Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for:

Rapid Evaluation of the Interaction Energies for Carbohydrate-Containing Hydrogen-Bonded Complexes via the Polarizable Dipole-Dipole Interaction Model Combined with NBO Charge or AM1 Charge

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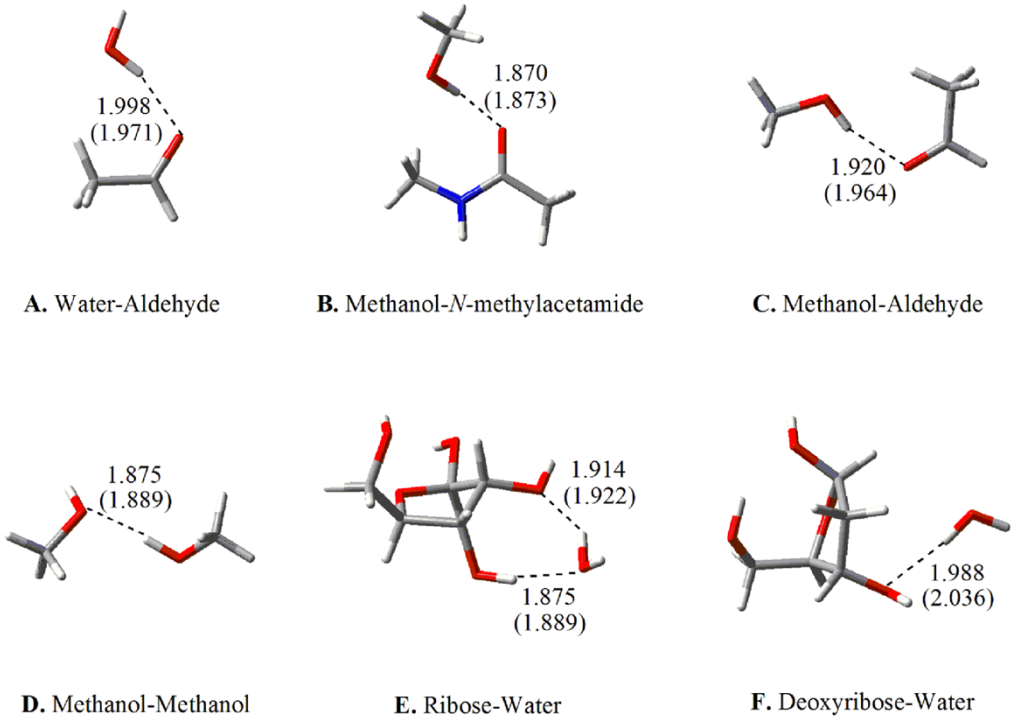

A. Water-Aldehyde **B.** Methanol-*N*-methylacetamide **C.** Methanol-Aldehyde

D. Methanol-Methanol **E.** Ribose-Water **F.** Deoxyribose-Water

Mean unsigned error (MUE) = 0.023 Å

Root mean squared error (RMSE) = 0.028 Å

Figure S1. The training dimers used to derive the parameters needed in this work. The equilibrium hydrogen bond distances predicted by eq (1) are given in the corresponding position. Values in parentheses are obtained from MP2/6-31+G(d,p) calculations. All distances are in Å.

Table S1. The interaction energies obtained by the CP-corrected MP2/aug-cc-pVTZ method (IE_{MP2}), and by eq (2) with NBO charge (IE) for the six training dimers.

Dimers	IE_{MP2}	eq (2) with NBO charge						
		E_{dd}^{perm}	E_{pol}	E_{vdw}	Δ_{mix}	IE	ΔE	δ(%)
A	-6.11	-3.94	-0.60	-0.22	-1.32	-6.08	0.03	0.4
B	-8.12	-4.95	-0.53	-0.52	-2.11	-8.11	0.01	0.1
C	-6.25	-4.41	-0.47	-0.29	-1.13	-6.30	-0.05	0.9
D	-5.63	-3.29	-0.29	-0.20	-1.47	-5.25	0.38	6.8
E	-9.10	-5.91	-0.91	0.41	-2.64	-9.05	0.05	0.6
F	-6.02	-3.54	-0.53	-0.74	-0.77	-5.58	0.44	7.4
Mean unsigned error (MUE)							0.16	
Root mean squared error (RMSE)							0.24	
Mean relative error (MRE)								2.7

$\Delta E = IE - IE_{MP2}$, $\delta = |\Delta E \div IE_{MP2}| \times 100\%$, All energies are in kcal/mol.

Table S2. The equilibrium hydrogen bond distances R_{eq}(H···O) obtained by MP2/6-31+G(d,p), by eq (1) and by eq (2).

Dimer	MP2	Eq (1)	Δ*R*	eq (2) with NBO charge	Δ*R*	eq (2) with AM1 charge	Δ*R*
1	2.061	2.072	0.011	2.050	-0.011	2.050	-0.011
	1.979	1.987	0.008	1.971	-0.008	1.971	-0.008
2	2.076	2.088	0.012	2.065	-0.011	2.070	-0.006
	1.967	1.975	0.008	1.959	-0.008	1.962	-0.005
3	1.865	1.882	0.017	1.855	-0.010	1.860	-0.005
4	1.881	1.855	-0.026	1.835	-0.046	1.840	-0.041
5	1.859	1.900	0.041	1.880	0.021	1.890	0.031
	1.796	1.836	0.040	1.816	0.020	1.826	0.030
6	1.870	1.910	0.040	1.890	0.020	1.895	0.025
	1.792	1.830	0.038	1.811	0.019	1.816	0.024
7	1.800	1.840	0.040	1.820	0.020	1.825	0.025
	1.989	2.026	0.037	2.007	0.018	2.012	0.023
8	1.850	1.857	0.007	1.840	-0.010	1.840	-0.010
	1.910	1.914	0.004	1.899	-0.011	1.899	-0.011
9	1.846	1.835	-0.011	1.820	-0.026	1.810	-0.036
10	1.872	1.897	0.025	1.884	0.012	1.884	0.012
	1.842	1.880	0.038	1.860	0.018	1.860	0.018
11	1.877	1.900	0.023	1.888	0.011	1.894	0.017
	1.833	1.870	0.037	1.850	0.017	1.860	0.027
12	1.770	1.800	0.030	1.770	0.000	1.780	0.010
	1.921	1.950	0.029	1.921	0.000	1.931	0.010
13	1.871	1.880	0.009	1.860	-0.011	1.865	-0.006
	1.884	1.890	0.006	1.879	-0.005	1.881	-0.003
14	1.918	1.925	0.007	1.918	0.000	1.918	0.000
	1.918	1.925	0.007	1.918	0.000	1.918	0.000
15	1.804	1.818	0.014	1.804	0.000	1.804	0.000
	1.841	1.865	0.024	1.841	0.000	1.841	0.000
16	1.838	1.887	0.049	1.865	0.027	1.870	0.032
17	1.812	1.845	0.033	1.820	0.008	1.830	0.018
	1.927	1.939	0.012	1.930	0.003	1.934	0.007
	2.165	2.191	0.026	2.171	0.006	2.179	0.014
18	1.825	1.875	0.050	1.855	0.030	1.855	0.030
	1.788	1.833	0.045	1.815	0.027	1.815	0.027
19	1.828	1.875	0.047	1.855	0.027	1.860	0.032
	1.793	1.832	0.039	1.816	0.023	1.820	0.027
20	1.913	1.932	0.019	1.900	-0.013	1.913	0.000
	1.806	1.815	0.009	1.800	-0.006	1.806	0.000
Mean unsigned error (MUE)			0.025		0.014		0.016
Root mean squared error (RMSE)			0.029		0.017		0.020

All distances are in Å.

Table S3. The equilibrium hydrogen bond distances R_{eq}(H···O) obtained by B3LYP/6-31+G(d,p), by eq (1) and by eq (2).

Dimer	B3LYP	Eq (1)	Δ*R*	eq (2) with NBO charge	Δ*R*	eq (2) with AM1 charge	Δ*R*
21	1.822	1.828	0.006	1.815	-0.007	1.810	-0.012
	1.969	1.972	0.003	1.966	-0.003	1.963	-0.006
22	1.824	1.812	-0.012	1.812	-0.012	1.800	-0.024
	1.966	1.957	-0.009	1.957	-0.009	1.948	-0.018
23	1.901	1.883	-0.018	1.882	-0.019	1.877	-0.024
	1.973	1.958	-0.015	1.956	-0.017	1.950	-0.023
	2.020	2.012	-0.008	2.011	-0.009	2.009	-0.011
24	1.820	1.820	0.000	1.800	-0.020	1.810	-0.010
	1.901	1.902	0.001	1.892	-0.009	1.897	-0.004
25	1.882	1.876	-0.006	1.864	-0.018	1.864	-0.018
	1.817	1.810	-0.007	1.790	-0.027	1.790	-0.027
26	2.066	2.036	-0.030	2.036	-0.030	2.033	-0.033
	1.787	1.740	-0.047	1.740	-0.047	1.735	-0.052
	1.930	1.887	-0.043	1.887	-0.043	1.882	-0.048
Mean unsigned error (MUE)			0.015		0.019		0.022
Root mean squared error (RMSE)			0.021		0.023		0.026

All distances are in Å.

The data in Table S2 and Table S3 indicate that both eq (1) and eq (2) can produce accurate equilibrium hydrogen bond distances. But eq (1) is more efficient than eq (2) and that is the reason why we use eq (1) to produce equilibrium hydrogen bond distances.

