Supporting Information

Energies and 2´-hydroxyl group orientations of RNA backbone conformations. Benchmark CCSD(T)/CBS database, electronic analysis and assessment of DFT methods and MD simulations

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Table S1 List of solvent relative energies (kcal.mol^{-1}) referenced against the **1a** conformation. Applied methods are tagged as follows: M1: B-LYP, M2: PBE, M3: revPBE, M4: TPSS, M5: oTPSS, M6: B3-LYP, M7: PW6B95, M8: MPW1B95, M9: PWPB95, M10: DSD-B-LYP, M11: MP2(D,T), and M12: MP2(T,Q). For further details see Methods. MAD and MAX (both in kcal.mol^{-1}) represent the mean absolute deviation and the maximum absolute deviation from the reference CBS(T) energies. MM labels force field calculations. Listed DFT energies include D3 correction; MAD and MAX values are quoted for DFs with and without D3 term.

Label	GGA			meta-GGA		Hybrid			Double-Hyb.		MP2/CBS		CBS(T)	MM
	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12		
1a	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	**0.00**	0.00
1m	-0.21	-0.05	-0.31	-0.17	-0.22	-0.05	0.14	0.15	0.15	0.21	0.42	0.28	**0.23**	2.13
1L	1.62	1.79	1.93	1.85	1.91	1.50	1.92	2.01	1.95	1.71	1.89	1.95	**1.80**	4.22
&a	-0.51	-0.30	-0.10	-0.22	0.01	-0.63	-0.60	-0.58	-0.70	-0.79	-0.69	-0.64	**-0.72**	-0.39
7a	2.30	2.36	2.43	2.29	2.36	2.31	2.55	2.63	2.60	2.46	2.77	2.59	**2.52**	6.30
3a	2.14	2.16	2.10	2.04	2.05	2.30	2.61	2.65	2.63	2.50	2.95	2.57	**2.50**	6.19
9a	1.45	1.41	1.44	1.38	1.42	1.55	1.77	1.81	1.81	1.73	2.01	1.82	**1.77**	4.26
1g	1.25	1.31	1.21	1.29	1.29	1.33	1.59	1.65	1.59	1.46	1.79	1.64	**1.54**	5.02
7d	0.68	0.75	0.76	0.64	0.61	0.80	1.06	1.09	1.18	1.15	1.60	1.33	**1.24**	2.30
3d	1.45	1.43	1.52	1.32	1.37	1.57	1.73	1.76	1.83	1.83	2.25	1.91	**1.81**	4.61
5d	0.03	0.09	-0.07	0.03	-0.01	0.13	0.31	0.34	0.27	0.21	0.50	0.27	**0.19**	1.45
1e	-1.30	-1.01	-0.51	-0.95	-0.55	-1.43	-0.55	-0.53	-0.70	-1.37	-1.19	-1.16	**-1.18**	2.51
1c	-0.17	-0.12	0.28	0.06	0.51	-0.03	0.42	0.44	0.29	-0.05	0.16	0.06	**-0.14**	4.44
1f	0.57	0.59	0.81	0.76	1.09	0.72	1.33	1.35	1.16	0.75	1.18	0.89	**0.61**	7.31
5j	0.62	0.70	0.54	0.64	0.68	0.71	1.13	1.22	1.12	1.00	1.55	1.14	**0.92**	3.80
1b	-0.52	-0.28	-0.37	-0.47	-0.36	-0.32	-0.33	-0.32	-0.39	-0.37	-0.59	-0.50	**-0.35**	0.16
1[	-1.48	-1.21	-1.49	-1.49	-1.44	-1.25	-1.30	-1.31	-1.37	-1.18	-1.17	-1.33	**-1.24**	0.92
3b	0.80	1.01	1.01	0.75	0.88	1.01	1.16	1.21	1.14	1.07	1.26	0.95	**1.05**	5.80
1z	-0.15	-0.03	0.08	-0.09	0.15	0.05	0.12	0.18	0.07	-0.02	-0.04	-0.10	**-0.01**	1.41
5z	1.72	2.18	1.97	1.97	2.06	1.94	2.40	2.49	2.32	2.06	2.28	2.17	**2.19**	4.31
7p	0.35	0.50	0.45	0.16	0.27	0.62	0.57	0.60	0.59	0.75	0.75	0.62	**0.68**	4.30
1t	-0.80	-0.76	-0.53	-0.69	-0.29	-0.49	0.03	0.04	-0.22	-0.63	-0.50	-0.76	**-0.82**	4.12
5q	-0.93	-0.83	-1.15	-0.98	-0.90	-0.69	-0.47	-0.42	-0.61	-0.63	-0.44	-0.80	**-0.89**	1.89
1o	-1.11	-0.97	-1.24	-1.27	-1.20	-0.92	-0.90	-0.87	-1.00	-0.95	-0.91	-1.11	**-1.08**	1.29
7r	-0.04	0.10	0.06	-0.24	-0.10	0.20	0.31	0.33	0.31	0.36	0.55	0.26	**0.24**	2.00
2a	0.82	0.89	0.66	0.68	0.72	0.90	1.10	1.12	1.07	1.01	1.30	1.05	**0.88**	2.02
4a	2.16	2.25	2.03	2.00	2.04	2.21	2.45	2.44	2.39	2.27	2.55	2.25	**2.21**	6.43
0a	1.58	1.43	1.39	1.12	1.22	1.66	1.61	1.56	1.61	1.73	1.99	1.73	**1.63**	7.96
#a	1.71	1.36	1.48	1.02	1.26	1.76	1.88	1.71	1.77	1.77	2.05	1.81	**1.66**	8.15
4g	5.28	5.34	5.16	5.14	5.18	5.34	5.56	5.56	5.51	5.41	5.80	5.41	**5.44**	10.71
6g	1.58	1.67	1.45	1.38	1.37	1.68	1.89	1.91	1.92	1.85	2.16	1.89	**1.92**	3.97
8d	1.35	1.49	1.28	1.21	1.27	1.44	1.63	1.65	1.62	1.62	1.95	1.66	**1.51**	2.81
4d	2.36	2.47	2.09	2.25	2.29	2.55	2.84	2.89	2.80	2.76	3.06	2.81	**2.64**	6.33
6d	0.78	0.77	0.61	0.54	0.52	0.92	1.13	1.13	1.16	1.11	1.42	1.21	**1.11**	4.20
2h	0.90	0.94	0.67	0.86	1.01	1.06	1.34	1.41	1.26	1.16	1.51	1.19	**0.85**	2.26
4n	4.29	3.91	3.82	3.65	3.71	4.26	3.76	3.69	3.77	4.26	4.47	4.32	**4.02**	10.77
0i	3.48	3.56	3.54	3.39	3.58	3.55	3.64	3.70	3.64	3.69	3.75	3.81	**3.63**	7.81
6n	0.05	0.09	-0.11	-0.11	-0.05	0.11	0.33	0.32	0.28	0.15	0.21	0.20	**0.15**	1.83
6j	0.45	0.49	0.09	0.35	0.35	0.69	1.12	1.16	1.07	0.97	1.42	1.05	**0.83**	5.67
2[	-0.57	-0.25	-0.55	-0.64	-0.48	-0.33	-0.08	-0.07	-0.25	-0.34	-0.30	-0.50	**-0.51**	2.55
4b	1.14	1.35	1.15	0.99	1.17	1.40	1.56	1.57	1.43	1.35	1.37	1.18	**1.25**	7.36
0b	1.19	1.44	1.26	1.11	1.25	1.49	1.81	1.83	1.77	1.66	1.81	1.60	**1.65**	5.94
4p	1.21	1.53	1.26	1.13	1.33	1.57	1.71	1.73	1.66	1.77	1.78	1.70	**1.65**	5.78
6p	-0.65	-0.43	-0.61	-0.87	-0.77	-0.39	-0.34	-0.35	-0.38	-0.39	-0.43	-0.46	**-0.36**	2.57
4s	2.06	2.26	1.77	1.93	2.05	2.46	2.87	2.88	2.68	2.51	2.46	2.33	**2.29**	7.32
2o	-0.80	-0.64	-0.91	-1.00	-0.81	-0.58	-0.34	-0.28	-0.53	-0.65	-0.64	-0.83	**-0.92**	0.30
MAD-D3	**0.22**	**0.16**	**0.29**	**0.32**	**0.31**	**0.15**	**0.22**	**0.24**	**0.16**	**0.10**	**N/A**		**N/A**	**N/A**
MAX-D3	**0.56**	**0.49**	**0.75**	**0.64**	**0.73**	**0.44**	**0.85**	**0.86**	**0.61**	**0.31**				
MAD	**0.88**	**0.55**	**1.04**	**0.79**	**0.89**	**0.70**	**0.28**	**0.30**	**0.19**	**0.19**	**0.28**	**0.11**	**0.00**	**3.26**
MAX	**2.25**	**1.39**	**2.54**	**1.79**	**2.14**	**1.82**	**0.62**	**0.69**	**0.47**	**0.57**	**0.66**	**0.34**	**0.00**	**6.74**

