0.606620	-0.674659
C	1.985797	-1.613277	-1.003546
C	1.783708	-2.251359	1.321806
C	3.461524	0.293395	-1.744309
H	0.725818	-3.204233	-0.292549
H	1.710136	-1.759669	-2.042493
H	2.689206	0.983799	-2.082150
H	4.307050	0.870980	-1.371967
H	3.800573	-0.282905	-2.605299
H	3.982132	0.315094	0.941556
H	2.989792	-1.118521	2.697890
H	1.337969	-2.872100	2.087461
H	-2.821977	-1.358985	-1.935802
H	-1.857424	0.886187	-2.276203
H	-1.212918	3.030588	-1.458929
H	-2.359476	3.674532	-0.285366
H	-0.786684	3.087901	0.255505
H	-2.614562	1.846210	1.833916
H	-3.572654	-0.407869	2.186092
H	-3.697615	-2.015984	0.296134
C	1.235005	-0.930657	-0.835888
C	0.415520	-1.204271	0.412807
O	1.243216	-0.902460	1.560491
C	1.654031	0.443731	1.618283
C	2.404504	0.879035	0.362877
C	1.594723	0.534679	-0.877363
H	2.293917	0.506665	2.502152
O	0.561443	1.348083	1.720406
H	0.023960	1.069191	2.474187
H	3.351435	0.338195	0.314787
O	2.731142	2.265740	0.389779
H	1.928054	2.707865	0.703118
H	0.671856	1.126875	-0.888330
O	2.353402	0.761584	-2.062644
H	2.708030	1.658315	-1.979055
H	2.160799	-1.513070	-0.760842
O	0.479983	-1.335926	-1.976604
H	0.956053	-0.970270	-2.737028
H	-0.471611	-0.567213	0.426146
C	-0.014502	-2.659840	0.498976
H	-0.939584	-2.768658	-0.071757
H	-0.221609	-2.900259	1.541485
O	0.979445	-3.572145	0.050247
H	0.986823	-3.486944	-0.912682

F-1p (E_t = -955.995892)

C	4.088853	-0.086849	0.585470
C	3.079881	0.888969	-1.377192
C	2.341503	-0.279435	-1.574923
C	2.470419	-1.369907	-0.704824
C	3.347382	-1.252090	0.382454
C	3.959382	0.988357	-0.296980
C	1.654921	-2.620599	-0.908046
H	4.768885	-0.020313	1.425732
H	3.459927	-2.086260	1.066113
H	1.461266	-2.786695	-1.967658
H	2.181537	-3.492935	-0.522057
H	0.692178	-2.560095	-0.396969
H	1.658639	-0.343842	-2.413903
H	2.973145	1.714303	-2.070655
H	4.541487	1.889115	-0.147220

C	-0.721675	1.321968	-0.599666
C	-0.247115	0.870147	0.776044
O	-1.421591	0.626117	1.575271
C	-2.202947	-0.440158	1.087434
C	-2.644105	-0.192371	-0.357905
C	-1.459743	0.168667	-1.233276
H	-3.073491	-0.473925	1.749231
O	-1.469863	-1.645479	1.158575
H	-1.880459	-2.224659	0.496630
H	-3.348944	0.646131	-0.375477
O	-3.267521	-1.393146	-0.813746
H	-3.359376	-1.290662	-1.771960
H	-0.779504	-0.689563	-1.295706
O	-1.984953	0.488957	-2.519293
H	-1.243440	0.871258	-3.009666
H	-1.410593	2.159985	-0.465193
O	0.350284	1.695757	-1.468667
H	0.613686	2.577780	-1.168333
H	0.336911	-0.048699	0.693613
C	0.598113	1.919872	1.461975
H	0.546171	1.755817	2.541139
H	1.634179	1.789004	1.137697
O	0.113596	3.217327	1.094691
H	0.562725	3.863843	1.651372

C	-1.060023	1.234377	-0.132624
C	-0.312362	0.316753	0.828419
O	-1.270235	-0.230904	1.761040
C	-2.257772	-1.032525	1.155749
C	-3.044175	-0.234385	0.117573
C	-2.098191	0.418583	-0.868029
H	-2.909550	-1.348604	1.975270
O	-1.649579	-2.148729	0.538040
H	-2.291366	-2.446908	-0.126774
H	-3.614963	0.550126	0.626619
O	-3.910456	-1.154161	-0.543923
H	-4.235901	-0.688625	-1.328031
H	-1.577573	-0.366130	-1.431593
O	-2.899429	1.210131	-1.739935
H	-2.272405	1.702182	-2.288798
H	-1.554343	2.023186	0.442540
O	-0.213799	1.791756	-1.140336
H	0.316623	2.481969	-0.721498
H	0.175094	-0.482785	0.270027
C	0.711167	1.037258	1.677845
H	1.512681	1.417939	1.046304
H	1.149762	0.320290	2.378076
O	0.136251	2.151612	2.353687
H	-0.588613	1.783895	2.877592

F-1q (E_t = -955.996371)

C	2.240396	-2.005943	-0.334603
C	2.986944	-0.098818	-1.611093
C	3.049212	0.658238	-0.438455
C	2.706516	0.097015	0.797928
C	2.301612	-1.243922	0.832944
C	2.585913	-1.434758	-1.562039
C	2.819404	0.893178	2.071728
H	1.936347	-3.044858	-0.284842
H	2.042191	-1.696912	1.784179
H	1.938417	0.758906	2.699887
H	3.688237	0.580014	2.652813
H	2.924803	1.956666	1.861907
H	3.358105	1.696373	-0.485933
H	3.266814	0.350367	-2.556762
H	2.550404	-2.027428	-2.467968
C	-1.441297	0.888234	1.071154
C	-0.964598	1.322372	-0.304152
O	-0.257584	0.228134	-0.928161
C	-1.024071	-0.944107	-1.100289
C	-1.559862	-1.452764	0.230586
C	-2.313901	-0.341299	0.940906
H	-0.335731	-1.660837	-1.551910
O	-2.167867	-0.742103	-1.913159

F-1r (E_t = -955.995609)

C	1.830560	-1.980119	-0.668083
C	2.001122	-1.524000	1.696664
C	2.898796	-0.490586	1.427971
C	3.273613	-0.183759	0.111658
C	2.726265	-0.940877	-0.930669
C	1.469835	-2.277526	0.646748
C	4.282860	0.899874	-0.165368
H	1.415828	-2.550927	-1.489699
H	2.992587	-0.710090	-1.955756
H	4.166826	1.732544	0.527976
H	5.301545	0.522916	-0.060905
H	4.176382	1.286390	-1.178605
H	3.308950	0.090482	2.246884
H	1.704675	-1.732329	2.716321
H	0.772726	-3.079479	0.853941
C	-0.923685	0.761812	-1.164743
C	-0.160817	1.001170	0.132850
O	-1.133159	1.283302	1.165594
C	-2.008003	0.209948	1.432716
C	-2.770104	-0.199205	0.171938
C	-1.808779	-0.447442	-0.971950
H	-2.697789	0.592105	2.191361
O	-1.274406	-0.889683	1.923969

H	-1.860527	-0.505117	-2.798040
H	-0.714180	-1.756946	0.849453
O	-2.386726	-2.601765	0.068098
H	-2.966913	-2.387780	-0.678286
H	-3.200991	-0.075215	0.352006
O	-2.687199	-0.736809	2.258215
H	-3.134234	-1.589374	2.157696
H	-0.562681	0.619176	1.675471
O	-2.152261	1.971924	1.652801
H	-2.586548	1.604313	2.435758
H	-1.821495	1.607073	-0.921285
C	0.042958	2.456372	-0.246845
H	0.800621	2.207313	0.503690
H	-0.458608	3.372784	0.057699
O	0.630965	2.685571	-1.517542
H	0.982573	1.822062	-1.777763
H	-1.831567	-1.662530	1.737456
H	-3.448287	0.612139	-0.115521
O	-3.496494	-1.384766	0.491546
H	-3.793046	-1.744485	-0.357047
H	-1.167616	-1.302018	-0.723072
O	-2.604753	-0.733195	-2.118803
H	-1.981256	-0.765447	-2.858284
H	-1.543875	1.637787	-1.377511
O	-0.064987	0.470637	-2.271456
H	0.240034	1.318482	-2.619049
H	0.424530	0.119309	0.393190
C	0.733108	2.218755	0.081512
H	1.513432	2.064692	-0.662921
H	1.213879	2.343669	1.056927
O	0.009121	3.382975	-0.303751
H	-0.715959	3.448460	0.333156

F-1s (E_t = -955.990530)

C	-1.674274	1.415502	-1.552311
C	-1.972927	2.131491	0.734128
C	-2.908292	1.114449	0.925244
C	-3.240534	0.234707	-0.114995
C	-2.607961	0.396279	-1.353214
C	-1.359843	2.289847	-0.511082
C	-4.294464	-0.823825	0.082485
H	-1.193206	1.520648	-2.516786
H	-2.837556	-0.285094	-2.164368
H	-5.292985	-0.422138	-0.097549
H	-4.275735	-1.212837	1.100459
H	-4.146796	-1.658208	-0.602850
H	-3.382002	0.996451	1.893784
H	-1.710913	2.786877	1.554253
H	-0.634853	3.079718	-0.662189
C	1.056889	-1.188895	-0.629906
C	0.252470	-0.904271	0.632952
O	1.191019	-0.701840	1.708071
C	1.997251	0.438131	1.520914
C	2.784377	0.352215	0.210770
C	1.862588	0.045711	-0.952683
H	2.680428	0.441352	2.375443
O	1.193635	1.600542	1.514692
H	1.715793	2.259199	1.029230
H	3.518642	-0.456993	0.289362
O	3.430228	1.612874	0.029861
H	3.749565	1.611776	-0.884009
H	1.171095	0.884444	-1.096166
O	2.691819	-0.123336	-2.100151
H	2.106285	-0.474959	-2.785834
H	1.738283	-2.018322	-0.422127

F-1t (E_t = -955.993839)

C	2.587160	1.312553	1.717850
C	2.726639	1.735973	-0.655262
C	3.517682	0.596544	-0.806794
C	3.843528	-0.208084	0.292334
C	3.373097	0.170012	1.556605
C	2.251630	2.092994	0.608735
C	4.587764	-1.502708	0.103699
H	2.235033	1.590468	2.703817
H	3.622712	-0.437178	2.419813
H	5.274610	-1.443850	-0.739901
H	5.162218	-1.761477	0.992635
H	3.883322	-2.313545	-0.091592
H	3.876494	0.319831	-1.791987
H	2.470500	2.333069	-1.520778
H	1.641485	2.979435	0.731068
C	-0.884947	0.586103	-0.686623
C	-0.715618	-0.921834	-0.606080
O	-1.235856	-1.393745	0.661439
C	-2.604720	-1.113896	0.867630
C	-2.884320	0.381761	0.786168
C	-2.347466	0.937926	-0.521741
H	-2.826626	-1.504327	1.864012
O	-3.442778	-1.704404	-0.109527
H	-3.358920	-2.663715	-0.030491
H	-2.374669	0.879779	1.612768
O	-4.271843	0.670129	0.929707
H	-4.721182	0.029419	0.357986
H	-2.906015	0.494791	-1.356101
O	-2.447266	2.359307	-0.550974
H	-3.366489	2.562295	-0.326010
H	-0.317458	1.047782	0.132515

O	0.235708	-1.484331	-1.760870
H	-0.041584	-2.402778	-1.634060
H	-0.352189	-0.005129	0.501228
C	-0.662564	-2.050739	0.998685
H	-1.594829	-1.932776	0.439659
H	-0.884534	-1.989361	2.067165
O	-0.021047	-3.284502	0.656101
H	-0.544440	-3.999703	1.035642

O	-0.393036	1.017343	-1.949575
H	-0.677933	1.938839	-2.031631
H	-1.257128	-1.401630	-1.425956
C	0.735786	-1.346544	-0.615406
H	1.258341	-0.814023	0.183028
H	1.186632	-1.068509	-1.565078
O	0.867279	-2.757513	-0.477377
H	0.393283	-2.971178	0.337186

(ii) Optimized coordinates of Tol : β-D-glucose complexes

F-2a (E_t = -955.998458)

C	-2.902134	0.429466	-0.966504
C	-3.233309	-1.528242	0.410563
C	-2.729588	-0.832766	1.510562
C	-2.306205	0.498999	1.390563
C	-2.390817	1.118515	0.136703
C	-3.329010	-0.895108	-0.833055
C	-1.739311	1.234357	2.576532
H	-2.982967	0.931625	-1.923378
H	-2.042475	2.136712	0.014750
H	-2.235410	0.929697	3.497542
H	-0.672470	1.034161	2.694939
H	-1.861697	2.310439	2.463084
H	-2.671341	-1.325096	2.474931
H	-3.565201	-2.552649	0.525112
H	-3.759126	-1.419406	-1.678846
C	2.415581	0.635894	0.144637
C	1.075048	1.193508	-0.310086
O	0.538811	0.357483	-1.349038
C	0.253332	-0.954966	-0.856603
C	1.558062	-1.623121	-0.467274
C	2.234421	-0.797706	0.605436
H	-0.412900	-0.875065	0.011887
O	-0.326816	-1.712687	-1.872260
H	-1.262162	-1.465074	-1.896190
H	2.192068	-1.661108	-1.361334
O	1.343490	-2.919141	0.078839
H	0.851519	-3.409240	-0.594563
H	1.583321	-0.791921	1.491387
O	3.524208	-1.297922	0.940380
H	3.397992	-2.229898	1.166810
H	3.109607	0.639078	-0.706633
O	2.894251	1.454275	1.203597
H	3.656969	0.982974	1.568379
H	0.384950	1.208488	0.542459
C	1.162628	2.581489	-0.910508
H	1.904474	2.569656	-1.717549