Table S4. The interaction energy components obtained by eq (2) with NBO charge

	E_{dd}^{perm}	E_{pol}	E_{vdw}	Δ_{mix}	IE
1	-5.75(55.5%)	-0.75(7.3%)	-2.43(23.5%)	-1.42(13.7%)	-10.35
2	-5.77(56.1%)	-0.75(7.3%)	-2.33(22.7%)	-1.43(13.9%)	-10.28
3	-4.82(50.4%)	-0.98(10.3%)	-1.74(18.2%)	-2.02(21.1%)	-9.56
4	-4.84(52.3%)	-0.84(9.1%)	-1.34(14.5%)	-2.24(24.1%)	-9.26
5	-7.31(51.3%)	-0.88(6.2%)	-1.34(9.4%)	-4.73(33.1%)	-14.26
6	-7.46(51.1%)	-0.9(6.2%)	-1.36(9.3%)	-4.88(33.4%)	-14.60
7	-11.50(63.2%)	-1.43(7.8%)	-2.64(14.5%)	-2.63(14.5%)	-18.20
8	-5.73(61.0%)	-0.64(6.9%)	-0.22(2.3%)	-2.80(29.8%)	-9.39
9	-7.02(54.7%)	-1.46(11.3%)	-1.95(15.2%)	-2.41(18.8%)	-12.84
10	-6.70(51.6%)	-0.93(7.2%)	-1.81(13.9%)	-3.55(27.3%)	-12.99
11	-6.82(51.4%)	-0.96(7.2%)	-1.74(13.1%)	-3.75(28.3%)	-13.27
12	-11.59(57.7%)	-2.40(11.9%)	-2.67(13.3%)	-3.43(17.1%)	-20.09
13	-5.18(58.1%)	-0.56(6.2%)	-0.41(4.6%)	-2.77(31.1%)	-8.92
14	-2.80(37.9%)	-0.49(6.6%)	-1.90(25.7%)	-2.20(29.8%)	-7.39
15	-5.88(47.9%)	-0.95(7.7%)	-1.85(15.1%)	-3.59(29.3%)	-12.27
16	-4.74(51.4%)	-0.79(8.6%)	-1.72(18.6%)	-1.98(21.5%)	-9.23
17	-14.18(59.2%)	-2.18(9.1%)	-3.63(15.1%)	-3.99(16.6%)	-23.98
18	-7.87(57.0%)	-1.06(7.7%)	-1.27(9.2%)	-3.61(26.1%)	-13.81
19	-8.01(57.7%)	-1.03(7.4%)	-1.23(8.8%)	-3.62(26.1%)	-13.89
20	-5.88(58.5%)	-0.80(8.0%)	-0.23(2.3%)	-3.13(31.2%)	-10.04
21	-5.51(57.7%)	-0.32(3.4%)	-0.94(9.9%)	-2.76(29.0%)	-9.53
22	-5.04(52.5%)	-0.03(0.3%)	-1.51(15.7%)	-3.02(31.5%)	-9.60
23	-5.55(53.5%)	-0.13(1.3%)	-1.40(13.5%)	-3.30(31.7%)	-10.38
24	-6.70(55.5%)	-0.88(7.3%)	-1.23(10.2%)	-3.27(27.0%)	-12.08
25	-6.93(54.6%)	-0.81(6.4%)	-1.36(10.7%)	-3.59(28.3%)	-12.69
26	-10.01(50.1%)	-0.27(1.4%)	-4.56(22.8%)	-5.13(25.7%)	-19.97

All energies are in kcal/mol.

Table S5. The interaction energy components obtained by eq (2) with AM1 charge

	E_{dd}^{perm}	E_{pol}	E_{vdw}	Δ_{mix}	IE
1	-5.75(54.6%)	-0.93(8.8%)	-2.43(23.1%)	-1.42(13.5%)	-10.53
2	-5.77(55.1%)	-0.93(8.9%)	-2.33(22.3%)	-1.43(13.7%)	-10.46
3	-4.82(50.4%)	-0.98(10.3%)	-1.74(18.2%)	-2.02(21.1%)	-9.56
4	-4.84(52.0%)	-0.89(9.5%)	-1.34(14.4%)	-2.24(24.1%)	-9.31
5	-7.31(50.8%)	-1.01(7.0%)	-1.34(9.3%)	-4.73(32.9%)	-14.39
6	-7.46(50.7%)	-1.01(6.9%)	-1.36(9.2%)	-4.88(33.2%)	-14.71
7	-11.50(63.0%)	-1.49(8.2%)	-2.64(14.5%)	-2.63(14.3%)	-18.26
8	-5.73(60.5%)	-0.72(7.6%)	-0.22(2.3%)	-2.80(29.6%)	-9.47
9	-7.02(53.8%)	-1.67(12.8%)	-1.95(14.9%)	-2.41(18.5%)	-13.05
10	-6.70(51.0%)	-1.08(8.2%)	-1.81(13.8%)	-3.55(27.0%)	-13.14
11	-6.82(50.8%)	-1.13(8.4%)	-1.74(12.9%)	-3.75(27.9%)	-13.44
12	-11.59(56.5%)	-2.84(13.8%)	-2.67(13.0%)	-3.43(16.7%)	-20.53
13	-5.18(57.4%)	-0.67(7.4%)	-0.41(4.5%)	-2.77(30.7%)	-9.03
14	-2.80(38.0%)	-0.47(6.4%)	-1.90(25.8%)	-2.20(29.8%)	-7.37
15	-5.88(46.9%)	-1.21(9.7%)	-1.85(14.8%)	-3.59(28.6%)	-12.53
16	-4.74(51.5%)	-0.77(8.4%)	-1.72(18.6%)	-1.98(21.5%)	-9.21
17	-14.18(58.4%)	-2.51(10.3%)	-3.63(14.9%)	-3.99(16.4%)	-24.31
18	-7.87(56.2%)	-1.26(9.0%)	-1.27(9.1%)	-3.61(25.7%)	-14.01
19	-8.01(56.9%)	-1.22(8.7%)	-1.23(8.7%)	-3.62(25.7%)	-14.08
20	-5.88(58.0%)	-0.90(8.9%)	-0.23(2.3%)	-3.13(30.8%)	-10.14
21	-5.51(54.9%)	-0.82(8.2%)	-0.94(9.4%)	-2.76(27.5%)	-10.03
22	-5.04(50.5%)	-0.41(4.1%)	-1.51(15.1%)	-3.02(30.3%)	-9.98
23	-5.55(51.9%)	-0.45(4.2%)	-1.40(13.1%)	-3.30(30.8%)	-10.70
24	-6.70(54.7%)	-1.05(8.6%)	-1.23(10.0%)	-3.27(26.7%)	-12.25
25	-6.93(53.8%)	-1.01(7.8%)	-1.36(10.6%)	-3.59(27.8%)	-12.89
26	-10.01(48.2%)	-1.08(5.2%)	-4.56(21.9%)	-5.13(24.7%)	-20.78

All energies are in kcal/mol.

Table S6. Cartesian coordinates for all the hydrogen-bonded complexes considered in this work

A. Water-Aldehyde

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.237812	-0.407194	0.003609
8	0	-0.293446	-1.196535	-0.003116
6	0	-1.105946	1.083696	-0.005309
1	0	-2.265622	-0.804984	0.018152
1	0	-1.639937	1.481410	-0.870291
1	0	-0.063319	1.388039	-0.032520
1	0	-1.594014	1.486760	0.884113
8	0	2.180690	0.310518	0.014840
1	0	3.026066	-0.138974	-0.084483
1	0	1.501421	-0.383133	0.001438

B. Methanol-*N*-methylacetamide

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	0.560965	1.935711	0.096049
7	0	1.557952	0.905305	-0.167646
6	0	1.317749	-0.404043	0.085876
6	0	2.434021	-1.372520	-0.225834
8	0	0.238699	-0.798129	0.565315
1	0	-0.281595	1.859562	-0.588497
1	0	0.187765	1.829621	1.112407
1	0	1.038749	2.905532	-0.013564
1	0	2.435162	1.163528	-0.588554
1	0	3.323298	-0.886566	-0.623733
1	0	2.693459	-1.904606	0.687354
1	0	2.069117	-2.101628	-0.946728
6	0	-3.302956	-0.632845	-0.131471
8	0	-2.265528	0.341934	-0.137881
1	0	-4.199469	-0.143884	-0.504844
1	0	-3.501403	-1.006940	0.875892
1	0	-3.067563	-1.479022	-0.781820
1	0	-1.447234	-0.080981	0.178416

C. Methanol-Aldehyde

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	-1.903374	-0.454773	0.003831
8	0	-0.913385	-1.186240	-0.007238
6	0	-1.860556	1.041345	0.017295
1	0	-2.905606	-0.913662	0.003807
1	0	-2.392975	1.418367	-0.858152

1	0	-0.837343	1.407692	0.022140
1	0	-2.396988	1.402953	0.896703
6	0	2.768020	-0.065350	0.035105
8	0	1.455648	0.482218	-0.060000
1	0	3.458983	0.773235	0.020210
1	0	2.994293	-0.721981	-0.808044
1	0	2.908276	-0.620021	0.965694
1	0	0.808716	-0.241741	-0.041834

D. Methanol- Methanol

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	2.270513	0.172713	0.327402
8	0	1.311475	-0.497339	-0.483098
6	0	3.206656	-0.369691	0.222372
1	0	1.982922	0.173708	1.381919
1	0	2.427052	1.205241	0.004608
1	0	0.459668	-0.040270	-0.385551
1	0	-2.186686	-0.402436	0.230758
6	0	-1.275633	0.654209	-0.110905
8	0	-1.699608	-0.976149	1.012459
6	0	-2.377922	-1.052768	-0.622781
1	0	-3.126134	-0.000171	0.609580
1	0	-1.662331	1.183478	-0.819537
1	0	2.270513	0.172713	0.327402
1	0	1.311475	-0.497339	-0.483098