Table S2 List of O2′H group acceptors and respective H-bond strengths estimated by AIM analysis for RNA backbone conformations. The (i+1) designates that respective H-bond acceptor belongs to the i+1-th (i.e. 5′-3′ downstream) nucleotide. Electronic densities (ρ) and magnitudes of electronic density Laplacians (Δρ) at the H-bond critical point are given in a.u.

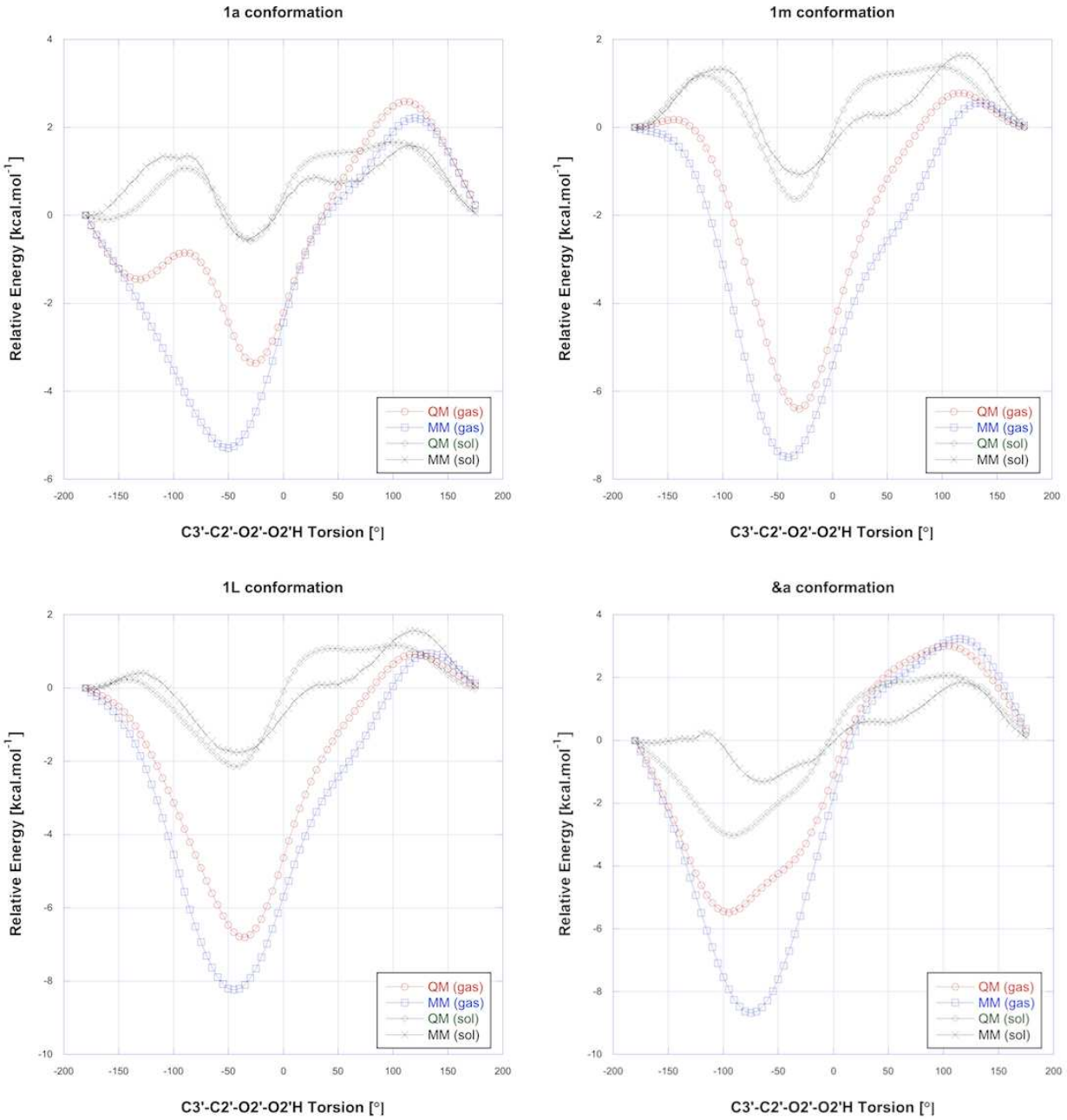
δ, δ + 1, γ + 1	Group	Label	ρ	Δρ	O2′H Acceptor
3, 3, p	**Group I**	1a	0.025	0.021	O3′
		1m	0.027	0.022	O3′
		1L	0.026	0.023	O3′
		&a	0.011	0.009	O5′ (i+1)
			0.012	0.010	O4′ (i+1)
		7a	0.022	0.020	O3′
		3a	0.026	0.022	O3′
		9a	0.025	0.022	O3′
		1g	0.027	0.022	O3′
		7d	0.036	0.029	O3′
		3d	0.033	0.027	O3′
		5d	0.021	0.019	O3′
3, 3, t		1e	0.028	0.020	O4′ (i+1)
		1c	0.026	0.020	O5′ (i+1)
		1f	0.026	0.020	O5′ (i+1)
		5j	0.029	0.024	O3′
3, 2, p	**Group II**	1b	0.026	0.022	O3′
		1[	0.027	0.022	O3′
		3b	0.028	0.023	O3′
		1z	0.026	0.022	O3′
		5z	0.031	0.021	O2P (i+1)
		7p	0.030	0.025	O3′
3, 2, t		1t	0.027	0.020	O5′ (i+1)
		5q	0.023	0.020	O3′
3, 2, m		1o	0.026	0.022	O3′
		7r	0.030	0.025	O3′
2, 3, p	**Group III**	2a	0.029	0.024	O3′
		4a	0.027	0.022	O3′
		0a	0.014	0.010	O1P (i+1)
			0.020	0.019	O3′
		#a	0.033	0.022	O1P (i+1)
		4g	0.026	0.022	O3′
		6g	0.028	0.023	O3′
		8d	0.032	0.026	O3′
		4d	0.026	0.022	O3′
		6d	0.026	0.021	O3′
2, 3, t		2h	0.030	0.024	O3′
		4n	0.028	0.017	O1P (i+1)
		0i	0.029	0.025	O3′
		6n	0.029	0.024	O3′