F-2b (E_t = -955.996582)

C	-2.082465	-1.394275	-1.506198
C	-3.030592	-1.019622	0.680651
C	-2.921528	0.359945	0.487584
C	-2.399798	0.885741	-0.701560
C	-1.981772	-0.013748	-1.694043
C	-2.606007	-1.902820	-0.314614
C	-2.265182	2.371322	-0.902309
H	-1.759770	-2.070856	-2.288047
H	-1.591998	0.373545	-2.629624
H	-1.258282	2.714197	-0.663743
H	-2.476821	2.643071	-1.936312
H	-2.962593	2.911773	-0.263110
H	-3.259748	1.039197	1.262171
H	-3.455170	-1.401718	1.601460
H	-2.686952	-2.972441	-0.169512
C	1.002891	0.699090	1.133126
C	1.459413	1.111734	-0.262548
O	2.446621	0.169485	-0.711850
C	1.894905	-1.132198	-0.862923
C	1.409394	-1.652156	0.486361
C	0.399164	-0.685876	1.061497
H	1.061056	-1.126936	-1.574237
O	2.874593	-1.973374	-1.408457
H	3.672152	-1.832114	-0.877698
H	2.276378	-1.714827	1.160444
O	0.771617	-2.913892	0.340955
H	1.391860	-3.469617	-0.152327
H	-0.463868	-0.649918	0.394755
O	-0.011109	-1.030722	2.382957
H	-0.525221	-1.845039	2.296389
H	1.880813	0.678842	1.793661
O	0.040785	1.637717	1.613199
H	-0.407609	1.189002	2.346449
H	0.592873	1.097474	-0.935237
C	2.093934	2.492651	-0.305491
H	2.522543	2.651984	-1.293858

H	1.484829	3.291915	-0.152352
O	-0.110710	3.001880	-1.386151
H	-0.418029	2.261683	-1.929172

H	2.908430	2.534132	0.427745
O	1.131093	3.515340	-0.095485
H	0.678978	3.295080	0.732887

F-2c (E_t = -955.995244)

C	-2.384245	-0.621960	-1.627217
C	-2.658375	0.245553	0.609701
C	-2.405739	-1.027414	1.129974
C	-2.151211	-2.114769	0.284789
C	-2.141310	-1.890572	-1.099711
C	-2.647725	0.450963	-0.771681
C	-1.843028	-3.480355	0.836248
H	-2.360242	-0.469311	-2.698394
H	-1.941713	-2.720598	-1.768546
H	-2.110290	-3.546783	1.890251
H	-2.394668	-4.251519	0.298488
H	-0.778209	-3.686658	0.730344
H	-2.421233	-1.181141	2.203439
H	-2.870316	1.070428	1.279739
H	-2.853271	1.433730	-1.177869
C	1.350369	0.703229	-1.271946
C	1.050181	-0.471760	-0.353762
O	1.627496	-0.209796	0.945934
C	1.006537	0.903754	1.576016
C	1.273409	2.152341	0.745019
C	0.761398	1.962017	-0.665709
H	-0.070170	0.740824	1.685843
O	1.523940	1.036256	2.872336
H	2.487823	1.025609	2.778056
H	2.362309	2.304989	0.708714
O	0.608609	3.285980	1.287997
H	0.857097	3.323051	2.222384
H	-0.327943	1.842081	-0.626258
O	1.119917	3.046871	-1.517655
H	0.759274	3.843641	-1.104917
H	2.440006	0.828881	-1.344728
O	0.780699	0.434493	-2.545473
H	0.830295	1.272571	-3.027844
H	-0.031492	-0.591290	-0.251661
C	1.664336	-1.777243	-0.809358
H	2.738730	-1.626802	-0.971282
H	1.210492	-2.082488	-1.749811
O	1.426610	-2.806137	0.142800
H	1.643447	-2.406265	0.997146

F-2d (E_t = -955.995320)

C	2.872097	0.146328	-1.141923
C	2.736993	0.540880	1.235536
C	1.926380	1.654233	1.000955
C	1.579737	2.034339	-0.302897
C	2.062928	1.261517	-1.369394
C	3.210740	-0.217637	0.163283
C	0.680571	3.218451	-0.549407
H	3.229534	-0.443119	-1.976439
H	1.814001	1.546076	-2.386329
H	0.880184	3.661008	-1.525043
H	-0.373626	2.934289	-0.520802
H	0.836322	3.987599	0.206834
H	1.569371	2.243255	1.838955
H	2.986514	0.262222	2.251422
H	3.829299	-1.088063	0.338926
C	-0.991323	-1.064486	1.367626
C	-0.097012	-1.391501	0.182578
O	-0.899609	-1.390977	-1.021582
C	-1.379134	-0.085727	-1.311501
C	-2.303445	0.365936	-0.187335
C	-1.591058	0.311026	1.146381
H	-0.547725	0.615244	-1.428697
O	-2.053901	-0.109066	-2.540740
H	-2.682512	-0.844032	-2.487231
H	-3.159434	-0.324047	-0.157205
O	-2.732907	1.709484	-0.385846
H	-3.071236	1.753034	-1.291956
H	-0.766246	1.034249	1.133123
O	-2.472204	0.570728	2.235784
H	-2.850951	1.445867	2.075135
H	-1.805385	-1.800991	1.420697
O	-0.199506	-1.087186	2.546998
H	-0.753782	-0.689326	3.233906
H	0.678939	-0.628726	0.095261
C	0.554023	-2.754674	0.239855
H	-0.226182	-3.518945	0.345817
H	1.208134	-2.804139	1.107934
O	1.350772	-2.976511	-0.914933
H	0.784353	-2.725076	-1.657667

F-2e (E_t = -955.990947)

F-2f (E_t = -955.991056)

C	2.748828	-1.263232	-1.332894
C	3.197916	0.201185	0.532174
C	2.374349	-0.584034	1.341378
C	1.726800	-1.718190	0.831709
C	1.922174	-2.040733	-0.518588
C	3.387110	-0.136918	-0.809554
C	0.812054	-2.540364	1.701514
H	2.890206	-1.533015	-2.372068
H	1.437479	-2.920117	-0.929087
H	0.745888	-3.564679	1.335453
H	1.179219	-2.572805	2.727270
H	-0.196790	-2.123307	1.720744
H	2.241643	-0.321613	2.385437
H	3.682678	1.076072	0.946414
H	4.025584	0.468594	-1.440065
C	-2.006075	0.194367	0.472538
C	-1.457570	-0.406283	-0.826399
O	-0.979515	0.631906	-1.684890
C	0.108751	1.322817	-1.086718
C	-0.410552	2.073934	0.126948
C	-0.953322	1.074067	1.119639
H	0.874162	0.600280	-0.779005
O	0.593109	2.194922	-2.067357
H	1.063428	2.886254	-1.578912
H	-1.216033	2.737754	-0.210497
O	0.679192	2.818447	0.664273
H	0.363176	3.176572	1.505618
H	-0.124998	0.430115	1.439472
O	-1.477514	1.803685	2.226022
H	-1.859783	1.140461	2.817666
H	-2.878560	0.816614	0.227335
O	-2.338067	-0.793258	1.446391
H	-2.894876	-1.441824	0.985765
H	-0.649583	-1.105200	-0.576965
C	-2.522421	-1.110319	-1.644799
H	-3.262852	-0.367637	-1.956237
H	-2.065376	-1.542404	-2.538080
O	-3.111230	-2.121712	-0.816198
H	-3.850672	-2.509827	-1.297878

C	3.177842	0.137384	0.521490
C	2.410383	0.289981	-1.762572
C	1.935715	-1.022542	-1.687241
C	2.077401	-1.772956	-0.513705
C	2.704373	-1.172680	0.587816
C	3.029407	0.874959	-0.656013
C	1.542105	-3.175288	-0.409359
H	3.662756	0.579414	1.383201
H	2.825091	-1.741057	1.503545
H	1.213850	-3.544026	-1.380331
H	2.302911	-3.857258	-0.028655
H	0.695779	-3.194127	0.276830
H	1.456548	-1.469606	-2.550930
H	2.303428	0.847610	-2.685267
H	3.409819	1.887368	-0.715492
C	-0.295737	0.600939	0.867753
C	-1.049257	1.723908	0.149221
O	-1.769782	1.200901	-0.972806
C	-2.732063	0.237120	-0.587663
C	-2.021551	-0.960570	0.021175
C	-1.261742	-0.504408	1.241567
H	-3.416095	0.674964	0.159137
O	-3.412465	-0.107732	-1.758862
H	-3.813859	-0.969785	-1.575325
H	-1.316142	-1.341822	-0.727615
O	-3.022374	-1.924554	0.332065
H	-2.583036	-2.607907	0.856811
H	-1.975867	-0.102407	1.973836
O	-0.587221	-1.635049	1.790720
H	0.015453	-1.270063	2.455682
H	0.456622	0.198194	0.183664
O	0.293573	1.020242	2.094487
H	0.869443	1.765384	1.861754
H	-1.729874	2.207756	0.863542
C	-0.115090	2.747292	-0.469947
H	-0.701573	3.555800	-0.913448
H	0.449473	2.242919	-1.257368
O	0.754106	3.236616	0.559474
H	1.417854	3.796430	0.140675

F-2g (E_t = -955.993907)

C	-2.012881	-2.060863	0.797247
C	-1.906773	-0.099861	2.201454
C	-2.671429	0.603866	1.268362
C	-3.116979	-0.009239	0.089599
C	-2.777442	-1.350282	-0.129759
C	-1.569501	-1.434564	1.964024
C	-3.868358	0.775245	-0.951999
H	-1.752648	-3.092590	0.600218

F-2h (E_t = -955.987012)

C	2.564415	-0.472808	1.896239
C	4.057192	-0.826821	0.032975
C	3.738441	0.440038	-0.459706
C	2.831588	1.268543	0.213719
C	2.252445	0.794110	1.398461
C	3.465473	-1.290029	1.210745
C	2.440441	2.606463	-0.355052
H	2.104368	-0.820365	2.812762

H	-3.117851	-1.845458	-1.032829
H	-4.580469	0.143641	-1.482648
H	-4.417366	1.602201	-0.503291
H	-3.168739	1.185722	-1.681065
H	-2.934807	1.638162	1.460862
H	-1.574931	0.391785	3.107674
H	-0.980857	-1.984160	2.688142
C	0.190492	0.197179	-0.966360
C	1.009117	1.426426	-0.601792
O	1.785881	1.133306	0.577688
C	2.725628	0.090208	0.344191
C	1.994119	-1.195608	0.005231
C	1.126919	-0.969443	-1.213981
H	3.387570	0.376481	-0.488435
O	3.446664	-0.146382	1.517309
H	3.997451	0.628282	1.687840
H	1.356067	-1.448148	0.860371
O	2.898025	-2.247848	-0.311883
H	3.447159	-2.378472	0.473079
H	1.777459	-0.722374	-2.065081
O	0.331441	-2.110604	-1.518125
H	0.952157	-2.848511	-1.599946
H	-0.460472	-0.050025	-0.124249
O	-0.570512	0.496626	-2.132222
H	-0.975964	-0.345023	-2.387261
H	1.680199	1.688496	-1.431202
C	0.165425	2.630403	-0.239962
H	-0.528060	2.337869	0.555825
H	-0.411943	2.943010	-1.107547
O	0.985190	3.723887	0.146914
H	1.562521	3.366437	0.834573
H	1.560521	1.428478	1.942021
H	3.266091	3.052802	-0.908545
H	1.596785	2.493997	-1.037252
H	2.149288	3.297738	0.435399
H	4.202331	0.793722	-1.373841
H	4.770609	-1.446973	-0.496411
H	3.713318	-2.270724	1.596912
C	-0.883462	0.765825	-0.705636
C	-0.745970	-0.725965	-1.001062
O	-1.114728	-1.457106	0.177968
C	-2.479011	-1.261616	0.510014
C	-2.708630	0.188499	0.891695
C	-2.303985	1.067348	-0.270135
H	-3.110400	-1.528673	-0.353109
O	-2.788743	-2.035535	1.632310
H	-2.640048	-2.959486	1.391781
H	-2.069192	0.402329	1.756284
O	-4.076652	0.466610	1.167160
H	-4.330468	-0.120662	1.892132
H	-2.974342	0.852108	-1.113991
O	-2.353580	2.452754	0.059329
H	-3.252158	2.618931	0.376793
H	-0.202801	1.016894	0.117067
O	-0.560163	1.507280	-1.878917
H	-0.885576	2.403630	-1.706490
H	-1.408917	-0.991397	-1.836272
C	0.668128	-1.114662	-1.349726
H	1.284075	-0.999718	-0.456858
H	1.034230	-0.429164	-2.119920
O	0.648101	-2.463743	-1.810005
H	1.559700	-2.776007	-1.789845