E. Ribose-Water

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-2.239723	-1.024403	1.416985
6	0	-2.095142	-1.618852	0.128257
6	0	-1.061428	-0.894179	-0.710247
8	0	-1.524228	0.479648	-0.850671
6	0	-0.447628	1.360105	-0.529577
6	0	0.351357	-0.823444	-0.107467
6	0	0.364864	0.581964	0.485627
8	0	1.681717	1.094347	0.682224
8	0	1.260395	-0.967910	-1.188630
8	0	-0.933113	2.530984	0.075155
1	0	-2.561231	-0.123202	1.262300
1	0	-3.048653	-1.622998	-0.408522
1	0	-1.785380	-2.650820	0.294403
1	0	-0.985949	-1.352276	-1.700177
1	0	0.135731	1.590081	-1.427573
1	0	0.506917	-1.591498	0.656063

1	0	-0.193838	0.579634	1.426017
1	0	1.592294	2.009070	0.987510
1	0	2.164609	-1.019671	-0.824718
1	0	-1.354584	3.078644	-0.601638
8	0	3.695359	-0.766753	0.253171
1	0	3.259276	-0.003059	0.667202
1	0	4.075414	-1.294770	0.963695

F. Water-Deoxyribose

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-2.575927	-0.309374	0.571820
6	0	-2.056198	-1.030913	-0.539767
6	0	-0.551562	-0.886513	-0.707050
8	0	-0.185731	0.425306	-1.190343
6	0	0.069412	1.284610	-0.088827
6	0	0.235185	-1.037555	0.589523
6	0	0.343676	0.392752	1.124929
8	0	1.523904	-1.574722	0.221781
8	0	-1.074961	2.089848	0.214383
1	0	-2.383123	0.634650	0.432402
1	0	-2.536651	-0.727840	-1.475721
1	0	-2.293253	-2.080100	-0.354771
1	0	-0.198750	-1.598410	-1.456164
1	0	0.900186	1.925430	-0.382226
1	0	-0.262273	-1.710504	1.291046
1	0	-0.407195	0.582210	1.890296
1	0	1.332742	0.586597	1.539242
1	0	2.006420	-1.764281	1.039594
1	0	-1.200179	2.710040	-0.519178
8	0	3.509209	0.506402	-0.228549
1	0	4.364375	0.197917	-0.554097
1	0	2.862679	-0.189672	-0.436010

2. Deoxyribose-Uracil

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-1.664902	-1.539291	1.694366
6	0	-1.060059	-1.960068	0.473206
6	0	-1.418182	-1.082840	-0.716110
8	0	-2.761673	-1.331940	-1.197098
6	0	-3.661789	-0.454102	-0.552307
6	0	-1.396179	0.411682	-0.399597
6	0	-2.853943	0.750549	-0.066696
8	0	-0.936417	1.088211	-1.582306
8	0	-4.257523	-1.068802	0.599686

1	0	-2.630203	-1.570557	1.572449
1	0	-1.320267	-2.996109	0.232773
1	0	0.018005	-1.905991	0.631134
1	0	-0.751709	-1.318497	-1.547958
1	0	-4.443314	-0.224991	-1.277161
1	0	-0.734436	0.631531	0.442291
1	0	-3.003250	0.883484	1.003937
1	0	-3.153000	1.662552	-0.582000
1	0	-0.706284	2.001160	-1.325592
1	0	-4.794846	-1.811935	0.286392
6	0	1.722610	2.139389	-0.065659
6	0	2.773376	2.318771	0.913986
6	0	3.593567	1.277115	1.208969
7	0	3.506485	0.053360	0.586288
6	0	2.513870	-0.208115	-0.354919
7	0	1.753082	0.894730	-0.700455
8	0	2.342300	-1.325256	-0.846863
8	0	0.852280	2.975647	-0.359772
6	0	4.331451	-1.081039	1.003754
1	0	2.858093	3.263962	1.426453
1	0	4.377487	1.359543	1.950043
1	0	0.980728	0.715500	-1.349136
1	0	4.694427	-1.600220	0.121628
1	0	3.749695	-1.775711	1.607834
1	0	5.168121	-0.696442	1.580246

3. Ribose-Acetone

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	3.268035	0.064224	-0.256334
8	0	2.700113	1.012169	-0.813919
6	0	3.068435	-0.218051	1.210150
6	0	4.158712	-0.868276	-1.031555
1	0	2.226866	-0.907140	1.319989
1	0	2.821185	0.699289	1.739506
1	0	3.951383	-0.682514	1.646805
1	0	5.184061	-0.774158	-0.669207
1	0	4.117488	-0.630915	-2.090745
1	0	3.849369	-1.901062	-0.863331
8	0	-1.209561	-2.020746	-1.052866
6	0	-2.522685	-1.461024	-1.076025
6	0	-2.605160	-0.120829	-0.366753
8	0	-2.354839	-0.287801	1.054994
6	0	-0.997085	-0.021041	1.339226
6	0	-1.576738	0.909609	-0.812821
6	0	-0.371859	0.620965	0.095734

8	0	0.328018	1.812797	0.437010
8	0	-2.095140	2.205443	-0.540758
8	0	-0.284453	-1.238696	1.605449
1	0	-0.956475	-2.147611	-0.122653
1	0	-3.248223	-2.142015	-0.620229
1	0	-2.780147	-1.333932	-2.128500
1	0	-3.614162	0.286200	-0.459335
1	0	-0.950009	0.630505	2.212915
1	0	-1.321168	0.806277	-1.872376
1	0	0.290694	-0.099260	-0.383279
1	0	1.201643	1.765841	0.001743
1	0	-1.330480	2.740782	-0.265590
1	0	-0.645046	-1.609085	2.425285

4. Ribose-Aldehyde

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	0	3.721297	-0.242619	-0.807228
8	0	3.066935	0.724805	-1.200224
6	0	3.508676	-0.950518	0.491594
1	0	4.530758	-0.628016	-1.447773
1	0	3.317379	-2.007166	0.294613
1	0	2.678334	-0.531667	1.052704
1	0	4.430554	-0.895195	1.074809
8	0	-1.320295	-1.651269	-1.527554
6	0	-2.591987	-1.171184	-1.074570
6	0	-2.359019	-0.037539	-0.100308
8	0	-1.851040	-0.564248	1.148571
6	0	-0.545204	-0.057955	1.411687
6	0	-1.338529	0.993153	-0.572346
6	0	-0.047378	0.528558	0.099518
8	0	0.846289	1.611740	0.326893
8	0	-1.718400	2.265740	-0.052131
8	0	0.318714	-1.099373	1.810883
1	0	-1.433137	-2.540686	-1.884485
1	0	-3.151393	-1.957400	-0.561869
1	0	-3.184658	-0.801017	-1.918748
1	0	-3.312322	0.458446	0.101980
1	0	-0.604445	0.706536	2.193244
1	0	-1.253477	1.026434	-1.662525
1	0	0.413662	-0.271229	-0.481686
1	0	1.640325	1.457233	-0.217059
1	0	-0.887458	2.758539	0.062248
1	0	-0.008881	-1.445345	2.652964

5. Ribose-Thymine

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-4.595078	-0.081497	2.044510
6	0	-4.749924	-1.075729	1.033142
6	0	-4.037170	-0.683640	-0.245453
8	0	-4.634720	0.567719	-0.687164
6	0	-3.589890	1.492935	-0.994339
6	0	-2.526550	-0.429398	-0.104111
6	0	-2.465057	1.095200	-0.059998
8	0	-1.192047	1.597076	-0.458740
8	0	-1.898193	-0.956375	-1.262573
8	0	-3.995834	2.802597	-0.695740
1	0	-5.003983	0.723969	1.692596
1	0	-5.808273	-1.247803	0.813995
1	0	-4.322693	-1.995728	1.432846
1	0	-4.183700	-1.447021	-1.014526
1	0	-3.293655	1.396835	-2.044510
1	0	-2.122452	-0.879486	0.807175
1	0	-2.726074	1.441803	0.944200
1	0	-1.185913	2.556396	-0.316513
1	0	-0.952911	-1.097076	-1.059998
1	0	-4.621292	3.096252	-1.372421
6	0	3.985397	-0.120270	0.066589
6	0	3.746460	1.207336	0.231262
6	0	2.364624	1.668762	0.159286
7	0	1.420227	0.647034	0.019730
6	0	1.662949	-0.684357	-0.215561
7	0	2.987152	-1.062851	-0.105667
8	0	0.761887	-1.503250	-0.468124
8	0	2.005371	2.850159	0.240128
6	0	4.829117	2.223724	0.420410
6	0	3.312271	-2.461533	-0.385406
1	0	4.989685	-0.524612	0.094864
1	0	0.445328	0.948792	-0.109314
1	0	4.680603	2.769058	1.352448
1	0	4.809769	2.955490	-0.387070
1	0	5.808182	1.746017	0.442368
1	0	3.297470	-2.657257	-1.457291
1	0	2.576660	-3.096268	0.098984
1	0	4.301086	-2.665924	0.016266

6. Ribose-Uracil

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-3.675618	-0.876214	2.108877
6	0	-3.784035	-1.779567	1.009868

6	0	-3.180199	-1.193494	-0.250338
8	0	-3.923639	0.023304	-0.538991
6	0	-2.995498	1.077291	-0.804531
6	0	-1.698049	-0.795244	-0.140943
6	0	-1.787244	0.718705	0.037133
8	0	-0.594798	1.383594	-0.371689
8	0	-1.067108	-1.153485	-1.361328
8	0	-3.515497	2.304122	-0.366016
1	0	-4.180433	-0.087609	1.857620
1	0	-4.830064	-2.038465	0.819027
1	0	-3.247519	-2.684409	1.296393
1	0	-3.285422	-1.890960	-1.086003
1	0	-2.748322	1.106605	-1.871348
1	0	-1.211276	-1.275846	0.712367
1	0	-2.026705	0.948820	1.079400
1	0	-0.651222	2.310597	-0.092880
1	0	-0.110931	-1.251366	-1.189903
1	0	-4.202315	2.589960	-0.983976
6	0	2.914098	1.671820	0.354031
6	0	4.291604	1.273946	0.587690
6	0	4.655644	-0.020229	0.407899
7	0	3.781087	-0.988846	-0.039359
6	0	2.446242	-0.692606	-0.266099
7	0	2.109787	0.631247	-0.133453
8	0	1.632046	-1.572330	-0.592910
8	0	2.440796	2.799461	0.527131
6	0	4.181748	-2.391668	-0.150380
1	0	4.995919	2.009834	0.942602
1	0	5.666421	-0.362921	0.584418
1	0	1.112598	0.852845	-0.256695
1	0	3.787480	-2.801749	-1.075459
1	0	3.793003	-2.970784	0.685996
1	0	5.267357	-2.432676	-0.158450