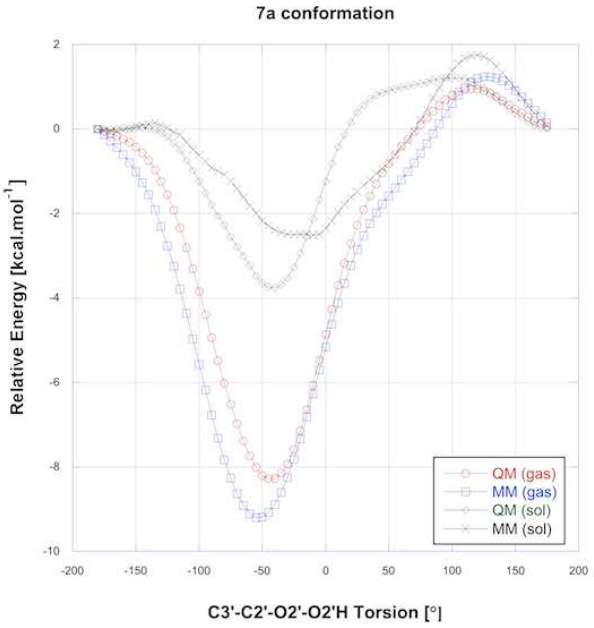
		6j	0.026	0.021	O3′
2, 2, p	**Group IV**	2[	0.028	0.023	O3′
		4b	0.024	0.021	O3′
		0b	0.027	0.022	O3′
		4p	0.028	0.022	O3′
		6p	0.028	0.023	O3′
2, 2, t		4s	0.024	0.021	O3′
2, 2, m		2o	0.028	0.023	O3′

