

Supporting material for

Evaluation of basis sets and density functionals for carbohydrates

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To be published in *Journal of Chemical Theory and Computation*

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Table S6. X,y,z coordinates (in Å) of the 15 conformers of the AnGol15 test set, minimized using B3LYP/6-31+G**

Table S1. Absolute and relative energies of conformers of the ALL15 test set, in Hartrees and kcal/mol, respectively.

Order number	1	2	3	4	5	6	7	8
Anomer	α	β	β	α	α	β	α	α
Hydroxymethyl rotamer	tg	gg	gt	gt	gg	tg	gg	tg
Ring shape	4C1	4C1	4C1	4C1	4C1	4C1	4C1	4C1
H-6 conformation	g-	g+	g-	g-	g+	g+	g+	g+
H1-H-4 conformation	c0cc	rrrr	rrrr	rcrr	rcrr	rrrr	c0cc	crrr
B3LYP/6-311++G(d,p)	0.000	0.253	0.294	0.335	0.393	0.488	0.647	1.724
B3LYP/6-311+G(d,p)	-687.40455	-687.40412	-687.40403	-687.40397	-687.40390	-687.40377	-687.40340	-687.40182
	0.000	0.268	0.325	0.363	0.405	0.485	0.721	1.708
B3LYP/6-31+G(d,p)	-687.23286	-687.23214	-687.23210	-687.23212	-687.23194	-687.23218	-687.23144	-687.23036
	0.000	0.449	0.477	0.461	0.575	0.425	0.890	1.564
B3LYP/6-31+G(d)	-687.19631	-687.19507	-687.19502	-687.19546	-687.19527	-687.19536	-687.19465	-687.19394
	0.000	0.779	0.812	0.533	0.653	0.596	1.044	1.490
B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d,p)	-687.40440	-687.40398	-687.40394	-687.40383	-687.40376	-687.40367	-687.40331	-687.40168
	0.000	0.263	0.287	0.361	0.402	0.457	0.683	1.705
B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d)	-687.40417	-687.40377	-687.40374	-687.40362	-687.40356	-687.40345	-687.40311	-687.40146
	0.000	0.250	0.274	0.349	0.387	0.455	0.667	1.705
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d)	-687.23276	-687.23205	-687.23201	-687.23204	-687.23186	-687.23207	-687.23136	-687.23027
	0.000	0.445	0.471	0.456	0.569	0.433	0.882	1.565
B3PW91/6-311+G(d,p)	-687.13889	-687.13801	-687.13791	-687.13832	-687.13829	-687.13769	-687.13778	-687.13638
	0.000	0.553	0.617	0.360	0.382	0.756	0.696	1.576
B3PW91/6-31+G(d,p)	-686.97275	-686.97156	-686.97152	-686.97197	-686.97180	-686.97160	-686.97129	-686.97040
	0.000	0.744	0.769	0.489	0.592	0.718	0.914	1.473
B3PW91/6-31+G(d)	-686.93705	-686.93522	-686.93515	-686.93611	-686.93593	-686.93553	-686.93531	-686.93478
	0.000	1.149	1.194	0.594	0.707	0.956	1.095	1.429
B3PW91/6-311+G(d,p)//B3PW91/6-31+G(d)	-687.13910	-687.13818	-687.13805	-687.13851	-687.13849	-687.13783	-687.13800	-687.13653
	0.000	0.579	0.659	0.373	0.387	0.798	0.694	1.614
B3PW91/6-31+G(d,p)//B3PW91/6-31+G(d)	-686.97311	-686.97181	-686.97175	-686.97227	-686.97212	-686.97184	-686.97161	-686.97069
	0.000	0.813	0.856	0.527	0.624	0.794	0.943	1.519
PBEh/6-311+G(d,p)	-686.65404	-686.65300	-686.65277	-686.65326	-686.65326	-686.65270	-686.65279	-686.65146
	0.000	0.656	0.799	0.489	0.491	0.841	0.787	1.620
LSDA/6-311+G(d,p)	-682.08638	-682.08110	-682.08033	-682.08348	-682.08412	-682.08171	-682.08337	-682.08340

	0.000	3.318	3.798	1.820	1.423	2.930	1.893	1.875
PBE/6-311+G(d,p)	-686.63197	-686.62997	-686.62980	-686.63128	-686.63136	-686.62982	-686.63055	-686.62978
	0.000	1.256	1.362	0.436	0.388	1.350	0.893	1.377
TPSS/6-311+G(d,p)	-687.48092	-687.47848	-687.47822	-687.48007	-687.48018	-687.47817	-687.47943	-687.47857
	0.000	1.531	1.692	0.532	0.463	1.721	0.936	1.474
HF/6-31G(d)	-683.33357	-683.33415	-683.33365	-683.33249	-683.33256	-683.33401	-683.33258	-683.33090
	0.000	-0.361	-0.051	0.681	0.634	-0.275	0.626	1.678
M05-2X/6-311+G(d,p)	-687.33565	-687.33455	-687.33391	-687.33475	-687.33514	-687.33368	-687.33510	-687.33285
	0.000	0.691	1.091	0.564	0.316	1.235	0.343	1.758
M05-2X/6-31+G(d,p)	-687.15767	-687.15623	-687.15575	-687.15658	-687.15687	-687.15579	-687.15676	-687.15513
	0.000	0.900	1.207	0.683	0.503	1.178	0.570	1.595
M05-2X/6-31+G(d)	-687.12086	-687.11870	-687.11822	-687.11954	-687.11982	-687.11860	-687.11964	-687.11842
	0.000	1.350	1.652	0.828	0.650	1.416	0.760	1.528
M05-2X/6-311+G(d,p)//M05-2X/6-31+G(d,p)	-687.33556	-687.33446	-687.33382	-687.33465	-687.33504	-687.33359	-687.33500	-687.33276
	0.000	0.692	1.097	0.574	0.330	1.238	0.353	1.760
M05-2X/6-311+G(d,p)//M05-2X/6-31+G(d)	-687.33539	-687.33431	-687.33366	-687.33449	-687.33488	-687.33343	-687.33486	-687.33257
	0.000	0.676	1.083	0.565	0.323	1.231	0.335	1.768
M05-2X/6-31+G(d,p)//M05-2X/6-31+G(d)	-687.15759	-687.15618	-687.15569	-687.15652	-687.15680	-687.15572	-687.15670	-687.15505
	0.000	0.883	1.191	0.671	0.491	1.172	0.555	1.591
HF/cc-pVTZ(-f)//B3LYP/6-31+G(d)	-683.58574	-683.58883	-683.58869	-683.58608	-683.58589	-683.58787	-683.58603	-683.58340
	0.000	-1.941	-1.852	-0.214	-0.095	-1.335	-0.184	1.470
LMP2/cc-pVTZ(-f)//B3LYP/6-31+G(d)	-685.78009	-685.77942	-685.77895	-685.77938	-685.77962	-685.77871	-685.77934	-685.77796
	0.000	0.420	0.719	0.447	0.296	0.871	0.475	1.337

Order number	9	10	11	12	13	14	15
Anomer	α	α	β	α	β	β	α
Hydroxymethyl rotamer	gt	gg	tg	gg	gt	tg	tg
Ring shape	4C1	4C1	4C1	4C1	4C1	1C4	1C4
H-6 conformation	g-	g-	t	t	t	t	t
H1-H-4 conformation	c0cc	rcrr	cccc	c0cc	rrrr	rcrr	ccrr
B3LYP/6-311++G(d,p)	1.960	2.561	2.665	3.053	3.842	4.851	5.474
B3LYP/6-311+G(d,p)	-687.40140	-687.40045	-687.40029	-687.39964	-687.39834	-687.39676	-687.39576
	1.973	2.568	2.671	3.076	3.894	4.884	5.511
B3LYP/6-31+G(d,p)	-687.22945	-687.22848	-687.22857	-687.22768	-687.22643	-687.22504	-687.22402
	2.139	2.745	2.692	3.249	4.031	4.902	5.542

