

Conformational and electronic effects on the regioselectivity of the glycosylation of different anomers of *N*-dimethylmaleoyl-protected glucosamine acceptors

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Supplementary Information

Supplementary Table 1. Relative zero-point energies (ΔE_{ZPE}), vibrational enthalpies (ΔH_{vib})^a and entropic terms^b ($-T\Delta S$) adding to the electronic energies to build the free energies of conformers **G1** and **T1** of DMM-protected glucosamine derivatives **7a**, **7b**, **8a** and **8b** and the three conformers of **12** calculated at the B3LYP/6-31+G** level. All energies are indicated in $\text{kJ}\cdot\text{mol}^{-1}$

Compound	ΔE	ΔE_{ZPE}	ΔH_{vib}	$-T\Delta S_{\text{vib}}$	$-T\Delta S_{\text{rot}}$	ΔG
7a G1-T1	-15.5	+0.5	-0.6	+2.4	-0.1	-13.2
8a G1-T1	-21.6	+1.3	-0.6	+1.8	-0.1	-19.2
7b G1-T1	+4.6	-2.2	+0.9	-2.0	-0.1	+1.2
8b G1-T1	-3.3	-1.2	+0.7	-1.7	-0.1	-5.7
12 G1- T1	+5.4	-0.8	-0.2	+1.0	-0.2	+5.1
12 G1' – T1	+8.7	-2.7	+1.2	-3.7	-0.2	+3.3

^a Relative change in vibrational enthalpies between 0 and 298.15 K (*i. e.*, excluding the zero-point energy). ^b At 298.15 K, splitted in rotational and vibrational terms.

Supplementary Table 2. Charge (q)^a and Fukui functions (f) on O3 and O4 calculated for the different conformers of DMM-protected glucosamine derivatives 7a, 7b, 8a and 8b at the B3LYP/6-31+G** level

	q_{O3}				q_{O4}				f_{O3}				f_{O4}			
	1 ^a	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
<u>7a</u>																
G1	-0.562	-0.691	-0.654	-0.721	-0.492	-0.671	-0.613	-0.671	0.055	0.011	0.000	0.007	0.040	0.027	0.024	0.029
G2	-0.560	-0.681	-0.693	-0.719	-0.492	-0.642	-0.630	-0.660	0.034	0.071	0.059	0.067	0.037	0.055	0.039	0.029
G3	-0.556	-0.700	-0.718	-0.709	-0.501	-0.684	-0.754	-0.688	0.050	0.067	0.060	0.070	0.035	0.044	0.031	0.045
T1	-0.500	-0.711	-0.667	-0.754	-0.482	-0.706	-0.754	-0.724	0.045	0.089	0.071	0.088	0.113	0.176	0.171	0.176
<u>8a</u>																
G1	-0.560	-0.676	-0.683	-0.732	-0.493	-0.638	-0.618	-0.668	0.047	0.071	0.054	0.069	0.051	0.065	0.060	0.066
G3	-0.555	-0.684	-0.757	-0.704	-0.495	-0.648	-0.688	0.663	0.052	0.071	0.065	0.071	0.058	0.073	0.062	0.073
T1	-0.496	-0.714	-0.694	-0.754	-0.465	-0.684	-0.709	-0.702	0.063	0.103	0.092	0.047	0.089	0.132	0.129	0.133
<u>7b</u>																
T1	-0.539	-0.660	-0.675	-0.719	-0.525	-0.690	-0.728	-0.702	0.059	0.075	0.066	0.077	0.052	0.101	0.084	0.099
G1	-0.527	-0.678	-0.663	-0.681	-0.503	-0.635	-0.692	-0.650	0.053	0.054	0.039	0.053	0.035	0.050	0.048	0.050
G2	-0.525	-0.660	-0.669	-0.679	-0.504	-0.641	-0.669	-0.654	0.041	0.054	0.042	0.052	0.021	0.038	0.024	0.033
G3	-0.522	-0.667	-0.657	-0.673	-0.511	-0.647	-0.713	-0.671	0.045	0.048	0.035	0.043	0.035	0.045	0.034	0.042
G4	-0.527	-0.659	-0.671	-0.710	-0.541	-0.654	-0.652	-0.663	0.036	0.050	0.044	0.054	0.023	0.053	0.037	0.051
G5	-0.526	-0.647	-0.700	-0.717	-0.541	-0.659	-0.689	-0.673	0.051	0.063	0.059	0.068	0.038	0.070	0.050	0.067
<u>8b</u>																
G1	-0.525	-0.651	-0.655	-0.666	-0.504	-0.615	-0.677	-0.648	0.056	0.090	0.059	0.078	0.044	0.077	0.070	0.068
T1	-0.532	-0.642	-0.657	-0.710	-0.516	-0.685	-0.691	-0.684	0.050	0.081	0.070	0.074	0.042	0.084	0.095	0.089
G3	-0.523	-0.644	-0.604	-0.671	-0.509	-0.624	-0.703	-0.648	0.056	0.056	0.040	-0.009	0.049	0.064	0.055	-0.003
G4	-0.523	-0.651	-0.695	-0.708	-0.545	-0.651	-0.667	-0.663	0.046	0.060	0.056	0.064	0.029	0.064	0.052	0.064

^a According to: (1) Mulliken, (2) Merz.Singh-Kollmann, (3) CHelp scheme and (4) CHelpG scheme of fitting charges (see text)

Supplementary Table 3. Charges (q)^a on O3 and O4 calculated for the different conformers of DMM-protected glucosamine derivatives **7a**, **7b**, **8a** and **8b** at the MP2/6-311++G**//B3LYP/6-31+G** level

	q_{O3} 1 ^a	2	3	4	q_{O4} 1	2	3	4
<u>7a</u>								
G1	-0.266	-0.744	-0.718	-0.775	-0.211	-0.723	-0.659	-0.721
G2	-0.262	-0.735	-0.756	-0.772	-0.199	-0.690	-0.670	-0.706
G3	-0.260	-0.754	-0.773	-0.764	-0.204	-0.736	-0.797	-0.738
T1	-0.225	-0.762	-0.721	-0.802	-0.176	-0.739	-0.781	-0.754
<u>8a</u>								
G1	-0.264	-0.734	-0.741	-0.788	-0.210	-0.691	-0.664	-0.719
G3	-0.262	-0.740	-0.810	-0.759	-0.190	-0.696	-0.727	.0.712
T1	-0.231	-0.761	-0.744	-0.799	-0.166	-0.723	-0.740	-0.737
<u>7b</u>								
T1	-0.228	-0.705	-0.713	-0.765	-0.231	-0.726	-0.754	-0.738
G1	-0.255	-0.726	-0.702	-0.725	-0.203	-0.685	-0.731	-0.695
G2	-0.245	-0.704	-0.712	-0.721	-0.198	-0.686	-0.712	-0.697
G3	-0.243	-0.714	-0.699	-0.716	-0.189	-0.698	-0.749	-0.717
G4	-0.231	-0.706	-0.726	-0.759	-0.248	-0.695	-0.696	-0.703
G5	-0.228	-0.697	-0.754	-0.769	-0.245	-0.701	-0.730	-0.712
<u>8b</u>								
G1	-0.252	-0.700	-0.699	-0.712	-0.202	-0.664	-0.726	-0.687
T1	-0.227	-0.686	-0.704	-0.754	-0.218	-0.726	-0.723	-0.727
G3	-0.249	-0.691	-0.649	-0.714	-0.178	-0.673	-0.738	-0.693
G4	-0.232	-0.702	-0.748	-0.758	-0.262	-0.692	-0.713	-0.704

^a According to: (1) Mulliken, (2) Merz.Singh-Kollmann, (3) CHelp scheme and (4) CHelpG scheme of fitting charges (see text)

Supplementary Table 4. Boltzmann-averaged charge (q) and Fukui functions on O3 and O4 calculated for DMM-protected glucosamine derivatives **7a**, **7b**, **8a** and **8b** at the B3LYP/6-31+G** level. Charges were also recalculated at the MP2/6-311++G** level.

	7a		8a		7b		8b	
	O3	O4	O3	O4	O3	O4	O3	O4
B3LYP/6-31+G**								
q Mulliken	-0.562	-0.492	-0.559	-0.493	-0.537	-0.521	-0.526	-0.509
q MK	-0.690	-0.668	-0.677	-0.639	-0.662	-0.681	-0.649	-0.630
q Chelp	-0.664	-0.625	-0.691	-0.625	-0.673	-0.721	-0.652	-0.682
q CHelpG	-0.720	-0.671	-0.729	-0.667	-0.712	-0.693	-0.677	-0.655
f Mulliken	0.0514	0.0398	0.0477	0.0517	0.0572	0.0490	0.0542	0.0430
f MK	0.0232	0.0323	0.0712	0.0661	0.0714	0.0915	0.0828	0.0761
f Chelp	0.0123	0.0270	0.0553	0.0602	0.0611	0.0767	0.0586	0.0714
f CHelpG	0.0202	0.0301	0.0694	0.0668	0.0725	0.0902	0.0668	0.0636
MP2/6-311++G**								
q Mulliken	-0.264	-0.207	-0.264	-0.205	-0.233	-0.224	-0.526	-0.509
q MK	-0.743	-0.716	-0.735	-0.692	-0.709	-0.717	-0.649	-0.630
q Chelp	-0.732	-0.675	-0.758	-0.679	-0.711	-0.748	-0.652	-0.682
q ChelpG	-0.773	-0.719	-0.781	-0.717	-0.756	-0.729	-0.677	-0.655
q_{O4}/q_{O3}^a								
Mulliken	0.877 (0.784)		0.882 (0.777)		0.972 (0.961)		0.968	
MK	0.968 (0.964)		0.944 (0.941)		1.029 (1.011)		0.971	
Chelp	0.942 (0.922)		0.904 (0.896)		1.071 (1.052)		1.046	
ChelpG	0.932 (0.930)		0.915 (0.918)		0.973 (0.964)		0.968	
f_{O4}/f_{O3}								
Mulliken	0.77		1.08		0.86		0.79	
MK	1.39		0.93		1.28		0.92	
Chelp	2.20		1.09		1.26		1.22	
ChelpG	1.49		0.96		1.24		0.95	
Rate_{O4/O3}^b								
	0.31		0.00		2.90		1.00	

^a In parentheses, value determined by the MP2/6-311++G** calculation. ^b Experimental rate for the analogs **2a**, **2b**, **3a** and **3b** (ref. 6).