7. Ribose-Gly dipeptide

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	2.670390	1.186642	2.221684
6	0	2.491303	2.113177	1.151123
6	0	2.315880	1.408736	-0.180715
8	0	3.515053	0.615204	-0.408732
6	0	3.140190	-0.735151	-0.687150
6	0	1.130230	0.428263	-0.264417
6	0	1.805392	-0.903938	0.014050
8	0	1.036150	-2.006540	-0.458453
8	0	0.594187	0.379215	-1.578545

8	0	4.065275	-1.627795	-0.119097
1	0	3.494481	0.712180	2.033140
1	0	3.342071	2.798095	1.082715
1	0	1.597457	2.692016	1.386515
1	0	2.219642	2.146187	-0.983042
1	0	3.054389	-0.888623	-1.767997
1	0	0.357038	0.668014	0.472206
1	0	2.002893	-0.991907	1.085873
1	0	1.528362	-2.812802	-0.243500
1	0	-0.096097	1.075539	-1.630029
1	0	4.881208	-1.600987	-0.638044
7	0	-3.378129	1.325039	0.114178
6	0	-3.413068	2.588659	0.831754
6	0	-2.442030	1.081186	-0.819929
8	0	-1.609769	1.942960	-1.187280
6	0	-2.452234	-0.334639	-1.392587
7	0	-1.869467	-1.285147	-0.458300
6	0	-2.606203	-1.796476	0.559483
8	0	-3.785461	-1.442021	0.766314
6	0	-1.929146	-2.831598	1.423174
1	0	-3.903670	0.521129	0.449931
1	0	-4.323043	2.620478	1.424384
1	0	-3.411105	3.412062	0.121293
1	0	-2.547519	2.695353	1.487144
1	0	-1.860610	-0.343093	-2.303686
1	0	-3.476484	-0.641556	-1.612597
1	0	-0.898794	-1.561909	-0.581700
1	0	-2.056740	-2.550805	2.466830
1	0	-0.870886	-2.931160	1.193223
1	0	-2.427907	-3.788091	1.270357

8. Ribose-Methanol

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-2.433831	-1.179634	1.383433
6	0	-2.478667	-1.627039	0.024507
6	0	-1.439532	-0.867133	-0.767916
8	0	-1.893578	0.497163	-0.959381
6	0	-0.881498	1.393680	-0.507834
6	0	-0.058591	-0.783883	-0.100382
6	0	-0.124596	0.599737	0.536921
8	0	1.166564	1.136801	0.837124
8	0	0.908456	-0.859356	-1.139431
8	0	-1.447634	2.526928	0.101096
1	0	-3.260393	-1.420285	1.819409
1	0	-3.458362	-1.440119	-0.422215

1	0	-2.255914	-2.698270	-0.034561
1	0	-1.320213	-1.338462	-1.747206
1	0	-0.234882	1.682679	-1.343831
1	0	0.088472	-1.572477	0.642627
1	0	-0.748682	0.551861	1.432398
1	0	1.024594	1.993976	1.264209
1	0	1.792155	-0.901548	-0.720059
1	0	-1.873116	3.062045	-0.582867
6	0	4.468061	-0.227523	-0.112323
8	0	3.226648	-0.688417	0.428648
1	0	4.943052	-1.085649	-0.578802
1	0	5.120888	0.157284	0.672555
1	0	4.309729	0.547324	-0.865057
1	0	2.748616	0.066713	0.813641

9. Fructose-Acetone				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-1.533478	2.486786	-0.595078
6	0	-0.520737	1.614914	-0.181244
6	0	-2.637253	1.833725	-1.256180
6	0	-1.058197	0.522705	0.768784
6	0	0.586868	2.483215	0.403610
6	0	-3.271698	0.766495	-0.370865
8	0	-4.303696	0.090729	-1.086761
6	0	-2.216888	-0.227539	0.108032
8	0	0.115158	3.127411	1.596329
8	0	0.022293	0.969421	-1.347595
8	0	-1.590851	1.040359	1.982468
8	0	-1.790390	-1.055176	-0.987473
1	0	-3.352158	2.624374	-1.471008
1	0	-2.302811	1.401321	-2.203491
1	0	-0.236465	-0.177612	0.971481
1	0	1.447372	1.844543	0.621185
1	0	0.851547	3.215652	-0.361526
1	0	-3.733170	1.238342	0.495636
1	0	-3.859116	-0.613754	-1.586456
1	0	-2.660248	-0.903748	0.840714
1	0	0.854630	3.589661	2.011887
1	0	0.810837	0.456314	-1.067947
1	0	-1.097992	1.849700	2.203506
1	0	-1.190353	-0.499100	-1.519150
6	0	2.344498	-1.718109	-0.141647
8	0	2.196228	-0.500412	-0.311569
6	0	1.321823	-2.715546	-0.615800
6	0	3.577728	-2.252991	0.534241

1	0	1.298004	-3.589676	0.033722
1	0	1.616547	-3.054840	-1.612167
1	0	0.332962	-2.265854	-0.677002
1	0	3.299026	-2.676056	1.501450
1	0	4.303711	-1.457703	0.677933
1	0	4.010056	-3.060547	-0.057922

10. Fructose-Thymine

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	3.512735	1.211802	-0.215894
6	0	3.470568	-0.086590	-0.715741
6	0	2.243567	1.715602	0.262184
6	0	2.894397	-1.096849	0.301372
6	0	4.877156	-0.406371	-1.212099
6	0	1.641719	0.805875	1.326240
8	0	0.400754	1.321159	1.779032
6	0	1.526237	-0.627000	0.806379
8	0	5.780435	-0.450329	-0.103396
8	0	2.614092	-0.068559	-1.884900
8	0	3.699198	-1.235905	1.464060
8	0	0.517458	-0.754947	-0.207409
1	0	2.468901	2.691774	0.684339
1	0	1.555025	1.850755	-0.577702
1	0	2.773213	-2.063888	-0.209576
1	0	4.852034	-1.373059	-1.727269
1	0	5.149334	0.380103	-1.918495
1	0	2.305767	0.786272	2.190423
1	0	-0.202298	1.413856	1.015154
1	0	1.211132	-1.284153	1.617605
1	0	6.661590	-0.683589	-0.423790
1	0	2.615049	-0.954502	-2.281006
1	0	4.628684	-1.096529	1.214657
1	0	0.831650	-0.280517	-0.995920
6	0	-4.843448	0.363319	-0.217337
6	0	-4.637686	-0.972924	-0.084973
6	0	-3.263058	-1.455340	0.013005
7	0	-2.295566	-0.443424	0.038630
6	0	-2.498641	0.903410	-0.149191
7	0	-3.821107	1.294755	-0.215947
8	0	-1.568334	1.726666	-0.226038
8	0	-2.940165	-2.645527	0.090581
6	0	-5.744685	-1.980603	-0.082415
6	0	-4.083290	2.719234	-0.417752
1	0	-5.839021	0.780529	-0.303939
1	0	-1.307234	-0.726851	0.039988

1	0	-5.724712	-2.564571	0.837779
1	0	-5.625574	-2.680555	-0.909410
1	0	-6.714010	-1.490381	-0.169632
1	0	-3.780776	3.027755	-1.417460
1	0	-3.520415	3.294634	0.312004
1	0	-5.148028	2.888154	-0.282848

11. Fructose-Uracil

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	3.362518	1.162950	-0.209807
6	0	3.261554	-0.134605	-0.703032
6	0	2.112722	1.733396	0.243700
6	0	2.623820	-1.108052	0.313008
6	0	4.656197	-0.527116	-1.180465
6	0	1.449387	0.862946	1.303971
8	0	0.225638	1.439778	1.729190
6	0	1.273832	-0.568769	0.796862
8	0	5.542502	-0.609983	-0.060330
8	0	2.420358	-0.081545	-1.881743
8	0	3.405514	-1.277532	1.487477
8	0	0.270213	-0.662986	-0.226225
1	0	2.379705	2.700217	0.663031
1	0	1.445911	1.896814	-0.608441
1	0	2.462434	-2.071962	-0.192808
1	0	4.589110	-1.494226	-1.691108
1	0	4.975816	0.240889	-1.887279
1	0	2.096262	0.819706	2.180342
1	0	-0.337121	1.598612	0.945413
1	0	0.920019	-1.201620	1.611462
1	0	6.416112	-0.883857	-0.368942
1	0	2.380222	-0.969464	-2.271199
1	0	4.343819	-1.184457	1.249809
1	0	0.607854	-0.199655	-1.011819
6	0	-2.623817	1.264635	-0.289689
6	0	-3.989831	1.708239	-0.464466
6	0	-4.998851	0.804108	-0.373972
7	0	-4.785975	-0.523186	-0.090268
6	0	-3.496051	-1.040478	0.047924
7	0	-2.492608	-0.087975	0.009097
8	0	-3.288494	-2.242412	0.213934
8	0	-1.618326	1.994848	-0.368301
6	0	-5.883157	-1.489479	-0.065424
1	0	-4.180134	2.746831	-0.683576
1	0	-6.035561	1.087960	-0.498467
1	0	-1.527839	-0.443501	0.051906

1	0	-5.776918	-2.126904	0.807683
1	0	-5.865766	-2.112672	-0.958244
1	0	-6.818053	-0.938469	-0.013627