B3LYP/6-31+G(d)	-687.19265	-687.19174	-687.19165	-687.19078	-687.18920	-687.18833	-687.18743
	2.297	2.869	2.924	3.467	4.462	5.005	5.570
B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d,p)	-687.40126	-687.40031	-687.40018	-687.39960	-687.39822	-687.39661	-687.39561
	1.970	2.569	2.650	3.014	3.876	4.887	5.514
B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d)	-687.40105	-687.40010	-687.39997	-687.39938	-687.39802	-687.39638	-687.39539
	1.958	2.553	2.639	3.007	3.863	4.890	5.509
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d)	-687.22936	-687.22840	-687.22846	-687.22759	-687.22635	-687.22495	-687.22393
	2.134	2.738	2.700	3.245	4.026	4.904	5.540
B3PW91/6-311+G(d,p)	-687.13581	-687.13484	-687.13417	-687.13382	-687.13220	-687.13090	-687.13046
	1.933	2.545	2.965	3.184	4.199	5.019	5.290
B3PW91/6-31+G(d,p)	-686.96932	-686.96836	-686.96798	-686.96737	-686.96574	-686.96465	-686.96414
	2.149	2.754	2.989	3.371	4.398	5.081	5.398
B3PW91/6-31+G(d)	-686.93332	-686.93242	-686.93179	-686.93126	-686.92923	-686.92881	-686.92842
	2.344	2.910	3.306	3.634	4.907	5.172	5.416
B3PW91/6-311+G(d,p)//B3PW91/6-31+G(d)	-687.13601	-687.13504	-687.13435	-687.13403	-687.13236	-687.13104	-687.13063
	1.942	2.551	2.983	3.184	4.233	5.062	5.316
B3PW91/6-31+G(d,p)//B3PW91/6-31+G(d)	-686.96963	-686.96866	-686.96824	-686.96766	-686.96599	-686.96500	-686.96450
	2.182	2.790	3.055	3.419	4.471	5.092	5.403
PBEh/6-311+G(d,p)	-686.65080	-686.64972	-686.64930	-686.64881	-686.64695	-686.64586	-686.64545
	2.032	2.713	2.975	3.283	4.449	5.133	5.391
LSDA/6-311+G(d,p)	-682.08142	-682.07994	-682.07906	-682.07888	-682.07413	-682.07594	-682.07630
	3.114	4.042	4.593	4.707	7.691	6.556	6.325
PBE/6-311+G(d,p)	-686.62871	-686.62797	-686.62614	-686.62653	-686.62418	-686.62399	-686.62374
	2.046	2.513	3.662	3.420	4.892	5.013	5.170
TPSS/6-311+G(d,p)	-687.47747	-687.47666	-687.47461	-687.47543	-687.47247	-687.47294	-687.47242
	2.165	2.673	3.955	3.441	5.302	5.003	5.334
HF/6-31G(d)	-683.32983	-683.32879	-683.32995	-683.32790	-683.32726	-683.32573	-683.32357
	2.351	2.998	2.275	3.557	3.964	4.923	6.276
M05-2X/6-311+G(d,p)	-687.33215	-687.33139	-687.33044	-687.33108	-687.32767	-687.32775	-687.32652
	2.195	2.671	3.269	2.868	5.008	4.955	5.728
M05-2X/6-31+G(d,p)	-687.15394	-687.15311	-687.15233	-687.15272	-687.14957	-687.15001	-687.14860
	2.340	2.862	3.350	3.103	5.083	4.804	5.691
M05-2X/6-31+G(d)	-687.11679	-687.11598	-687.11509	-687.11547	-687.11185	-687.11294	-687.11173
	2.551	3.058	3.621	3.378	5.649	4.965	5.727
M05-2X/6-311+G(d,p)//M05-2X/6-31+G(d,p)	-687.33205	-687.33129	-687.33035	-687.33098	-687.32758	-687.32766	-687.32643
	2.204	2.682	3.275	2.877	5.013	4.958	5.730
M05-2X/6-311+G(d,p)//M05-2X/6-31+G(d)	-687.33189	-687.33114	-687.33020	-687.33083	-687.32741	-687.32748	-687.32624
	2.198	2.670	3.255	2.861	5.006	4.961	5.741
M05-2X/6-31+G(d,p)//M05-2X/6-31+G(d)	-687.15388	-687.15304	-687.15226	-687.15266	-687.14950	-687.14993	-687.14852

	2.326	2.852	3.339	3.088	5.072	4.802	5.691
HF/cc-pVTZ(-f)//B3LYP/6-31+G(d)	-683.58359	-683.58278	-683.58427	-683.58221	-683.58332	-683.57927	-683.57762
	1.351	1.856	0.919	2.211	1.517	4.062	5.092
LMP2/cc-pVTZ(-f)//B3LYP/6-31+G(d)	-685.77680	-685.77659	-685.77510	-685.77553	-685.77327	-685.77361	-685.77216
	2.066	2.200	3.132	2.866	4.283	4.070	4.979

Table S2. Absolute and relative energies of conformers of the AnGol15 test set, in Hartrees and kcal/mol, respectively (Over yellow background, data from Ref. 50).

Order number	1	2	3	4	5	6	7	8
Original name	S1-	S2-	S4-	S3-	N1-	N2-	S1+	S2+
Ring shape	S	S	S	S	N	N	S	S
Dihedral w3	g-	g-	g-	g-	g-	g-	g+	g+
Dihedrals w2/c1/c2	g-/g+/t	g-/g+/t	t/t/g-	t/t/g-	g-/g+/t	g-/g+/t	g-/g-/g+	g-/g-/g+
Dihedrals c4/c5	g-/t	g+/t	g-/t	g+/t	g+/g-	g-/g+	g+/g+	g+/g-
B3LYP/6-311++G(d,p)	-651.45781	-651.45623	-651.45479	-651.45317	-651.45159	-651.45110	-651.45066	-651.45041
	0.000	0.991	1.897	2.914	3.903	4.209	4.483	4.640
B3LYP/6-31+G(d,p)	-651.30177	-651.30022	-651.29839	-651.29693	-651.29520	-651.29469	-651.29409	-651.29393
	0.000	0.973	2.120	3.033	4.121	4.438	4.817	4.918
B3LYP/6-31+G(d)	-651.27147	-651.26998	-651.26739	-651.26590	-651.26434	-651.26372	-651.26288	-651.26276
	0.000	0.930	2.560	3.493	4.473	4.859	5.387	5.465
B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d)	-651.45735	-651.45578	-651.45429	-651.45277	-651.45113	-651.45068	-651.45002	-651.44973
	0.000	0.986	1.917	2.876	3.903	4.182	4.601	4.779
B3PW91/6-31+G(d,p)	-651.05493	-651.05348	-651.05090	-651.04949	-651.04782	-651.04729	-651.04659	-651.04653
	0.000	0.913	2.530	3.414	4.465	4.797	5.235	5.274
B3PW91/6-311+G(d,p)//B3PW91/6-31+G(d,p)	-651.20554	-651.20399	-651.20187	-651.20035	-651.19871	-651.19824	-651.19765	-651.19741
	0.000	0.973	2.304	3.258	4.286	4.581	4.948	5.097
LSDA/6-31+G(d,p)	-646.12370	-646.12245	-646.11525	-646.11405	-646.11003	-646.10915	-646.10880	-646.10856
	0.000	0.786	5.300	6.053	8.577	9.132	9.349	9.497
LSDA/6-311+G(d,p)//B3PW91/6-31+G(d,p)	-646.28326	-646.28194	-646.27512	-646.27376	-646.26991	-646.26910	-646.26897	-646.26861
	0.000	0.831	5.110	5.960	8.374	8.887	8.965	9.195
HF/6-31G(d)	-647.49036	-647.48890	-647.48738	-647.48605	-647.48473	-647.48462	-647.48460	-647.48443
	0.000	0.920	1.873	2.705	3.537	3.603	3.614	3.727
M05-2X/6-311+G(d,p)	-651.38194	-651.38062	-651.37795	-651.37669	-651.37376	-651.37331	-651.37519	-651.37456
	0.000	0.829	2.503	3.295	5.134	5.415	4.237	4.629

M05-2X/6-31+G(d,p)	-651.22042	-651.21917	-651.21627	-651.21517	-651.21214	-651.21166	-651.21334	-651.21290
	0.000	0.786	2.607	3.298	5.196	5.497	4.443	4.720
M05-2X/6-31+G(d)	-651.18965	-651.18842	-651.18470	-651.18362	-651.18070	-651.18009	-651.18143	-651.18106
	0.000	0.770	3.106	3.785	5.614	6.001	5.158	5.393
M05-2X/6-311+G(d,p)//M05-2X/6-31+G(d,p)	-651.38187	-651.38054	-651.37788	-651.37662	-651.37371	-651.37322	-651.37508	-651.37448
	0.000	0.835	2.501	3.291	5.120	5.429	4.259	4.636
M05-2X/6-311+G(d,p)//M05-2X/6-31+G(d)	-651.38177	-651.38044	-651.37780	-651.37653	-651.37362	-651.37311	-651.37499	-651.37440
	0.000	0.831	2.489	3.283	5.110	5.432	4.249	4.625
M05-2X/6-31+G(d,p)//M05-2X/6-31+G(d)	-651.22037	-651.21912	-651.21622	-651.21513	-651.21211	-651.21162	-651.21331	-651.21287
	0.000	0.782	2.599	3.288	5.181	5.489	4.427	4.703
MP2/6-311+G(d,p)//B3LYP/6-31+G(d,p)	-649.73026	-649.72859	-649.72690	-649.72537	-649.72205	-649.72148	-649.72351	-649.72302
	0.000	1.049	2.107	3.068	5.152	5.511	4.234	4.543
HF/cc-pVTZ//B3LYP/6-311++G(d,p)	-647.73979	-647.73812	-647.73889	-647.73751	-647.73628	-647.73651	-647.73667	-647.73649
	0.000	1.054	0.569	1.431	2.206	2.062	1.961	2.073
HF/cc-pVTZ++//B3LYP/6-311++G(d,p)	-647.74683	-647.74555	-647.74675	-647.74544	-647.74426	-647.74416	-647.74468	-647.74431
	0.000	0.805	0.052	0.876	1.616	1.674	1.353	1.586
LMP2/cc-pVTZ//B3LYP/6-311++G(d,p)	-650.08202	-650.08021	-650.07811	-650.07664	-650.07411	-650.07428	-650.07530	-650.07522
	0.000	1.135	2.455	3.377	4.963	4.856	4.219	4.269
LMP2/cc-pVTZ++//B3LYP/6-311++G(d,p)	-650.14421	-650.14249	-650.14106	-650.13948	-650.13660	-650.13638	-650.13792	-650.13770
	0.000	1.077	1.977	2.966	4.770	4.911	3.947	4.079
HF/cc-pVTZ(-f)//B3LYP/6-311++G(d,p)	-647.72138	-647.71990	-647.72031	-647.71897	-647.71804	-647.71815	-647.71820	-647.71795
	0.000	0.925	0.670	1.513	2.096	2.027	1.995	2.153
LMP2/cc-pVTZ(-f)//B3LYP/6-311++G(d,p)	-649.85674	-649.85521	-649.85304	-649.85160	-649.84950	-649.84942	-649.85046	-649.85031
	0.000	0.962	2.324	3.222	4.543	4.593	3.938	4.035