Supplementary Table 5. Charge determined by Mulliken analysis on selected atoms of several conformers of different compounds at the B3LYP/6-31+G** level

	Conf	Char ^a	C1	C2	C3	C4	C5	O5	O1	O3	O4
7a	Avg	$\alpha/132$	0.01	-0.30	-0.46	0.49	0.06	-0.27	-0.23	-0.56	-0.49
8a	Avg	$\beta/131$	0.01	-0.29	-0.46	0.49	0.01	-0.26	-0.23	-0.56	-0.49
7b	Avg	$\beta/182$	0.36	-1.36	0.51	0.02	-0.11	-0.35	-0.25	-0.54	-0.52
8b	Avg	$\beta/186$	0.41	-1.15	0.33	-0.03	0.06	-0.35	-0.25	-0.53	-0.51
10a	-	$\alpha/158$	0.00	-0.40	-0.04	-0.37	-0.01	-0.29	-0.27	-	-
10b	-	$\beta/189$	0.24	-0.90	0.09	-0.31	-0.09	-0.36	-0.28	-	-
11a	Avg	$\alpha/158$	0.15	-0.38	-0.49	0.23	-0.29	-0.27	-0.25	-	-0.49
11b	Avg	$\beta/189$	0.35	-1.15	-0.10	0.13	-0.17	-0.35	-0.25	-	-0.49
12	G1	-/128	0.02	-0.29	-0.35	0.34	0.04	-0.31	-	-0.58	-0.50
12	G1'	-/176	0.07	-0.56	0.15	-0.09	0.01	-0.30	-	-0.53	-0.51
12	T	-/172	0.10	-0.88	0.49	0.05	-0.15	-0.31	-	-0.55	-0.54
13a	G1	$\alpha/-$	-0.01	-0.09	0.02	0.02	0.00	-0.30	-0.33	-0.55	-0.54
13b	G1	$\beta/-$	0.36	-0.40	0.14	-0.16	0.05	-0.35	-0.28	-0.55	-0.53

^aCharacteristics: α or β refer to the anomeric configuration, and the number after refers to the χ_2 angle (in °) of the DMM group

Supplementary Table 6. Charge determined by Mulliken analysis on selected atoms of several conformers of different compounds at the MP2/6-311++G**//B3LYP/6-31+G** level

	Conf	Char ^a	C1	C2	C3	C4	C5	O5	O1	O3	O4
7a	Avg	α /132	-0.54	-0.30	-0.40	-0.59 ^b	0.01	0.01	0.01	-0.26	-0.21
8a	Avg	β /131	-0.54	-0.28	-0.39	-0.60 ^b	-0.10	0.01	0.01	-0.26	-0.21
7b	Avg	β /182	-0.43	-0.71	-0.06	-0.60 ^b	-0.30	-0.12	-0.10	-0.23	-0.22
8b	Avg	β /186	-0.20	-0.96	-0.18	-0.59 ^b	-0.12	-0.11	-0.10	-0.25	-0.20
10a	-	α /158	-0.88	-0.12	0.02	-0.61	-0.14	-0.10	-0.07	-	-
10b	-	β /189	-0.39	-1.02	0.21	-0.58	-0.20	-0.19	-0.12	-	-
11a	Avg	α /158	-0.60	-0.38	-0.14	-0.57	-0.33	-0.02	-0.02	-	-0.18
11b	Avg	β /189	-0.31	-1.30	0.23	-0.58	-0.35	-0.12	-0.10	-	-0.19
12	G1	-/128	-0.17	-0.28	-0.27	-0.44	-0.23	-0.08	-	-0.28	-0.23
12	G1'	-/176	-0.04	-0.86	-0.26	-0.33	-0.21	-0.08	-	-0.25	-0.22
12	T	-/172	-0.08	-1.08	0.16	-0.57	-0.37	-0.11	-	-0.23	-0.24
13a	G1	α /-	-0.33	-0.57	-0.40	-0.13	-0.30	-0.03	-0.11	-0.29	-0.23
13b	G1	β /-	-0.10	-0.47	-0.48	-0.26	-0.30	-0.08	-0.16	-0.26	-0.23

^aCharacteristics: α or β refer to the anomeric configuration, and the number after refers to the χ_2 angle of the DMM group. ^balthough the average is similar for α - and β -anomers, the range is different: -0.67 to -0.32 for **7a/8a** and -1.06 to -0.49 for **7b/8b**.

Cartesian coordinates for the different conformers, as minimized at B3LYP/6-31+G** level

Compound **7a** - Conformer **G1**

C 0	-0.555644	-1.042418	-0.130910
C 0	0.212656	0.189286	-0.673312
C 0	-0.456137	1.473757	-0.157380
C 0	-1.936535	1.460691	-0.552741
C 0	-2.612678	0.206852	0.012435
C 0	-4.066807	0.083216	-0.402088
O 0	-1.921299	-0.954616	-0.480325
O 0	-0.338137	-1.106135	1.256516
N 0	1.649591	0.095989	-0.374334
O 0	0.108932	2.656850	-0.714841
O 0	-2.592158	2.609374	-0.034633
O 0	-4.687164	-0.913786	0.394428
C 0	2.443600	0.864453	0.475662
C 0	3.825924	0.266901	0.471937
C 0	3.832927	-0.773565	-0.382107
C 0	2.448398	-0.908338	-0.947938
O 0	2.110730	1.872749	1.083293
O 0	2.059713	-1.728170	-1.759277
C 0	-0.847313	-2.294454	1.866682
C 0	4.906968	0.864221	1.308137
C 0	4.921051	-1.704494	-0.799034
C 0	-6.046812	-1.115736	0.058167
H 0	-0.209106	-1.959587	-0.619833
H 0	0.119636	0.161523	-1.764206
H 0	-0.395421	1.511403	0.934474
H 0	-2.008604	1.446001	-1.652712
H 0	-2.562307	0.236486	1.108153
H 0	-4.121800	-0.186243	-1.469404
H 0	-4.561013	1.054730	-0.257708
H 0	0.869107	2.883517	-0.154374
H 0	-2.022150	3.366732	-0.237951
H 0	-0.578530	-2.238367	2.922954
H 0	-0.387381	-3.186504	1.418912
H 0	-1.935376	-2.358840	1.762866
H 0	5.855828	0.341586	1.170662
H 0	4.637574	0.829053	2.369758
H 0	5.047654	1.921545	1.058184
H 0	5.864800	-1.469000	-0.302767
H 0	5.072577	-1.658085	-1.883231
H 0	4.651472	-2.741001	-0.567235
H 0	-6.432349	-1.888123	0.727473
H 0	-6.157338	-1.455309	-0.983306
H 0	-6.636928	-0.195799	0.193286

Compound **7a** - Conformer **G2**

C 0	-0.657778	-0.959722	-0.027670
C 0	0.138773	0.218864	-0.639781
C 0	-0.472506	1.545739	-0.161536
C 0	-1.959120	1.569961	-0.531158
C 0	-2.679293	0.363256	0.082132
C 0	-4.145152	0.290815	-0.333154
O 0	-2.028084	-0.844781	-0.360189
O 0	-0.417153	-0.963050	1.356959
N 0	1.578004	0.083993	-0.371137
O 0	0.122176	2.684442	-0.777129
O 0	-2.566416	2.757390	-0.043234
O 0	-4.886012	-0.681696	0.389717
C 0	2.421810	0.858221	0.424552
C 0	3.783252	0.214776	0.404625
C 0	3.730639	-0.858246	-0.406555
C 0	2.326014	-0.968958	-0.925669
O 0	2.139575	1.898941	1.001812
O 0	1.885860	-1.807514	-1.690461
C 0	-0.927662	-2.110795	2.035808
C 0	4.907884	0.807612	1.184581
C 0	4.774846	-1.841213	-0.816422
C 0	-4.960325	-1.964763	-0.219578
H 0	-0.349067	-1.910119	-0.476864
H 0	0.017213	0.150120	-1.726042
H 0	-0.388877	1.623872	0.926560
H 0	-2.047942	1.521721	-1.629260
H 0	-2.627643	0.431399	1.176048
H 0	-4.214042	0.107989	-1.416372
H 0	-4.600002	1.260984	-0.114642
H 0	0.901069	2.907022	-0.241354
H 0	-1.979430	3.488711	-0.288795
H 0	-0.614702	-2.019100	3.077265
H 0	-0.509653	-3.032839	1.608134
H 0	-2.020915	-2.151483	1.983154
H 0	5.836064	0.251997	1.035929
H 0	4.672446	0.817051	2.254814
H 0	5.070843	1.850985	0.893177
H 0	5.744579	-1.607530	-0.372131
H 0	4.881511	-1.856638	-1.906715
H 0	4.487954	-2.855916	-0.518012
H 0	-5.611792	-2.571170	0.414597
H 0	-3.975825	-2.439603	-0.298543
H 0	-5.405677	-1.898531	-1.223835