F-2i (E_t = -955.984502)

C	-2.228824	1.467338	-1.076789
C	-3.616458	1.042811	0.849077
C	-4.072157	-0.136562	0.256373
C	-3.614125	-0.532152	-1.007241
C	-2.688904	0.287988	-1.666080
C	-2.688204	1.847421	0.186242
C	-4.074417	-1.825013	-1.627737
H	-1.523243	2.094746	-1.607817
H	-2.329829	0.002449	-2.648680
H	-3.385056	-2.638901	-1.397150
H	-5.059411	-2.108133	-1.258495
H	-4.132093	-1.739799	-2.712259
H	-4.800623	-0.751615	0.773744
H	-3.986625	1.333916	1.824503
H	-2.318985	2.751744	0.650582

C	0.928164	0.915899	0.496928
C	0.779746	-0.464686	1.130789
O	1.243853	-1.446451	0.192245
C	2.629825	-1.300655	-0.069466
C	2.883159	0.023453	-0.765328
C	2.377815	1.143657	0.115731
H	3.189357	-1.340554	0.879380
O	3.034874	-2.310228	-0.947593
H	2.867077	-3.154381	-0.508372
H	2.318005	0.010330	-1.704633
O	4.268520	0.261020	-0.988752
H	4.583437	-0.473684	-1.532726
H	2.978440	1.156179	1.035912
O	2.443934	2.410075	-0.534794
H	3.363734	2.517605	-0.814407
H	0.318610	0.940393	-0.414195
O	0.497264	1.904548	1.424921
H	0.812466	2.744630	1.060457
H	1.378270	-0.507870	2.051283
C	-0.653396	-0.789785	1.464179
H	-1.219698	-0.867034	0.531541
H	-1.063043	0.038532	2.047285
O	-0.660447	-2.012727	2.196350
H	-1.584559	-2.232574	2.360564

(iii) Optimized coordinates of Tol : β-D-galactose complexes

F-3a (E_t = -955.996107)				**F-3b** (E_t = -955.988458)			
C	-2.441566	-1.623019	-1.306542	C	-3.020279	0.964751	-1.045658
C	-3.291634	0.626083	-1.097382	C	-2.869697	0.924679	1.363534
C	-3.181648	0.534026	0.292973	C	-2.595338	-0.444254	1.320040
C	-2.709910	-0.634900	0.906222	C	-2.534346	-1.131470	0.098943
C	-2.337776	-1.709073	0.083815	C	-2.744301	-0.404229	-1.081422
C	-2.919779	-0.452870	-1.902502	C	-3.084573	1.633911	0.178806
C	-2.583661	-0.732614	2.404362	C	-2.225115	-2.605217	0.056323
H	-2.161465	-2.470003	-1.920877	H	-3.192681	1.502896	-1.969636
H	-1.983095	-2.627340	0.539475	H	-2.709187	-0.918812	-2.035402
H	-2.864082	-1.727140	2.750378	H	-1.149615	-2.788438	0.012229
H	-1.560598	-0.545603	2.736224	H	-2.610974	-3.106388	0.943625
H	-3.234301	-0.009509	2.894997	H	-2.679643	-3.070105	-0.818138
H	-3.488630	1.370128	0.912003	H	-2.444217	-0.990641	2.244563
H	-3.678834	1.531847	-1.548383	H	-2.927267	1.431700	2.319040
H	-3.013501	-0.388414	-2.979264	H	-3.315276	2.691638	0.210770
C	0.428291	0.965679	0.811812	C	1.298124	0.710028	1.105435
C	0.285094	0.938622	-0.705408	C	0.490479	1.181952	-0.111760
O	1.516089	0.530895	-1.326166	O	1.056824	0.659333	-1.321900
C	1.876556	-0.785040	-0.923933	C	0.968601	-0.755554	-1.346860
C	2.093095	-0.865495	0.585283	C	1.683979	-1.368772	-0.149682

C	0.850527	-0.402850	1.332316
H	1.099535	-1.499297	-1.221387
O	3.034497	-1.161410	-1.619113
H	3.701906	-0.491077	-1.412014
H	2.927296	-0.197864	0.842307
O	2.358645	-2.211974	0.943503
H	3.057740	-2.508552	0.343731
H	0.058646	-1.129956	1.143789
O	1.037837	-0.359686	2.737741
H	1.535237	0.457341	2.896021
H	-0.546654	1.227198	1.242618
O	1.439835	1.865822	1.263372
H	1.389606	2.653179	0.695365
H	-0.515159	0.232853	-0.957703
C	-0.036247	2.287218	-1.320473
H	-0.232318	2.160795	-2.388575
H	-0.921489	2.713519	-0.850842
O	1.034581	3.216318	-1.110392
H	1.813842	2.780713	-1.487215

C	1.165225	-0.803477	1.156864
H	-0.079151	-1.075741	-1.355916
O	1.527537	-1.214152	-2.550468
H	2.391322	-0.780377	-2.615004
H	2.752397	-1.138910	-0.220976
O	1.454232	-2.779619	-0.116225
H	1.737320	-3.116167	-0.978318
H	0.095516	-1.043310	1.233797
O	1.875694	-1.323635	2.266300
H	1.923146	-2.277711	2.112666
H	0.852025	1.140072	2.014368
O	2.675298	1.020849	0.998665
H	2.717587	1.921414	0.641955
H	-0.536396	0.815133	-0.002574
C	0.395741	2.681644	-0.266536
H	-0.137003	2.900814	-1.196013
H	-0.187885	3.073844	0.573218
O	1.713051	3.239103	-0.286608
H	1.635851	4.199754	-0.299562

F-3c (E_t = -955.988965)

C	3.253496	0.871916	-0.110074
C	2.355073	0.072720	1.981816
C	2.133912	-1.180378	1.405096
C	2.469983	-1.429592	0.066284
C	3.030319	-0.383884	-0.680737
C	2.912728	1.105389	1.223745
C	2.209719	-2.777368	-0.555512
H	3.694766	1.664487	-0.701650
H	3.314656	-0.562864	-1.712365
H	1.176026	-2.872001	-0.894423
H	2.860723	-2.940389	-1.413877
H	2.393758	-3.576455	0.162133
H	1.713926	-1.980764	2.004955
H	2.098914	0.238989	3.021084
H	3.081387	2.079126	1.664809
C	-0.548719	-0.200711	-1.327039
C	-0.281343	1.071960	-0.533521
O	-1.469817	1.502987	0.143183
C	-1.917614	0.549517	1.113946
C	-2.300477	-0.733135	0.401746
C	-1.101015	-1.253784	-0.383784
H	-1.097148	0.352898	1.823453
O	-3.043134	1.066757	1.741520
H	-2.760351	1.838930	2.247577
H	-3.118717	-0.487220	-0.285459
O	-2.686305	-1.700230	1.364752
H	-2.707343	-2.535975	0.875943
H	-0.326362	-1.525807	0.335492

F-3d (E_t = -955.995353)

C	-2.757492	1.510612	-0.566722
C	-3.858850	-0.575864	-1.087747
C	-3.591470	-1.035911	0.204445
C	-2.911322	-0.230470	1.128862
C	-2.505269	1.048148	0.725922
C	-3.440924	0.701476	-1.476805
C	-2.671051	-0.710498	2.536222
H	-2.408037	2.489973	-0.866160
H	-1.975325	1.683092	1.426928
H	-3.525753	-0.487761	3.176777
H	-2.510082	-1.787761	2.561805
H	-1.796880	-0.226943	2.971226
H	-3.910515	-2.029997	0.496923
H	-4.387646	-1.211022	-1.787549
H	-3.637236	1.056236	-2.480335
C	2.575035	0.420095	0.671956
C	1.199279	1.087206	0.640017
O	0.423336	0.636272	-0.467445
C	0.201641	-0.766957	-0.409644
C	1.530777	-1.479075	-0.553614
C	2.434783	-1.093955	0.596492
H	-0.269977	-1.021266	0.554403
O	-0.591624	-1.158724	-1.482774
H	-1.481334	-0.801795	-1.341349
H	1.974608	-1.142613	-1.496245
O	1.394427	-2.895494	-0.508812
H	0.762305	-3.119052	-1.206269
H	1.986067	-1.467940	1.526193

O	-1.448176	-2.451800	-1.076084
H	-1.906464	-2.141161	-1.873356
H	0.391694	-0.559189	-1.761095
O	-1.550459	-0.042049	-2.340304
H	-1.143916	0.374475	-3.109213
H	0.506020	0.852555	0.197131
C	0.150363	2.259575	-1.367806
H	1.081347	2.026468	-1.885746
H	-0.628627	2.472393	-2.108966
O	0.401276	3.387055	-0.544504
H	-0.389756	3.459860	0.007609

O	3.745745	-1.627139	0.421501
H	3.618560	-2.537898	0.118232
H	3.074575	0.688695	1.612632
O	3.339494	0.879332	-0.439758
H	4.060556	0.237642	-0.536434
H	0.696532	0.819435	1.585664
C	1.267638	2.607952	0.558155
H	0.262067	3.005729	0.701240
H	1.887680	2.957080	1.396486
O	1.720113	3.095733	-0.685078
H	2.491254	2.559770	-0.920465

F-3e (E_t = -955.997143)

C	-2.903368	-1.385375	0.915678
C	-2.333517	-1.559303	-1.422873
C	-2.384457	-0.167307	-1.534323
C	-2.702551	0.636275	-0.430214
C	-2.952998	0.004768	0.796346
C	-2.594533	-2.173150	-0.195746
C	-2.750953	2.137359	-0.549852
H	-3.105432	-1.850536	1.872327
H	-3.205055	0.608026	1.661599
H	-3.525270	2.549823	0.096736
H	-1.802740	2.599563	-0.267872
H	-2.976139	2.436118	-1.573391
H	-2.202274	0.301240	-2.495657
H	-2.101303	-2.162031	-2.292506
H	-2.559771	-3.251615	-0.107801
C	0.629471	0.777959	0.884508
C	0.968707	1.247235	-0.526142
O	2.103908	0.560939	-1.073031
C	1.915774	-0.844917	-1.099765
C	1.788444	-1.355461	0.320426
C	0.560868	-0.736984	0.949729
H	1.007085	-1.087762	-1.675488
O	3.052481	-1.443059	-1.651952
H	3.140270	-1.119478	-2.557718
H	2.686105	-1.036117	0.860395
O	1.608725	-2.767198	0.376715
H	2.385353	-3.154482	-0.049660
H	-0.319576	-1.077640	0.397144
O	0.457127	-1.090758	2.329205
H	0.638109	-2.041161	2.365500
H	-0.353935	1.176640	1.154449
O	1.628676	1.275455	1.774792
H	1.532262	0.734989	2.574847
H	0.086432	1.064569	-1.153316
C	1.355536	2.724027	-0.533223
H	2.390914	2.788882	-0.195016

F-3f (E_t = -955.994073)

C	2.648071	-0.232496	-1.878829
C	1.870017	-2.054695	-0.498877
C	2.463449	-1.458624	0.616323
C	3.152855	-0.242808	0.503896
C	3.242527	0.356569	-0.759546
C	1.960758	-1.441904	-1.751981
C	3.821609	0.373225	1.704360
H	2.730710	0.245309	-2.847452
H	3.780169	1.292407	-0.866919
H	4.799348	-0.077519	1.880902
H	3.969881	1.443333	1.564787
H	3.222520	0.227825	2.602583
H	2.389490	-1.940353	1.585295
H	1.341746	-2.994336	-0.391492
H	1.503203	-1.903670	-2.617897
C	-1.174231	0.648456	-1.162957
C	-0.188306	0.983637	-0.050031
O	-0.810654	0.858098	1.240474
C	-1.227809	-0.483048	1.467533
C	-2.260089	-0.922696	0.433625
C	-1.729428	-0.761509	-0.985466
H	-0.364998	-1.157362	1.438009
O	-1.747260	-0.573785	2.767278
H	-2.469213	0.070044	2.813106
H	-3.142952	-0.277473	0.547430
O	-2.570780	-2.290960	0.644818
H	-2.779015	-2.368374	1.586579
H	-0.931117	-1.492723	-1.132489
O	-2.718320	-1.030904	-1.963255
H	-3.271614	-0.235537	-1.978583
H	-0.642482	0.701164	-2.123236
O	-2.317129	1.503054	-1.169021
H	-2.003525	2.395313	-0.944768
H	0.655251	0.291983	-0.122756
C	0.337261	2.405299	-0.090991
H	1.119325	2.521324	0.664449

H	1.293675	3.123305	-1.544173
O	0.484338	3.501167	0.280855
H	0.730704	3.274533	1.189645

H	0.762332	2.624956	-1.069684
O	-0.718036	3.350740	0.124666
H	-1.111748	3.087301	0.970106

F-3g (E_t = -955.995732)