Order number	9	10	11	12	13	14	15
Original name	N3-	N1+	S4+	S3+	N3+	N2+	N4+
Ring shape	N	N	S	S	N	N	N
Dihedral w3	g-	g+	g+	g+	g+	g+	g+
Dihedrals w2/c1/c2	t/g+/t	t/g+/g+	t/g+/g+	t/g+/g+	g+/g-/g+	g-/g-/g+	t/g+/g+
Dihedrals c4/c5	g+/g-	g-/g+	g+/g-	g+/g+	g-/g+	g-/g+	g+/g-
B3LYP/6-311++G(d,p)	-651.44923	-651.44877	-651.44872	-651.44868	-651.44849	-651.44818	-651.44802
	5.383	5.674	5.701	5.728	5.844	6.043	6.140
B3LYP/6-31+G(d,p)	-651.29290	-651.29251	-651.29232	-651.29220	-651.29266	-651.29186	-651.29200
	5.562	5.806	5.927	6.004	5.716	6.213	6.127
B3LYP/6-31+G(d)	-651.26177	-651.26134	-651.26120	-651.26099	-651.26174	-651.26066	-651.26094

	6.086	6.352	6.441	6.571	6.101	6.778	6.607
B3LYP/6-311+G(d,p)//B3LYP/6-31+G(d)	-651.44860	-651.44826	-651.44808	-651.44805	-651.44797	-651.44764	-651.44757
	5.490	5.705	5.815	5.833	5.886	6.090	6.138
B3PW91/6-31+G(d,p)	-651.04542	-651.04483	-651.04482	-651.04470	-651.04480	-651.04448	-651.04464
	5.971	6.339	6.348	6.424	6.359	6.557	6.460
B3PW91/6-311+G(d,p)//B3PW91/6-31+G(d,p)	-651.19617	-651.19559	-651.19564	-651.19557	-651.19504	-651.19504	-651.19496
	5.877	6.241	6.210	6.255	6.587	6.589	6.636
LSDA/6-31+G(d,p)	-646.10462	-646.10344	-646.10558	-646.10544	-646.10705	-646.10489	-646.10513
	11.973	12.711	11.368	11.455	10.447	11.805	11.653
LSDA/6-311+G(d,p)//B3PW91/6-31+G(d,p)	-646.26431	-646.26285	-646.26541	-646.26538	-646.26628	-646.26443	-646.26458
	11.889	12.807	11.201	11.222	10.654	11.814	11.724
HF/6-31G(d)	-647.48230	-647.48225	-647.48187	-647.48170	-647.48255	-647.48171	-647.47969
	5.057	5.094	5.329	5.440	4.903	5.429	6.698
M05-2X/6-311+G(d,p)	-651.37023	-651.37030	-651.37165	-651.37189	-651.37085	-651.36986	-651.37000
	7.349	7.302	6.457	6.305	6.958	7.578	7.491
M05-2X/6-31+G(d,p)	-651.20883	-651.20886	-651.21018	-651.21028	-651.20977	-651.20866	-651.20897
	7.275	7.257	6.429	6.365	6.686	7.380	7.189
M05-2X/6-31+G(d)	-651.17705	-651.17699	-651.17837	-651.17840	-651.17814	-651.17679	-651.17722
	7.907	7.942	7.077	7.061	7.220	8.067	7.799
M05-2X/6-311+G(d,p)//M05-2X/6-31+G(d,p)	-651.37015	-651.37023	-651.37157	-651.37181	-651.37077	-651.36978	-651.36991
	7.356	7.306	6.460	6.310	6.963	7.588	7.506
M05-2X/6-311+G(d,p)//M05-2X/6-31+G(d)	-651.37005	-651.37012	-651.37149	-651.37172	-651.37068	-651.36970	-651.36982
	7.351	7.305	6.446	6.303	6.954	7.574	7.494
M05-2X/6-31+G(d,p)//M05-2X/6-31+G(d)	-651.20879	-651.20883	-651.21014	-651.21024	-651.20972	-651.20863	-651.20893
	7.263	7.238	6.414	6.355	6.678	7.365	7.178
MP2/6-311+G(d,p)//B3LYP/6-31+G(d,p)	-649.71925	-649.71926	-649.72062	-649.72072	-649.71945	-649.71903	-649.71895
	6.907	6.902	6.050	5.986	6.785	7.048	7.100
HF/cc-pVTZ//B3LYP/6-311++G(d,p)	-647.73535	-647.73508	-647.73470	-647.73466	-647.73391	-647.73404	-647.73281
	2.788	2.958	3.194	3.224	3.694	3.614	4.381
HF/cc-pVTZ++//B3LYP/6-311++G(d,p)	-647.74356	-647.74385	-647.74315	-647.74316	-647.74186	-647.74234	-647.74186
	2.054	1.874	2.311	2.303	3.120	2.821	3.123
LMP2/cc-pVTZ//B3LYP/6-311++G(d,p)	-650.07198	-650.07154	-650.07280	-650.07260	-650.07215	-650.07183	-650.07075
	6.303	6.576	5.789	5.911	6.195	6.393	7.069
LMP2/cc-pVTZ++//B3LYP/6-311++G(d,p)	-650.13441	-650.13474	-650.13576	-650.13536	-650.13471	-650.13482	-650.13409
	6.144	5.937	5.300	5.552	5.956	5.889	6.345
HF/cc-pVTZ(-f)//B3LYP/6-311++G(d,p)	-647.71699	-647.71685	-647.71605	-647.71603	-647.71564	-647.71578	-647.71449
	2.753	2.842	3.341	3.354	3.599	3.511	4.325

LMP2/cc-pVTZ(-f)//B3LYP/6-311++G(d,p)	-649.84716	-649.84715	-649.84778	-649.84761	-649.84758	-649.84730	-649.84615
	6.008	6.017	5.620	5.728	5.750	5.921	6.646

Table S3. Absolute and relative energies of conformers of the GLC4 test set, in Hartrees and kcal/mol, respectively.

Order number	1	2	3	4
Anomer	β	β	β	β
Hydroxymethyl rotamer	gt	tg	gt	gg
Ring shape	4C1	4C1	1C4	1C4
H-6 conformation	g-	g+	g+	g-
B3LYP/6-311+G(d,p)	-687.40340	-687.40314	-687.39186	-687.39449
	0.000	0.160	7.241	5.590
B3LYP/6-31+G(d,p)	-687.23154	-687.23144	-687.22002	-687.22293
	0.000	0.062	7.225	5.400
B3PW91/6-311+G(d,p)	-687.13735	-687.13704	-687.12672	-687.12903
	0.000	0.194	6.672	5.222
B3PW91/6-31+G(d,p)	-686.97094	-686.97080	-686.96038	-686.96295
	0.000	0.089	6.630	5.019
PBE1PBE/6-311+G(d,p)	-686.65269	-686.65255	-686.64290	-686.64504
	0.000	0.088	6.145	4.801
PBE1PBE/6-31+G(d,p)	-686.49054	-686.49058	-686.48101	-686.48340
	0.000	-0.025	5.982	4.485
M05-2X/6-311+G(d,p)	-687.33168	-687.33151	-687.32428	-687.32437
	0.000	0.102	4.643	4.585
M05-2X/6-31+G(d,p)	-687.15372	-687.15366	-687.14624	-687.14676
	0.000	0.033	4.692	4.368
HF/cc-pVTZ(-f)//B3LYP/6-31+G(d)	-683.58869	-683.58794	-683.57175	-683.57171
	0.000	0.471	10.632	10.657
LMP2/cc-pVTZ(-f)//B3LYP/6-31+G(d)	-685.77778	-685.77732	-685.76835	-685.76880
	0.000	0.290	5.920	5.633

Table S4. Main geometrical features of the 15 conformers of the AnGol test set. The acronyms for the exo-cyclic angles (χ_n and ω_n) were defined in ref. 50. Q and ϕ are Cremer-Pople puckering parameters.