Compound **7a** - Conformer **G3**

C 0	-0.538436	-1.095011	-0.274817
C 0	0.207528	0.183264	-0.733603
C 0	-0.534288	1.422037	-0.206644
C 0	-1.990152	1.371152	-0.679964
C 0	-2.650675	0.071991	-0.206738
C 0	-4.073351	-0.093613	-0.735723
O 0	-1.887282	-1.047244	-0.690479
O 0	-0.389666	-1.202774	1.119986
N 0	1.630427	0.130544	-0.365386
O 0	0.013543	2.645989	-0.687510
O 0	-2.717419	2.468523	-0.144562
O 0	-4.802211	-1.114493	-0.067220
C 0	2.351389	0.893520	0.551891
C 0	3.753854	0.346899	0.597009
C 0	3.842697	-0.659759	-0.292366
C 0	2.494281	-0.822228	-0.933239
O 0	1.950149	1.864267	1.179180
O 0	2.177627	-1.623881	-1.792448
C 0	-0.848435	-2.446579	1.653323
C 0	4.768476	0.951060	1.508148
C 0	4.984424	-1.534942	-0.685892
C 0	-5.449135	-0.682039	1.118511
H 0	-0.130549	-1.979414	-0.776313
H 0	0.169728	0.192753	-1.828142
H 0	-0.531464	1.417858	0.887640
H 0	-2.005761	1.405924	-1.781812
H 0	-2.658894	0.069094	0.891012
H 0	-4.021898	-0.388725	-1.788897
H 0	-4.596123	0.869199	-0.660679
H 0	0.736579	2.875757	-0.081003
H 0	-2.173085	3.257270	-0.290379
H 0	-0.655458	-2.413089	2.727043
H 0	-0.296069	-3.286067	1.208750
H 0	-1.919414	-2.586104	1.471845
H 0	5.741062	0.465689	1.404072
H 0	4.445780	0.870773	2.552268
H 0	4.884547	2.020425	1.300210
H 0	5.891433	-1.287866	-0.130322
H 0	5.191214	-1.438920	-1.757632
H 0	4.740634	-2.588643	-0.509911
H 0	-5.984503	-1.546101	1.518768
H 0	-6.169790	0.122735	0.909020
H 0	-4.737937	-0.323960	1.877207

Compound **7a** - Conformer **T1**

C 0	-0.399064	-1.318164	-0.070834
C 0	0.202636	-0.027066	-0.661660
C 0	-0.628825	1.211706	-0.272824
C 0	-2.088667	0.980940	-0.672047
C 0	-2.603852	-0.361471	-0.115910
C 0	-3.978271	-0.748613	-0.679924
O 0	-1.747566	-1.452619	-0.485919
O 0	-0.255657	-1.272549	1.326127
N 0	1.626550	0.091571	-0.327925
O 0	-0.138485	2.358970	-0.950685
O 0	-2.852722	2.056231	-0.145224
O 0	-4.993063	0.210265	-0.381257
C 0	2.276931	0.969818	0.542439
C 0	3.743559	0.621295	0.518882
C 0	3.924805	-0.388822	-0.352149
C 0	2.580916	-0.751733	-0.915581
O 0	1.774848	1.879036	1.183324
O 0	2.333679	-1.620509	-1.733199
C 0	-0.546917	-2.504558	1.983078
C 0	4.710254	1.380255	1.363954
C 0	5.154718	-1.113453	-0.785039
C 0	-5.626882	0.027495	0.881739
H 0	0.100761	-2.202608	-0.482330
H 0	0.154111	-0.135593	-1.750496
H 0	-0.596464	1.363575	0.808744
H 0	-2.148379	0.964729	-1.773024
H 0	-2.648040	-0.279618	0.978669
H 0	-4.260923	-1.741568	-0.304553
H 0	-3.915611	-0.802131	-1.771604
H 0	0.419790	2.842511	-0.326210
H 0	-3.785558	1.861713	-0.332703
H 0	-0.341052	-2.348073	3.043401
H 0	0.094214	-3.311539	1.601734
H 0	-1.596667	-2.790620	1.850851
H 0	5.732356	1.020705	1.227582
H 0	4.445512	1.294781	2.423821
H 0	4.677823	2.448250	1.121542
H 0	6.045125	-0.732346	-0.280556
H 0	5.296581	-1.018425	-1.867410
H 0	5.064746	-2.185478	-0.576574
H 0	-4.926663	0.157727	1.717163
H 0	-6.084728	-0.969325	0.944534
H 0	-6.409114	0.785980	0.952823

Compound **7b** - Conformer **G1**

C 0	0.582630	0.928355	-0.003738
C 0	-0.194594	-0.314858	-0.480786
C 0	0.475846	-1.577991	0.089246
C 0	1.967858	-1.597509	-0.252896
C 0	2.627967	-0.283784	0.192897
C 0	4.089762	-0.203003	-0.207840
O 0	1.934395	0.802387	-0.428410
O 0	0.019846	2.050193	-0.594267
N 0	-1.618825	-0.252909	-0.161131
O 0	-0.068951	-2.780639	-0.459261
O 0	2.616254	-2.682729	0.398139
O 0	4.695513	0.877929	0.481050
C 0	-2.182044	-0.075349	1.105777
C 0	-3.659027	0.140275	0.915202
C 0	-3.918608	0.126320	-0.407188
C 0	-2.622611	-0.103119	-1.136312
O 0	-1.575129	-0.101905	2.163837
O 0	-2.453948	-0.165671	-2.337231
C 0	0.561791	3.289895	-0.130640
C 0	-4.555472	0.326524	2.093174
C 0	-5.193759	0.291275	-1.163167
C 0	6.061935	1.040905	0.150231
H 0	0.560994	1.013468	1.096623
H 0	-0.143209	-0.336637	-1.573379
H 0	0.373055	-1.587027	1.182254
H 0	2.068805	-1.691544	-1.345728
H 0	2.562260	-0.197722	1.288737
H 0	4.159020	-0.055074	-1.297856
H 0	4.582216	-1.151403	0.050858
H 0	-0.963077	-2.911826	-0.118504
H 0	2.100585	-3.479692	0.206604
H 0	-0.004093	4.076638	-0.632080
H 0	1.622501	3.373663	-0.384811
H 0	0.436809	3.384986	0.957066
H 0	-5.594443	0.471218	1.789825
H 0	-4.238352	1.192515	2.684950
H 0	-4.502457	-0.540870	2.760753
H 0	-6.040808	0.460098	-0.494957
H 0	-5.397987	-0.596093	-1.772893
H 0	-5.120097	1.134567	-1.858801
H 0	6.193234	1.258782	-0.920976
H 0	6.647864	0.142974	0.401478
H 0	6.435081	1.885202	0.734125

Compound **7b** - Conformer **G2**

C 0	-0.676180	-0.850820	0.086308
C 0	0.125052	0.348301	-0.457544
C 0	-0.489537	1.650605	0.084446
C 0	-1.986140	1.706344	-0.228876
C 0	-2.687521	0.432406	0.268879
C 0	-4.164280	0.407757	-0.116499
O 0	-2.036411	-0.705143	-0.315392
O 0	-0.153926	-2.010619	-0.467143
N 0	1.554327	0.251207	-0.173093
O 0	0.082103	2.815155	-0.515710
O 0	-2.586952	2.831499	0.399091
O 0	-4.899025	-0.618379	0.531969
C 0	2.145957	0.097817	1.083766
C 0	3.611617	-0.161121	0.862235
C 0	3.836181	-0.195767	-0.466262
C 0	2.527238	0.043281	-1.168754
O 0	1.566949	0.170353	2.155329
O 0	2.327077	0.069784	-2.366098
C 0	-0.666958	-3.219926	0.093006
C 0	4.534075	-0.332829	2.022193
C 0	5.086264	-0.417177	-1.249185
C 0	-4.987324	-1.845328	-0.180965
H 0	-0.633595	-0.890362	1.188215
H 0	0.044548	0.333141	-1.548550
H 0	-0.362742	1.691564	1.174160
H 0	-2.104538	1.770202	-1.322410
H 0	-2.614242	0.381789	1.366400
H 0	-4.255268	0.324055	-1.210175
H 0	-4.604577	1.357796	0.198180
H 0	0.983152	2.935219	-0.189441
H 0	-2.055214	3.606684	0.166768
H 0	-0.100518	-4.033595	-0.362848
H 0	-1.730801	-3.340800	-0.134645
H 0	-0.521704	-3.237439	1.182008
H 0	5.560078	-0.517236	1.697136
H 0	4.209283	-1.168788	2.651744
H 0	4.523096	0.557903	2.660433
H 0	5.946411	-0.586241	-0.598015
H 0	5.296053	0.444975	-1.892281
H 0	4.973312	-1.279860	-1.915124
H 0	-4.005169	-2.311477	-0.317974
H 0	-5.450657	-1.695298	-1.167830
H 0	-5.626391	-2.503136	0.413048