C	2.235734	-1.788362	1.264027
C	1.957129	-1.823828	-1.134298
C	2.764019	-0.688435	-1.240833
C	3.315635	-0.086064	-0.101732
C	3.043830	-0.655005	1.150304
C	1.691014	-2.378515	0.120284
C	4.230503	1.104323	-0.224040
H	2.039445	-2.214935	2.240072
H	3.466901	-0.205328	2.041952
H	4.137943	1.762258	0.639427
H	5.272988	0.789298	-0.289621
H	4.004057	1.684060	-1.118200
H	2.969920	-0.266733	-2.218601
H	1.543606	-2.277036	-2.026931
H	1.069598	-3.261308	0.205063
C	-0.789050	0.701818	-1.146893
C	-0.100472	0.876764	0.204259
O	-1.051505	0.836459	1.277272
C	-1.740604	-0.420415	1.353956
C	-2.528761	-0.636616	0.079410
C	-1.598115	-0.583332	-1.128621
H	-0.991901	-1.219191	1.475209
O	-2.621077	-0.356841	2.425956
H	-2.089059	-0.299541	3.229776
H	-3.257135	0.179525	0.010119
O	-3.157400	-1.907137	0.137562
H	-3.458159	-2.066312	-0.769418
H	-0.923496	-1.441682	-1.075731
O	-2.361620	-0.741460	-2.322472
H	-2.742534	0.136891	-2.481421
H	-0.011623	0.632913	-1.920583
O	-1.717936	1.736256	-1.461320
H	-1.389873	2.552966	-1.047327
H	0.631749	0.071405	0.314692
C	0.595276	2.215108	0.369407
H	1.269476	2.403318	-0.465574
H	1.177303	2.208549	1.295477
O	-0.362131	3.280856	0.381453
H	-1.002686	3.021170	1.062616

F-3h (E_t = -955.989571)

C	2.163648	-1.897682	0.971946
C	2.016129	-1.598492	-1.420059
C	2.849773	-0.481310	-1.328045
C	3.350684	-0.056289	-0.089914
C	2.997695	-0.781000	1.056851
C	1.672911	-2.312536	-0.269073
C	4.297818	1.111672	0.000673
H	1.900447	-2.443776	1.869311
H	3.375999	-0.466640	2.023334
H	4.147594	1.805300	-0.826110
H	5.335396	0.776180	-0.034465
H	4.160069	1.658161	0.933316
H	3.116946	0.064454	-2.226473
H	1.642017	-1.914244	-2.386311
H	1.028920	-3.180493	-0.337289
C	-0.905155	0.897766	-1.064549
C	-0.112296	0.933098	0.242716
O	-0.959134	0.707771	1.368523
C	-1.522667	-0.609274	1.343163
C	-2.408599	-0.720267	0.111602
C	-1.609062	-0.445181	-1.157698
H	-0.723092	-1.357735	1.307756
O	-2.201728	-0.816757	2.536789
H	-2.987901	-0.254768	2.514828
H	-3.184298	0.053962	0.199782
O	-2.970771	-2.021582	0.056738
H	-3.332057	-2.087779	-0.839851
H	-0.873424	-1.243725	-1.280382
O	-2.474027	-0.511685	-2.290254
H	-2.922488	0.348989	-2.297809
H	-0.203623	1.005992	-1.904273
O	-1.944309	1.868993	-1.142854
H	-1.616013	2.667238	-0.698265
H	0.642345	0.140165	0.180692
C	0.635569	2.224573	0.484654
H	1.122197	2.164456	1.461781
H	1.404410	2.329202	-0.288261
O	-0.290771	3.316186	0.441440
H	0.201021	4.137960	0.550529

F-3i (E_t = -955.995471)

F-3j (E_t = -955.993662)

C	1.777297	-1.645542	-1.546137
C	2.565370	0.620937	-1.816668
C	3.210880	0.538993	-0.581485
C	3.145428	-0.627176	0.192722
C	2.421659	-1.717209	-0.308632
C	1.841172	-0.471334	-2.300976
C	3.768816	-0.677230	1.561196
H	1.235305	-2.504621	-1.923086
H	2.372094	-2.633107	0.270151
H	3.069397	-0.278541	2.296586
H	4.018582	-1.699260	1.843543
H	4.680673	-0.081997	1.599790
H	3.770915	1.391031	-0.212265
H	2.626109	1.533343	-2.396565
H	1.349446	-0.416022	-3.264355
C	-0.793197	-0.624805	1.204688
C	-1.673132	-0.986195	0.015368
O	-2.465356	0.136812	-0.415702
C	-1.651346	1.231051	-0.814779
C	-0.858284	1.722291	0.378608
C	0.035475	0.604185	0.868588
H	-0.967402	0.908978	-1.616832
O	-2.471216	2.285585	-1.226267
H	-2.931327	2.006131	-2.027886
H	-1.577024	1.994122	1.158245
O	-0.001363	2.810330	0.042798
H	-0.578458	3.518197	-0.274871
H	0.745638	0.358945	0.076793
O	0.724565	0.991926	2.059585
H	1.055772	1.884922	1.882862
H	-0.110079	-1.464381	1.397232
O	-1.619024	-0.370819	2.332197
H	-1.044697	0.099267	2.955685
H	-1.019437	-1.303605	-0.808652
C	-2.678391	-2.081860	0.308337
H	-2.157326	-2.991070	0.608053
H	-3.317270	-1.757245	1.132587
O	-3.428445	-2.395215	-0.857993
H	-3.804677	-1.550669	-1.138946
C	-2.776898	-0.793893	-1.281888
C	-3.291002	-0.288066	1.021888
C	-2.892943	1.034313	0.817411
C	-2.431501	1.463153	-0.434906
C	-2.382488	0.531684	-1.481239
C	-3.235911	-1.206534	-0.029150
C	-2.057719	2.905022	-0.661847
H	-2.728853	-1.499872	-2.101707
H	-2.035957	0.847840	-2.459341
H	-2.946654	3.519172	-0.813669
H	-1.519542	3.312410	0.194273
H	-1.425864	3.014309	-1.542685
H	-2.938340	1.741257	1.638639
H	-3.639371	-0.599650	1.998535
H	-3.537818	-2.234133	0.127392
C	0.916638	0.598798	1.018975
C	1.343052	1.022708	-0.385407
O	2.045259	-0.016724	-1.076448
C	1.288042	-1.207177	-1.186666
C	0.982711	-1.738777	0.203836
C	0.168140	-0.721138	0.967540
H	0.353432	-1.046002	-1.739138
O	2.037059	-2.135632	-1.927299
H	2.945110	-2.049326	-1.600660
H	1.938952	-1.898265	0.717906
O	0.211598	-2.934322	0.147962
H	0.693409	-3.531955	-0.441492
H	-0.783893	-0.580417	0.453165
O	-0.042951	-1.133748	2.318700
H	-0.311335	-2.062437	2.266879
H	0.248290	1.370899	1.423442
O	2.071608	0.461402	1.847190
H	1.770969	-0.050823	2.614293
H	0.416628	1.260109	-0.929054
C	2.240165	2.253817	-0.401525
H	2.381345	2.565501	-1.436506
H	1.703094	3.058155	0.121719
O	3.527565	2.030774	0.131842
H	3.393574	1.565769	0.970295

(iv) Optimized coordinates of Tol : α-D-mannose complexes

F-4a (E_t = -956.000091)			
C	2.972750	0.000975	1.725450
C	3.389776	1.144656	-0.357646
C	3.042780	-0.012137	-1.057093
C	2.644477	-1.175146	-0.381527
C	2.617508	-1.152440	1.018457
C	3.351569	1.157010	1.039145

F-4b (E_t = -956.000091)			
C	-3.219891	-0.671529	-1.676221
C	-2.438979	-2.422634	-0.211636
C	-2.487618	-1.536794	0.869717
C	-2.902980	-0.210784	0.695445
C	-3.274813	0.205033	-0.591591
C	-2.796470	-1.990223	-1.490759

C	2.194782	-2.387539	-1.151669
H	2.975570	-0.012397	2.809800
H	2.314977	-2.041459	1.559572
H	1.190453	-2.226819	-1.546133
H	2.859381	-2.584532	-1.992797
H	2.180782	-3.272089	-0.516207
H	3.076585	-0.015069	-2.141096
H	3.697760	2.030338	-0.899660
H	3.630039	2.049794	1.584745
C	-1.502524	-0.229662	-1.019957
C	-0.435678	0.705017	-0.476500
O	-0.950574	1.389616	0.694468
C	-1.315568	0.501945	1.748938
C	-2.455011	-0.394219	1.286346
C	-2.018154	-1.176543	0.054212
H	-1.642576	1.167131	2.553960
O	-0.263635	-0.339317	2.135605
H	0.532713	0.203792	2.234642
H	-2.752338	-1.075262	2.083944
O	-3.604595	0.397607	0.973403
H	-3.265028	1.179247	0.512037
H	-1.221795	-1.873521	0.318869
O	-3.092674	-1.953402	-0.472464
H	-3.863618	-1.366455	-0.420293
H	-2.336392	0.383116	-1.384763
O	-0.930758	-0.966432	-2.097682
H	-1.589216	-1.645694	-2.307933
H	0.454247	0.131136	-0.214115
C	-0.074411	1.811142	-1.447408
H	0.228019	1.369551	-2.395195
H	0.765905	2.380584	-1.038386
O	-1.193120	2.650315	-1.711997
H	-1.426388	3.033165	-0.856138

C	-2.889309	0.768427	1.838335
H	-3.515067	-0.330034	-2.660761
H	-3.606251	1.226580	-0.742600
H	-2.020529	1.423236	1.757388
H	-2.846550	0.251656	2.796227
H	-3.783115	1.392138	1.828912
H	-2.198406	-1.878719	1.856697
H	-2.144818	-3.453719	-0.049359
H	-2.762589	-2.675365	-2.328447
C	1.003881	1.523946	0.220998
C	0.297564	0.605415	-0.761116
O	1.220970	-0.422110	-1.204371
C	1.711099	-1.234079	-0.139682
C	2.514796	-0.374814	0.825289
C	1.632318	0.743056	1.366236
H	2.352451	-1.966809	-0.638922
O	0.682901	-1.831082	0.602072
H	0.045616	-2.210379	-0.021585
H	2.904046	-0.981848	1.642833
O	3.647662	0.185384	0.155021
H	3.327732	0.450655	-0.720422
H	0.836276	0.323496	1.982917
O	2.376537	1.632945	2.196734
H	3.217754	1.754064	1.728474
H	1.793945	2.057737	-0.321942
O	0.043757	2.451042	0.720889
H	0.497345	2.908579	1.444827
H	-0.567400	0.148895	-0.277820
C	-0.129993	1.318318	-2.028258
H	-0.750600	2.172903	-1.765013
H	-0.719059	0.628705	-2.640737
O	0.994745	1.819011	-2.742401
H	1.514820	1.037129	-2.969699

F-4c (E_t = -955.993842)

C	2.499528	-1.857813	-0.659900
C	3.278802	-0.504825	1.182513
C	3.180246	0.634166	0.381419
C	2.733172	0.549628	-0.944479
C	2.391292	-0.711460	-1.449755
C	2.934347	-1.756054	0.663936
C	2.549322	1.788288	-1.778773
H	2.236949	-2.822716	-1.075142
H	2.050298	-0.798352	-2.475510
H	1.529232	2.158588	-1.669551
H	3.235436	2.575659	-1.468371
H	2.727087	1.579582	-2.833414
H	3.462891	1.600024	0.785345
H	3.631193	-0.417868	2.202990

F-4d (E_t = -955.997685)

C	-3.058380	-0.458332	1.317108
C	-2.615651	-1.170361	-0.945761
C	-2.346614	0.152346	-1.306591
C	-2.431242	1.186837	-0.367541
C	-2.792975	0.861349	0.948445
C	-2.969709	-1.480225	0.367264
C	-2.125547	2.612762	-0.739960
H	-3.344339	-0.687474	2.336804
H	-2.883358	1.654815	1.683741
H	-1.959060	2.710210	-1.811965
H	-2.948375	3.273828	-0.465302
H	-1.231053	2.952105	-0.218189
H	-2.054257	0.379649	-2.324779
H	-2.533326	-1.957142	-1.684194