12. Fructose-Gly dipeptide				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	3.143299	-0.378249	-0.985059
6	0	2.017657	-0.886159	-0.325996
6	0	3.013028	1.002908	-1.378077
6	0	1.689533	-0.072245	0.944862
6	0	2.276514	-2.366777	-0.080480
6	0	2.723507	1.907044	-0.183432
8	0	2.520560	3.248627	-0.621799
6	0	1.507308	1.404352	0.588331
8	0	3.356362	-2.515474	0.853659
8	0	0.892947	-0.796244	-1.220074
8	0	2.727680	-0.090886	1.915867
8	0	0.310171	1.632339	-0.188339
1	0	3.966661	1.266578	-1.828997
1	0	2.231196	1.103491	-2.136857
1	0	0.755505	-0.473871	1.358671
1	0	1.358204	-2.813807	0.310158
1	0	2.527249	-2.811035	-1.045824
1	0	3.582609	1.914645	0.485776
1	0	1.597367	3.296939	-0.917776
1	0	1.389240	1.984469	1.505076
1	0	3.420893	-3.445823	1.106028
1	0	0.152313	-1.316648	-0.831526
1	0	3.167537	-0.957630	1.860682
1	0	0.301934	0.914976	-0.857286
7	0	-3.422276	-1.658888	-0.353365
6	0	-3.491316	-2.567102	-1.487835
6	0	-2.268934	-1.440924	0.296623
8	0	-1.208291	-2.054718	0.026035
6	0	-2.323541	-0.365463	1.375185
7	0	-2.336641	0.963304	0.785020
6	0	-3.493431	1.499143	0.315369
8	0	-4.579086	0.888091	0.381485
6	0	-3.391969	2.887339	-0.264955
1	0	-4.188647	-1.021836	-0.148077
1	0	-4.530396	-2.653761	-1.791949
1	0	-3.112597	-3.545284	-1.199859
1	0	-2.895347	-2.196476	-2.322151
1	0	-1.439514	-0.464466	2.000682
1	0	-3.217606	-0.481675	1.989549

1	0	-1.440997	1.398584	0.566846
1	0	-3.866415	2.892698	-1.244273
1	0	-2.361731	3.227638	-0.350979
1	0	-3.944309	3.570795	0.378731

13. Fructose-Methanol

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	1.360593	-0.130707	1.339456
6	0	1.628061	0.584621	0.177919
6	0	-0.037968	-0.440271	1.557624
6	0	1.061290	-0.092917	-1.091319
6	0	3.133628	0.830271	0.157219
6	0	-0.622648	-1.198679	0.373659
8	0	-1.968731	-1.570036	0.615409
6	0	-0.431892	-0.394978	-0.912907
8	0	3.818432	-0.415562	0.009082
8	0	0.995422	1.885574	0.315282
8	0	1.672289	-1.341445	-1.382676
8	0	-1.211679	0.815298	-0.931345
1	0	-0.052403	-1.061650	2.449221
1	0	-0.595773	0.478588	1.761651
1	0	1.187111	0.608095	-1.929907
1	0	3.367040	1.499358	-0.679158
1	0	3.387834	1.316713	1.100969
1	0	-0.067046	-2.128899	0.252899
1	0	-2.537126	-0.774581	0.661937
1	0	-0.772708	-0.985378	-1.764193
1	0	4.770860	-0.253569	-0.005365
1	0	1.335927	2.473689	-0.377140
1	0	2.591357	-1.319124	-1.066124
1	0	-0.739331	1.459536	-0.374179
6	0	-4.910210	0.339747	-0.334579
8	0	-3.676831	0.666742	0.311551
1	0	-5.611085	0.068411	0.449642
1	0	-4.790500	-0.506522	-1.013953
1	0	-5.305555	1.194510	-0.885615
1	0	-3.006130	0.885139	-0.360454

14. Fructose-Fructose

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	4.366516	-1.238323	0.546263
6	0	4.394745	0.152442	0.575954
6	0	3.038882	-1.816251	0.535322
6	0	3.582638	0.790916	-0.572597

6	0	5.865016	0.556368	0.626303
6	0	2.207942	-1.291244	-0.629286
8	0	0.914463	-1.874861	-0.611142
6	0	2.156572	0.233202	-0.593724
8	0	6.508342	0.183936	-0.595645
8	0	3.809059	0.569380	1.837207
8	0	4.117921	0.508005	-1.857836
8	0	1.376362	0.694989	0.518927
1	0	3.198867	-2.886969	0.436569
1	0	2.541469	-1.625234	1.490728
1	0	3.539792	1.876250	-0.396297
1	0	5.922653	1.640333	0.776855
1	0	6.305215	0.041771	1.482593
1	0	2.681367	-1.591788	-1.564215
1	0	0.338724	-1.378109	0.001159
1	0	1.649562	0.607508	-1.484318
1	0	7.431051	0.469001	-0.565548
1	0	3.916251	1.530012	1.923323
1	0	5.082921	0.419890	-1.778615
1	0	1.910499	0.580675	1.322738
8	0	-4.366868	1.238029	0.546079
6	0	-4.394679	-0.152748	0.575992
6	0	-3.039461	1.816491	0.535102
6	0	-3.582176	-0.791199	-0.572295
6	0	-5.864869	-0.557036	0.626068
6	0	-2.208330	1.291633	-0.629429
8	0	-0.914921	1.875433	-0.611305
6	0	-2.156414	-0.232766	-0.593530
8	0	-6.508002	-0.184260	-0.595859
8	0	-3.809026	-0.569330	1.837358
8	0	-4.117615	-0.509212	-1.857678
8	0	-1.376007	-0.693713	0.519377
1	0	-3.199892	2.887135	0.436262
1	0	-2.541963	1.625745	1.490518
1	0	-3.538763	-1.876442	-0.395591
1	0	-5.922318	-1.641076	0.776199
1	0	-6.305319	-0.042837	1.482465
1	0	-2.681783	1.591917	-1.564427
1	0	-0.339443	1.378859	0.001388
1	0	-1.649145	-0.607086	-1.483973
1	0	-7.430917	-0.468653	-0.565742
1	0	-3.916569	-1.529882	1.923943
1	0	-5.082509	-0.420009	-1.778229
1	0	-1.910737	-0.580446	1.322949

15. Fructose-Deoxyribose

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-4.038162	0.088654	-1.015930
6	0	-2.663223	0.303207	-0.754883
6	0	-4.382538	-1.302979	-1.007614
6	0	-2.274826	-0.268616	0.630219
6	0	-2.451660	1.810516	-0.882050
6	0	-4.198532	-1.854736	0.397827
8	0	-4.465408	-3.266693	0.455444
6	0	-2.749161	-1.708923	0.840683
8	0	-3.278824	2.525085	0.050217
8	0	-1.903290	-0.265747	-1.798737
8	0	-2.878662	0.443222	1.708054
8	0	-1.921753	-2.626648	0.108307
1	0	-5.428070	-1.345322	-1.314438
1	0	-3.769516	-1.855652	-1.722626
1	0	-1.182205	-0.228729	0.719864
1	0	-1.391983	2.015533	-0.701797
1	0	-2.704529	2.069855	-1.911194
1	0	-4.832092	-1.305069	1.097595
1	0	-5.383713	-3.427536	0.199280
1	0	-2.672318	-1.921921	1.911209
1	0	-3.055649	3.464310	0.006607
1	0	-1.089111	-0.703369	-1.471069
1	0	-3.121338	1.334183	1.395340
1	0	-2.413620	-3.464294	0.076157
8	0	3.098602	0.357086	1.668655
6	0	2.347610	1.019913	0.657669
6	0	1.911500	0.101700	-0.473785
8	0	3.018051	-0.259705	-1.331680
6	0	3.599060	-1.467270	-0.871704
6	0	1.344666	-1.235367	-0.002304
6	0	2.557739	-2.171173	0.000946
8	0	0.363754	-1.646881	-0.965988
8	0	4.748260	-1.211853	-0.054947
1	0	3.897186	-0.014008	1.253525
1	0	2.905151	1.858932	0.227707
1	0	1.458923	1.414581	1.155045
1	0	1.194992	0.624298	-1.112152
1	0	3.906600	-2.019196	-1.760132
1	0	0.894089	-1.155746	0.990616
1	0	2.956802	-2.304779	1.005371
1	0	2.284332	-3.143478	-0.406509
1	0	-0.232941	-2.296875	-0.546204
1	0	5.428085	-0.816116	-0.620773

16. Glucose-Acetone				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	2.177446	1.438689	0.095401
6	0	2.462663	0.096811	-0.340558
6	0	0.840110	1.804682	-0.221102
6	0	1.551880	-0.845448	0.435860
6	0	3.941791	-0.152741	-0.080500
8	0	1.833215	-2.187792	0.035743
8	0	0.624615	3.126748	0.194864
6	0	-0.159419	0.940912	0.535045
8	0	-1.493306	1.296886	0.157588
6	0	0.086020	-0.519220	0.197373
8	0	4.403431	-1.323043	-0.745214
8	0	-0.660219	-1.415905	1.015095
1	0	2.271816	-0.003101	-1.418040
1	0	0.685902	1.701541	-1.306633
1	0	1.763800	-0.720812	1.506249
1	0	4.514746	0.681975	-0.481513
1	0	4.115030	-0.204707	1.000316
1	0	1.133576	-2.732524	0.432694
1	0	1.236360	3.701366	-0.287523
1	0	-0.004582	1.101402	1.608200
1	0	-1.555562	2.256701	0.285619
1	0	-0.151885	-0.688199	-0.860629
1	0	3.816475	-2.050147	-0.484618
1	0	-1.507686	-1.593238	0.562957
6	0	-3.757282	-0.649321	-0.342286
8	0	-2.910535	-1.505763	-0.621589
6	0	-4.163569	-0.380145	1.082527
6	0	-4.408471	0.179160	-1.415826
1	0	-5.229366	-0.164477	1.153058
1	0	-3.609278	0.495244	1.424038
1	0	-3.908324	-1.227382	1.714383
1	0	-5.472502	-0.059277	-1.468895
1	0	-3.937249	-0.017670	-2.374566
1	0	-4.320798	1.236605	-1.163409