Compound **7b** - Conformer **G3**

C 0	0.583830	0.956438	-0.180941
C 0	-0.178554	-0.338325	-0.526183
C 0	0.559580	-1.537992	0.094759
C 0	2.030275	-1.543628	-0.328347
C 0	2.677049	-0.183141	-0.027355
C 0	4.108739	-0.092403	-0.552752
O 0	1.913450	0.839285	-0.672634
O 0	-0.046528	2.017801	-0.813010
N 0	-1.585241	-0.291604	-0.133273
O 0	0.022170	-2.791965	-0.331706
O 0	2.749224	-2.551426	0.372755
O 0	4.817348	1.034820	-0.059919
C 0	-2.083727	-0.021257	1.144470
C 0	-3.572924	0.152931	1.018861
C 0	-3.902569	0.028359	-0.282008
C 0	-2.642906	-0.235513	-1.060934
O 0	-1.420405	0.049026	2.166158
O 0	-2.536586	-0.388366	-2.260753
C 0	0.485310	3.301686	-0.474545
C 0	-4.409060	0.418827	2.225669
C 0	-5.219962	0.109921	-0.976560
C 0	5.430659	0.830067	1.202447
H 0	0.620124	1.117507	0.910743
H 0	-0.184187	-0.437469	-1.615732
H 0	0.516534	-1.467453	1.189788
H 0	2.075632	-1.725600	-1.413822
H 0	2.669839	-0.025205	1.062944
H 0	4.068940	0.018916	-1.641299
H 0	4.638375	-1.023226	-0.309217
H 0	-0.854902	-2.912588	0.054547
H 0	2.257227	-3.378939	0.269129
H 0	-0.136621	4.034991	-0.990282
H 0	1.523851	3.395653	-0.805085
H 0	0.427968	3.471074	0.609915
H 0	-5.462283	0.544515	1.966182
H 0	-4.063476	1.321895	2.740837
H 0	-4.321384	-0.402044	2.946487
H 0	-6.033165	0.314570	-0.277041
H 0	-5.436518	-0.826190	-1.503490
H 0	-5.203238	0.897329	-1.738238
H 0	6.150693	-0.001319	1.165752
H 0	4.698127	0.622888	1.996141
H 0	5.961309	1.752687	1.448041

Compound **7b** - Conformer **G4**

C 0	0.635923	0.991657	-0.004697
C 0	-0.203791	-0.202260	-0.496893
C 0	0.393119	-1.507281	0.050103
C 0	1.885143	-1.602027	-0.284464
C 0	2.617019	-0.331745	0.192116
C 0	4.084494	-0.305389	-0.199105
O 0	1.989858	0.798322	-0.414940
O 0	0.148989	2.145480	-0.596601
N 0	-1.615080	-0.068519	-0.170648
O 0	-0.328395	-2.595272	-0.509942
O 0	2.351032	-2.788400	0.374078
O 0	4.742939	0.710000	0.532471
C 0	-2.177329	-0.004250	1.102085
C 0	-3.669125	0.096519	0.926942
C 0	-3.937521	0.091837	-0.393093
C 0	-2.632236	-0.015515	-1.135189
O 0	-1.561347	-0.020457	2.156169
O 0	-2.469418	-0.050016	-2.338794
C 0	0.726565	3.352189	-0.093788
C 0	-4.567409	0.179714	2.115266
C 0	-5.227709	0.169377	-1.137483
C 0	6.106000	0.853127	0.176235
H 0	0.606973	1.070932	1.095515
H 0	-0.157344	-0.209389	-1.590379
H 0	0.296228	-1.517210	1.145246
H 0	1.994626	-1.700904	-1.373728
H 0	2.547354	-0.267631	1.289391
H 0	4.166045	-0.120611	-1.282792
H 0	4.542597	-1.283847	0.023719
H 0	0.073709	-3.405818	-0.166137
H 0	3.108618	-3.151484	-0.099746
H 0	0.210589	4.170728	-0.598204
H 0	1.797811	3.396854	-0.312806
H 0	0.570173	3.434478	0.990867
H 0	-5.616844	0.256063	1.822633
H 0	-4.310592	1.047318	2.733373
H 0	-4.444698	-0.703012	2.752935
H 0	-6.079829	0.261643	-0.460607
H 0	-5.366996	-0.722912	-1.758266
H 0	-5.226067	1.025756	-1.820980
H 0	6.217200	1.126598	-0.884049
H 0	6.671402	-0.073256	0.364091
H 0	6.516484	1.652364	0.796727

Compound **7b** - Conformer **G5**

C 0	-0.731896	-0.908869	0.069876
C 0	0.135848	0.241910	-0.472429
C 0	-0.399628	1.578366	0.059723
C 0	-1.891944	1.721250	-0.250636
C 0	-2.669174	0.491474	0.261424
C 0	-4.146805	0.534885	-0.120655
O 0	-2.090516	-0.683215	-0.318637
O 0	-0.291883	-2.093722	-0.497021
N 0	1.548750	0.063605	-0.176616
O 0	0.351552	2.626775	-0.535405
O 0	-2.303669	2.935942	0.391800
O 0	-4.942798	-0.424946	0.550939
C 0	2.138276	0.007067	1.084042
C 0	3.621950	-0.140863	0.877174
C 0	3.859558	-0.170223	-0.448554
C 0	2.541059	-0.038779	-1.162957
O 0	1.546714	0.059879	2.150918
O 0	2.350449	-0.024390	-2.362827
C 0	-0.843602	-3.274328	0.084633
C 0	4.544906	-0.227619	2.046136
C 0	5.129232	-0.301406	-1.220182
C 0	-5.085930	-1.673415	-0.117669
H 0	-0.682563	-0.956825	1.170784
H 0	0.062553	0.226246	-1.564401
H 0	-0.281318	1.605534	1.152435
H 0	-2.015472	1.803962	-1.339955
H 0	-2.594135	0.449521	1.359372
H 0	-4.243466	0.430511	-1.212756
H 0	-4.546775	1.511554	0.173855
H 0	-0.013537	3.458870	-0.201814
H 0	-3.044759	3.327148	-0.085855
H 0	-0.331955	-4.115810	-0.385303
H 0	-1.919187	-3.346395	-0.107977
H 0	-0.663671	-3.296022	1.168347
H 0	5.584994	-0.335672	1.731121
H 0	4.280748	-1.078152	2.684574
H 0	4.459251	0.668259	2.671357
H 0	5.994217	-0.402103	-0.561053
H 0	5.278492	0.571893	-1.865130
H 0	5.087847	-1.173060	-1.882852
H 0	-4.129226	-2.197642	-0.214149
H 0	-5.519777	-1.535380	-1.119320
H 0	-5.773408	-2.268952	0.487335

Compound **7b** - Conformer **T1**

C 0	0.478753	1.280457	0.019906
C 0	-0.183321	0.008801	-0.545731
C 0	0.620895	-1.228461	-0.119615
C 0	2.088178	-1.064432	-0.514984
C 0	2.645162	0.259800	0.035272
C 0	4.062054	0.562661	-0.469155
O 0	1.838713	1.342723	-0.427430
O 0	-0.200817	2.383371	-0.468059
N 0	-1.585497	-0.094760	-0.171027
O 0	0.043024	-2.369236	-0.739315
O 0	2.773158	-2.202841	0.002464
O 0	4.996225	-0.460695	-0.120851
C 0	-2.101479	-0.190260	1.118902
C 0	-3.596341	-0.316119	0.994301
C 0	-3.911809	-0.287390	-0.314990
C 0	-2.635738	-0.142452	-1.100314
O 0	-1.450777	-0.164078	2.152084
O 0	-2.516872	-0.073302	-2.307313
C 0	0.169095	3.624724	0.132400
C 0	-4.450211	-0.440763	2.211479
C 0	-5.226479	-0.371468	-1.014305
C 0	5.606352	-0.295716	1.157169
H 0	0.474011	1.271045	1.122995
H 0	-0.178845	0.089113	-1.637204
H 0	0.574889	-1.333349	0.973928
H 0	2.155370	-1.043396	-1.614473
H 0	2.632926	0.219005	1.137116
H 0	4.392269	1.537384	-0.086096
H 0	4.046954	0.612093	-1.562554
H 0	0.619226	-3.121861	-0.541695
H 0	3.723600	-2.061128	-0.142343
H 0	-0.512296	4.375252	-0.271467
H 0	1.200766	3.893317	-0.117144
H 0	0.054731	3.577930	1.224432
H 0	-5.511233	-0.486207	1.956588
H 0	-4.286228	0.407315	2.885540
H 0	-4.187168	-1.342164	2.776722
H 0	-6.054512	-0.460945	-0.307824
H 0	-5.246843	-1.233503	-1.690567
H 0	-5.388212	0.515453	-1.637067
H 0	4.873950	-0.347536	1.973358
H 0	6.139837	0.662941	1.209937
H 0	6.323409	-1.111262	1.270365