H	3.034829	-2.644616	1.275962
C	-1.407681	0.996155	-0.145115
C	-0.426138	0.399538	0.843618
O	-1.114190	-0.655743	1.548334
C	-1.539679	-1.699452	0.701232
C	-2.441162	-1.231443	-0.443703
C	-1.807290	-0.050503	-1.167175
H	-2.087364	-2.375049	1.369060
O	-0.459965	-2.355601	0.068397
H	0.254149	-2.412436	0.719622
H	-2.586769	-2.063519	-1.139791
O	-3.693051	-0.739405	0.040511
H	-4.221430	-1.489721	0.337935
H	-0.919681	-0.380721	-1.709439
O	-2.697939	0.513328	-2.128603
H	-3.561190	0.514362	-1.685743
H	-2.296805	1.298733	0.417005
O	-0.804505	2.127253	-0.776161
H	-1.360772	2.296403	-1.552709
H	0.438074	-0.012363	0.315244
C	0.058832	1.425839	1.854523
H	0.901889	1.961279	1.410430
H	0.415543	0.900467	2.740141
O	-0.955373	2.325513	2.281751
H	-1.104907	2.917121	1.532047
H	-3.176387	-2.505391	0.647539
C	1.419685	-0.621285	-0.729002
C	0.581513	-0.891285	0.515384
O	1.233995	-0.331757	1.670417
C	1.472020	1.059744	1.586495
C	2.277632	1.454944	0.357458
C	1.635871	0.869911	-0.888634
H	2.035665	1.285271	2.495523
O	0.265954	1.793732	1.511340
H	-0.331500	1.409029	2.167516
H	2.284555	2.548960	0.287430
O	3.589600	0.940143	0.523699
H	3.973694	0.972556	-0.365561
H	0.660887	1.337385	-1.061461
O	2.528891	1.125892	-1.973337
H	2.228955	0.544332	-2.687373
H	2.397534	-1.103156	-0.601973
O	0.785744	-1.041565	-1.935846
H	0.511190	-1.959374	-1.782425
H	-0.411967	-0.461776	0.382105
C	0.481149	-2.366760	0.857257
H	-0.190420	-2.494248	1.710303
H	1.478806	-2.716290	1.138577
O	-0.007657	-3.069907	-0.294113
H	0.074256	-4.014474	-0.117795

F-4e (E_t = -955.996284)

C	1.511595	-0.996438	-1.423559
C	2.667316	-2.129964	0.371350
C	3.550704	-1.054239	0.478232
C	3.436210	0.059054	-0.364787
C	2.406954	0.069249	-1.314814
C	1.638974	-2.097460	-0.573906
C	4.337763	1.252182	-0.193100
H	0.699406	-0.958828	-2.135999
H	2.307240	0.919674	-1.981501
H	5.302340	0.961752	0.221562
H	4.515388	1.751358	-1.145555
H	3.876869	1.969615	0.486936
H	4.342568	-1.080316	1.218572
H	2.776619	-2.984605	1.027874
H	0.950473	-2.929372	-0.659816
C	-1.459314	-0.438565	1.070345
C	-0.790025	0.916482	0.908267
O	-0.621729	1.187545	-0.496721
C	-1.834326	1.208086	-1.229900
C	-2.605944	-0.099890	-1.121696
C	-2.790765	-0.472627	0.341745
H	-1.517291	1.370006	-2.263412

F-4f (E_t = -955.994527)

C	3.868768	1.126775	-0.268488
C	2.145644	0.783570	-1.921921
C	1.882208	-0.479612	-1.387164
C	2.610345	-0.955447	-0.289904
C	3.610576	-0.139881	0.257298
C	3.141462	1.589770	-1.367929
C	2.355078	-2.336162	0.255707
H	4.637457	1.748299	0.173681
H	4.179138	-0.493406	1.110688
H	2.491926	-2.364845	1.336813
H	1.338337	-2.650841	0.027726
H	3.038304	-3.065366	-0.183216
H	1.081322	-1.084577	-1.792740
H	1.572755	1.133639	-2.772559
H	3.341344	2.572227	-1.776752
C	-0.859618	-0.221551	1.472857
C	-0.859646	1.095065	0.715782
O	-0.903450	0.818164	-0.699469
C	-2.053530	0.109439	-1.109485
C	-2.210403	-1.221734	-0.385732
C	-2.102517	-1.013995	1.120423
H	-1.899707	-0.061548	-2.178661

O	-2.710985	2.214474	-0.773587
H	-2.232196	3.051778	-0.838213
H	-3.584739	0.034605	-1.595437
O	-1.847679	-1.099369	-1.785860
H	-2.221431	-1.936621	-1.470074
H	-3.475300	0.246421	0.811212
O	-3.337627	-1.789754	0.371109
H	-3.145047	-2.125822	1.259264
H	-0.804169	-1.199314	0.644189
O	-1.640189	-0.809918	2.443088
H	-2.168376	-0.111393	2.856488
H	-1.409651	1.703721	1.356905
C	0.605925	0.956636	1.503798
H	1.172411	0.097146	1.140241
H	0.540843	0.897521	2.588996
O	1.254506	2.182031	1.185399
H	1.253268	2.207569	0.218480
O	-3.244352	0.822138	-0.848098
H	-3.134531	1.697104	-1.244753
H	-3.196987	-1.630886	-0.639303
O	-1.175389	-2.086572	-0.833217
H	-1.120525	-2.774965	-0.152267
H	-2.975955	-0.471478	1.492036
O	-1.967454	-2.286567	1.783530
H	-2.853223	-2.655850	1.895624
H	0.022610	-0.793932	1.164190
O	-0.828908	0.072197	2.864152
H	-0.919858	-0.782720	3.307249
H	-1.733750	1.687164	1.003245
C	0.403560	1.904160	0.944705
H	1.274735	1.270411	0.761731
H	0.424905	2.240594	1.979489
O	0.422074	3.061721	0.120459
H	0.465040	2.715232	-0.780429

F-4g (E_t = -955.997798)

C	2.253677	0.006300	1.999500
C	1.834412	1.949204	0.628422
C	2.587699	1.378264	-0.400170
C	3.181630	0.119445	-0.249049
C	3.001883	-0.557551	0.965138
C	1.660741	1.260189	1.829828
C	3.925661	-0.525554	-1.386779
H	2.120806	-0.535479	2.927248
H	3.457286	-1.532356	1.101120
H	4.385511	0.223680	-2.030615
H	4.711920	-1.184311	-1.019361
H	3.236794	-1.117917	-1.989404
H	2.724221	1.921818	-1.329104
H	1.373289	2.918186	0.485686
H	1.078816	1.700085	2.630027
C	-1.175329	0.221096	-1.039167
C	-1.989957	0.628518	0.178280
O	-2.661735	-0.553853	0.671805
C	-1.749438	-1.544220	1.142889
C	-0.860185	-2.018343	0.000903
C	-0.155040	-0.836688	-0.652664
H	-2.396185	-2.359905	1.479361
O	-0.913549	-1.071227	2.165273
H	-1.487452	-0.786229	2.889747
H	-0.128481	-2.739032	0.366346
O	-1.658150	-2.701099	-0.974051
H	-2.488483	-2.204678	-1.029867
H	0.566618	-0.399955	0.033858
O	0.570434	-1.249755	-1.812173
H	-0.018681	-1.883292	-2.253857

F-4h (E_t = -955.996394)

C	-3.482412	1.351153	-0.913236
C	-3.106996	-0.957880	-1.506690
C	-3.202201	-1.313853	-0.159389
C	-3.432488	-0.348362	0.829061
C	-3.571241	0.987961	0.431854
C	-3.242007	0.378500	-1.886982
C	-3.461150	-0.722687	2.285853
H	-3.595267	2.389395	-1.199832
H	-3.753231	1.748478	1.182877
H	-4.170357	-0.105711	2.836724
H	-3.745006	-1.766119	2.419298
H	-2.473299	-0.574746	2.722306
H	-3.111575	-2.355994	0.128666
H	-2.925900	-1.718624	-2.255441
H	-3.169465	0.657890	-2.930280
C	2.332825	0.795742	0.216533
C	2.627472	-0.653599	-0.139693
O	1.555620	-1.471378	0.382321
C	0.291489	-1.159733	-0.208884
C	-0.102188	0.264574	0.145749
C	0.977798	1.233740	-0.316611
H	-0.402476	-1.868606	0.249711
O	0.311026	-1.258114	-1.607745
H	0.531896	-2.173872	-1.826211
H	-1.064230	0.516037	-0.292506
O	-0.254927	0.373675	1.569195
H	0.444158	-0.181462	1.948738
H	1.018567	1.259233	-1.406816
O	0.705630	2.562981	0.124902
H	0.356661	2.449838	1.023506

H	-1.866375	-0.204850	-1.782264
O	-0.536781	1.370641	-1.587991
H	0.190780	1.027085	-2.128718
H	-1.319476	1.033599	0.940391
C	-3.065485	1.656519	-0.134694
H	-3.726215	1.749588	0.726757
H	-3.666309	1.299640	-0.981070
O	-2.504211	2.935731	-0.373613
H	-1.818061	2.807742	-1.044903

F-4i (E_t = -955.996296)

C	-1.839206	1.944037	-0.891751
C	-2.804400	1.264673	1.211342
C	-3.208608	0.059119	0.631002
C	-2.936948	-0.220855	-0.712798
C	-2.248213	0.741139	-1.466451
C	-2.114954	2.210033	0.452565
C	-3.331609	-1.534501	-1.332306
H	-1.310020	2.676448	-1.489468
H	-2.031798	0.540540	-2.510036
H	-3.781892	-1.384312	-2.313949
H	-2.452984	-2.166886	-1.458033
H	-4.052595	-2.061542	-0.708616
H	-3.740012	-0.672136	1.229550
H	-3.028782	1.460790	2.252624
H	-1.789460	3.139881	0.900167
C	1.499627	0.464166	0.755497
C	1.925004	0.230780	-0.689381
O	2.215884	-1.159633	-0.890947
C	1.125754	-2.021662	-0.613364
C	0.555144	-1.837170	0.785982
C	0.272153	-0.370316	1.055873
H	1.551403	-3.023430	-0.709411
O	0.057776	-1.809708	-1.515544
H	0.417689	-1.950843	-2.401653
H	-0.379770	-2.405717	0.853918
O	1.525932	-2.330295	1.697821
H	1.266924	-1.951204	2.551526
H	-0.547731	-0.026674	0.423650
O	-0.074153	-0.271495	2.438125
H	-0.093593	0.678871	2.622233
H	2.317029	0.140959	1.411701
O	1.133388	1.819157	1.010729
H	1.894818	2.353831	0.735249
H	1.109451	0.557535	-1.348318
C	3.220310	0.942780	-1.049499
H	3.503408	0.698475	-2.076595
H	4.010879	0.593508	-0.387251
O	3.133201	2.360256	-0.850980
H	2.311817	0.874620	1.313504
O	3.369591	1.623812	-0.306032
H	3.049775	2.531869	-0.193958
H	2.691552	-0.756948	-1.225393
C	3.916551	-1.167028	0.483501
H	3.970074	-2.246220	0.343238
H	3.890801	-0.970591	1.563304
O	5.057598	-0.605057	-0.139522
H	4.916484	0.353003	-0.152783

F-4j (E_t = -955.991840)

C	-3.639529	1.097496	1.153802
C	-2.225975	-0.752265	1.787987
C	-2.386191	-1.304593	0.516818
C	-3.170544	-0.667800	-0.454927
C	-3.794723	0.538061	-0.117072
C	-2.850736	0.455877	2.109406
C	-3.294576	-1.258697	-1.833473
H	-4.129871	2.032860	1.393508
H	-4.404520	1.045923	-0.855683
H	-3.994866	-0.690014	-2.443753
H	-2.321537	-1.258110	-2.324112
H	-3.647798	-2.289633	-1.787850
H	-1.897907	-2.241088	0.270802
H	-1.613019	-1.259363	2.523429
H	-2.727939	0.887566	3.094760
C	0.822834	-0.618946	-0.586622
C	0.928609	0.882396	-0.773187
O	1.608741	1.441897	0.376193
C	2.917273	0.947562	0.563200
C	2.951542	-0.572924	0.711263
C	2.209417	-1.226918	-0.442750
H	3.254599	1.431314	1.487140
O	3.769168	1.241730	-0.521195
H	3.706878	2.194167	-0.676034
H	3.993156	-0.907687	0.724013
O	2.259147	-0.990736	1.890953
H	2.829345	-0.826522	2.651656
H	2.761079	-1.068645	-1.370487
O	2.105973	-2.638279	-0.261369
H	1.864767	-2.743854	0.672095
H	0.251465	-0.811596	0.328278
O	0.168107	-1.173803	-1.723736
H	0.353282	-2.123977	-1.672218
H	1.494866	1.105940	-1.682164
C	-0.408266	1.591451	-0.818796
H	-0.981889	1.331623	0.075699
H	-0.964761	1.260743	-1.693303
O	-0.224280	2.997686	-0.939321