	B3LYP 6-311++G**	B3LYP 6-31+G**	B3LYP 6-31+G*	B3PW91 6-31+G**	SVWN 6-31+G**	M05-2X 6-311+G**	M05-2X 6-31+G**	M05-2X 6-31+G*	HF 6-31G*
S1+									
ω_3	49.4	49.5	49.6	48.0	41.5	49.0	48.5	48.8	51.4
ω_2	-60.0	-60.0	-59.9	-60.7	-64.4	-60.2	-60.2	-60.2	-59.2
χ_1	-52.9	-52.4	-52.2	-51.0	-43.1	-51.4	-51.1	-50.9	-53.4
χ_2	76.9	76.3	76.4	77.2	82.5	76.4	76.0	75.9	73.8
χ_4	48.0	47.6	47.5	47.9	51.4	48.5	48.2	48.3	44.7
χ_5	67.7	66.6	66.6	67.4	73.1	73.4	69.7	69.3	67.2
Q	0.354	0.353	0.352	0.360	0.382	0.383	0.381	0.381	0.353
ϕ	115.5	115.2	116.0	114.7	114.5	122.1	120.9	121.7	116.3
S2+									
ω_3	49.0	49.0	49.0	47.0	40.6	48.9	48.4	48.6	50.8
ω_2	-59.8	-59.9	-60.0	-60.9	-64.4	-60.1	-60.1	-60.2	-59.1
χ_1	-53.2	-52.3	-52.0	-50.6	-42.9	-51.4	-51.0	-50.8	-53.3
χ_2	76.3	75.9	76.0	77.2	82.3	75.8	75.3	75.2	73.4
χ_4	48.7	48.4	48.4	48.6	51.4	48.4	48.4	48.5	45.3
χ_5	-49.8	-49.4	-50.0	-50.0	-54.0	-50.6	-48.9	-49.8	-50.6
Q	0.343	0.342	0.341	0.349	0.369	0.368	0.370	0.370	0.341
ϕ	116.1	116.2	117.0	114.9	113.1	121.5	121.1	121.9	117.7
S3+									
ω_3	49.9	49.5	49.5	48.8	45.2	48.9	48.5	48.8	51.0
ω_2	-178.2	-178.4	-178.0	-178.1	-172.4	-176.8	-177.1	-176.6	-177.8
χ_1	48.9	48.8	48.7	48.3	42.1	47.9	47.8	47.7	50.2
χ_2	70.5	70.1	70.8	70.2	75.0	71.2	70.4	70.8	68.2
χ_4	46.3	46.2	46.1	46.5	50.0	46.3	46.3	46.5	43.4
χ_5	67.6	66.7	66.4	67.4	71.9	70.0	68.5	68.4	66.6
Q	0.357	0.355	0.354	0.362	0.385	0.382	0.382	0.381	0.355
ϕ	115.4	115.5	116.2	115.9	115.1	118.0	118.4	119.2	116.4
S4+									

ω_3	48.8	48.6	48.5	48.0	44.4	48.6	48.1	48.1	50.1
ω_2	-179.2	-179.4	-179.1	-179.3	-173.6	-177.7	-178.1	-177.7	-178.8
χ_1	49.3	49.1	49.0	48.6	42.7	48.3	48.1	48.1	50.5
χ_2	70.6	70.2	70.8	70.4	74.7	71.0	70.2	70.6	68.1
χ_4	47.1	46.8	46.9	47.1	50.3	46.3	46.3	46.6	44.2
χ_5	-51.2	-50.8	-51.3	-51.2	-54.3	-52.1	-50.4	-51.5	-51.8
Q	0.347	0.347	0.346	0.353	0.378	0.370	0.373	0.373	0.345
ϕ	113.5	113.5	114.2	113.6	113.4	115.7	117.4	117.2	113.7
S1-									
ω_3	-62.5	-62.9	-62.9	-63.7	-67.4	-62.6	-63.4	-63.5	-60.6
ω_2	-76.8	-77.4	-77.3	-77.8	-77.9	-76.6	-77.4	-77.6	-76.3
χ_1	58.6	59.0	59.0	59.1	57.8	58.6	59.8	60.0	60.8
χ_2	-141.2	-141.1	-141.9	-141.1	-141.1	-142.1	-141.5	-142.1	-143.2
χ_4	-42.2	-42.1	-42.1	-42.2	-45.9	-41.7	-41.6	-41.7	-39.6
χ_5	-160.6	-160.2	-160.1	-159.7	-157.3	-158.9	-158.4	-158.2	-161.5
Q	0.361	0.361	0.362	0.369	0.395	0.382	0.383	0.383	0.363
ϕ	118.8	118.4	118.2	119.2	115.8	123.8	124.2	123.9	118.1
S2-									
ω_3	-61.3	-62.0	-61.9	-62.6	-66.1	-61.8	-62.7	-62.9	-59.9
ω_2	-76.9	-77.4	-77.3	-77.7	-77.7	-76.6	-77.6	-77.7	-76.4
χ_1	58.5	58.9	58.8	58.9	57.6	58.4	59.6	59.9	60.7
χ_2	-141.1	-141.0	-141.8	-141.1	-141.2	-141.8	-141.1	-141.7	-142.9
χ_4	44.0	43.7	43.7	44.1	48.0	44.4	44.2	44.4	41.5
χ_5	-160.5	-159.9	-159.8	-159.5	-157.1	-157.6	-157.2	-157.0	-160.6
Q	0.360	0.361	0.362	0.368	0.397	0.383	0.384	0.384	0.361
ϕ	114.9	114.7	114.5	115.5	113.3	122.0	122.2	122.0	114.0
S3-									
ω_3	-66.2	-66.9	-66.5	-67.2	-71.6	-67.3	-67.9	-67.7	-65.2
ω_2	-176.7	-176.9	-177.0	-175.9	-168.4	-176.5	-176.5	-176.4	-178.6
χ_1	164.2	164.1	164.5	163.2	158.8	165.1	164.6	164.8	167.9
χ_2	-78.2	-78.1	-77.3	-79.5	-87.7	-77.7	-77.7	-77.0	-73.3
χ_4	44.4	44.1	44.1	44.6	48.5	44.8	44.6	44.8	41.8
χ_5	-165.5	-165.4	-165.4	-165.1	-160.4	-164.8	-165.2	-165.0	-168.3
Q	0.367	0.368	0.367	0.377	0.407	0.395	0.398	0.398	0.369
ϕ	117.9	118.5	118.3	119.7	119.0	125.0	126.1	125.8	118.1

S4-

ω_3	-67.1	-67.3	-66.9	-67.8	-72.2	-67.8	-68.4	-68.0	-65.4
ω_2	-176.5	-176.7	-176.8	-175.7	-168.2	-176.2	-176.2	-176.1	-178.3
χ_1	164.7	164.6	165.2	163.9	159.3	165.7	165.3	165.6	168.5
χ_2	-78.2	-78.1	-77.3	-79.5	-87.7	-77.8	-77.8	-77.1	-73.4
χ_4	-41.8	-41.6	-41.6	-41.6	-45.3	-41.3	-40.9	-41.0	-39.5
χ_5	-165.9	-166.0	-165.9	-165.8	-161.3	-165.8	-166.2	-166.0	-169.1
Q	0.368	0.369	0.368	0.378	0.405	0.394	0.397	0.396	0.370
ϕ	121.2	121.7	121.2	122.6	120.9	126.2	127.5	127.1	121.6

N1+

ω_3	54.6	54.6	54.7	54.2	50.5	55.6	55.3	55.4	55.6
ω_2	179.6	179.4	179.9	179.9	185.2	181.6	181.4	181.8	180.7
χ_1	51.8	51.6	51.5	51.1	45.6	50.4	50.4	50.4	52.5
χ_2	70.8	70.5	70.9	71.1	79.1	71.4	70.8	71.2	66.6
χ_4	-44.2	-44.8	-45.1	-45.7	-51.5	-49.6	-50.4	-50.5	-44.4
χ_5	50.0	50.4	51.1	51.5	55.3	53.3	52.9	52.5	48.8
Q	0.361	0.362	0.360	0.368	0.379	0.384	0.383	0.381	0.363
ϕ	302.3	302.3	302.4	305.5	319.8	306.5	307.6	307.3	302.1

N2+

ω_3	48.9	48.6	48.8	47.5	41.2	49.1	48.9	49.1	50.3
ω_2	-65.0	-65.0	-65.0	-65.1	-67.7	-65.8	-65.4	-65.3	-64.6
χ_1	-51.0	-50.2	-50.2	-49.2	-42.6	-49.8	-49.8	-49.5	-52.3
χ_2	82.3	82.3	82.2	83.8	91.4	82.5	81.8	81.7	76.0
χ_4	-45.6	-46.4	-46.7	-47.3	-52.5	-50.9	-50.6	-51.4	-44.9
χ_5	49.9	50.3	50.6	51.1	54.8	52.1	51.0	51.1	48.0
Q	0.356	0.357	0.356	0.361	0.372	0.377	0.379	0.377	0.357
ϕ	315.1	316.3	316.3	319.9	332.9	317.0	316.7	317.3	316.3

N3+

ω_3	49.6	50.0	50.2	50.0	49.2	51.7	51.5	51.9	52.7
ω_2	66.0	66.6	66.7	66.0	62.7	64.9	64.6	65.0	66.2
χ_1	-69.1	-68.7	-68.2	-68.3	-64.8	-74.2	-73.7	-73.1	-74.5
χ_2	73.6	72.8	72.9	73.3	76.1	73.8	72.8	72.9	70.3
χ_4	-50.2	-49.9	-50.2	-51.0	-49.2	-50.9	-50.4	-51.9	-50.1
χ_5	52.7	53.0	53.2	53.5	56.5	55.4	54.4	54.3	50.3
Q	0.367	0.367	0.366	0.373	0.387	0.386	0.386	0.385	0.369
ϕ	282.3	282.0	281.8	286.6	290.8	295.6	294.6	294.0	281.6

N4+

ω_3	52.7	52.3	52.1	51.5	48.2	53.5	52.8	52.8	55.1
ω_2	-178.2	-178.4	-178.6	-177.9	-172.1	-176.8	-177.1	-176.8	-177.9
χ_1	50.2	50.0	50.0	49.5	43.6	49.0	49.3	49.3	51.0
χ_2	76.8	76.4	77.4	78.1	83.0	76.8	76.4	76.7	71.5
χ_4	48.0	48.1	48.1	48.8	52.7	50.1	49.7	50.0	46.7
χ_5	-45.6	-46.0	-46.7	-46.4	-48.9	-47.9	-46.6	-47.1	-50.4
Q	0.348	0.351	0.349	0.354	0.371	0.375	0.372	0.371	0.352
ϕ	326.4	326.3	326.1	328.3	325.9	325.0	325.6	325.7	326.3