Compound **8a** - Conformer **G1**

C 0	-0.358102	-1.001439	-0.053354
C 0	0.423921	0.201674	-0.637657
C 0	-0.198548	1.511256	-0.125184
C 0	-1.686792	1.529985	-0.489243
C 0	-2.382436	0.299347	0.103841
C 0	-3.836941	0.217443	-0.309316
O 0	-1.732616	-0.889227	-0.373517
O 0	-0.112825	-1.043179	1.328846
N 0	1.864713	0.076016	-0.376862
O 0	0.379979	2.670519	-0.714381
O 0	-2.309938	2.693085	0.033323
O 0	-4.469767	-0.797824	0.509704
C 0	2.702861	0.840210	0.434358
C 0	4.071065	0.212823	0.393983
C 0	4.027487	-0.840882	-0.442899
C 0	2.622371	-0.955341	-0.959444
O 0	2.410085	1.863295	1.037558
O 0	2.187436	-1.780212	-1.741501
C 0	-0.595981	-2.225741	1.969884
C 0	5.192051	0.799072	1.184117
C 0	5.081200	-1.801460	-0.880395
C 0	-5.742819	-1.095625	0.211611
O 0	-6.402657	-0.594883	-0.669502
H 0	-0.045848	-1.935221	-0.533033
H 0	0.299067	0.158610	-1.724931
H 0	-0.112008	1.563257	0.964419
H 0	-1.781661	1.506447	-1.587139
H 0	-2.318739	0.350174	1.198321
H 0	-3.931196	-0.059529	-1.362795
H 0	-4.333470	1.175637	-0.140947
H 0	1.160008	2.887672	-0.177787
H 0	-1.741231	3.442555	-0.200301
H 0	-0.299942	-2.152140	3.017638
H 0	-0.142254	-3.121157	1.523222
H 0	-1.686183	-2.299881	1.897647
H 0	6.124716	0.254942	1.021926
H 0	4.958801	0.783988	2.254736
H 0	5.345475	1.849681	0.914274
H 0	6.047461	-1.574179	-0.425446
H 0	5.191792	-1.780716	-1.970262
H 0	4.801545	-2.827502	-0.616092
H 0	-6.102914	-1.875280	0.898512

Compound **8a** - Conformer **G3**

C 0	-0.366213	-1.054490	-0.325614
C 0	0.417749	0.211269	-0.754698
C 0	-0.310197	1.462523	-0.235950
C 0	-1.752888	1.444781	-0.752384
C 0	-2.450972	0.157580	-0.296981
C 0	-3.856044	0.053150	-0.867153
O 0	-1.706305	-0.974070	-0.775402
O 0	-0.256473	-1.174845	1.069764
N 0	1.828905	0.123825	-0.352802
O 0	0.273534	2.676138	-0.697138
O 0	-2.475170	2.556892	-0.251399
O 0	-4.536143	-1.136382	-0.394049
C 0	2.546351	0.870083	0.581788
C 0	3.936814	0.296423	0.651628
C 0	4.023953	-0.708135	-0.240513
C 0	2.685499	-0.843165	-0.907510
O 0	2.150694	1.845409	1.204791
O 0	2.369246	-1.636129	-1.775082
C 0	-0.727849	-2.420784	1.585417
C 0	4.944601	0.877304	1.585105
C 0	5.156780	-1.602583	-0.616067
C 0	-5.284249	-1.026932	0.716418
O 0	-5.437230	-0.032313	1.386224
H 0	0.032751	-1.943405	-0.825687
H 0	0.406410	0.231345	-1.849771
H 0	-0.336791	1.452466	0.857905
H 0	-1.730157	1.468651	-1.854753
H 0	-2.497667	0.146199	0.798837
H 0	-3.815788	-0.063380	-1.952180
H 0	-4.427687	0.941111	-0.593647
H 0	0.983020	2.891567	-0.069681
H 0	-1.909869	3.334588	-0.375462
H 0	-0.558007	-2.394230	2.663001
H 0	-0.168795	-3.258607	1.146498
H 0	-1.795596	-2.556979	1.383074
H 0	5.911081	0.377433	1.494060
H 0	4.602380	0.793849	2.622754
H 0	5.080850	1.946295	1.387981
H 0	6.057979	-1.372859	-0.043913
H 0	5.384168	-1.507621	-1.683706
H 0	4.891585	-2.652271	-0.447168
H 0	-5.749441	-2.000690	0.928881

Compound 8a - Conformer T1				Compound 8b - Conformer G1			
C 0	-0.236840	-1.247033	-0.214030	C 0	-0.369268	-0.898898	0.033595
C 0	0.426996	0.053896	-0.706308	C 0	0.417685	0.330933	-0.461561
C 0	-0.376084	1.290999	-0.259906	C 0	-0.217637	1.607979	0.118967
C 0	-1.835432	1.142487	-0.702332	C 0	-1.714805	1.654913	-0.196465
C 0	-2.410367	-0.222117	-0.266228	C 0	-2.388937	0.352772	0.262515
C 0	-3.763337	-0.555926	-0.899134	C 0	-3.851762	0.310024	-0.129132
O 0	-1.572375	-1.304446	-0.693985	O 0	-1.731998	-0.751210	-0.361550
O 0	-0.154222	-1.281519	1.184435	O 0	0.159700	-2.028853	-0.568151
N 0	1.842326	0.103452	-0.321461	N 0	1.845457	0.244102	-0.168776
O 0	0.161175	2.462761	-0.853565	O 0	0.337111	2.798129	-0.442883
O 0	-2.557345	2.208324	-0.097331	O 0	-2.338270	2.743521	0.470308
O 0	-4.783209	0.402101	-0.507805	O 0	-4.462305	-0.798115	0.576552
C 0	2.496312	0.913769	0.610209	C 0	2.428164	0.054698	1.087646
C 0	3.947676	0.507161	0.618980	C 0	3.897916	-0.181860	0.870484
C 0	4.119885	-0.468095	-0.292861	C 0	4.134229	-0.169920	-0.456531
C 0	2.783700	-0.749669	-0.917285	C 0	2.829388	0.079667	-1.162607
O 0	2.008514	1.814436	1.274167	O 0	1.838499	0.085878	2.155447
O 0	2.531383	-1.565247	-1.786275	O 0	2.638454	0.144977	-2.359717
C 0	-0.526321	-2.531847	1.766758	C 0	-0.378975	-3.262340	-0.084567
C 0	4.912979	1.187094	1.530265	C 0	4.812382	-0.382826	2.032063
C 0	5.335035	-1.221164	-0.718638	C 0	5.393197	-0.352591	-1.235107
C 0	-5.541656	0.095086	0.566879	C 0	-5.747640	-1.050747	0.288736
O 0	-5.456304	-0.907507	1.232506	O 0	-6.432334	-0.440468	-0.499436
H 0	0.245694	-2.125154	-0.657835	H 0	-0.327168	-0.983288	1.133196
H 0	0.409234	0.014998	-1.800805	H 0	0.345276	0.351928	-1.553113
H 0	-0.364087	1.372539	0.829791	H 0	-0.094499	1.616299	1.209921
H 0	-1.872635	1.222135	-1.800868	H 0	-1.833893	1.752229	-1.286995
H 0	-2.505027	-0.224269	0.827209	H 0	-2.308555	0.274702	1.358245
H 0	-4.072442	-1.559294	-0.603797	H 0	-3.961695	0.156746	-1.206144
H 0	-3.707078	-0.487372	-1.987698	H 0	-4.349739	1.238798	0.157285
H 0	0.731012	2.880193	-0.192263	H 0	1.239129	2.916920	-0.118699
H 0	-3.471127	2.176379	-0.411187	H 0	-1.830888	3.540674	0.258786
H 0	-0.342108	-2.440556	2.838326	H 0	0.174866	-4.055478	-0.589009
H 0	0.085131	-3.347956	1.357923	H 0	-1.443889	-3.344900	-0.321387
H 0	-1.584989	-2.754303	1.594545	H 0	-0.235756	-3.348774	1.001495
H 0	5.923536	0.789897	1.414230	H 0	5.842282	-0.549258	1.709768
H 0	4.605716	1.068255	2.575283	H 0	4.489038	-1.240430	2.632533
H 0	4.933991	2.264812	1.333885	H 0	4.789617	0.487495	2.697589
H 0	6.221467	-0.899473	-0.167962	H 0	6.248778	-0.538039	-0.582443
H 0	5.517867	-1.083014	-1.790158	H 0	5.601453	0.533989	-1.844623
H 0	5.196293	-2.296984	-0.563324	H 0	5.293596	-1.191456	-1.932811
H 0	-6.262947	0.905924	0.739558	H 0	-6.090643	-1.908570	0.885072