H	2.516484	2.702314	-1.511206	H	0.325012	3.238183	-0.181882

(v) Optimized coordinates of Tol : α-L-Fucose complexes

F-5a (E_t = -880.971685)				**F-5b** (E_t = -880.968121)			
C	2.583278	-0.060624	-1.550228	C	3.143247	1.470290	-0.278929
C	2.815684	1.229272	0.475175	C	2.984762	-0.424400	1.208673
C	2.557089	0.084046	1.230413	C	2.436197	-1.185344	0.174186
C	2.303866	-1.149609	0.612028	C	2.232412	-0.635352	-1.098535
C	2.321167	-1.202759	-0.787633	C	2.590798	0.704048	-1.307687
C	2.827891	1.160474	-0.920731	C	3.339845	0.907671	0.985065
C	2.016212	-2.371634	1.442856	C	1.601954	-1.445436	-2.200932
H	2.595024	-0.124553	-2.631269	H	3.429575	2.498127	-0.466999
H	2.142022	-2.150447	-1.284227	H	2.450605	1.143824	-2.289232
H	1.081065	-2.243400	1.987777	H	0.518232	-1.312322	-2.219055
H	2.810329	-2.543638	2.170089	H	1.809413	-2.507156	-2.069208
H	1.935809	-3.260327	0.817750	H	1.988940	-1.145064	-3.174307
H	2.566092	0.140882	2.314188	H	2.168642	-2.220033	0.356897
H	3.013250	2.170149	0.974342	H	3.131815	-0.871391	2.183741
H	3.022314	2.047207	-1.509631	H	3.776380	1.496718	1.782039
C	-1.270440	-0.319136	-1.305889	C	-0.447190	0.777559	0.736146
C	-1.475550	-1.440196	-0.295182	C	-0.866207	1.323888	-0.627366
O	-2.345483	-0.935451	0.745978	O	-2.264773	1.104718	-0.876569
C	-1.759560	0.110466	1.501615	C	-2.659098	-0.239209	-0.808069
C	-1.448371	1.298527	0.595323	C	-2.349030	-0.822515	0.565080
C	-0.623238	0.864553	-0.608210	C	-0.868136	-0.673029	0.869152
H	-2.515650	0.369015	2.248297	H	-3.737005	-0.232333	-0.994041
O	-0.577843	-0.341912	2.122787	O	-1.987323	-0.995212	-1.805053
H	0.001220	0.436360	2.170930	H	-2.080466	-1.916547	-1.513107
H	-2.395699	1.727991	0.247334	H	-2.934084	-0.282688	1.316639
O	-0.719159	2.249707	1.368217	O	-2.700019	-2.205939	0.527010
H	-0.304385	2.834437	0.715686	H	-2.260449	-2.595427	1.297695
H	0.371371	0.586530	-0.266823	H	-0.305845	-1.273872	0.155280
O	-0.451403	1.976189	-1.486502	O	-0.577386	-1.202055	2.161922
H	-1.285093	2.020766	-1.982033	H	-0.831883	-0.489049	2.768909
H	-0.634236	-0.647242	-2.131052	H	0.639403	0.849165	0.832322
O	-2.515070	0.094807	-1.886914	O	-1.096468	1.449461	1.828363
H	-3.163544	0.016588	-1.169764	H	-0.628160	2.277771	1.985291
H	-0.508410	-1.700194	0.140046	H	-0.275597	0.796681	-1.381787
C	-2.153059	-2.666681	-0.864135	C	-0.652103	2.816916	-0.750939
H	-3.103060	-2.400637	-1.321924	H	-1.270032	3.338005	-0.021690
H	-1.518386	-3.120445	-1.624797	H	0.397965	3.059021	-0.584456
H	-2.330315	-3.390751	-0.072139	H	-0.938840	3.153357	-1.744596

F-5c (E_t = -880.971016)	**F-5d** (E_t = -880.970864)

C	3.173191	-1.090257	-0.298775
C	2.330680	-0.262789	1.806549
C	2.096370	0.980803	1.217331
C	2.392007	1.210865	-0.134218
C	2.926870	0.154569	-0.883706
C	2.868875	-1.304409	1.047082
C	2.101085	2.546326	-0.767897
H	3.602906	-1.888495	-0.891698
H	3.174045	0.316211	-1.927368
H	2.340093	3.359981	-0.083158
H	1.046835	2.638276	-1.035854
H	2.692490	2.684016	-1.672485
H	1.695939	1.791555	1.817060
H	2.088929	-0.420539	2.849826
H	3.057724	-2.268305	1.502337
C	-0.724328	-0.114774	-1.280978
C	-0.484962	-1.402796	-0.505299
O	-1.738002	-1.771931	0.124848
C	-2.159340	-0.843781	1.103255
C	-2.401498	0.520009	0.462435
C	-1.176649	0.972377	-0.318809
H	-3.089591	-1.258368	1.503562
O	-1.179941	-0.729746	2.112393
H	-1.344342	0.135282	2.520527
H	-3.253569	0.439262	-0.222924
O	-2.688422	1.440012	1.513506
H	-2.609745	2.317816	1.111155
H	-0.375087	1.188914	0.387489
O	-1.470199	2.195378	-0.997525
H	-1.937264	1.914635	-1.801503
H	0.187449	0.199399	-1.792445
O	-1.728499	-0.283685	-2.292488
H	-2.363164	-0.911199	-1.912408
H	0.266516	-1.218657	0.263294
C	-0.078863	-2.572885	-1.372052
H	0.886459	-2.365586	-1.831490
H	0.004887	-3.469458	-0.761668
H	-0.811631	-2.744499	-2.157619

C	2.582020	-1.986905	-0.250774
C	3.323072	-0.178979	1.166541
C	2.955429	0.739881	0.181266
C	2.402300	0.312297	-1.034096
C	2.220379	-1.062760	-1.233303
C	3.133806	-1.546988	0.954201
C	1.973161	1.310500	-2.077650
H	2.429413	-3.044261	-0.426196
H	1.798011	-1.414976	-2.167795
H	1.987223	0.864034	-3.071656
H	2.637607	2.174166	-2.087064
H	0.961789	1.674405	-1.884802
H	3.114247	1.799789	0.348777
H	3.762214	0.170992	2.092917
H	3.420772	-2.261249	1.715514
C	-0.480118	-0.358309	0.984552
C	-0.435687	1.153045	1.165215
O	-1.785007	1.662351	1.024168
C	-2.323709	1.462860	-0.265217
C	-2.402868	-0.027147	-0.580470
C	-1.047437	-0.690668	-0.387386
H	-3.321403	1.910226	-0.228316
O	-1.519679	2.111031	-1.231777
H	-1.742196	1.672033	-2.068893
H	-3.128737	-0.490719	0.098210
O	-2.831990	-0.153253	-1.934511
H	-2.644806	-1.073474	-2.173426
H	-0.369106	-0.327786	-1.159581
O	-1.174344	-2.097679	-0.586031
H	-1.504156	-2.427571	0.265367
H	0.516428	-0.788973	1.084409
O	-1.302106	-0.980481	1.984910
H	-2.028746	-0.357175	2.139844
H	0.193285	1.582641	0.384282
C	0.050314	1.589019	2.529057
H	-0.558085	1.144473	3.313385
H	1.081751	1.266256	2.663399
H	-0.000694	2.672600	2.610401

F-5e (E_t = -880.971399)

C	3.249852	-0.958308	-0.474529
C	2.461389	-0.408467	1.738981
C	2.123300	0.871782	1.296317
C	2.346048	1.260215	-0.031969
C	2.907816	0.323626	-0.910691
C	3.025742	-1.329077	0.853256
C	1.961352	2.637077	-0.507769
H	3.694825	-1.662301	-1.166962
H	3.096541	0.608584	-1.939980

F-5f (E_t = -880.970787)

C	2.721775	0.768125	1.359074
C	3.240532	0.384878	-0.966437
C	2.714182	-0.903327	-0.868001
C	2.184648	-1.377656	0.340975
C	2.194679	-0.523629	1.450150
C	3.246355	1.226149	0.149874
C	1.625493	-2.772446	0.430072
H	2.728069	1.409517	2.231949
H	1.794709	-0.874716	2.395043

H	2.121353	3.375734	0.277600
H	0.910062	2.682689	-0.798065
H	2.559109	2.929778	-1.370347
H	1.696328	1.583952	1.993958
H	2.291140	-0.681765	2.773167
H	3.297949	-2.319751	1.195286
C	-0.739671	-0.053776	-1.312551
C	-0.408249	-1.372058	-0.628451
O	-1.533652	-1.865736	0.136724
C	-2.027133	-0.964618	1.092619
C	-2.414233	0.369675	0.473953
C	-1.228382	0.944437	-0.278498
H	-2.896751	-1.460508	1.531969
O	-1.072349	-0.640783	2.099014
H	-0.827807	-1.467591	2.535262
H	-3.231288	0.206016	-0.227480
O	-2.884024	1.296741	1.452119
H	-2.250129	1.230510	2.182274
H	-0.422005	1.150932	0.432178
O	-1.612132	2.134405	-0.971898
H	-2.168711	2.622946	-0.346338
H	0.180367	0.327345	-1.775481
O	-1.749618	-0.268688	-2.290649
H	-2.057373	0.620619	-2.521992
H	0.428855	-1.184283	0.049197
C	-0.060259	-2.470773	-1.607346
H	-0.897703	-2.642674	-2.278234
H	0.813020	-2.180536	-2.190392
H	0.166206	-3.388815	-1.068255
H	1.292328	-2.997374	1.442539
H	2.375219	-3.513602	0.150660
H	0.776577	-2.880462	-0.244550
H	2.725275	-1.556528	-1.734356
H	3.651162	0.730195	-1.907390
H	3.660090	2.224006	0.077596
C	-1.012094	1.121417	0.839007
C	-0.323444	1.375978	-0.494201
O	-1.182033	1.029384	-1.608057
C	-1.663807	-0.286937	-1.584240
C	-2.398310	-0.602759	-0.291834
C	-1.501631	-0.315799	0.899832
H	-2.333172	-0.364257	-2.445133
O	-0.625739	-1.261236	-1.671326
H	-0.127365	-1.072765	-2.477847
H	-3.275495	0.039902	-0.227411
O	-2.869569	-1.949611	-0.256250
H	-2.119687	-2.487488	-0.551179
H	-0.639835	-0.991884	0.876414
O	-2.238232	-0.471713	2.113057
H	-2.775162	-1.267576	1.982361
H	-0.275284	1.283048	1.637605
O	-2.114477	2.008786	0.977050
H	-2.626243	1.644982	1.715520
H	0.569698	0.748060	-0.526816
C	0.043726	2.828776	-0.696901
H	0.720936	3.151341	0.092894
H	0.540221	2.953833	-1.657441
H	-0.854251	3.440266	-0.670481

F-5g (E_t = -880.970688)

C	-2.892454	-0.851745	-1.332349
C	-3.335752	0.997662	0.154119
C	-2.724173	0.300198	1.198286
C	-2.193743	-0.981209	0.996599
C	-2.285194	-1.544269	-0.283402
C	-3.419146	0.423561	-1.116408
C	-1.499448	-1.715134	2.113988
H	-2.948803	-1.304812	-2.313982
H	-1.883176	-2.535908	-0.459258
H	-1.893866	-1.411153	3.083422
H	-0.426014	-1.514785	2.109689
H	-1.637712	-2.791886	2.017559
H	-2.671739	0.748111	2.184816
H	-3.750261	1.982173	0.333631
H	-3.894408	0.961314	-1.926974
C	0.377018	0.814556	-0.796615
C	0.642705	1.422077	0.573567
O	2.048432	1.387979	0.912317

F-5h (E_t = -880.970688)

C	-3.335756	0.997656	0.154143
C	-2.892452	-0.851723	-1.332357
C	-2.285187	-1.544262	-0.283423
C	-2.193736	-0.981222	0.996588
C	-2.724172	0.300178	1.198297
C	-3.419150	0.423576	-1.116394
C	-1.499436	-1.715162	2.113965
H	-3.750270	1.982163	0.333671
H	-2.671739	0.748076	2.184834
H	-0.426003	-1.514811	2.109664
H	-1.637699	-2.791913	2.017521
H	-1.893851	-1.411195	3.083404
H	-1.883164	-2.535896	-0.459296
H	-2.948800	-1.304775	-2.313998
H	-3.894416	0.961341	-1.926950
C	0.377017	0.814565	-0.796610
C	0.642706	1.422077	0.573576
O	2.048434	1.387973	0.912324

C	2.629553	0.112856	0.849380
C	2.442791	-0.535225	-0.512916
C	0.967665	-0.583619	-0.866154
H	3.689407	0.267629	1.066384
O	2.062385	-0.805657	1.783370
H	2.250272	-0.465003	2.668005
H	2.958852	0.070500	-1.256720
O	3.020101	-1.839313	-0.567041
H	2.718558	-2.280062	0.241559
H	0.445621	-1.232868	-0.155647
O	0.797492	-1.061204	-2.200796
H	1.433325	-1.786818	-2.291721
H	-0.707321	0.754635	-0.940748
O	0.980769	1.635514	-1.791298
H	0.956815	1.094591	-2.595046
H	0.087851	0.825509	1.304568
C	0.227787	2.874112	0.657130
H	0.777892	3.452385	-0.080093
H	-0.839315	2.960209	0.455106
H	0.434951	3.264765	1.651682

C	2.629551	0.112849	0.849380
C	2.442787	-0.535224	-0.512920
C	0.967661	-0.583611	-0.866158
H	3.689406	0.267618	1.066385
O	2.062381	-0.805667	1.783364
H	2.250268	-0.465019	2.668002
H	2.958850	0.070504	-1.256720
O	3.020093	-1.839313	-0.567052
H	2.718548	-2.280065	0.241547
H	0.445615	-1.232862	-0.155654
O	0.797486	-1.061188	-2.200802
H	1.433318	-1.786804	-2.291731
H	-0.707322	0.754647	-0.940743
O	0.980770	1.635528	-1.791287
H	0.956813	1.094612	-2.595040
H	0.087852	0.825506	1.304573
C	0.227792	2.874112	0.657148
H	-0.839310	2.960214	0.455128
H	0.434961	3.264759	1.651701
H	0.777896	3.452387	-0.080074

F-5i (E_t = -880.968719)