N1-

ω_3	-69.0	-69.9	-69.9	-70.6	-75.5	-69.7	-70.6	-71.4	-66.6
ω_2	-76.5	-76.8	-76.8	-77.2	-77.1	-76.8	-77.4	-77.7	-76.1
χ_1	60.4	60.9	60.9	61.0	60.2	61.0	62.2	62.7	62.6
χ_2	-149.2	-149.5	-149.2	-148.5	-145.8	-149.0	-149.1	-148.8	-152.5
χ_4	32.0	30.0	31.2	30.7	38.6	29.1	27.2	28.4	22.8
χ_5	-54.5	-54.3	-55.3	-55.6	-61.8	-58.6	-57.4	-58.4	-54.9
Q	0.379	0.384	0.384	0.387	0.400	0.410	0.412	0.412	0.380
ϕ	262.4	258.9	260.9	262.2	263.0	262.5	260.0	258.2	262.8

N2-

ω_3	-63.8	-64.4	-64.4	-65.0	-66.9	-60.9	-61.5	-61.9	-60.1
ω_2	-75.0	-75.5	-75.5	-75.7	-75.2	-74.4	-75.2	-75.4	-74.5
χ_1	58.2	58.6	58.6	58.6	56.8	57.2	58.5	58.8	60.1
χ_2	-149.9	-149.6	-149.3	-148.9	-145.8	-149.0	-147.9	-147.5	-152.1
χ_4	-40.1	-40.8	-40.8	-41.0	-47.8	-46.0	-47.7	-48.6	-41.5
χ_5	49.1	50.1	50.5	50.0	55.1	52.9	52.8	52.9	48.4
Q	0.360	0.362	0.361	0.366	0.382	0.385	0.383	0.381	0.365
ϕ	284.3	284.8	285.1	286.8	299.7	295.7	298.7	299.3	287.9

N3-

ω_3	-50.8	-51.5	-51.2	-51.2	-46.6	-52.0	-52.5	-52.7	-52.0
ω_2	178.7	179.1	179.7	179.5	189.2	180.4	180.8	181.2	178.7
χ_1	48.5	48.1	47.7	46.5	39.3	48.0	46.5	46.4	48.8
χ_2	165.6	164.8	164.9	164.5	160.1	166.9	166.1	166.0	167.1
χ_4	30.7	28.7	29.8	29.5	47.2	30.1	30.0	30.2	19.0
χ_5	-51.4	-51.6	-52.5	-53.0	-58.4	-56.1	-55.1	-55.1	-52.2
Q	0.378	0.382	0.382	0.387	0.380	0.397	0.398	0.400	0.379

ϕ	251.4	249.0	249.6	251.5	262.2	259.7	256.8	255.6	253.6
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Table S5. X,y,z coordinates (in Å) of the 15 conformers of the ALL15 test set, minimized using B3LYP/6-31+G**

Conformer 1			Conformer 2				
C	1.615227	0.911489	0.468348	C	1.228730	0.841176	0.535675
C	1.118382	1.339969	-0.929847	C	0.582927	1.414951	-0.725097
C	-0.366259	0.997471	-1.098607	C	-0.885559	0.997782	-0.808441
C	-0.621985	-0.480382	-0.783185	C	-1.050812	-0.517182	-0.628442
C	-0.011763	-0.866289	0.578791	C	-0.266865	-1.029705	0.599054
C	-0.039117	-2.375675	0.829045	C	-0.193908	-2.552739	0.664198
O	1.077590	1.696531	1.499046	O	2.588711	1.172048	0.489018
O	1.397004	2.698650	-1.210226	O	0.612876	2.839483	-0.729615
O	-1.111627	1.831058	-0.192323	O	-1.647306	1.615706	0.235058
O	-2.037028	-0.656367	-0.803580	O	-2.425121	-0.860105	-0.523071
O	1.362706	-0.488790	0.636138	O	1.099863	-0.572850	0.541275
O	-1.385016	-2.883954	0.806788	O	0.517373	-3.107279	-0.435283
H	0.138028	1.863466	1.302650	H	3.016351	0.877918	1.305025
H	0.939754	3.245762	-0.555474	H	1.527406	3.122290	-0.587273
H	-2.019880	1.489436	-0.181740	H	-1.488938	2.569813	0.190341
H	-2.227491	-1.530812	-0.421434	H	-2.851904	-0.172944	0.012333
H	-1.765506	-2.822210	1.692228	H	1.399092	-2.708186	-0.440097
H	2.700370	1.003010	0.537599	H	0.749444	1.254273	1.437165
H	1.685053	0.762392	-1.667053	H	1.128947	1.008007	-1.588537
H	-0.682264	1.215209	-2.127078	H	-1.292408	1.296160	-1.784385
H	-0.144608	-1.089327	-1.567164	H	-0.665589	-1.028182	-1.516306
H	-0.578830	-0.363758	1.376860	H	-0.745779	-0.652183	1.515776
H	0.456907	-2.601699	1.778797	H	-1.206230	-2.961376	0.624062
H	0.500053	-2.895182	0.031318	H	0.268601	-2.846875	1.617465

Conformer 3

C	1.493661	-0.383001	0.098413
C	0.647551	-1.248984	1.032374
C	-0.808109	-1.283366	0.561961
C	-1.350763	0.129254	0.297176
C	-0.370764	0.946009	-0.569442
C	-0.762135	2.413247	-0.683539
O	2.776464	-0.311797	0.654546
O	1.103906	-2.598270	1.062427
O	-0.927244	-1.997486	-0.671401
O	-2.639468	0.069084	-0.294658
O	0.938499	0.923232	0.036393
O	0.133561	3.139061	-1.515223
H	3.364738	0.155483	0.045834
H	2.048969	-2.592880	1.270940
H	-0.496623	-2.857134	-0.556318
H	-2.623517	-0.649183	-0.946486
H	1.019421	3.038739	-1.139857
H	1.521836	-0.816322	-0.913729
H	0.698136	-0.794952	2.032654
H	-1.424567	-1.771323	1.329673
H	-1.471971	0.641696	1.258968
H	-0.312097	0.506225	-1.575938
H	-0.807926	2.854774	0.323858
H	-1.751561	2.487793	-1.138824

Conformer 4

C	1.387022	0.846066	0.334160
C	0.697211	1.468495	-0.893112
C	-0.778511	1.049667	-0.949369
C	-0.917335	-0.481556	-0.851882
C	-0.129854	-1.040587	0.346802
C	-0.031154	-2.560192	0.337034
O	0.815191	1.444550	1.494409
O	0.874517	2.869192	-0.956644
O	-1.561308	1.692343	0.067268
O	-2.284883	-0.852580	-0.771950
O	1.237166	-0.557355	0.331585
O	0.642680	-3.059449	1.485048
H	1.304725	1.163207	2.279617
H	0.274588	3.278935	-0.316042
H	-1.086797	1.622534	0.913675
H	-2.733629	-0.161268	-0.257957
H	1.528468	-2.671201	1.492805
H	2.466002	1.026042	0.306510
H	1.204410	1.057742	-1.772613
H	-1.215029	1.387899	-1.894178
H	-0.520089	-0.927348	-1.772949
H	-0.608178	-0.727754	1.284235
H	0.472364	-2.884223	-0.586556
H	-1.037678	-2.983057	0.349906

Conformer 5

C	1.381047	0.840262	0.451558
C	0.725980	1.421445	-0.814201
C	-0.755911	1.031774	-0.878015
C	-0.925138	-0.489844	-0.724581
C	-0.158169	-1.034017	0.496553
C	-0.060190	-2.557156	0.509239
O	0.798413	1.495523	1.576227
O	0.935774	2.814378	-0.932347
O	-1.538825	1.734510	0.100405
O	-2.301291	-0.826969	-0.623221
O	1.211500	-0.558692	0.514206
O	0.682415	-3.062481	-0.592715
H	1.286434	1.258349	2.376594
H	0.317731	3.262527	-0.336107
H	-1.077568	1.690721	0.955741
H	-2.734834	-0.096254	-0.152475
H	1.569368	-2.679148	-0.545117
H	2.462824	1.004063	0.437905
H	1.238602	0.961364	-1.665732
H	-1.171652	1.342170	-1.841531
H	-0.538783	-0.984685	-1.622212
H	-0.666921	-0.711411	1.415730
H	-1.065813	-2.976865	0.432366
H	0.384807	-2.879463	1.461529

Conformer 6

C	1.458657	0.752685	0.434268
C	0.798374	1.394245	-0.787479
C	-0.688118	1.035095	-0.853146
C	-0.898414	-0.473204	-0.676063
C	-0.126881	-1.010626	0.548331
C	-0.191316	-2.536038	0.667455
O	2.829588	1.019492	0.343675
O	0.877534	2.816213	-0.748002
O	-1.419387	1.669619	0.198498
O	-2.290764	-0.780422	-0.594005
O	1.257311	-0.653101	0.408290
O	-1.481559	-2.989602	1.046738
H	3.277633	0.642660	1.113657
H	1.804462	3.064229	-0.622260
H	-1.201547	2.613137	0.182066
H	-2.703740	-0.097211	-0.041506
H	-2.125445	-2.573397	0.450993
H	1.033909	1.162835	1.364665
H	1.307673	0.997310	-1.677413
H	-1.093564	1.350170	-1.824860
H	-0.522668	-0.988867	-1.567408
H	-0.539266	-0.565925	1.466232
H	0.503099	-2.858048	1.448297
H	0.134430	-2.991247	-0.281125