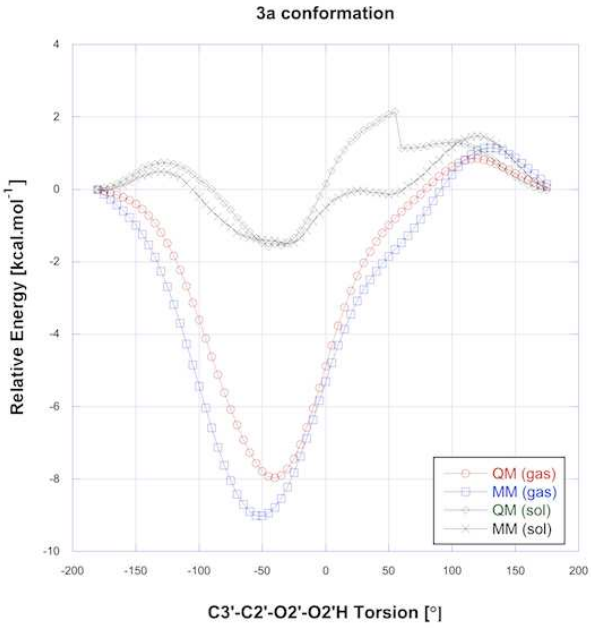
Comment on MD simulation protocol

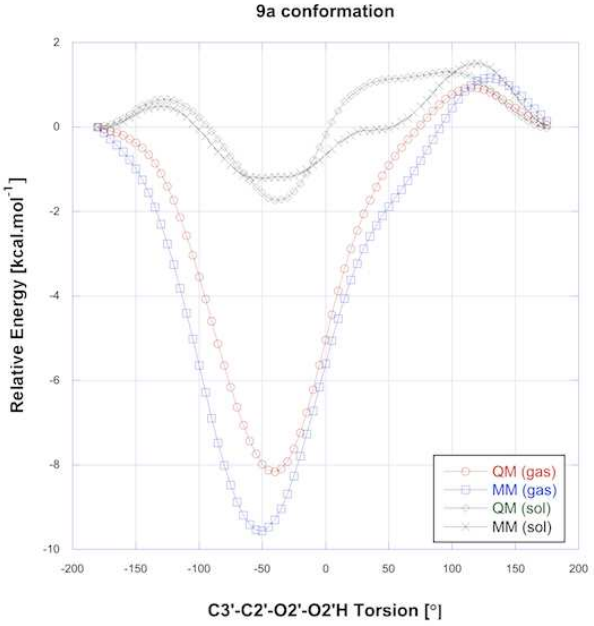
The simulation protocol was as follows – both systems (SRL and *glmS*, for more details see main text) were minimized, by first optimizing the waters and ions, while the positions of the RNA molecule remained constrained. Subsequently, all RNA atoms were frozen and the solvent molecules with counter-ions were allowed to move during a 1000-step minimization, followed by 10 ps long MD runs under [NpT] conditions (p = 1 atm., T = 298.16 K) in order to relax the total density. After this, the solute and nucleobases were relaxed by several minimization runs, with decreasing force constants applied to the sugar-phosphate backbone atoms. After the relaxation, each system was heated from 10.00 K to 298.16 K for 100 ps. The particle-mesh Ewald (PME) method for treating electrostatic interactions was used, and all simulations were performed under periodic boundary conditions in the [NpT] ensemble at 298.16 K using weak-coupling Berendsen thermostat with coupling time of 1 ps. The SHAKE algorithm, with a tolerance of 10^{-5} Å, was used to fix the positions of all hydrogen atoms, and a 10.0 Å cutoff was applied to non-bonding interactions to allow a 2 fs integration step. The simulation lengths of production phases of the simulations were 1 μs.

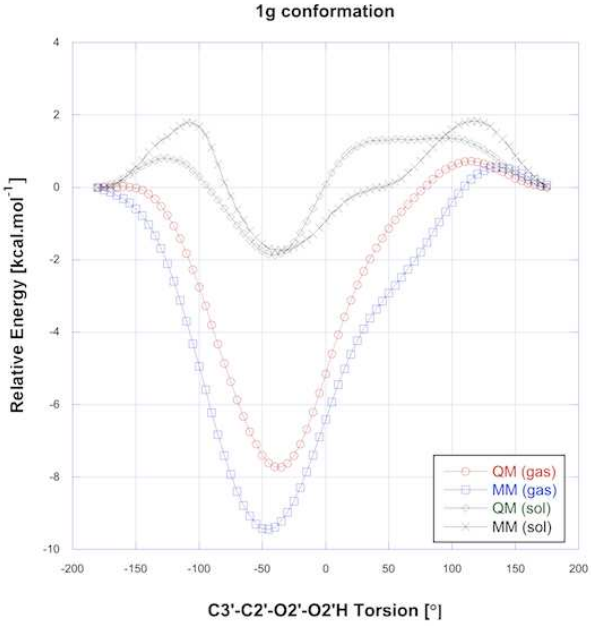
Figure S1 Hydroxyl group rotation energy profiles (kcal.mol^{-1}). The zero energy refers to C3′-C2′-O2′-O2′H torsion of 180°. The sequence of conformations corresponds to that in Table 1 in the main text. For methodology details, see Methods in the main text.