C	-2.200920	-2.018922	0.093169
C	-2.013616	-0.430749	1.903732
C	-2.830606	0.459605	1.202664
C	-3.342643	0.127096	-0.058640
C	-3.019109	-1.124801	-0.599812
C	-1.700357	-1.674741	1.350961
C	-4.257585	1.070544	-0.793974
H	-1.943461	-2.971676	-0.350533
H	-3.402091	-1.395535	-1.577497
H	-5.303105	0.864963	-0.558849
H	-4.053990	2.105698	-0.522246
H	-4.134594	0.973668	-1.871934
H	-3.075815	1.421445	1.639866
H	-1.630602	-0.157446	2.879466
H	-1.073543	-2.370154	1.895215
C	0.348482	0.349660	-0.730796
C	0.714490	1.462909	0.240405
O	2.127721	1.742594	0.085094
C	2.951338	0.655268	0.455336
C	2.661487	-0.551439	-0.432082
C	1.177034	-0.886978	-0.418299
H	3.974644	1.013604	0.307772
O	2.722464	0.318255	1.806198
H	3.032539	-0.597732	1.887846
H	2.963859	-0.312979	-1.458734
O	3.425439	-1.644470	0.073375
H	3.049510	-2.431172	-0.349147

F-5j (E_t = -880.969513)

C	2.316391	-1.914760	-0.579398
C	1.713492	-1.171238	1.634786
C	2.506039	-0.033341	1.464444
C	3.208178	0.183855	0.271946
C	3.106195	-0.775498	-0.744581
C	1.618214	-2.118411	0.613298
C	4.097667	1.387659	0.106305
H	2.257690	-2.648304	-1.374907
H	3.645174	-0.624830	-1.673550
H	4.103904	1.730512	-0.927693
H	5.126588	1.155469	0.385739
H	3.761825	2.212351	0.733819
H	2.577540	0.695391	2.264487
H	1.180317	-1.320837	2.565753
H	0.999854	-2.997356	0.740174
C	-0.895652	1.273831	0.507187
C	-0.173670	0.906462	-0.781251
O	-1.099895	0.458428	-1.799656
C	-1.918938	-0.612391	-1.410503
C	-2.706875	-0.297251	-0.149854
C	-1.759127	0.110205	0.964804
H	-2.586685	-0.785336	-2.258830
O	-1.184282	-1.792737	-1.101026
H	-0.643447	-2.001384	-1.874367
H	-3.377502	0.535528	-0.358018
O	-3.523019	-1.394041	0.260440
H	-2.944723	-2.169825	0.208030

H	0.912311	-1.262147	0.571084
O	0.922807	-1.946999	-1.339904
H	0.856488	-1.500164	-2.199251
H	-0.711500	0.109695	-0.663710
O	0.597520	0.739965	-2.090867
H	1.396739	1.288319	-2.053491
H	0.527272	1.118593	1.259446
C	-0.014424	2.761605	-0.021462
H	-1.083334	2.610152	0.123663
H	0.336327	3.528508	0.665661
H	0.153327	3.095252	-1.043011
H	-1.114949	-0.739000	1.219098
O	-2.503480	0.545386	2.103154
H	-3.237090	-0.082824	2.180100
H	-0.135913	1.479551	1.274147
O	-1.711581	2.416118	0.281658
H	-2.302159	2.446077	1.049786
H	0.516938	0.093519	-0.548588
C	0.570015	2.074320	-1.389429
H	1.086035	1.753820	-2.292897
H	-0.131732	2.867134	-1.634701
H	1.304806	2.454449	-0.680653

F-5k (E_t = -880.969378)

C	1.833371	-2.008034	0.288825
C	2.150578	-0.319272	1.985352
C	2.981685	0.392173	1.117953
C	3.246007	-0.079112	-0.174808
C	2.665636	-1.290655	-0.573069
C	1.574367	-1.523268	1.572555
C	4.172952	0.672763	-1.093037
H	1.386281	-2.937398	-0.040006
H	2.869072	-1.673926	-1.567543
H	4.110813	1.746048	-0.917531
H	3.926105	0.486573	-2.137633
H	5.209765	0.370013	-0.937934
H	3.426514	1.325655	1.444717
H	1.958915	0.060275	2.981566
H	0.935006	-2.079492	2.246586
C	-1.102734	1.102926	0.788615
C	-0.190945	1.116333	-0.429790
O	-0.930368	0.864954	-1.648910
C	-1.672695	-0.325718	-1.644192
C	-2.638959	-0.389828	-0.473041
C	-1.885558	-0.198771	0.831785
H	-2.208780	-0.332928	-2.597087
O	-0.860128	-1.488713	-1.516924
H	-0.211634	-1.461081	-2.232970
H	-3.364504	0.416045	-0.576645
O	-3.376703	-1.611592	-0.453278
H	-2.716239	-2.305326	-0.600015
H	-1.189793	-1.033642	0.972657
O	-2.807580	-0.113253	1.918868
H	-3.472842	-0.794464	1.739683
H	-0.471071	1.171080	1.685228
O	-2.002881	2.201139	0.716862
H	-2.683233	1.998825	1.377061
H	0.547266	0.323440	-0.293727
C	0.495567	2.448069	-0.635145

H	1.140910	2.399438	-1.510645
H	-0.249642	3.226235	-0.777506
H	1.102756	2.688718	0.236765

(vi) Optimized coordinates of Tol : β-L-fucose complexes

F-6a (E_t = -880.964512)				**F-6b** (E_t = -880.967603)			
C	2.982262	-0.342419	-1.303546	C	3.074498	-0.762341	1.055700
C	2.997327	-1.472352	0.831739	C	2.792795	-0.993186	-1.330199
C	2.747696	-0.257417	1.470894	C	2.399959	0.344819	-1.409706
C	2.603154	0.928989	0.736794	C	2.340848	1.150515	-0.263417
C	2.716758	0.868091	-0.657535	C	2.677674	0.574176	0.969429
C	3.125604	-1.517324	-0.559629	C	3.132024	-1.551226	-0.095155
C	2.400484	2.245851	1.439580	C	1.897606	2.587794	-0.351581
H	3.090663	-0.362938	-2.381696	H	3.339575	-1.183913	2.017341
H	2.608396	1.773993	-1.242661	H	2.646463	1.183061	1.866368
H	3.357399	2.680569	1.732602	H	2.338181	3.178399	0.451159
H	1.804880	2.121588	2.343604	H	0.812033	2.678498	-0.276300
H	1.894328	2.962480	0.794112	H	2.201930	3.029008	-1.300437
H	2.658230	-0.228806	2.551138	H	2.155793	0.775875	-2.374698
H	3.102086	-2.377809	1.415909	H	2.843678	-1.593815	-2.230166
H	3.344249	-2.455189	-1.055744	H	3.446052	-2.585497	-0.032003
C	-2.306387	1.052820	0.329052	C	-1.241239	-1.167906	-0.934253
C	-0.917377	1.402004	-0.191959	C	-0.511342	-1.507891	0.361244
O	-0.586814	0.424226	-1.194879	O	-1.109313	-0.836691	1.488364
C	-0.413408	-0.855264	-0.574071	C	-1.054313	0.567396	1.351999
C	-1.724487	-1.362110	0.004888	C	-1.847694	0.988719	0.125466
C	-2.327608	-0.340570	0.963462	C	-1.286389	0.341540	-1.120014
H	0.335302	-0.757082	0.223425	H	-0.019646	0.920704	1.277726
O	-0.006761	-1.775543	-1.540743	O	-1.591158	1.153213	2.512382
H	0.931946	-1.604206	-1.699914	H	-2.391745	0.643752	2.707529
H	-2.414668	-1.513853	-0.836264	H	-2.880656	0.646123	0.262893
O	-1.500407	-2.570084	0.712734	O	-1.789766	2.401242	-0.068778
H	-1.082059	-3.164101	0.073966	H	-2.035390	2.793766	0.781728
H	-1.727270	-0.345412	1.878152	H	-0.268733	0.714268	-1.281170
O	-3.650982	-0.679077	1.339853	O	-2.111349	0.609403	-2.254034
H	-4.191964	-0.394391	0.587228	H	-2.317558	1.554048	-2.212745
H	-2.651117	1.785331	1.062233	H	-0.680252	-1.610001	-1.769943
O	-3.253459	1.082681	-0.746941	O	-2.561555	-1.688460	-0.875575
H	-2.776065	0.704730	-1.503195	H	-3.032294	-1.241352	-1.595266
H	-0.194621	1.329153	0.632045	H	0.521785	-1.159420	0.254869
C	-0.829873	2.764259	-0.843696	C	-0.536071	-2.985318	0.681225
H	-1.567963	2.847697	-1.637620	H	-1.565116	-3.316989	0.791979
H	0.163073	2.908141	-1.264921	H	0.007199	-3.169908	1.605688
H	-1.022299	3.545134	-0.108426	H	-0.066201	-3.549156	-0.124064

F-6c (E_t = -880.967507)

C	-3.194832	-1.492791	0.165317
C	-2.290625	-0.297722	2.056915
C	-2.256250	0.871935	1.294270
C	-2.679201	0.878554	-0.042842
C	-3.153747	-0.319631	-0.591546
C	-2.754479	-1.487537	1.490639
C	-2.580792	2.128688	-0.875207
H	-3.571116	-2.406667	-0.277939
H	-3.501666	-0.330911	-1.618501
H	-3.297388	2.106663	-1.695562
H	-1.581456	2.228712	-1.299914
H	-2.780785	3.015385	-0.274107
H	-1.913038	1.796567	1.746212
H	-1.965808	-0.277644	3.090126
H	-2.789354	-2.394827	2.080551
C	1.509446	-1.504300	-0.126600
C	0.257991	-0.954817	-0.804100
O	0.479450	0.368730	-1.336574
C	0.893811	1.292926	-0.352063
C	2.205233	0.837382	0.262667
C	2.019625	-0.515727	0.911609
H	0.135614	1.415962	0.428826
O	1.034369	2.550407	-0.969233
H	1.488881	2.371936	-1.806372
H	2.943312	0.743668	-0.542814
O	2.644763	1.735001	1.277124
H	2.650034	2.613305	0.871311
H	1.282685	-0.416252	1.719888
O	3.256529	-1.019403	1.411765
H	3.677690	-0.275673	1.866266
H	1.238784	-2.442369	0.378282
O	2.512747	-1.729212	-1.107099
H	3.328745	-1.849124	-0.597747
H	-0.530985	-0.896285	-0.046483
C	-0.195611	-1.805001	-1.969015
H	-1.093221	-1.373757	-2.405804
H	-0.419752	-2.815475	-1.628386
H	0.592547	-1.849162	-2.715974

F-6d (E_t = -880.967018)

C	-3.230254	-1.195386	0.298401
C	-2.389397	-0.638158	-1.894075
C	-2.209207	0.684784	-1.484304
C	-2.537893	1.090357	-0.182548
C	-3.044178	0.128958	0.702540
C	-2.900676	-1.583780	-1.001730
C	-2.321882	2.514754	0.258494
H	-3.635806	-1.919142	0.994667
H	-3.314627	0.425704	1.710072
H	-1.295346	2.681054	0.590605
H	-2.985299	2.769534	1.084269
H	-2.521636	3.206979	-0.559246
H	-1.828316	1.417226	-2.188076
H	-2.139674	-0.927236	-2.907600
H	-3.048836	-2.608221	-1.319005
C	0.590617	0.145919	1.343216
C	0.403773	-1.242234	0.739096
O	1.584432	-1.669782	0.030700
C	1.926337	-0.792310	-1.021624
C	2.235793	0.584149	-0.453850
C	1.018237	1.122271	0.259388
H	1.122543	-0.720199	-1.766301
O	3.043970	-1.316872	-1.693745
H	3.639779	-1.622821	-0.994006
H	3.053715	0.472562	0.268075
O	2.564881	1.512643	-1.482299
H	3.264502	1.093641	-2.003312
H	0.211128	1.228623	-0.473517
O	1.293650	2.373693	0.891969
H	1.785900	2.893424	0.239578
H	-0.374957	0.469124	1.754376
O	1.582480	0.084978	2.359610
H	1.811394	1.010376	2.533846
H	-0.429102	-1.176338	0.028808
C	0.121462	-2.301969	1.779883
H	-0.788012	-2.051460	2.324644
H	0.951766	-2.356717	2.478954
H	-0.010815	-3.267513	1.295972

F-6e (E_t = -880.967183)

C	-2.772035	-1.044625	1.420008
C	-2.369370	-1.451532	-0.925042
C	-2.488410	-0.082225	-1.179291
C	-2.750718	0.823435	-0.143065
C	-2.893850	0.320640	1.157764
C	-2.503584	-1.935814	0.377998
C	-2.810881	2.304337	-0.401911

F-6f (E_t = -880.963849)

C	-2.070116	-1.929881	0.747604
C	-1.880024	-1.269270	-1.566572
C	-2.734166	-0.190601	-1.324881
C	-3.266655	0.035366	-0.048491
C	-2.926217	-0.851783	0.981738
C	-1.545602	-2.144197	-0.529871
C	-4.227687	1.168055	0.199205