Conformer 7

C	1.484074	0.984526	0.365337
C	0.782209	1.376885	-0.952816
C	-0.693452	0.961022	-0.918268
C	-0.828666	-0.525027	-0.573595
C	-0.042392	-0.869454	0.704367
C	0.039594	-2.366072	0.987452
O	1.064417	1.762164	1.454753
O	0.954016	2.743871	-1.272658
O	-1.345570	1.767550	0.080027
O	-2.230563	-0.771092	-0.396199
O	1.314540	-0.420093	0.575346
O	0.624366	-3.095714	-0.085914
H	0.097383	1.867053	1.408926
H	0.592316	3.274574	-0.548132
H	-2.255994	1.448005	0.168602
H	-2.435841	-1.685072	-0.627107
H	1.524087	-2.760046	-0.206431
H	2.563423	1.123247	0.282720
H	1.269268	0.819309	-1.759338
H	-1.154573	1.158008	-1.894576
H	-0.434127	-1.119035	-1.406412
H	-0.525011	-0.385331	1.564671
H	0.601975	-2.514734	1.918748
H	-0.965285	-2.774448	1.130698

Conformer 8

C	1.547139	-0.844860	0.557471
C	0.290586	-1.270232	1.345826
C	-0.989184	-0.839027	0.614479
C	-0.932676	0.639754	0.230046
C	0.366125	0.960766	-0.534087
C	0.553771	2.460190	-0.786731
O	1.743588	-1.681663	-0.565662
O	0.270882	-2.675778	1.575177
O	-1.142434	-1.573861	-0.619435
O	-2.092367	1.023884	-0.509012
O	1.491611	0.533428	0.248649
O	-0.354971	2.959865	-1.755681
H	0.912405	-1.721000	-1.070075
H	0.886084	-3.083077	0.945211
H	-1.388311	-2.481696	-0.392821
H	-2.257621	0.330913	-1.167893
H	-1.249166	2.697136	-1.485996
H	2.444682	-0.960204	1.168818
H	0.317297	-0.771655	2.321986
H	-1.863353	-1.023245	1.251439
H	-0.946660	1.238119	1.148434
H	0.362602	0.452666	-1.508442
H	1.560949	2.624404	-1.178066
H	0.468720	3.005072	0.166665

Conformer 9

C	1.499193	-0.783736	0.538863
C	0.316388	-1.168236	1.453831
C	-1.016282	-0.941347	0.729241
C	-1.109777	0.493415	0.194322
C	0.136128	0.848786	-0.636607
C	0.230422	2.328266	-0.999115
O	1.678137	-1.677246	-0.525685
O	0.433994	-2.479643	1.968759
O	-1.079140	-1.882090	-0.356213
O	-2.310701	0.527275	-0.585244
O	1.323479	0.574130	0.121399
O	1.365626	2.604497	-1.799463
H	0.806397	-1.890871	-0.903468
H	0.490909	-3.096168	1.224281
H	-1.866285	-1.674959	-0.882169
H	-2.517162	1.431086	-0.853337
H	2.130746	2.207729	-1.357044
H	2.434260	-0.779674	1.101546
H	0.347180	-0.502818	2.322524
H	-1.848636	-1.130372	1.419142
H	-1.185942	1.179194	1.051228
H	0.136579	0.259475	-1.562805
H	-0.639886	2.629939	-1.592062
H	0.244274	2.923566	-0.072023

Conformer 10

C	1.463604	0.885915	0.472512
C	0.806767	1.477225	-0.788216
C	-0.665375	1.050282	-0.874862
C	-0.779910	-0.476319	-0.744489
C	-0.048971	-0.990558	0.507234
C	-0.013360	-2.516469	0.608686
O	0.862788	1.529906	1.599461
O	0.983436	2.876752	-0.882061
O	-1.484914	1.706709	0.103749
O	-2.142841	-0.884184	-0.733117
O	1.314214	-0.513200	0.522063
O	0.382634	-3.175341	-0.589416
H	1.348371	1.292492	2.401211
H	0.390905	3.299375	-0.243291
H	-1.027198	1.673592	0.961464
H	-2.637411	-0.201685	-0.250876
H	-0.396336	-3.299549	-1.146379
H	2.542649	1.065584	0.467859
H	1.337607	1.046630	-1.643609
H	-1.077625	1.360895	-1.839972
H	-0.315560	-0.935674	-1.623870
H	-0.564573	-0.621061	1.406332
H	-1.000274	-2.862380	0.937497
H	0.721372	-2.788838	1.372092

Conformer 11

C	1.449829	0.947313	0.509262
C	0.817796	1.517611	-0.770280
C	-0.642952	1.082872	-0.891881
C	-0.796946	-0.430334	-0.673694
C	-0.023098	-0.897644	0.578373
C	0.048816	-2.417046	0.708065
O	2.821702	1.218053	0.568466
O	0.955178	2.934600	-0.803493
O	-1.368832	1.815836	0.096545
O	-2.198573	-0.666705	-0.569485
O	1.333196	-0.465855	0.497102
O	-1.297450	-2.915855	0.770605
H	2.942582	2.127603	0.255503
H	0.219200	3.307459	-0.292556
H	-2.247412	1.410123	0.160251
H	-2.322897	-1.562398	-0.212158
H	-1.286596	-3.880227	0.798428
H	0.934995	1.343682	1.401236
H	1.391813	1.125838	-1.617314
H	-1.024858	1.338209	-1.890944
H	-0.379462	-0.950582	-1.550487
H	-0.509309	-0.477615	1.471935
H	0.604457	-2.674950	1.616877
H	0.578820	-2.829987	-0.160155

Conformer 12

C	1.568329	-0.900393	0.519367
C	0.357829	-1.248077	1.413253
C	-0.954924	-0.972735	0.668166
C	-0.970313	0.460816	0.135030
C	0.293075	0.741721	-0.698838
C	0.386641	2.183152	-1.183791
O	1.731371	-1.813146	-0.538560
O	0.424430	-2.563745	1.929783
O	-1.045916	-1.917475	-0.415453
O	-2.159457	0.596821	-0.652286
O	1.455750	0.455042	0.086809
O	-0.076857	3.074282	-0.162850
H	0.856736	-2.005418	-0.920377
H	0.479667	-3.180168	1.185318
H	-1.827692	-1.689748	-0.940173
H	-2.396377	1.531956	-0.701508
H	0.293902	3.951982	-0.310654
H	2.493439	-0.930571	1.097392
H	0.394771	-0.584374	2.282845
H	-1.803869	-1.124100	1.347012
H	-0.989082	1.152054	0.984235
H	0.284702	0.102253	-1.592258
H	1.432237	2.382262	-1.444695
H	-0.227990	2.297511	-2.087467

Conformer 13

C	1.361522	-0.885052	-0.142462
C	0.542059	-1.325901	1.077365
C	-0.932016	-0.956806	0.904382
C	-1.097306	0.515727	0.498679
C	-0.147239	0.881149	-0.665419
C	-0.158316	2.369019	-0.960545
O	2.726835	-1.163742	0.035006
O	0.602734	-2.736246	1.267656
O	-1.528968	-1.731068	-0.139139
O	-2.451599	0.792934	0.175012
O	1.199330	0.506940	-0.321978
O	0.450637	2.583419	-2.232453
H	3.102619	-0.462266	0.588641
H	1.528766	-3.009035	1.187512
H	-1.316004	-2.661036	0.028368
H	-2.786414	0.036241	-0.331523
H	0.493143	3.531892	-2.404761
H	1.049501	-1.439364	-1.037170
H	0.941603	-0.797135	1.957806
H	-1.469041	-1.135710	1.846608
H	-0.848005	1.145556	1.361426
H	-0.453691	0.339986	-1.571766
H	0.391458	2.891400	-0.163724
H	-1.201509	2.708899	-0.957521

Conformer 14

C	1.218631	-0.879246	0.937231
C	1.487462	0.614685	0.705844
C	0.599320	1.161429	-0.421104
C	-0.879732	0.810465	-0.168344
C	-1.081392	-0.677143	0.134508
C	-1.102910	-1.556709	-1.124674
O	1.781454	-1.573959	-0.164851
O	1.298276	1.359980	1.906449
O	0.749261	2.575580	-0.539899
O	-1.373257	1.542614	0.967698
O	-0.152180	-1.169315	1.119128

O	-2.317010	-1.244655	-1.812779
H	1.742259	-2.522189	0.020467
H	0.346357	1.340549	2.114649
H	1.093469	2.895136	0.309645
H	-1.363220	2.479563	0.724197
H	-2.336569	-1.714672	-2.655270
H	1.684836	-1.189616	1.878183
H	2.542177	0.733750	0.442109
H	0.916896	0.717329	-1.370264
H	-1.476873	1.061851	-1.052726
H	-2.059349	-0.780965	0.612981
H	-1.088554	-2.606120	-0.801177
H	-0.229350	-1.378241	-1.761902

Conformer 15

C	1.203530	-1.009992	0.721819
C	1.501866	0.484719	0.508950
C	0.588235	1.085355	-0.566130
C	-0.890627	0.786245	-0.254750
C	-1.121449	-0.696067	0.065696
C	-1.168980	-1.598048	-1.177181
O	1.944537	-1.526458	1.773156
O	1.374178	1.192549	1.746147
O	0.792332	2.492109	-0.686576
O	-1.302964	1.531311	0.906452
O	-0.184505	-1.194537	1.026921
O	-2.266897	-1.159344	-1.977097
H	1.896859	-0.882598	2.499483
H	0.420088	1.250154	1.946280
H	1.185186	2.797574	0.146101
H	-1.303271	2.466692	0.657473
H	-2.393792	-1.771544	-2.712280
H	1.481154	-1.590283	-0.168339
H	2.551178	0.591350	0.213853
H	0.842826	0.640555	-1.536501
H	-1.515490	1.061788	-1.111242
H	-2.093743	-0.769241	0.560901
H	-1.307191	-2.630009	-0.830677
H	-0.233160	-1.552381	-1.752458