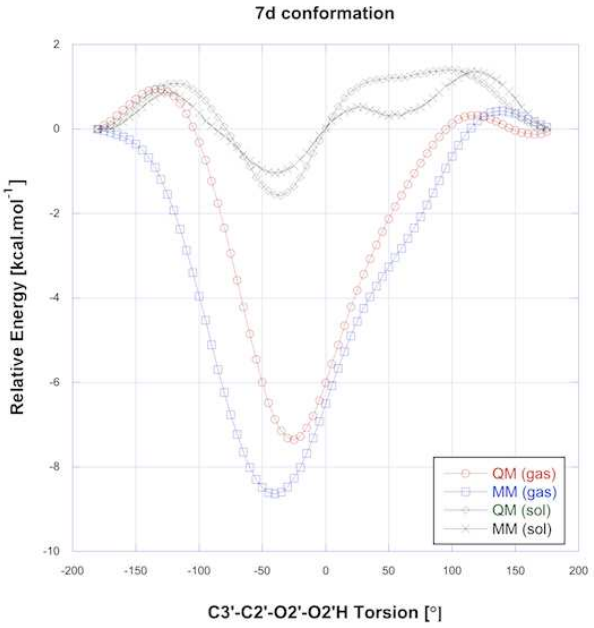


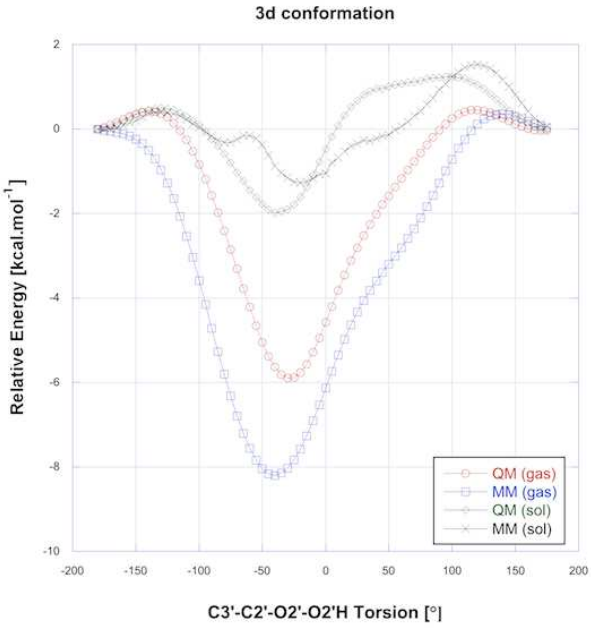

7a conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

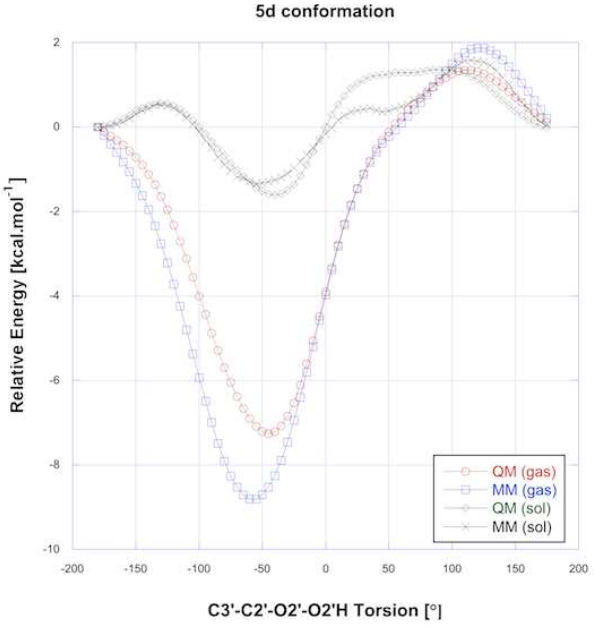

3a conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

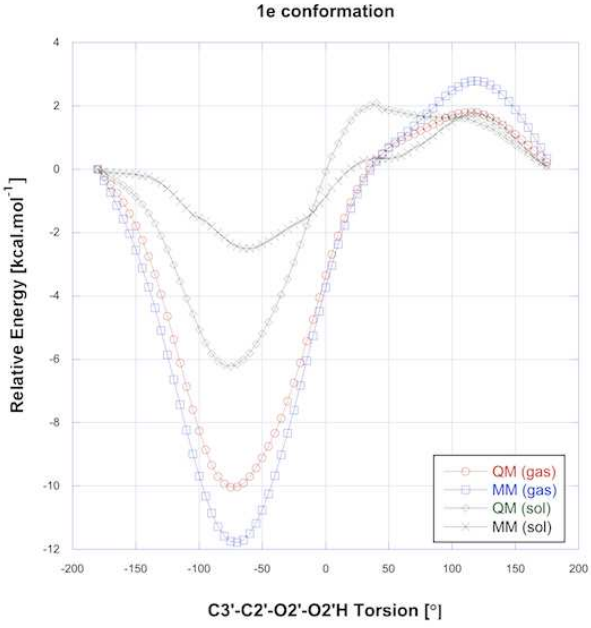

9a conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

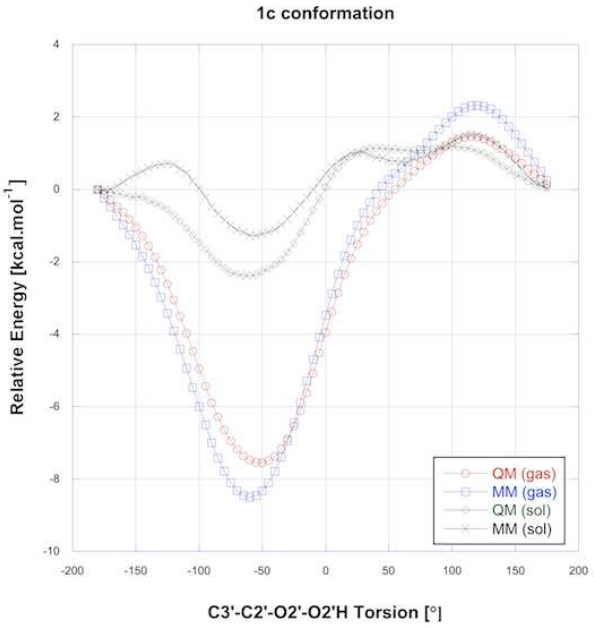

1g conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

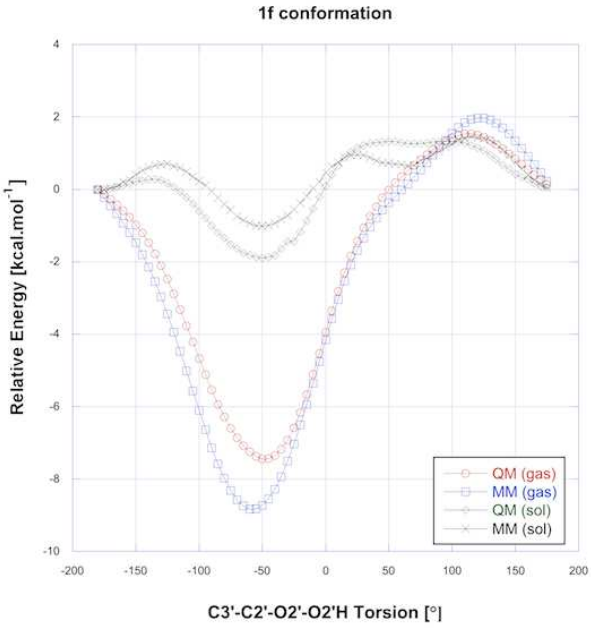

7d conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

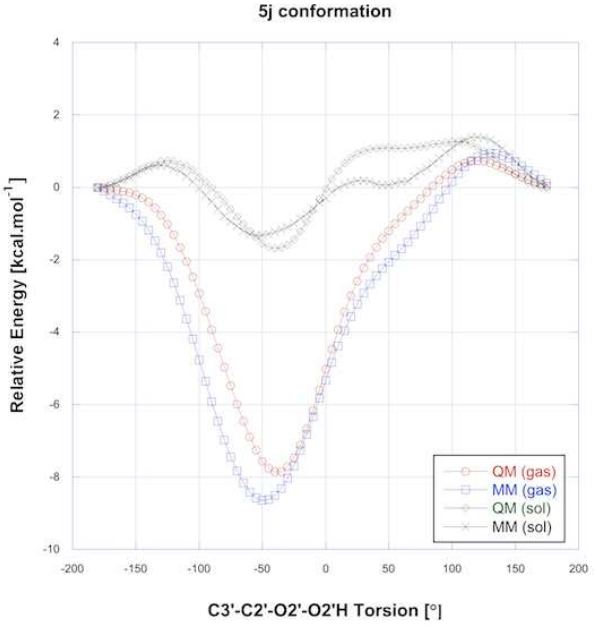