17. Glucose-Gly dipeptide				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	3.189109	-0.871704	0.350127
6	0	2.644972	0.447951	0.518640
6	0	2.154047	-1.844963	0.401848
6	0	1.761496	0.771790	-0.684793
6	0	3.823108	1.402687	0.670070

8	0	1.234878	2.085234	-0.455171
8	0	2.721871	-3.120005	0.286455
6	0	1.213741	-1.678317	-0.778029
8	0	0.098643	-2.571050	-0.656024
6	0	0.657895	-0.269401	-0.845322
8	0	3.421209	2.665927	1.187683
8	0	-0.008132	-0.173051	-2.100514
1	0	2.040186	0.493302	1.435987
1	0	1.605029	-1.737067	1.350749
1	0	2.379708	0.764379	-1.591479
1	0	4.523594	0.978751	1.388131
1	0	4.334012	1.504465	-0.294031
1	0	0.397861	2.216623	-0.938953
1	0	3.332295	-3.249003	1.026688
1	0	1.778663	-1.884982	-1.692942
1	0	0.442857	-3.472656	-0.743812
1	0	-0.050399	-0.136334	-0.012665
1	0	2.697822	2.983667	0.624410
1	0	-0.505262	0.669299	-2.116027
7	0	-2.611492	1.870329	0.563982
6	0	-1.949982	3.022518	1.162014
6	0	-2.303803	1.443245	-0.665091
8	0	-1.464352	2.029170	-1.399148
6	0	-3.015003	0.172160	-1.126459
7	0	-2.564863	-1.003184	-0.396828
6	0	-3.071874	-1.293170	0.830653
8	0	-3.893931	-0.539998	1.392221
6	0	-2.618067	-2.588777	1.452571
1	0	-3.255471	1.292049	1.101008
1	0	-2.367883	3.174230	2.152924
1	0	-2.121349	3.909958	0.555151
1	0	-0.876585	2.852257	1.237690
1	0	-2.802658	0.028894	-2.182573
1	0	-4.091606	0.279158	-0.980793
1	0	-1.815919	-1.568589	-0.785604
1	0	-2.541000	-2.448798	2.528043
1	0	-1.666652	-2.921065	1.043752
1	0	-3.376289	-3.349077	1.262617

18. Glucose-Thymine

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	2.443750	-1.378875	-0.226680
6	0	3.768888	-0.910991	0.077551
6	0	1.443809	-0.712584	0.541864
6	0	3.850093	0.556908	-0.327083

6	0	4.738828	-1.798772	-0.690391
8	0	5.170408	1.032239	-0.042602
8	0	0.206488	-1.265358	0.174382
6	0	1.420092	0.774257	0.209117
8	0	0.537646	1.501446	1.051200
6	0	2.809130	1.349291	0.430774
8	0	6.078081	-1.633710	-0.238221
8	0	2.888705	2.700447	-0.019977
1	0	3.973846	-1.010506	1.152389
1	0	1.640479	-0.864825	1.613125
1	0	3.645225	0.633772	-1.402601
1	0	4.474759	-2.840348	-0.514425
1	0	4.644440	-1.593853	-1.762789
1	0	5.158032	1.992904	-0.176169
1	0	0.190492	-2.206731	0.406773
1	0	1.143324	0.877074	-0.846744
1	0	-0.319336	1.625356	0.590674
1	0	3.039276	1.301008	1.504174
1	0	6.277005	-0.685041	-0.272541
1	0	2.162183	3.175000	0.414208
6	0	-5.077850	0.237945	-0.214634
6	0	-4.213372	1.284948	-0.309936
6	0	-2.795314	0.999888	-0.187236
7	0	-2.469981	-0.342275	-0.089613
6	0	-3.337887	-1.409598	0.068253
7	0	-4.677895	-1.074155	-0.072198
8	0	-2.950899	-2.561708	0.281133
8	0	-1.903922	1.872835	-0.200454
6	0	-4.651006	2.708688	-0.463160
6	0	-5.653069	-2.148636	0.114230
1	0	-6.149349	0.382103	-0.279273
1	0	-1.479565	-0.582266	0.026644
1	0	-4.198287	3.152368	-1.349794
1	0	-4.332822	3.302415	0.393763
1	0	-5.735127	2.770325	-0.552711
1	0	-5.751805	-2.402909	1.168999
1	0	-5.315257	-3.025838	-0.429222
1	0	-6.608496	-1.811578	-0.278149

19. Glucose-Uracil

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	2.117653	-1.372042	-0.244317
6	0	3.463211	-0.993991	0.094404
6	0	1.146403	-0.625918	0.485473
6	0	3.659662	0.458951	-0.324647

6	0	4.390381	-1.958156	-0.633225
8	0	5.001434	0.843717	-0.006234
8	0	-0.117137	-1.093101	0.086509
6	0	1.237191	0.853960	0.135211
8	0	0.381302	1.649264	0.943617
6	0	2.655860	1.333366	0.392379
8	0	5.723680	-1.881831	-0.141689
8	0	2.844725	2.668968	-0.071657
1	0	3.628843	-1.092944	1.176032
1	0	1.300144	-0.777040	1.563982
1	0	3.492013	0.535266	-1.406627
1	0	4.047983	-2.976058	-0.453704
1	0	4.342954	-1.761545	-1.710272
1	0	5.061188	1.800962	-0.151158
1	0	-0.202097	-2.029590	0.324995
1	0	0.997960	0.961845	-0.929040
1	0	-0.445930	1.838646	0.451528
1	0	2.850605	1.283593	1.472669
1	0	5.990636	-0.950218	-0.181248
1	0	2.145064	3.201679	0.338374
6	0	-2.947357	1.346010	-0.265199
6	0	-4.340066	1.652543	-0.505361
6	0	-5.265129	0.663274	-0.403283
7	0	-4.947496	-0.621985	-0.031762
6	0	-3.625709	-1.002687	0.187248
7	0	-2.715130	0.038516	0.142288
8	0	-3.302027	-2.167064	0.430606
8	0	-2.005628	2.153314	-0.375662
6	0	-5.951123	-1.686651	-0.010085
1	0	-4.614703	2.652221	-0.802045
1	0	-6.316305	0.842060	-0.586540
1	0	-1.737249	-0.259496	0.232388
1	0	-5.820355	-2.279120	0.890713
1	0	-5.840090	-2.335360	-0.877497
1	0	-6.934228	-1.224625	-0.013101

20. Glucose-Methanol

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-1.691708	1.388547	-0.002090
6	0	-1.899164	0.008835	0.352336
6	0	-0.370649	1.804887	0.318552
6	0	-0.964939	-0.831158	-0.508074
6	0	-3.370718	-0.299494	0.112804
8	0	-1.168730	-2.210821	-0.197671
8	0	-0.228048	3.157469	-0.018394
6	0	0.658029	1.042470	-0.504182

8	0	1.978345	1.430847	-0.093914
6	0	0.489970	-0.452154	-0.282889
8	0	-3.753844	-1.531324	0.712723
8	0	1.241974	-1.250150	-1.186532
1	0	-1.674630	-0.149837	1.416211
1	0	-0.192162	1.641756	1.392921
1	0	-1.209357	-0.642560	-1.561742
1	0	-3.972860	0.477687	0.580884
1	0	-3.571449	-0.292156	-0.964371
1	0	-0.466214	-2.693141	-0.664078
1	0	-0.853453	3.672593	0.511346
1	0	0.500676	1.278696	-1.561585
1	0	2.049187	2.387388	-0.237106
1	0	0.758140	-0.689256	0.756626
1	0	-3.146385	-2.211558	0.382309
1	0	2.179580	-1.242060	-0.896404
6	0	4.183088	-1.208911	1.147045
8	0	3.736687	-0.742394	-0.130060
1	0	4.473007	-2.247330	1.016381
1	0	3.388439	-1.149469	1.893764
1	0	5.046388	-0.638827	1.492182
1	0	3.419981	0.173829	-0.043383

21. Maltose-Deoxyribose

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-4.387334	0.555740	-0.566998
6	0	-5.507251	0.366358	0.318302
6	0	-3.285347	-0.315037	-0.305713
6	0	-6.043340	-1.056786	0.104847
6	0	-6.535920	1.458870	0.002726
8	0	-7.160380	-1.256689	0.970993
8	0	-2.314598	-0.017880	-1.272683
6	0	-3.713805	-1.780559	-0.474611
8	0	-2.700731	-2.678291	-0.054435
6	0	-4.942608	-2.072325	0.382437
8	0	-7.535921	1.548332	1.003736
8	0	-5.481317	-3.365813	0.122754
8	0	0.254293	2.393296	-0.112491
6	0	-1.100400	1.940642	-0.287288
6	0	1.020254	1.603618	0.784482
6	0	-1.040666	0.528001	-0.909731
6	0	-1.816968	2.983123	-1.165204
8	0	2.290777	2.201901	0.878540
6	0	1.173050	0.180479	0.234722
8	0	1.817654	-0.712293	1.123485