Compound **8b** - Conformer **G3**

C 0	-0.417671	-0.906326	-0.279639
C 0	0.384783	0.381580	-0.553381
C 0	-0.344698	1.579922	0.082197
C 0	-1.798222	1.633502	-0.395644
C 0	-2.481966	0.281358	-0.138309
C 0	-3.898881	0.262462	-0.690741
O 0	-1.734274	-0.739326	-0.802031
O 0	0.203247	-1.956700	-0.936249
N 0	1.774967	0.284822	-0.117492
O 0	0.235654	2.831066	-0.289815
O 0	-2.520899	2.648738	0.283293
O 0	-4.562601	-0.996608	-0.422424
C 0	2.223938	-0.040014	1.165970
C 0	3.712988	-0.238677	1.084358
C 0	4.089210	-0.075819	-0.199719
C 0	2.862293	0.239570	-1.010973
O 0	1.523182	-0.134174	2.160181
O 0	2.798759	0.434440	-2.207670
C 0	-0.352197	-3.242985	-0.650115
C 0	4.502067	-0.562398	2.308602
C 0	5.427822	-0.160123	-0.852075
C 0	-5.220461	-1.115757	0.742803
O 0	-5.301868	-0.277176	1.609787
H 0	-0.489970	-1.108165	0.802992
H 0	0.429496	0.518581	-1.638015
H 0	-0.342638	1.476466	1.175259
H 0	-1.794397	1.823658	-1.480975
H 0	-2.511523	0.093030	0.945446
H 0	-3.878193	0.336885	-1.779821
H 0	-4.470547	1.084679	-0.257891
H 0	1.086798	2.935232	0.154543
H 0	-2.000791	3.463246	0.221172
H 0	0.279076	-3.969205	-1.164393
H 0	-1.379573	-3.317700	-1.019024
H 0	-0.333382	-3.441840	0.430523
H 0	5.561649	-0.696293	2.081246
H 0	4.124589	-1.477565	2.778034
H 0	4.401757	0.233136	3.055648
H 0	6.212312	-0.405888	-0.133336
H 0	5.680684	0.789156	-1.337640
H 0	5.422014	-0.919963	-1.641402
H 0	-5.685756	-2.111053	0.789500

Compound **8b** - Conformer **G4**

C 0	0.408473	0.987618	-0.000041
C 0	-0.430722	-0.208778	-0.487674
C 0	0.152775	-1.512845	0.077426
C 0	1.646803	-1.620144	-0.245706
C 0	2.377009	-0.349767	0.234655
C 0	3.843864	-0.351164	-0.142903
O 0	1.771528	0.782276	-0.385920
O 0	-0.061697	2.133703	-0.615921
N 0	-1.842970	-0.063028	-0.174470
O 0	-0.570988	-2.599868	-0.478835
O 0	2.116565	-2.798074	0.423257
O 0	4.490091	0.735685	0.559430
C 0	-2.414527	0.013068	1.093536
C 0	-3.904503	0.114152	0.906564
C 0	-4.163492	0.097248	-0.415503
C 0	-2.853441	-0.019128	-1.147450
O 0	-1.804726	0.005092	2.151498
O 0	-2.680483	-0.066746	-2.348869
C 0	0.502804	3.348105	-0.116579
C 0	-4.811491	0.210087	2.087265
C 0	-5.448248	0.169216	-1.169665
C 0	5.810197	0.866860	0.354719
O 0	6.489796	0.157621	-0.350774
H 0	0.364752	1.082098	1.098343
H 0	-0.374823	-0.227486	-1.580753
H 0	0.047245	-1.511422	1.171845
H 0	1.764712	-1.721299	-1.333227
H 0	2.288962	-0.282656	1.330800
H 0	3.968096	-0.206203	-1.220278
H 0	4.320019	-1.290114	0.152139
H 0	-0.200000	-3.410383	-0.101917
H 0	2.788021	-3.236972	-0.112434
H 0	-0.011300	4.159031	-0.634689
H 0	1.576189	3.397826	-0.324163
H 0	0.332516	3.439113	0.965174
H 0	-5.858814	0.280659	1.785990
H 0	-4.561205	1.085869	2.696482
H 0	-4.691768	-0.664435	2.736642
H 0	-6.305013	0.269007	-0.499841
H 0	-5.584168	-0.728829	-1.782821
H 0	-5.440654	1.018957	-1.861333
H 0	6.184339	1.723759	0.932543

Compound **8b** - Conformer **T1**

C 0	0.311074	1.232984	-0.129622
C 0	-0.410723	-0.049167	-0.584059
C 0	0.371215	-1.277995	-0.096884
C 0	1.830871	-1.198488	-0.548804
C 0	2.450156	0.146763	-0.124175
C 0	3.840109	0.406012	-0.708718
O 0	1.653174	1.211836	-0.638813
O 0	-0.346860	2.325111	-0.663086
N 0	-1.800688	-0.084594	-0.158357
O 0	-0.262364	-2.439362	-0.613740
O 0	2.476972	-2.324574	0.046119
O 0	4.782448	-0.617971	-0.289304
C 0	-2.273833	-0.091959	1.151798
C 0	-3.774185	-0.189295	1.084261
C 0	-4.133706	-0.232531	-0.213477
C 0	-2.882805	-0.167370	-1.048025
O 0	-1.585849	-0.021671	2.158072
O 0	-2.802476	-0.179555	-2.260105
C 0	0.084245	3.588628	-0.152975
C 0	-4.588142	-0.220978	2.334239
C 0	-5.473213	-0.328060	-0.862361
C 0	5.568100	-0.342329	0.776864
O 0	5.561987	0.679634	1.416274
H 0	0.357052	1.295165	0.970473
H 0	-0.441164	-0.043621	-1.678132
H 0	0.360010	-1.301980	1.002226
H 0	1.862504	-1.273482	-1.646854
H 0	2.499732	0.191719	0.975407
H 0	4.201010	1.386473	-0.396422
H 0	3.810884	0.346362	-1.798740
H 0	0.275690	-3.199697	-0.349919
H 0	3.404237	-2.334044	-0.228618
H 0	-0.579571	4.336480	-0.589320
H 0	1.118195	3.799978	-0.443671
H 0	-0.003523	3.615741	0.941770
H 0	-5.657829	-0.260976	2.117781
H 0	-4.385970	0.663596	2.948335
H 0	-4.322016	-1.090885	2.945455
H 0	-6.278538	-0.346390	-0.124908
H 0	-5.538562	-1.233460	-1.476303
H 0	-5.633867	0.518367	-1.539304
H 0	6.225300	-1.202069	0.967546

Compound **9**

C 0	1.851384	0.047288	-1.249948
C 0	1.161894	-0.470566	0.027293
C 0	1.850936	0.095157	1.281056
C 0	3.364136	-0.167957	1.202067
C 0	3.923748	0.317476	-0.135971
O 0	3.234950	-0.282720	-1.234532
N 0	-0.279675	-0.201484	0.003047
C 0	-0.907482	1.047531	0.001772
C 0	-2.394345	0.801206	0.000448
C 0	-2.600189	-0.530052	0.002355
C 0	-1.256403	-1.207587	0.008177
O 0	-0.349202	2.131461	-0.000164
O 0	-1.035901	-2.404857	0.018561
C 0	-3.350488	1.946222	-0.005381
C 0	-3.856623	-1.334562	0.000027
H 0	1.718657	1.135743	-1.337047
H 0	1.427973	-0.433955	-2.135963
H 0	1.241076	-1.562355	0.032219
H 0	1.421780	-0.363308	2.179497
H 0	1.663351	1.173534	1.338100
H 0	3.882073	0.338487	2.025854
H 0	3.565377	-1.242227	1.301390
H 0	4.974396	0.040182	-0.256519
H 0	3.844671	1.415418	-0.208385
H 0	-4.387873	1.605017	-0.005970
H 0	-3.188022	2.579123	-0.885013
H 0	-3.191154	2.585685	0.870035
H 0	-4.743713	-0.697550	-0.003540
H 0	-3.897042	-1.988427	0.878395
H 0	-3.892005	-1.990985	-0.876676

Compound **10a**

C 0	-1.639034	-0.410155	0.796497
C 0	-0.876006	-0.614680	-0.532035
C 0	-1.565496	0.103039	-1.701616
C 0	-3.041136	-0.323862	-1.747646
C 0	-3.699781	-0.094542	-0.390170
O 0	-2.995471	-0.791185	0.653810
O 0	-1.486245	0.927987	1.197691
N 0	0.546585	-0.294192	-0.390707
C 0	1.477139	-1.250918	0.035466
C 0	2.814159	-0.574006	0.139914
C 0	2.649276	0.718096	-0.200094
C 0	1.198034	0.939068	-0.550448
O 0	1.223540	-2.419620	0.272855
O 0	0.707100	1.986196	-0.925115
C 0	-1.956211	1.198475	2.515457
C 0	4.024811	-1.338849	0.559476
C 0	3.621035	1.846971	-0.278629
H 0	-1.246614	-1.086652	1.568367
H 0	-0.902756	-1.694273	-0.713761
H 0	-1.055362	-0.153834	-2.636821
H 0	-1.486906	1.184718	-1.572666
H 0	-3.123293	-1.386266	-2.012017
H 0	-3.576937	0.246330	-2.516219
H 0	-3.737273	0.978107	-0.156717
H 0	-4.716650	-0.493645	-0.359263
H 0	-1.735038	2.248703	2.714519
H 0	-1.435962	0.570379	3.253047
H 0	-3.035215	1.026338	2.599941
H 0	4.905441	-0.695952	0.623260
H 0	4.233980	-2.149391	-0.147955
H 0	3.862834	-1.812226	1.534180
H 0	4.625291	1.536157	0.017535
H 0	3.302710	2.673731	0.366033
H 0	3.663523	2.248264	-1.297470