3d conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

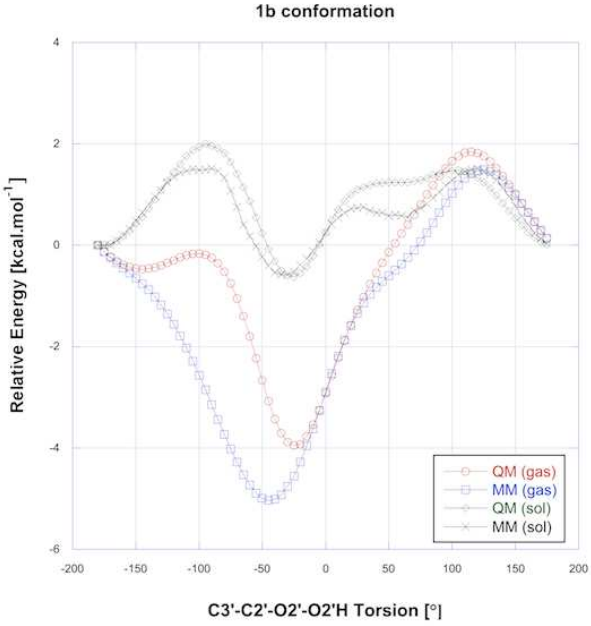

5d conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

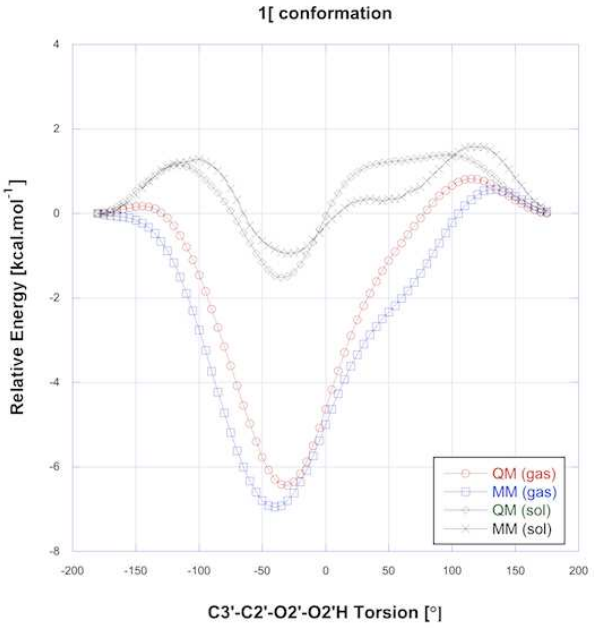

1e conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

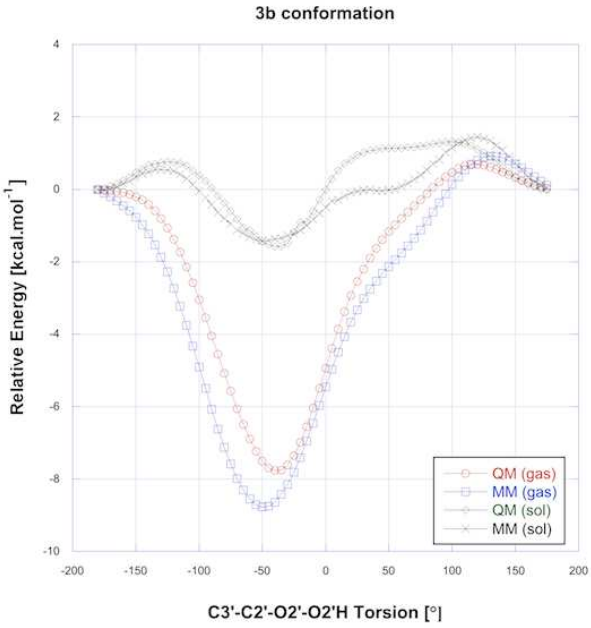

1c conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

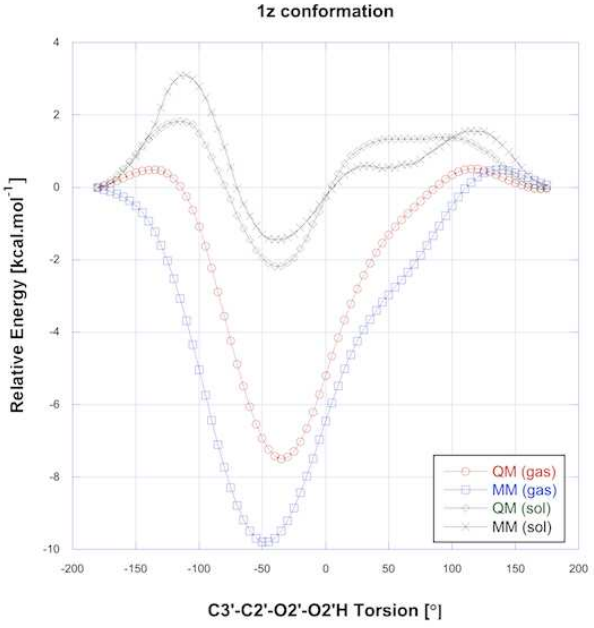

1f conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

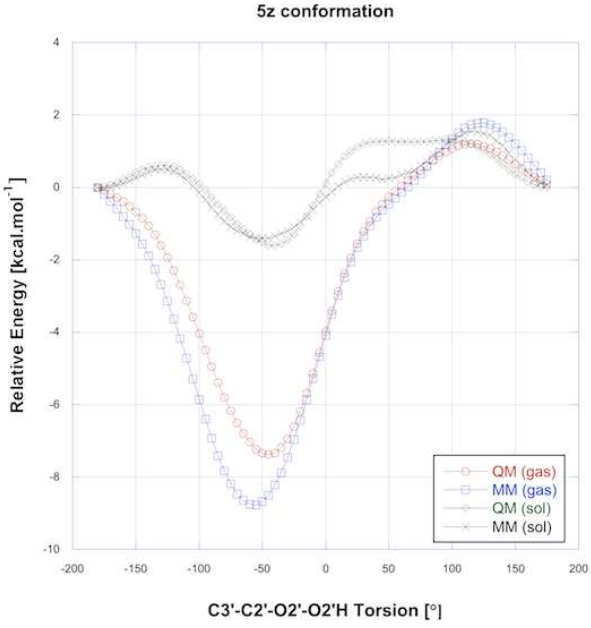

5j conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