Table S6. X,y,z coordinates (in Å) of the 15 conformers of the AnGol15 test set, minimized using B3LYP/6-31+G**

S1-	(Conformer 1)			S2-	(Conformer 2)		
C	-2.681567	-1.118532	-0.112948	C	-2.476785	-1.267188	-0.110394
C	-1.324927	-0.927278	0.586447	C	-1.183599	-0.892770	0.634679
C	-0.189586	-0.645824	-0.406453	C	-0.027156	-0.578630	-0.325869
C	1.180361	-0.339927	0.237920	C	1.285846	-0.084462	0.337135
C	1.331584	1.190879	0.053553	C	1.274782	1.434509	0.067165
O	0.787652	1.909170	1.147974	O	0.604049	2.153225	1.087150
C	0.572663	1.415527	-1.254932	C	0.563812	1.499154	-1.285366
O	-3.230497	0.138249	-0.503569	O	-3.116508	-0.102137	-0.625625
O	2.163251	-1.081116	-0.477651	O	2.434808	-0.630230	-0.302508
O	-1.444211	0.129723	1.548986	O	-1.455799	0.213566	1.504871
O	-0.544277	0.507955	-1.200168	O	-0.442867	0.466355	-1.232220
C	3.416301	-1.179255	0.187194	C	2.776389	-1.939040	0.126067
H	-2.574485	-1.797759	-0.969720	H	-2.261051	-1.995560	-0.904245
H	-3.401072	-1.555025	0.585481	H	-3.189872	-1.717533	0.585945
H	-1.072228	-1.845013	1.133350	H	-0.876934	-1.738393	1.264707
H	-0.068575	-1.515619	-1.066214	H	0.186989	-1.484437	-0.911433
H	1.210207	-0.603172	1.304146	H	1.318229	-0.289170	1.415587
H	2.380045	1.488259	-0.031996	H	2.295527	1.819438	0.014611
H	-0.020211	1.448092	1.444797	H	-0.172393	1.634369	1.371585
H	0.181707	2.431319	-1.344979	H	0.060756	2.454636	-1.449228
H	1.202916	1.176089	-2.122463	H	1.260514	1.292471	-2.108463
H	-2.586436	0.555482	-1.102224	H	-2.480202	0.329479	-1.222772
H	-2.195703	0.672933	1.250850	H	-2.238895	0.656271	1.131068
H	3.890776	-0.198594	0.326839	H	2.963654	-1.964172	1.209751
H	3.304339	-1.660020	1.169945	H	1.993714	-2.673514	-0.115265
H	4.057626	-1.796940	-0.444723	H	3.690540	-2.215856	-0.402949

S4- (Conformer 3)

C	2.690450	-0.471693	0.623347
C	1.423964	-0.635104	-0.209173
C	0.153742	-0.437445	0.617181
C	-1.145686	-0.406411	-0.224001
C	-1.557904	1.087861	-0.181827
O	-0.998765	1.828775	-1.253820
C	-1.018651	1.505880	1.186056
O	3.786882	-0.605803	-0.295340
O	-2.092807	-1.253943	0.420563
O	1.429117	0.304036	-1.289707
O	0.230816	0.812367	1.319471
C	-3.202991	-1.606165	-0.393343
H	2.691237	0.515613	1.096662
H	2.733131	-1.249591	1.397726
H	1.404800	-1.656484	-0.621350
H	0.072872	-1.263024	1.337823
H	-0.984567	-0.735097	-1.258824
H	-2.641960	1.209726	-0.250308
H	-0.065765	1.565908	-1.357807
H	-0.819445	2.577942	1.250611
H	-1.708355	1.203961	1.987874
H	4.595284	-0.276971	0.115974
H	2.333827	0.333007	-1.637290
H	-3.798800	-0.730735	-0.685652
H	-2.874493	-2.128169	-1.304146
H	-3.826723	-2.277385	0.200857

S3- (Conformer 4)

C	-2.542240	0.522906	0.665091
C	-1.327285	0.555042	-0.255558
C	-0.010471	0.425763	0.511878
C	1.248258	0.243316	-0.384361
C	1.599463	-1.249065	-0.197449
O	0.944731	-2.082706	-1.137650
C	1.138933	-1.486852	1.240539
O	-3.691404	0.578360	-0.195166
O	2.349992	1.009925	0.093077
O	-1.419876	-0.501698	-1.215335
O	-0.067842	-0.717305	1.377891
C	2.326764	2.371725	-0.302333
H	-2.531209	-0.402500	1.250019
H	-2.522208	1.385809	1.344674
H	-1.316957	1.520464	-0.786920
H	0.113719	1.332073	1.123047
H	1.053539	0.472065	-1.439769
H	2.672931	-1.404268	-0.324530
H	0.014678	-1.800669	-1.210600
H	0.895265	-2.533522	1.436083
H	1.894344	-1.136195	1.957974
H	-4.477473	0.313380	0.297494
H	-2.345524	-0.547204	-1.500694
H	2.312491	2.465883	-1.398404
H	1.460117	2.910097	0.109449
H	3.239214	2.829463	0.085593

N1- (Conformer 5)

C	2.830331	0.359206	-0.552393
C	1.454570	0.890994	-0.112946
C	0.303129	0.008319	-0.615417
C	-1.082380	0.251559	0.005126
C	-1.769256	-1.094788	-0.234931
O	-2.845165	-1.379950	0.644218
C	-0.634679	-2.092672	-0.008815
O	3.222523	-0.758762	0.240605
O	-1.840633	1.288906	-0.595410
O	1.431018	1.060297	1.298911
O	0.583708	-1.380769	-0.314802
C	-1.737065	2.560750	0.039909
H	3.589494	1.127939	-0.384206
H	2.819117	0.109786	-1.622990
H	1.310635	1.884432	-0.557979
H	0.229976	0.131179	-1.708239
H	-0.978747	0.419957	1.084963
H	-2.113410	-1.120186	-1.279334
H	-3.565652	-0.766418	0.446032
H	-0.699507	-2.975588	-0.651525
H	-0.620329	-2.410346	1.040328
H	2.549638	-1.447196	0.102320
H	2.009116	0.372466	1.668172
H	-2.032021	2.500547	1.096139
H	-0.720628	2.969714	-0.017263
H	-2.420894	3.227679	-0.489496

N2- (Conformer 6)

C	-2.878988	-0.732774	-0.430942
C	-1.469594	-1.007000	0.118044
C	-0.395870	-0.184213	-0.607001
C	1.015240	-0.301302	-0.016104
C	1.603086	1.096855	-0.245132
O	2.650186	1.358296	0.684866
C	0.369285	1.988371	-0.058323
O	-3.369555	0.527762	0.025852
O	1.689762	-1.361210	-0.667778
O	-1.448795	-0.787914	1.524827
O	-0.729764	1.228971	-0.584641
C	2.835085	-1.850075	0.027715
H	-3.576173	-1.482447	-0.047026
H	-2.879062	-0.789635	-1.529006
H	-1.221566	-2.063576	-0.049279
H	-0.362033	-0.507229	-1.656997
H	0.961424	-0.483183	1.066684
H	1.977203	1.154866	-1.276970
H	3.107501	2.171729	0.435359
H	0.419179	2.935665	-0.604964
H	0.221655	2.194252	1.010750
H	-2.737332	1.202020	-0.276431
H	-2.096271	-0.086372	1.702818
H	3.616850	-1.086378	0.109010
H	2.564884	-2.190360	1.037203
H	3.207557	-2.698067	-0.550840

S1+ (Conformer 7)

C	2.315280	0.108133	0.923936
C	1.250525	-0.848541	0.390021
C	0.171580	-0.160779	-0.457918
C	-0.877818	0.652113	0.339453
C	-2.099717	-0.278018	0.374506
O	-1.928703	-1.126640	1.511692
C	-1.963872	-1.019934	-0.953206
O	3.013775	0.777443	-0.120272
O	-1.268794	1.840406	-0.332740
O	1.954964	-1.801503	-0.412540
O	-0.559399	-1.206011	-1.146117
C	-0.339061	2.910715	-0.205814
H	1.863338	0.885176	1.547345
H	3.010292	-0.467227	1.551726
H	0.765553	-1.354785	1.237540
H	0.648176	0.474219	-1.212186
H	-0.549108	0.879824	1.362609
H	-3.026649	0.302734	0.445165
H	-2.615165	-1.806146	1.509509
H	-2.442685	-2.005001	-0.958106
H	-2.384755	-0.411787	-1.766614
H	3.333388	0.090198	-0.724006
H	1.291163	-2.277960	-0.934275
H	-0.222511	3.203708	0.848128
H	0.647145	2.653757	-0.613942
H	-0.752294	3.750810	-0.767346

S2+ (Conformer 8)