Compound **10b**

C 0	1.725375	0.664351	-0.048278
C 0	0.921906	-0.626019	-0.295586
C 0	1.497006	-1.779065	0.548668
C 0	3.009820	-1.911435	0.313408
C 0	3.693829	-0.555731	0.488756
O 0	3.095336	0.425026	-0.363128
O 0	1.235175	1.658128	-0.885834
N 0	-0.510523	-0.436498	-0.073260
C 0	-1.124129	0.036916	1.086264
C 0	-2.597609	0.157345	0.796516
C 0	-2.805675	-0.216177	-0.480815
C 0	-1.477408	-0.602212	-1.074675
O 0	-0.562798	0.300422	2.137436
O 0	-1.264286	-1.001830	-2.203759
C 0	1.792269	2.952158	-0.656376
C 0	-3.540906	0.627000	1.852707
C 0	-4.052719	-0.292336	-1.295871
H 0	1.655713	0.974591	1.009075
H 0	1.018492	-0.855689	-1.361265
H 0	0.978266	-2.708461	0.289890
H 0	1.299633	-1.577477	1.608276
H 0	3.442171	-2.640272	1.009894
H 0	3.201900	-2.275488	-0.703512
H 0	4.748507	-0.592606	0.204118
H 0	3.631226	-0.224362	1.538785
H 0	1.257807	3.637714	-1.316371
H 0	2.860779	2.970213	-0.893188
H 0	1.642968	3.260971	0.388026
H 0	-4.566909	0.681047	1.482412
H 0	-3.246459	1.616837	2.218766
H 0	-3.515732	-0.043888	2.718969
H 0	-4.932095	-0.003093	-0.716348
H 0	-4.201415	-1.308345	-1.678177
H 0	-3.979162	0.361052	-2.172569

Compound 11a - Conformer G1				Compound 11a - Conformer T1			
C 0	-0.541946	-0.934625	-0.117850	C 0	-0.405197	-1.187219	0.274931
C 0	0.238277	0.257655	-0.712059	C 0	0.208941	-0.152064	-0.690750
C 0	-0.431218	1.590833	-0.348629	C 0	-0.631732	1.129955	-0.750736
C 0	-1.915617	1.555387	-0.734794	C 0	-2.078957	0.772316	-1.087021
C 0	-2.588362	0.338789	-0.084675	C 0	-2.610477	-0.269182	-0.086440
C 0	-4.045976	0.180179	-0.476130	C 0	-3.993703	-0.815937	-0.461130
O 0	-1.900761	-0.852850	-0.507299	O 0	-1.761409	-1.430723	-0.072765
O 0	-0.363984	-0.944486	1.271671	O 0	-0.254770	-0.728183	1.589975
N 0	1.663970	0.206405	-0.385671	N 0	1.626113	0.079746	-0.408330
O 0	-2.605450	2.719992	-0.276475	O 0	-2.841660	1.972398	-1.048590
O 0	-4.652101	-0.769096	0.387311	O 0	-4.993674	0.202788	-0.521315
C 0	2.337880	0.721172	0.733917	C 0	2.218731	1.009625	0.462394
C 0	3.779995	0.295240	0.612042	C 0	3.708090	0.773010	0.407774
C 0	3.919207	-0.422930	-0.518360	C 0	3.948759	-0.241393	-0.444208
C 0	2.573243	-0.505877	-1.179481	C 0	2.628116	-0.715691	-0.979340
O 0	1.868158	1.406741	1.620817	O 0	1.654651	1.859782	1.121902
O 0	2.296048	-1.079820	-2.218600	O 0	2.436031	-1.625662	-1.767898
C 0	-0.908549	-2.095404	1.919566	C 0	-0.562742	-1.696225	2.589617
C 0	4.771048	0.697334	1.651758	C 0	4.631621	1.619019	1.217772
C 0	5.111771	-1.075090	-1.133942	C 0	5.222891	-0.883744	-0.880816
C 0	-6.011276	-1.005322	0.073800	C 0	-5.608964	0.503530	0.728399
H 0	-0.191597	-1.878296	-0.558575	H 0	0.081159	-2.164116	0.149755
H 0	0.194151	0.116668	-1.797052	H 0	0.196033	-0.635355	-1.673306
H 0	0.077002	2.407840	-0.877715	H 0	-0.233976	1.804749	-1.515936
H 0	-0.345550	1.782597	0.722833	H 0	-0.603951	1.658400	0.203938
H 0	-2.018471	1.465590	-1.828807	H 0	-2.123676	0.324171	-2.095267
H 0	-2.524346	0.441360	1.005861	H 0	-2.631420	0.188342	0.912401
H 0	-4.109471	-0.157341	-1.523636	H 0	-4.285356	-1.603340	0.247194
H 0	-4.547506	1.154542	-0.388350	H 0	-3.944941	-1.258865	-1.461266
H 0	-2.120085	3.506038	-0.559519	H 0	-3.777802	1.721844	-1.120953
H 0	-0.663227	-1.996818	2.978389	H 0	-0.339415	-1.230655	3.551122
H 0	-0.454009	-3.014872	1.523522	H 0	0.056975	-2.596025	2.467449
H 0	-1.994882	-2.146872	1.792267	H 0	-1.619669	-1.985011	2.557509
H 0	5.770471	0.320226	1.424498	H 0	5.672664	1.312775	1.094505
H 0	4.468504	0.323508	2.636310	H 0	4.370252	1.564807	2.280325
H 0	4.817738	1.788798	1.736654	H 0	4.539306	2.672520	0.930279
H 0	6.005974	-0.938626	-0.521994	H 0	6.087385	-0.447178	-0.376038
H 0	5.304088	-0.665192	-2.131927	H 0	5.358581	-0.775971	-1.962989
H 0	4.937694	-2.148541	-1.267847	H 0	5.201930	-1.959950	-0.676529
H 0	-6.386499	-1.733316	0.796661	H 0	-6.383995	1.245584	0.525994
H 0	-6.124505	-1.416447	-0.941372	H 0	-4.894725	0.920890	1.449963
H 0	-6.609400	-0.083567	0.149113	H 0	-6.073754	-0.395047	1.157018

Compound 11b - Conformer G1				Compound 11b - Conformer T1			
C 0	0.596039	0.820877	-0.031779	C 0	0.471231	1.112814	0.027725
C 0	-0.213936	-0.395295	-0.512193	C 0	-0.172853	-0.142097	-0.585393
C 0	0.424335	-1.684441	0.036727	C 0	0.649627	-1.389101	-0.218847
C 0	1.925206	-1.748742	-0.281980	C 0	2.120424	-1.203703	-0.591446
C 0	2.612652	-0.447536	0.163876	C 0	2.650965	0.121371	-0.009670
C 0	4.078515	-0.388976	-0.227382	C 0	4.058980	0.476177	-0.504334
O 0	1.944312	0.650710	-0.461552	O 0	1.822132	1.204646	-0.436896
O 0	0.074800	1.963672	-0.621387	O 0	-0.227041	2.230037	-0.404813
N 0	-1.633146	-0.297648	-0.183677	N 0	-1.579032	-0.278951	-0.214669
O 0	2.561230	-2.828576	0.405566	O 0	2.837332	-2.326553	-0.091562
O 0	4.698462	0.680585	0.466997	O 0	5.026817	-0.521350	-0.174022
C 0	-2.191943	-0.096116	1.079283	C 0	-2.109978	-0.304339	1.075090
C 0	-3.681524	0.030026	0.893762	C 0	-3.607800	-0.390884	0.940305
C 0	-3.952037	-0.083798	-0.421108	C 0	-3.911536	-0.396047	-0.372124
C 0	-2.651084	-0.295023	-1.147544	C 0	-2.624193	-0.319542	-1.148108
O 0	-1.577626	-0.036755	2.131302	O 0	-1.470375	-0.258921	2.113142
O 0	-2.491133	-0.453925	-2.343184	O 0	-2.491765	-0.307082	-2.357272
C 0	0.656245	3.182105	-0.151508	C 0	0.154113	3.451742	0.227654
C 0	-4.575360	0.244005	2.068797	C 0	-4.474492	-0.450668	2.153223
C 0	-5.241059	-0.037662	-1.170517	C 0	-5.222077	-0.465156	-1.081150
C 0	6.067067	0.826294	0.139007	C 0	5.615429	-0.370790	1.115168
H 0	0.579492	0.902191	1.068111	H 0	0.482126	1.056584	1.128941
H 0	-0.173038	-0.385946	-1.605714	H 0	-0.177100	0.005150	-1.669967
H 0	-0.090592	-2.553391	-0.391865	H 0	0.246949	-2.266339	-0.735041
H 0	0.299683	-1.724216	1.124779	H 0	0.583264	-1.578156	0.858493
H 0	2.070201	-1.855580	-1.368680	H 0	2.214152	-1.146456	-1.689201
H 0	2.538510	-0.362941	1.259497	H 0	2.638353	0.047024	1.090622
H 0	4.157074	-0.238865	-1.316674	H 0	4.357105	1.454164	-0.103004
H 0	4.555386	-1.345127	0.032177	H 0	4.045412	0.545064	-1.596857
H 0	2.136250	-3.658866	0.153850	H 0	3.782908	-2.145145	-0.222747
H 0	0.119600	3.989875	-0.651955	H 0	-0.538841	4.213591	-0.133437
H 0	1.720451	3.231291	-0.400794	H 0	1.178653	3.731935	-0.037775
H 0	0.530044	3.277803	0.935988	H 0	0.067184	3.368145	1.320066
H 0	-5.623185	0.317839	1.770033	H 0	-5.534185	-0.480457	1.890819
H 0	-4.296894	1.159622	2.602499	H 0	-4.295451	0.417847	2.796679
H 0	-4.471980	-0.576968	2.787254	H 0	-4.237162	-1.336013	2.754030
H 0	-6.091347	0.113963	-0.502138	H 0	-6.057984	-0.512544	-0.379991
H 0	-5.394897	-0.967192	-1.730041	H 0	-5.260941	-1.344581	-1.733791
H 0	-5.226784	0.770742	-1.910129	H 0	-5.355079	0.408258	-1.729275
H 0	6.203148	1.046678	-0.931209	H 0	4.877360	-0.477714	1.920874
H 0	6.640816	-0.080443	0.387408	H 0	6.108475	0.606975	1.203677
H 0	6.451027	1.663078	0.726772	H 0	6.364187	-1.159556	1.212378