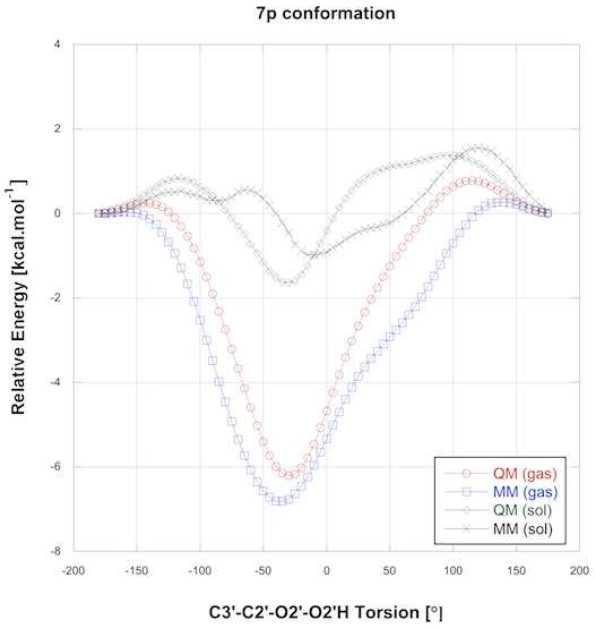

1b conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

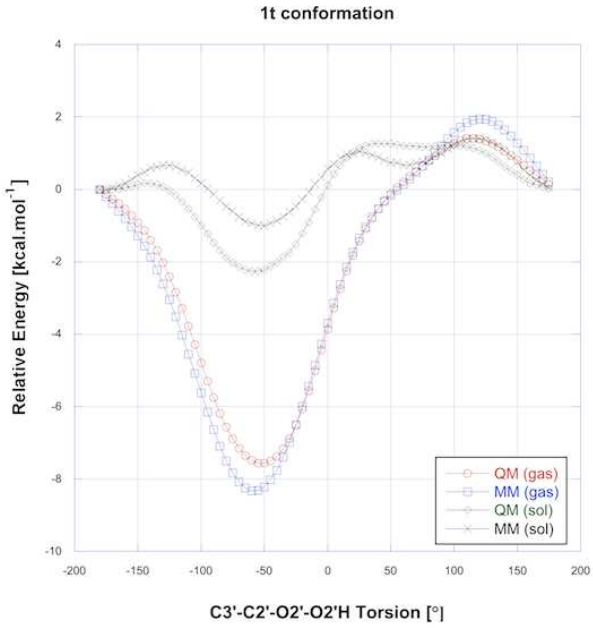

1[conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

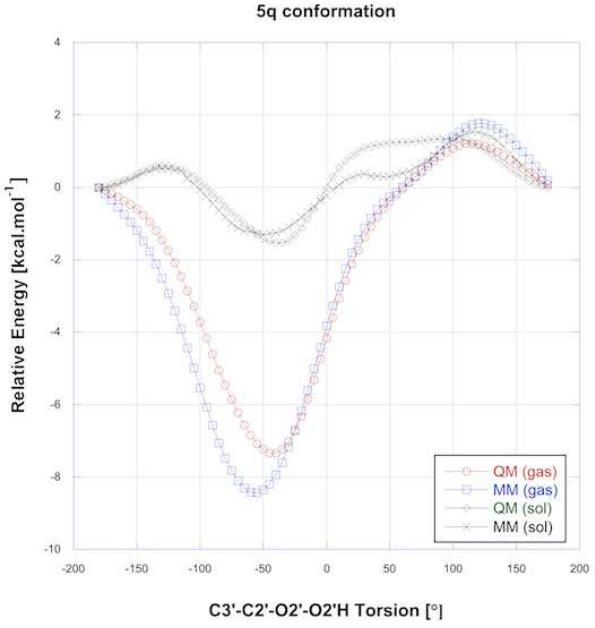

3b conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

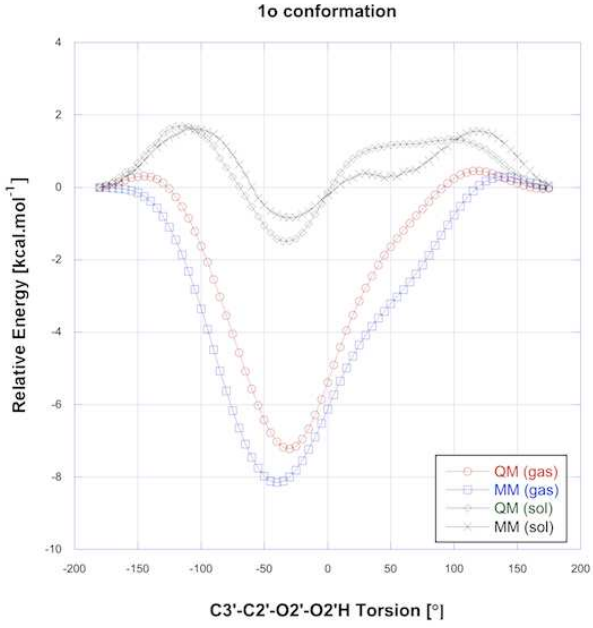

1z conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

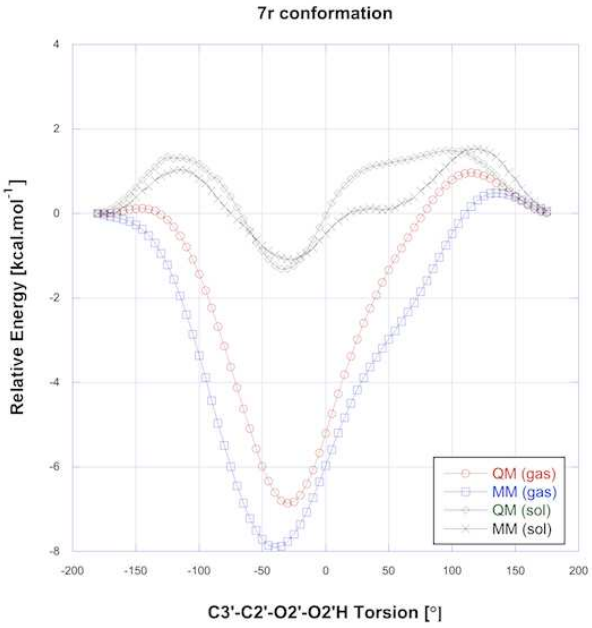

5z conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

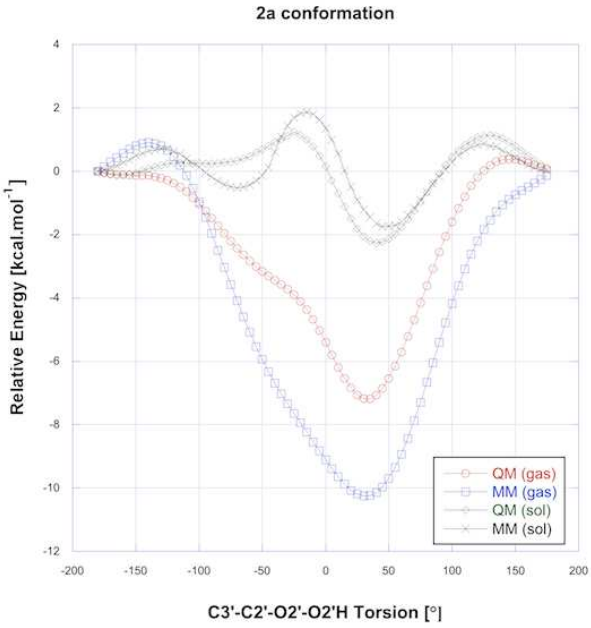