H	-2.882309	-1.411458	2.432703
H	-3.102727	1.007202	1.970837
H	-1.851397	2.757875	-0.152812
H	-3.578727	2.778628	0.208788
H	-3.031608	2.513042	-1.448033
H	-2.390697	0.285883	-2.194934
H	-2.182281	-2.137020	-1.742980
H	-2.416133	-2.996508	0.577337
C	1.354406	-1.325907	0.439038
C	1.490380	-1.279442	-1.080735
O	2.057750	-0.033325	-1.526468
C	1.295586	1.086857	-1.123079
C	1.247146	1.144440	0.394184
C	0.591971	-0.106564	0.931480
H	0.276526	1.052742	-1.529681
O	1.896480	2.243202	-1.650312
H	2.846941	2.123095	-1.506686
H	2.279278	1.194519	0.761549
O	0.482515	2.261699	0.846021
H	0.860890	3.033550	0.400310
H	-0.436902	-0.147883	0.568788
O	0.625071	-0.134429	2.359065
H	0.322478	0.739843	2.643059
H	0.782966	-2.226657	0.704354
O	2.651304	-1.357879	1.019186
H	2.504494	-1.135972	1.951355
H	0.476700	-1.370330	-1.495063
C	2.387237	-2.370662	-1.622401
H	3.383081	-2.258473	-1.202701
H	2.440372	-2.302229	-2.706810
H	1.996248	-3.349316	-1.346363

F-6g (E_t = -880.966802)

C	2.332674	1.696000	0.882041
C	1.963526	-0.372154	2.072242
C	2.542305	-1.079175	1.015461
C	3.025256	-0.413545	-0.118993
C	2.916131	0.982626	-0.166533
C	1.850144	1.019015	2.004873
C	3.570967	-1.181892	-1.291967
H	2.251432	2.773846	0.820756
H	3.288387	1.515493	-1.034580
H	4.356681	-0.621514	-1.797903
H	2.771445	-1.371769	-2.008703
H	3.985337	-2.139259	-0.978255
H	2.629097	-2.158627	1.074902
H	1.610138	-0.903764	2.947693
H	1.406777	1.570121	2.824983
C	-0.994779	-1.387830	-0.405093
H	-1.820518	-2.606371	1.555941
H	-3.331134	-0.693249	1.975239
H	-4.076885	1.974624	-0.517243
H	-5.261036	0.830443	0.106048
H	-4.101894	1.577193	1.201014
H	-2.991933	0.482052	-2.135650
H	-1.482508	-1.430054	-2.561349
H	-0.882265	-2.980179	-0.713738
C	0.914029	1.247681	-0.854974
C	0.129585	1.113934	0.444545
O	1.088501	0.812278	1.479438
C	1.633859	-0.506136	1.312983
C	2.443572	-0.551964	0.032191
C	1.610845	-0.071834	-1.154743
H	0.801576	-1.223978	1.260821
O	2.484139	-0.755017	2.384220
H	1.942495	-0.734770	3.183797
H	3.292993	0.129900	0.175183
O	2.887221	-1.879626	-0.195289
H	3.252099	-1.863480	-1.092261
H	0.863526	-0.837903	-1.372158
O	2.446058	0.024784	-2.306713
H	2.887998	0.883027	-2.204543
H	0.258597	1.517513	-1.686170
O	1.898385	2.284333	-0.753584
H	2.229579	2.216621	0.156725
H	-0.577362	0.285013	0.348533
C	-0.597748	2.372941	0.858193
H	0.098280	3.205308	0.934757
H	-1.080571	2.220803	1.821548
H	-1.357522	2.619602	0.117367

F-6h (E_t = -880.965390)

C	-2.803381	-1.735615	0.572865
C	-1.785679	-1.330810	-1.578467
C	-2.245129	-0.011787	-1.543560
C	-2.980673	0.466235	-0.450953
C	-3.260149	-0.416682	0.601212
C	-2.063379	-2.197278	-0.518406
C	-3.506224	1.877604	-0.432487
H	-3.024110	-2.400450	1.398672
H	-3.831440	-0.064677	1.453115
H	-3.554701	2.264239	0.585030
H	-4.511658	1.926691	-0.853610
H	-2.869213	2.540684	-1.016737
H	-2.026534	0.655057	-2.370619
H	-1.218707	-1.681442	-2.432486
H	-1.708968	-3.220064	-0.543124
C	0.692482	1.410924	0.331891

C	-1.717404	-1.098688	0.908447
O	-2.584739	0.044482	0.797519
C	-1.895180	1.218228	0.413574
C	-1.268711	1.011008	-0.955091
C	-0.286853	-0.134598	-0.888448
H	-1.119988	1.491369	1.141005
O	-2.812761	2.282384	0.391689
H	-3.600435	1.930169	-0.048511
H	-2.072178	0.760028	-1.658668
O	-0.543985	2.163290	-1.375722
H	-1.157825	2.906554	-1.289665
H	0.505616	0.130843	-0.187335
O	0.259465	-0.420142	-2.179698
H	0.505819	0.440684	-2.548898
H	-0.241671	-2.166478	-0.216819
O	-1.942419	-1.820979	-1.371398
H	-1.478803	-1.741411	-2.218842
H	-0.942627	-0.880002	1.657069
C	-2.588219	-2.248875	1.363785
H	-3.346985	-2.444564	0.611164
H	-3.068697	-1.998646	2.307140
H	-1.985138	-3.146082	1.498561
C	0.197685	0.279308	1.227488
O	1.253803	-0.654909	1.528441
C	1.782291	-1.249705	0.361597
C	2.399882	-0.172263	-0.514753
C	1.349094	0.837541	-0.915560
H	1.012937	-1.799077	-0.195669
O	2.750326	-2.196000	0.742288
H	3.264459	-1.764777	1.440884
H	3.168884	0.337145	0.079031
O	2.939185	-0.717442	-1.715023
H	3.521884	-1.438760	-1.438199
H	0.592809	0.328577	-1.524639
O	1.930211	1.926275	-1.633404
H	2.544484	1.524300	-2.264363
H	-0.177675	2.011733	0.030603
O	1.629846	2.200118	1.050700
H	2.079553	2.723565	0.369904
H	-0.588410	-0.249106	0.680026
C	-0.330083	0.770632	2.556242
H	-0.688819	-0.072445	3.143256
H	-1.154338	1.464814	2.394594
H	0.462179	1.281024	3.097660

F-6i (E_t = -880.965303)

C	2.965148	-1.008663	0.917074
C	2.271447	-1.212658	-1.385717
C	2.243095	0.179517	-1.496979
C	2.566850	0.996393	-0.404630
C	2.932391	0.382329	0.800784
C	2.634970	-1.811083	-0.177169
C	2.581178	2.496887	-0.538608
H	3.242926	-1.462522	1.860075
H	3.184610	0.998234	1.656918
H	1.903582	2.828368	-1.324890
H	3.580212	2.857737	-0.788491
H	2.280405	2.976871	0.392490
H	1.965832	0.637717	-2.440382
H	2.012834	-1.827278	-2.239145
H	2.649479	-2.889631	-0.087750
C	-0.932835	0.982950	1.050161
C	-1.261532	1.487711	-0.352500
O	-2.201433	0.626923	-1.020451
C	-1.731074	-0.702003	-1.139102
C	-1.512000	-1.286595	0.246013
C	-0.481969	-0.466458	0.987031
H	-0.800056	-0.753132	-1.717736
O	-2.685034	-1.445799	-1.854641
H	-3.540266	-1.193745	-1.476055
H	-2.466466	-1.238655	0.785043

F-6j (E_t = -880.965303)

C	2.271144	-1.212465	-1.386033
C	2.965057	-1.009129	0.916751
C	2.932548	0.381897	0.800785
C	2.567017	0.996305	-0.404455
C	2.243035	0.179740	-1.496971
C	2.634643	-1.811236	-0.177648
C	2.581588	2.496827	-0.538096
H	2.012361	-1.826840	-2.239585
H	1.965786	0.638207	-2.440248
H	1.903684	2.828627	-1.323979
H	3.580575	2.857530	-0.788379
H	2.281359	2.976656	0.393255
H	3.184938	0.997557	1.657044
H	3.242830	-1.463256	1.859625
H	2.648948	-2.889807	-0.088474
C	-0.932853	0.983234	1.049930
C	-1.261604	1.487658	-0.352839
O	-2.201486	0.626678	-1.020571
C	-1.731087	-0.702261	-1.138919
C	-1.511957	-1.286517	0.246327
C	-0.481932	-0.466170	0.987121
H	-0.800084	-0.753501	-1.717565
O	-2.685045	-1.446256	-1.854254
H	-3.540274	-1.194141	-1.475701
H	-2.466409	-1.238482	0.785374

O	-1.016740	-2.620670	0.174414
H	-1.628644	-3.098025	-0.403719
H	0.465154	-0.531781	0.449001
O	-0.329952	-0.923228	2.331999
H	-0.255151	-1.886262	2.269652
H	-0.107090	1.590374	1.448270
O	-2.088595	1.100856	1.868219
H	-1.899165	0.538901	2.635172
H	-0.320873	1.484860	-0.920683
C	-1.877327	2.869423	-0.349144
H	-2.804778	2.848031	0.216513
H	-2.081846	3.186638	-1.369506
H	-1.196715	3.582116	0.115634

O	-1.016655	-2.620593	0.175028
H	-1.628558	-3.098104	-0.402978
H	0.465174	-0.531578	0.449073
O	-0.329853	-0.922621	2.332189
H	-0.255021	-1.885667	2.270064
H	-0.107123	1.590783	1.447881
O	-2.088599	1.101281	1.867987
H	-1.899126	0.539516	2.635068
H	-0.320959	1.484717	-0.921044
C	-1.877463	2.869341	-0.349781
H	-2.804905	2.848027	0.215893
H	-2.082010	3.186323	-1.370210
H	-1.196879	3.582169	0.114832

F-6k (E_t = -880.965001)

C	1.805346	-0.301087	-2.021039
C	2.517453	-1.862700	-0.323167
C	3.197939	-0.834513	0.332329
C	3.186779	0.472999	-0.171335
C	2.486479	0.723071	-1.359000
C	1.820767	-1.599309	-1.504972
C	3.950291	1.571000	0.520705
H	1.270767	-0.088268	-2.938919
H	2.471467	1.728261	-1.766088
H	3.491900	2.541995	0.337522
H	4.980409	1.617189	0.163851
H	3.979199	1.408273	1.597432
H	3.736385	-1.046191	1.249497
H	2.537580	-2.866866	0.082315
H	1.296867	-2.396000	-2.018180
C	-1.086074	-1.140667	0.894989
C	-0.177453	0.041231	1.221915
O	-0.894089	1.286569	1.122526
C	-1.385584	1.492776	-0.188232
C	-2.403853	0.422952	-0.522363
C	-1.740172	-0.935343	-0.464669
H	-0.548727	1.460424	-0.906158
O	-2.055937	2.721578	-0.236813
H	-1.422412	3.401985	0.025145
H	-3.188508	0.476799	0.238775
O	-2.931465	0.565924	-1.839217
H	-3.345580	1.439144	-1.867914
H	-0.972504	-0.978577	-1.246814
O	-2.700256	-1.976526	-0.640766
H	-3.269521	-1.682115	-1.366425
H	-0.465263	-2.047010	0.853479
O	-2.083772	-1.253598	1.898612
H	-2.761284	-1.824560	1.505512
H	0.635433	0.038721	0.487973

F-6l (E_t = -880.965063)

C	3.045881	0.330224	-1.285505
C	2.833286	-1.182667	0.583497
C	2.364845	-0.132986	1.375484
C	2.222597	1.158969	0.850390
C	2.571542	1.375249	-0.489649
C	3.179790	-0.952325	-0.749764
C	1.759176	2.295785	1.723832
H	3.303578	0.515431	-2.320663
H	2.468342	2.368539	-0.912655
H	0.981284	1.970465	2.414996
H	1.359634	3.113596	1.124811
H	2.583025	2.692570	2.319227
H	2.100177	-0.319529	2.410632
H	2.921885	-2.175459	1.005950
H	3.538446	-1.764891	-1.368378
C	-2.085501	0.807780	0.539944
C	-1.339004	1.286699	-0.703893
O	-1.132049	0.215846	-1.639874
C	-0.377410	-0.843277	-1.077131
C	-1.153556	-1.443029	0.082891
C	-1.374437	-0.393059	1.147832
H	0.606388	-0.504558	-0.747223
O	-0.149813	-1.806759	-2.075421
H	-1.004354	-1.924621	-2.516834
H	-2.129195	-1.770401	-0.298348
O	-0.443123	-2.517903	0.691374
H	-0.160883	-3.088948	-0.037488
H	-0.393156	-0.089650	1.532181
O	-2.201209	-0.890008	2.200202
H	-1.871858	-1.779659	2.392744
H	-2.092799	1.626831	1.273758
O	-3.409274	0.447731	0.173422
H	-3.734519	-0.075304	0.922119
H	-0.356814	1.652705	-0.372909

C	0.383731	-0.021053	2.624533
H	-0.431316	-0.009202	3.343294
H	1.034316	0.834182	2.798898
H	0.961056	-0.935898	2.753909

C	-2.085331	2.369919	-1.451377
H	-3.046915	1.983656	-1.777999
H	-1.507833	2.684809	-2.317899
H	-2.251969	3.229478	-0.802950