6	0	-0.217639	-0.406818	-0.022652
8	0	-3.184782	3.134286	-0.840418
8	0	-0.103218	-1.680561	-0.657024
1	0	-5.183019	0.487231	1.363457
1	0	-2.916853	-0.142879	0.717700
1	0	-6.362267	-1.153886	-0.943843
1	0	-6.027955	2.426726	-0.022658
1	0	-6.970783	1.275883	-0.992053
1	0	-7.402774	-2.193530	0.926999
1	0	-3.961517	-1.928457	-1.535966
1	0	-1.856798	-2.467786	-0.500492
1	0	-4.655008	-1.999102	1.443356
1	0	-7.910069	0.662644	1.133455
1	0	-4.772216	-4.013316	0.245464
1	0	-1.604787	1.920818	0.691940
1	0	0.531033	1.583227	1.773302
1	0	-0.532128	0.615346	-1.875545
1	0	-1.343070	3.949824	-0.975828
1	0	-1.677512	2.738563	-2.228441
1	0	2.173378	3.124492	1.146986
1	0	1.714499	0.253163	-0.720285
1	0	2.781882	-0.532723	1.120122
1	0	-0.710055	-0.535848	0.954086
1	0	-3.650177	2.289369	-0.971878
1	0	0.565268	-2.173623	-0.153861
8	0	7.189970	-0.883841	-2.039197
6	0	6.416318	-1.781956	-1.258348
6	0	6.000868	-1.231817	0.108720
8	0	7.109815	-1.187963	1.034618
6	0	7.725242	0.079374	0.995808
6	0	5.462158	0.207504	0.068600
6	0	6.678623	1.072156	0.462434
8	0	4.396384	0.305722	1.026362
8	0	8.844038	0.091622	0.100946
1	0	7.986189	-0.637337	-1.535578
1	0	6.942497	-2.734853	-1.100475
1	0	5.511853	-1.990402	-1.840945
1	0	5.261645	-1.907231	0.551712
1	0	8.079556	0.290023	2.009307
1	0	5.091410	0.464636	-0.929122
1	0	7.087174	1.611680	-0.394785
1	0	6.397827	1.797045	1.230794
1	0	3.971122	1.179632	0.967662
1	0	9.529035	-0.488836	0.462716

22. Maltose-Ribose

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	4.445007	-0.567184	-0.011594
6	0	5.100156	0.263098	0.971121
6	0	3.268609	0.050008	-0.539033
6	0	5.593083	1.514572	0.252104
6	0	6.222940	-0.566412	1.581901
8	0	6.268388	2.343635	1.201744
8	0	2.728566	-0.872434	-1.451462
6	0	3.646817	1.320287	-1.288517
8	0	2.498258	2.043495	-1.708834
6	0	4.422040	2.245009	-0.369990
8	0	6.738466	0.042264	2.759366
8	0	4.954748	3.368678	-1.071470
8	0	-0.015129	-2.798116	0.124546
6	0	1.309020	-2.227066	0.090384
6	0	-1.024973	-1.798587	0.209471
6	0	1.417830	-1.404421	-1.201201
6	0	2.302559	-3.389198	0.158114
8	0	-2.264268	-2.452279	0.313740
6	0	-1.031898	-0.976130	-1.067289
8	0	-1.966039	0.094255	-1.037888
6	0	0.334891	-0.339989	-1.252439
8	0	3.480344	-3.054317	0.876264
8	0	0.405558	0.324584	-2.517588
1	0	4.391902	0.537256	1.764673
1	0	2.572150	0.278268	0.280517
1	0	6.285170	1.207096	-0.542287
1	0	5.825305	-1.535338	1.881225
1	0	7.004658	-0.726432	0.830431
1	0	6.459071	3.184018	0.756082
1	0	4.273956	1.026787	-2.139141
1	0	1.930143	1.461797	-2.252253
1	0	3.753380	2.587941	0.431644
1	0	6.996025	0.947794	2.526563
1	0	4.212200	3.807152	-1.514484
1	0	1.455462	-1.599653	0.980991
1	0	-0.838406	-1.162467	1.089018
1	0	1.266445	-2.085548	-2.042822
1	0	1.825445	-4.198597	0.709005
1	0	2.533420	-3.742655	-0.852509
1	0	-2.184315	-3.114792	1.018673
1	0	-1.233537	-1.661742	-1.898837
1	0	-2.860770	-0.251777	-1.235774
1	0	0.477926	0.395184	-0.448125
1	0	3.935325	-2.328399	0.413361

1	0	-0.409077	0.853258	-2.576698
8	0	-5.907333	3.149329	0.726430
6	0	-5.869228	2.454409	1.971494
6	0	-5.861515	0.950940	1.774739
8	0	-7.080628	0.610002	1.053501
6	0	-6.745769	-0.163440	-0.098189
6	0	-4.698824	0.400865	0.940149
6	0	-5.332999	0.270865	-0.436754
8	0	-4.620987	-0.665584	-1.251659
8	0	-4.374941	-0.873375	1.486544
8	0	-7.588638	0.160324	-1.174413
1	0	-6.753600	2.919994	0.313292
1	0	-6.724969	2.725694	2.596909
1	0	-4.955747	2.770063	2.476078
1	0	-5.864556	0.441626	2.742400
1	0	-6.797875	-1.231616	0.137362
1	0	-3.833533	1.069428	0.937924
1	0	-5.380730	1.251082	-0.917897
1	0	-5.103065	-0.754850	-2.087884
1	0	-3.719761	-1.313488	0.913922
1	0	-8.465421	-0.212172	-1.005576

23. Maltose-Glucose

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-3.710014	-0.671408	0.079785
6	0	-3.675202	-1.772932	1.007263
6	0	-2.445237	-0.390749	-0.517183
6	0	-3.283719	-3.040145	0.230615
6	0	-5.055508	-1.866468	1.668529
8	0	-3.237811	-4.134404	1.144246
8	0	-2.624493	0.687900	-1.390136
6	0	-1.982197	-1.600239	-1.341929
8	0	-0.680306	-1.392840	-1.877048
6	0	-1.937544	-2.844520	-0.461370
8	0	-5.038053	-2.707089	2.809741
8	0	-1.672764	-4.029665	-1.205331
8	0	-2.087164	4.018397	0.143986
6	0	-2.669979	2.706261	0.083940
6	0	-0.692055	3.991081	0.401788
6	0	-2.038905	1.971733	-1.119308
6	0	-4.195736	2.884896	-0.025102
8	0	-0.215235	5.300959	0.484065
6	0	0.043790	3.319720	-0.758352
8	0	1.442570	3.201179	-0.478710
6	0	-0.508478	1.914824	-1.003629

8	0	-4.922151	1.878788	0.654608
8	0	0.021807	1.353009	-2.198251
1	0	-2.928846	-1.576836	1.792610
1	0	-1.713807	-0.164586	0.274313
1	0	-4.049558	-3.226232	-0.537553
1	0	-5.349162	-0.871432	2.013320
1	0	-5.796082	-2.202044	0.926237
1	0	-2.874388	-4.897705	0.671103
1	0	-2.709120	-1.746694	-2.152689
1	0	-0.657987	-0.517270	-2.314518
1	0	-1.161283	-2.709423	0.308695
1	0	-4.658934	-3.560935	2.548632
1	0	-0.810691	-3.934507	-1.634778
1	0	-2.460573	2.172381	1.025284
1	0	-0.508223	3.441806	1.342724
1	0	-2.288391	2.543413	-2.019297
1	0	-4.448765	3.831844	0.458344
1	0	-4.492072	2.952211	-1.082169
1	0	-0.623907	5.745362	1.239905
1	0	-0.107354	3.931415	-1.657037
1	0	1.795880	4.092487	-0.342022
1	0	-0.215906	1.288945	-0.148022
1	0	-4.688857	1.006704	0.293494
1	0	0.923651	1.046172	-1.989954
8	0	5.650653	-1.147024	0.320844
6	0	4.994446	-0.088878	1.029376
6	0	4.834140	-2.301515	0.188666
6	0	3.766242	0.373294	0.222256
6	0	6.022434	1.026301	1.246974
8	0	3.115892	1.396075	0.972368
8	0	5.553486	-3.292529	-0.484945
6	0	3.602030	-1.982503	-0.659234
8	0	2.707464	-3.090294	-0.723646
6	0	2.833526	-0.809726	-0.052263
8	0	5.584660	1.975513	2.206153
8	0	1.797384	-0.366404	-0.924358
1	0	4.661783	-0.446885	2.017368
1	0	4.529661	-2.646183	1.192966
1	0	4.117570	0.772884	-0.740925
1	0	6.943972	0.580690	1.631492
1	0	6.255155	1.503318	0.282041
1	0	2.484729	1.883163	0.409423
1	0	6.327818	-3.536716	0.040752
1	0	3.952799	-1.707684	-1.664053
1	0	3.185062	-3.834283	-1.116977
1	0	2.394310	-1.132354	0.903964

1	0	4.669939	2.210302	1.978317
1	0	1.141927	-1.075226	-1.064201

24. Sucrose-Deoxyribose

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
8	0	-5.099934	0.219921	1.063004
6	0	-6.092689	-0.716557	0.589542
6	0	-4.102685	0.474806	0.094244
6	0	-6.042848	-0.606876	-0.943691
6	0	-5.793804	-2.104132	1.158839
6	0	-4.558558	-0.273660	-1.208572
8	0	-6.904147	0.393904	-1.458505
6	0	-4.031177	2.009412	-0.057951
8	0	-3.761153	-1.451095	-1.377392
8	0	-5.322075	2.547135	-0.357970
8	0	-1.168710	1.458281	0.654259
6	0	0.115940	1.866004	0.162093
6	0	-1.667094	0.282967	0.030702
6	0	1.160251	0.775109	0.470962
6	0	0.448017	3.212935	0.815602
8	0	2.411683	1.224305	-0.037408
8	0	-2.891903	-0.050952	0.628155
6	0	-0.716721	-0.889527	0.284295
8	0	-1.098157	-2.064042	-0.419875
6	0	0.701246	-0.538940	-0.163569
8	0	1.514275	3.875249	0.158480
8	0	1.593850	-1.605830	0.194955
8	0	-6.850880	-2.966104	0.732577
1	0	-7.065697	-0.377080	0.956010
1	0	-6.336739	-1.546525	-1.417706
1	0	-5.756395	-2.023893	2.253094
1	0	-4.819777	-2.460857	0.802407
1	0	-4.465164	0.371672	-2.089262
1	0	-6.535482	1.267281	-1.228971
1	0	-3.372205	2.300788	-0.878425
1	0	-3.635563	2.427484	0.871089
1	0	-3.999501	-1.860728	-2.219650
1	0	-5.825678	2.545026	0.468648
1	0	0.069600	2.018478	-0.928713
1	0	-1.781997	0.456125	-1.052662
1	0	1.215241	0.646568	1.562200
1	0	-0.429007	3.862031	0.740380
1	0	0.662621	3.057958	1.884559
1	0	3.131072	0.684222	0.356700
1	0	-0.720361	-1.075756	1.368423