C	2.318434	0.097595	0.931161
C	1.244446	-0.855391	0.408665
C	0.174696	-0.170064	-0.453937
C	-0.872188	0.659573	0.328671
C	-2.116969	-0.253536	0.344632
O	-2.067541	-1.193924	1.418739
C	-1.965343	-1.019526	-0.961389
O	3.026256	0.742882	-0.121210
O	-1.236522	1.857235	-0.341843
O	1.940029	-1.828191	-0.374391
O	-0.556673	-1.216519	-1.132140
C	-0.278679	2.904532	-0.230928
H	1.874142	0.890119	1.540932
H	3.005620	-0.475431	1.569708
H	0.751053	-1.344518	1.262504
H	0.661460	0.454723	-1.210629
H	-0.540538	0.889362	1.353299
H	-3.033529	0.346322	0.376792
H	-2.261382	-0.738039	2.248112
H	-2.449550	-1.998218	-0.929094
H	-2.368001	-0.429293	-1.795439
H	3.337286	0.043317	-0.715262
H	1.270953	-2.309165	-0.885804
H	-0.141316	3.198615	0.820564
H	0.695670	2.621915	-0.649671
H	-0.677997	3.752906	-0.790003

N3- (Conformer 9)

C	2.755749	-0.325678	-0.657870
C	1.532784	0.269898	0.047880
C	0.209376	-0.222514	-0.539508
C	-1.083255	0.393019	0.026706
C	-2.104902	-0.703928	-0.289796
O	-3.243840	-0.720576	0.557064
C	-1.298881	-1.991392	-0.101505
O	3.960158	0.175407	-0.093848
O	-1.492965	1.609831	-0.575706
O	1.604902	-0.007097	1.450377
O	0.092450	-1.622872	-0.218917
C	-1.113225	2.797949	0.113221
H	2.760906	-0.037912	-1.714383
H	2.718019	-1.423512	-0.600612
H	1.585176	1.360192	-0.042157
H	0.220973	-0.076981	-1.631702
H	-1.000224	0.507483	1.116477
H	-2.413488	-0.581267	-1.337922
H	-3.783050	0.055842	0.354350
H	-1.531421	-2.755074	-0.850573
H	-1.478253	-2.404578	0.897107
H	3.874829	0.093330	0.867982
H	1.318268	-0.928340	1.561270
H	-1.469157	2.784129	1.152423
H	-0.026566	2.948723	0.113134
H	-1.584724	3.627424	-0.418003

N1+ (Conformer 10)

C	2.273292	1.029746	0.067602
C	1.616970	-0.342761	0.184505
C	0.301801	-0.457368	-0.589956
C	-0.862514	0.366872	-0.009473
C	-2.039690	-0.622052	-0.004581
O	-2.955811	-0.293078	1.035716
C	-1.321192	-1.961615	0.191786
O	3.481636	1.089167	0.813876
O	-1.037297	1.525815	-0.801167
O	2.567772	-1.279910	-0.326051
O	-0.119238	-1.844740	-0.574325
C	-1.872699	2.523815	-0.218421
H	1.617716	1.806168	0.470614
H	2.455393	1.250534	-0.994655
H	1.427524	-0.557671	1.249081
H	0.463898	-0.178143	-1.636950
H	-0.665108	0.654081	1.037080
H	-2.529762	-0.586158	-0.987291
H	-3.757562	-0.823274	0.939650
H	-1.875377	-2.826406	-0.185249
H	-1.107223	-2.112775	1.260746
H	4.017584	0.328118	0.546578
H	2.127934	-2.141611	-0.376338
H	-2.903894	2.172719	-0.097733
H	-1.488884	2.833305	0.764181
H	-1.851860	3.377162	-0.898962

S4+ (Conformer 11)

C	2.269706	0.829267	0.276488
C	1.395560	-0.388516	-0.010816
C	0.039390	-0.035291	-0.637364
C	-1.007889	0.535069	0.351007
C	-1.920724	-0.676096	0.641036
O	-1.381721	-1.513695	1.662902
C	-1.856797	-1.437968	-0.674269
O	3.516169	0.452146	0.842288
O	-1.825748	1.541568	-0.230705
O	2.153349	-1.196749	-0.913731
O	-0.520547	-1.258092	-1.161614
C	-1.218931	2.823173	-0.311345
H	2.420105	1.390121	-0.659582
H	1.789449	1.491516	1.003483
H	1.222474	-0.944167	0.922395
H	0.187722	0.656078	-1.477641
H	-0.545890	0.914026	1.275399
H	-2.935297	-0.341689	0.885823
H	-1.481941	-1.078220	2.519522
H	-2.034866	-2.507819	-0.543638
H	-2.578165	-1.022373	-1.390122
H	3.875648	-0.253579	0.284168
H	1.572220	-1.912813	-1.211837
H	-0.931208	3.187745	0.686095
H	-0.330908	2.821336	-0.958521
H	-1.964212	3.497062	-0.738288

S3+ (Conformer 12)

C	2.268494	0.808902	0.286250
C	1.391320	-0.406390	-0.003220
C	0.038143	-0.048700	-0.630928
C	-1.008009	0.543840	0.348066
C	-1.937862	-0.644289	0.638854
O	-1.354030	-1.356542	1.729969
C	-1.879418	-1.411860	-0.679575
O	3.521747	0.425714	0.832520
O	-1.800281	1.560579	-0.250888
O	2.148722	-1.214224	-0.909694
O	-0.532483	-1.276624	-1.141049
C	-1.175873	2.835039	-0.302314
H	2.408318	1.380145	-0.645330
H	1.795847	1.461366	1.026456
H	1.215772	-0.961952	0.928792
H	0.189787	0.630128	-1.480670
H	-0.556728	0.906918	1.281005
H	-2.947056	-0.293267	0.883563
H	-1.841909	-2.177468	1.875146
H	-2.098329	-2.480033	-0.577708
H	-2.578781	-0.969089	-1.403062
H	3.872200	-0.276808	0.264827
H	1.568993	-1.930275	-1.209044
H	-0.912760	3.186779	0.706055
H	-0.269540	2.827389	-0.924039
H	-1.900075	3.521752	-0.744815

N3+ (Conformer 13)

C	2.551851	0.865389	0.040777
C	1.812353	-0.446455	0.332531
C	0.490664	-0.593840	-0.436296
C	-0.692076	0.259411	0.055054
C	-1.898452	-0.656140	-0.187179
O	-2.981841	-0.291242	0.662527
C	-1.301739	-2.033951	0.123981
O	1.865167	2.018565	0.507847
O	-0.698733	1.491015	-0.655633
O	2.703275	-1.487951	-0.055501
O	0.057924	-1.971215	-0.320218
C	-1.638380	2.458146	-0.169373
H	2.758660	0.926065	-1.037880
H	3.512565	0.833498	0.560655
H	1.600216	-0.506596	1.412397
H	0.668883	-0.384325	-1.500436
H	-0.620121	0.456032	1.136104
H	-2.190056	-0.583407	-1.244468
H	-3.763536	-0.808905	0.429245
H	-1.795192	-2.857483	-0.402471
H	-1.352666	-2.220363	1.206182
H	1.064543	2.128911	-0.032456
H	2.200913	-2.316145	-0.040567
H	-2.667762	2.110305	-0.294360
H	-1.460221	2.673768	0.892330
H	-1.476297	3.362244	-0.759038

N2+ (Conformer 14)

C	2.306416	0.945095	0.776885
C	1.582981	-0.389867	0.583181
C	0.444935	-0.321342	-0.447384
C	-0.830610	0.376334	0.066231
C	-1.943415	-0.669176	-0.146751
O	-2.918764	-0.564878	0.887734
C	-1.161980	-1.988261	-0.142113
O	2.989078	1.352946	-0.398834
O	-1.005237	1.589583	-0.640214
O	2.574236	-1.321782	0.150132
O	0.063685	-1.675254	-0.805923
C	-1.995606	2.454503	-0.093970
H	3.005911	0.841220	1.619429
H	1.592577	1.737886	1.020066
H	1.172867	-0.711152	1.555559
H	0.800841	0.167225	-1.357618
H	-0.768571	0.581876	1.148108
H	-2.394599	-0.495723	-1.133113
H	-3.684032	-1.111111	0.665953
H	-1.644122	-2.797855	-0.697679
H	-0.994350	-2.316561	0.895335
H	3.517568	0.593824	-0.688264
H	2.103763	-2.061053	-0.266604
H	-3.000059	2.017490	-0.152355
H	-1.777337	2.690173	0.957763
H	-1.961814	3.372263	-0.684284

N4+ (Conformer 15)

C	2.297899	0.742135	0.312003
C	1.421932	-0.495516	0.137878
C	0.135798	-0.254021	-0.669061
C	-0.978102	0.520212	0.085748
C	-2.144713	-0.485905	0.174242
O	-2.830569	-0.493772	1.416742
C	-1.468943	-1.833059	-0.056614
O	3.482836	0.439245	1.031983
O	-1.457279	1.680415	-0.580724
O	2.238211	-1.453362	-0.537430
O	-0.429399	-1.546877	-0.998139
C	-0.615595	2.820652	-0.489708
H	1.775889	1.510194	0.889613
H	2.538254	1.152807	-0.681572
H	1.156659	-0.880131	1.136731
H	0.379367	0.226743	-1.622664
H	-0.655339	0.785005	1.104716
H	-2.830524	-0.261492	-0.652928
H	-3.401542	0.283901	1.464334
H	-2.124113	-2.584431	-0.501226
H	-1.068847	-2.221990	0.891509
H	3.879162	-0.338339	0.611318
H	1.651874	-2.162559	-0.843729
H	-0.418494	3.088604	0.558747
H	0.342894	2.666687	-1.004528
H	-1.146728	3.641736	-0.975371