Compound 12 - Conformer G1				H O	-0.422576	1.397928	0.957407
C O	-0.624902	-1.165049	0.413545	H O	-2.109137	1.135403	-1.567215
C O	0.137856	-0.142493	-0.459239	H O	-2.587263	0.031793	1.256173
C O	-0.538879	1.225108	-0.292619	H O	-4.205662	-0.491292	-1.265515
C O	-2.027261	1.098585	-0.643244	H O	-4.615893	0.808319	-0.106714
C O	-2.686849	0.009956	0.217580	H O	0.864481	2.623752	-0.428891
C O	-4.143133	-0.214715	-0.147383	H O	-2.149159	3.128011	-0.285080
O O	-1.986158	-1.221634	0.028348	H O	5.589434	-0.250089	1.822519
N O	1.576253	-0.152305	-0.131810	H O	4.253506	-0.754548	2.881513
O O	-0.001736	2.239251	-1.136057	H O	4.486253	0.949370	2.532655
O O	-2.687010	2.334436	-0.406985	H O	6.019584	-0.756996	-0.410695
O O	-4.764853	-0.966601	0.881125	H O	5.337524	-0.052446	-1.893562
C O	2.381939	0.835618	0.433866	H O	5.108874	-1.760637	-1.561982
C O	3.783518	0.292078	0.516819	H O	-6.226112	-1.740023	-0.682483
C O	3.792967	-0.935625	-0.035734	H O	-6.689535	-0.418061	0.430473
C O	2.393402	-1.245707	-0.484170	H O	-6.475300	-2.078782	1.053240
O O	2.036454	1.958350	0.777718	Compound 12 - Conformer T1			
O O	2.007216	-2.246054	-1.056872	C O	0.507344	-0.327541	-1.602929
C O	4.874743	1.111756	1.118760	C O	-0.174967	-0.610153	-0.251713
C O	4.894794	-1.919104	-0.242255	C O	0.606253	0.070933	0.877434
C O	-6.118035	-1.267311	0.598345	C O	2.071952	-0.358936	0.812043
H O	-0.220492	-2.167556	0.269060	C O	2.652842	-0.098084	-0.590643
H O	-0.528795	-0.888761	1.477038	C O	4.070134	-0.661639	-0.755634
H O	0.054224	-0.455258	-1.505837	O O	1.865449	-0.762354	-1.577528
H O	-0.469026	1.544240	0.754895	N O	-1.584105	-0.226929	-0.267972
H O	-2.115006	0.817164	-1.705082	O O	0.014116	-0.290792	2.119002
H O	-2.635780	0.310592	1.276218	O O	2.751931	0.376840	1.826958
H O	-4.194250	-0.755022	-1.106808	O O	4.992930	-0.108799	0.185489
H O	-4.637182	0.760541	-0.264928	C O	-2.102951	1.069410	-0.308993
H O	0.761748	2.611108	-0.665541	C O	-3.594380	0.959094	-0.135834
H O	-2.137242	3.022568	-0.811800	C O	-3.906198	-0.343628	0.008533
H O	5.837467	0.599430	1.065085	C O	-2.631530	-1.138920	-0.064217
H O	4.655555	1.335970	2.168869	O O	-1.458335	2.092216	-0.469704
H O	4.959285	2.076232	0.606317	O O	-2.508836	-2.345863	0.019164
H O	5.853350	-1.529186	0.106196	C O	-4.449453	2.181522	-0.147597
H O	4.983683	-2.179301	-1.302677	C O	-5.216425	-1.027888	0.208681
H O	4.682257	-2.853250	0.290031	C O	5.616679	1.101278	-0.238340
H O	-6.212441	-1.877294	-0.313444	H O	0.019622	-0.894305	-2.399281
H O	-6.718192	-0.352217	0.473428	H O	0.453154	0.743839	-1.841248
H O	-6.505191	-1.834421	1.447814	H O	-0.176954	-1.690499	-0.075767
Compound 12 - Conformer G1'				H O	0.565204	1.161066	0.745704
C O	-0.619841	-1.253710	0.099590	H O	2.129804	-1.439586	1.020311
C O	0.153889	-0.075152	-0.526304	H O	2.649507	0.988835	-0.776635
C O	-0.518641	1.246880	-0.124518	H O	4.416451	-0.495116	-1.784087
C O	-2.009471	1.201607	-0.471908	H O	4.047727	-1.740713	-0.572757
C O	-2.663541	-0.038627	0.159737	H O	0.587239	0.053673	2.819304
C O	-4.129020	-0.171707	-0.213266	H O	3.703357	0.208681	1.719788
O O	-1.979292	-1.206758	-0.300992	H O	-5.508551	1.933873	-0.049462
N O	1.579382	-0.110771	-0.190373	H O	-4.303466	2.745016	-1.075792
O O	0.019071	2.375553	-0.823353	H O	-4.169742	2.854120	0.671207
O O	-2.667506	2.365869	0.012065	H O	-6.045670	-0.317351	0.217337
O O	-4.736472	-1.124767	0.642238	H O	-5.219132	-1.581850	1.154200
C O	2.159921	0.051947	1.071996	H O	-5.391542	-1.764582	-0.583259
C O	3.641259	-0.171629	0.917172	H O	4.891058	1.914221	-0.371875
C O	3.890185	-0.465886	-0.374192	H O	6.162624	0.945709	-1.178566
C O	2.581254	-0.453506	-1.115856	H O	6.324198	1.380795	0.544887
O O	1.567271	0.336797	2.099081				
O O	2.398036	-0.695024	-2.292979				
C O	4.550363	-0.052802	2.094122				
C O	5.163176	-0.774381	-1.087836				
C O	-6.100418	-1.344019	0.337214				
H O	-0.220180	-2.203888	-0.263808				
H O	-0.535806	-1.228608	1.195997				
H O	0.117746	-0.171268	-1.615604				

Compound **13a**

C 0	0.873287	1.262567	0.590246
C 0	1.961765	0.173851	0.663024
C 0	1.586911	-0.997677	-0.253743
C 0	0.182567	-1.505706	0.053116
C 0	-0.809120	-0.340110	-0.063750
C 0	-2.227472	-0.733466	0.302900
O 0	-0.408283	0.714241	0.833650
O 0	0.974844	1.886283	-0.669621
N 0	3.320765	0.607872	0.332915
O 0	2.492548	-2.084483	-0.083632
O 0	-0.205841	-2.528355	-0.858961
O 0	-3.112429	0.293046	-0.118582
C 0	0.127254	3.025769	-0.828425
C 0	-4.461971	0.021409	0.208793
H 0	1.003850	2.008020	1.389012
H 0	1.970218	-0.201961	1.692777
H 0	1.607807	-0.658431	-1.300753
H 0	0.167163	-1.893073	1.084716
H 0	-0.805720	0.029405	-1.096961
H 0	-2.297417	-0.878256	1.393289
H 0	-2.472456	-1.682361	-0.195274
H 0	3.753296	1.114499	1.099352
H 0	3.302109	1.222675	-0.477884
H 0	3.382414	-1.694831	-0.088346
H 0	0.528910	-3.156759	-0.912965
H 0	0.331364	3.427792	-1.822401
H 0	0.359409	3.788759	-0.071792
H 0	-0.928521	2.747871	-0.748385
H 0	-5.058225	0.856907	-0.164981
H 0	-4.603051	-0.061341	1.297659
H 0	-4.812548	-0.909706	-0.263260

Compound **13b**

C 0	-0.926964	1.171929	0.180773
C 0	-1.984335	0.112892	-0.192111
C 0	-1.471168	-1.285004	0.201729
C 0	-0.047268	-1.561135	-0.274257
C 0	0.868224	-0.422023	0.193261
C 0	2.297861	-0.583165	-0.291816
O 0	0.353901	0.800966	-0.329943
O 0	-1.285732	2.377526	-0.396858
N 0	-3.276753	0.431571	0.405368
O 0	-2.283196	-2.333438	-0.337023
O 0	0.432347	-2.793698	0.254126
O 0	3.129298	0.318617	0.420040
C 0	-0.518532	3.496303	0.045287
C 0	4.479944	0.264319	0.001672
H 0	-0.852237	1.273362	1.282536
H 0	-2.089833	0.156294	-1.281499
H 0	-1.467391	-1.360706	1.303577
H 0	-0.043485	-1.589760	-1.374896
H 0	0.879493	-0.393080	1.294971
H 0	2.337437	-0.373963	-1.373243
H 0	2.618876	-1.620819	-0.121403
H 0	-3.423737	0.044810	1.331229
H 0	-4.072384	0.253856	-0.192315
H 0	-3.185237	-2.231679	-0.004608
H 0	-0.240537	-3.464961	0.069486
H 0	-0.944885	4.372998	-0.445490
H 0	0.535312	3.390818	-0.231633
H 0	-0.600222	3.616220	1.135136
H 0	4.583882	0.539996	-1.059231
H 0	4.908320	-0.739690	0.147946
H 0	5.034397	0.980826	0.611884