1	0	-2.064940	-2.057729	-0.532375
1	0	0.713130	-0.421245	-1.257200
1	0	2.236351	3.230418	0.069645
1	0	1.178795	-2.434068	-0.089732
1	0	-6.731578	-3.837281	1.129881
8	0	8.238054	-1.650722	0.261318
6	0	7.784316	-0.711853	1.225172
6	0	6.404506	-0.117122	0.932588
8	0	6.439233	0.826502	-0.164163
6	0	6.150646	0.167999	-1.378590
6	0	5.340237	-1.144266	0.519882
6	0	5.378083	-1.113960	-1.022856
8	0	4.085306	-0.699335	1.053963
8	0	7.349951	-0.211751	-2.064529
1	0	8.256068	-1.218014	-0.610891
1	0	8.496960	0.117648	1.344166
1	0	7.735908	-1.251983	2.177330
1	0	6.070173	0.445362	1.810132
1	0	5.596766	0.878396	-1.999461
1	0	5.571305	-2.139611	0.913181
1	0	5.905272	-1.981550	-1.425711
1	0	4.366847	-1.098472	-1.436893
1	0	3.371369	-1.317164	0.805043
1	0	7.813463	0.594735	-2.332342

25. Sucrose-Fructose

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-5.419166	-0.121428	1.298407
6	0	-6.348231	-1.124627	0.830134
6	0	-4.578322	0.348964	0.265555
6	0	-6.486844	-0.863308	-0.679316
6	0	-5.830995	-2.512656	1.210586
6	0	-5.087774	-0.329196	-1.055692
8	0	-7.505228	0.069943	-0.993060
6	0	-4.701970	1.887850	0.272107
8	0	-4.187382	-1.382286	-1.420010
8	0	-6.071189	2.285900	0.168523
8	0	-1.722789	1.637961	0.589432
6	0	-0.562920	2.238314	-0.002493
6	0	-2.163044	0.464458	-0.082502
6	0	0.625370	1.259514	0.083291
6	0	-0.305060	3.558002	0.735371
8	0	1.749089	1.897250	-0.517319
8	0	-3.258926	-0.062629	0.614391
6	0	-1.063641	-0.600042	-0.049442

8	0	-1.389584	-1.752172	-0.814411
6	0	0.237806	-0.041809	-0.620402
8	0	0.575881	4.406276	0.020189
8	0	1.279990	-1.023942	-0.474996
8	0	-6.825061	-3.453930	0.801672
1	0	-7.304651	-0.944867	1.329170
1	0	-6.728131	-1.782318	-1.219182
1	0	-5.677833	-2.534843	2.297357
1	0	-4.870449	-2.708517	0.718726
1	0	-5.164185	0.398059	-1.871811
1	0	-7.213968	0.955119	-0.704405
1	0	-4.180435	2.335368	-0.576514
1	0	-4.250313	2.262211	1.194300
1	0	-4.480810	-1.753428	-2.262854
1	0	-6.471349	2.148904	1.039176
1	0	-0.757970	2.472457	-1.061853
1	0	-2.428034	0.709875	-1.124717
1	0	0.826167	1.051100	1.144591
1	0	-1.254273	4.091879	0.833223
1	0	0.067965	3.344744	1.749193
1	0	2.564162	1.414951	-0.273364
1	0	-0.913021	-0.872140	1.005745
1	0	-2.357924	-1.852709	-0.828161
1	0	0.100639	0.166780	-1.691366
1	0	1.360239	3.880255	-0.206458
1	0	0.912107	-1.877391	-0.751787
1	0	-6.571177	-4.335948	1.099447
8	0	5.827372	0.827167	-0.443867
6	0	4.944770	-0.210926	-0.723342
6	0	6.324726	0.885006	0.909752
6	0	5.525279	-1.607064	-0.350727
6	0	4.525173	-0.057895	-2.194158
6	0	6.974505	-0.433135	1.348325
8	0	7.348640	-0.356856	2.716746
6	0	6.021871	-1.615727	1.107636
8	0	5.631334	-0.340632	-3.053405
8	0	3.751292	-0.002321	0.076559
8	0	6.642488	-1.978311	-1.139385
8	0	4.957864	-1.602642	2.064608
1	0	7.056905	1.693549	0.912760
1	0	5.509995	1.157012	1.592574
1	0	4.713259	-2.346390	-0.454102
1	0	3.695008	-0.748907	-2.394299
1	0	4.176219	0.972217	-2.327412
1	0	7.886902	-0.598200	0.769758
1	0	6.568334	-0.618228	3.232389

1	0	6.562499	-2.551640	1.274213
1	0	5.371479	-0.213773	-3.974095
1	0	3.026296	-0.611659	-0.185666
1	0	6.543066	-1.605803	-2.031907
1	0	4.302068	-0.950846	1.766628

26. Sucrose-Maltose

Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
8	0	-1.334741	3.037220	-1.284224
6	0	-0.405505	3.921084	-0.609514
6	0	-2.430522	2.678997	-0.473333
6	0	-1.178998	4.492848	0.593591
6	0	0.874590	3.157363	-0.262812
6	0	-2.197958	3.375535	0.909624
8	0	-1.823620	5.724220	0.325061
6	0	-3.705499	3.141250	-1.214010
8	0	-1.670097	2.411257	1.834887
8	0	-3.630559	4.528969	-1.545278
8	0	-4.327113	0.190737	-0.984508
6	0	-5.449419	-0.625301	-0.618667
6	0	-3.499006	0.549890	0.111793
6	0	-4.919336	-1.956467	-0.062123
6	0	-6.319371	-0.797317	-1.869920
8	0	-6.032179	-2.780545	0.278544
8	0	-2.391155	1.254781	-0.375669
6	0	-2.932439	-0.699641	0.797009
8	0	-2.237319	-0.345873	1.997655
6	0	-4.037162	-1.690211	1.153313
8	0	-7.610733	-1.289948	-1.557414
8	0	-3.498766	-2.955168	1.580475
8	0	1.782560	4.095270	0.289297
1	0	-0.155606	4.730318	-1.301897
1	0	-0.504928	4.676570	1.434335
1	0	1.258200	2.709877	-1.191000
1	0	0.648626	2.342785	0.440814
1	0	-3.124820	3.803596	1.307503
1	0	-2.538812	5.565717	-0.319178
1	0	-4.598161	3.017431	-0.596590
1	0	-3.814240	2.527450	-2.111672
1	0	-1.489964	2.864781	2.669623
1	0	-3.039879	4.609251	-2.307889
1	0	-6.053169	-0.120051	0.152466
1	0	-4.080186	1.150569	0.833014
1	0	-4.315513	-2.440215	-0.844356
1	0	-6.457981	0.183073	-2.333147

1	0	-5.799341	-1.443341	-2.593347
1	0	-5.691247	-3.595792	0.674333
1	0	-2.244170	-1.170607	0.083769
1	0	-1.900639	0.570832	1.906309
1	0	-4.658575	-1.274049	1.957877
1	0	-7.503045	-2.112892	-1.055918
1	0	-3.235361	-2.893216	2.509026
1	0	2.676876	3.709240	0.341839
8	0	2.552238	-3.170076	-0.225528
6	0	1.211218	-3.376914	-0.705810
6	0	2.721305	-1.964588	0.522242
6	0	0.246141	-3.472734	0.494151
6	0	1.229292	-4.641631	-1.572687
8	0	-1.075154	-3.566625	-0.035247
8	0	4.080777	-1.851040	0.809960
6	0	1.885294	-2.091822	1.796443
8	0	2.045166	-0.922456	2.598558
6	0	0.418864	-2.243960	1.389205
8	0	0.039899	-4.784116	-2.332001
8	0	-0.390597	-2.309456	2.561511
8	0	5.741268	0.510356	-1.520193
6	0	4.910247	-0.616852	-1.211555
6	0	5.195641	1.770562	-1.126836
6	0	4.813126	-0.704929	0.326117
6	0	5.545434	-1.850979	-1.875605
8	0	6.070970	2.767869	-1.535756
6	0	5.074906	1.814031	0.393981
8	0	4.422150	3.020785	0.792894
6	0	4.280727	0.611404	0.909098
8	0	4.592824	-2.829095	-2.253236
8	0	4.353742	0.659627	2.324031
1	0	0.908975	-2.527186	-1.337669
1	0	2.360317	-1.114982	-0.077607
1	0	0.487181	-4.375312	1.076196
1	0	2.053768	-4.567385	-2.286698
1	0	1.409608	-5.519295	-0.932422
1	0	-1.736249	-3.547512	0.680044
1	0	2.232574	-2.976045	2.346930
1	0	1.376657	-0.977223	3.298890
1	0	0.135740	-1.353777	0.808963
1	0	-0.713603	-4.659322	-1.733633
1	0	-1.059042	-1.595390	2.491308
1	0	3.915545	-0.469798	-1.663759
1	0	4.201286	1.886825	-1.597136
1	0	5.820365	-0.875388	0.718089
1	0	6.028089	-1.516280	-2.797312

1	0	6.320443	-2.273713	-1.219711
1	0	6.159943	2.725517	-2.498159
1	0	6.092288	1.786293	0.805525
1	0	4.368794	2.991819	1.760851
1	0	3.236244	0.753278	0.588193
1	0	4.105491	-3.136977	-1.470711
1	0	3.651592	0.079270	2.671190