7p conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

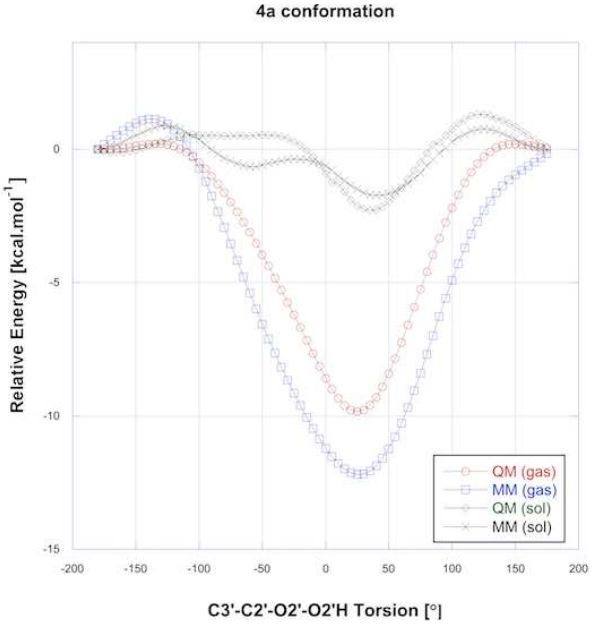

1t conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

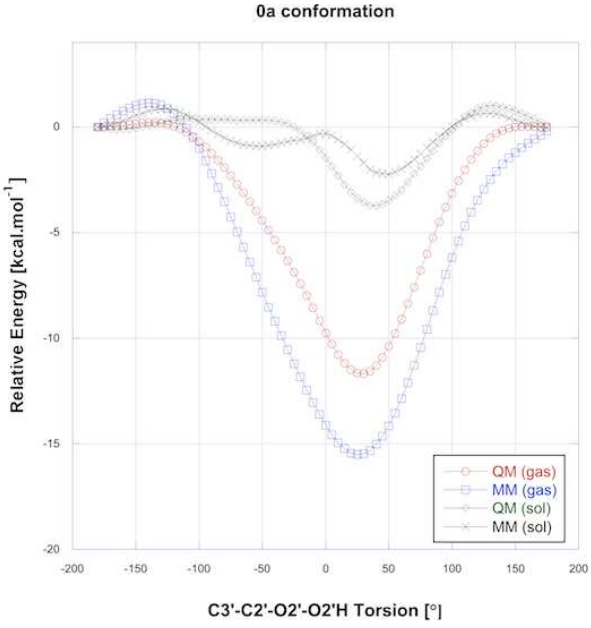

5q conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

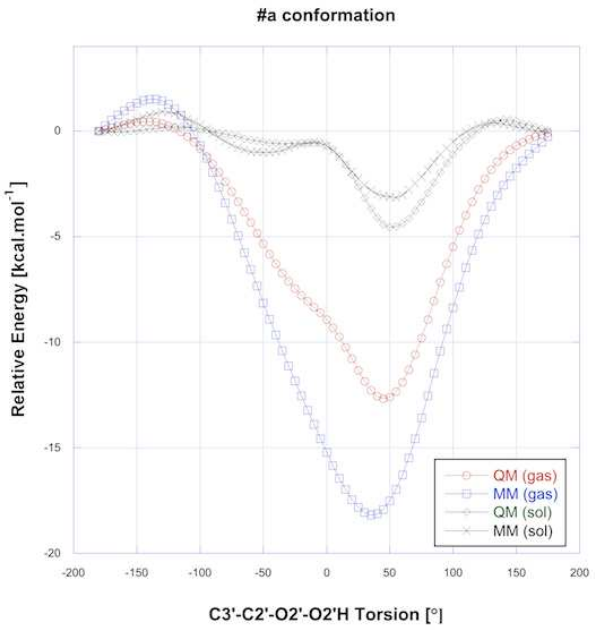

1o conformation
Relative Energy [kcal.mol^{-1}]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

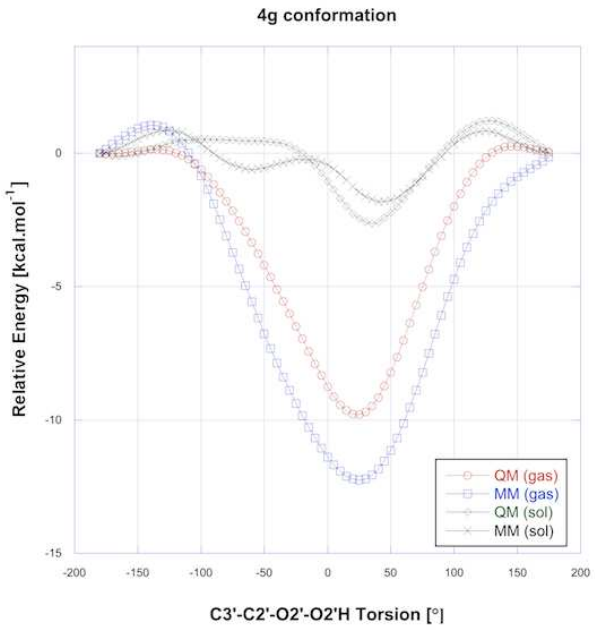

7r conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

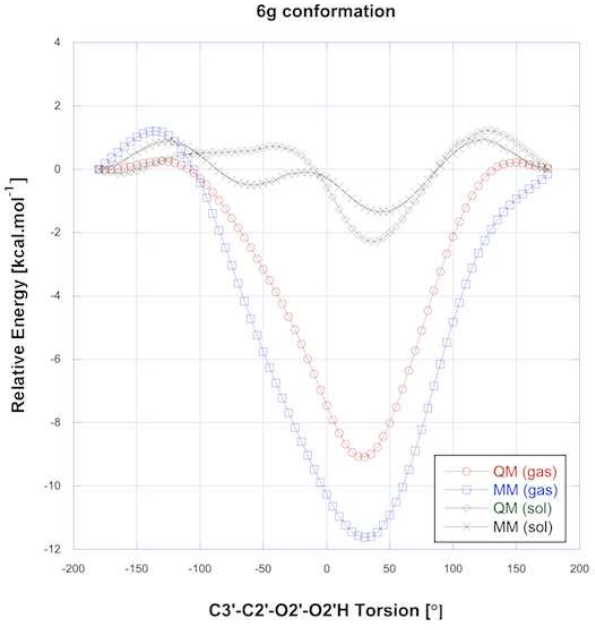

2a conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

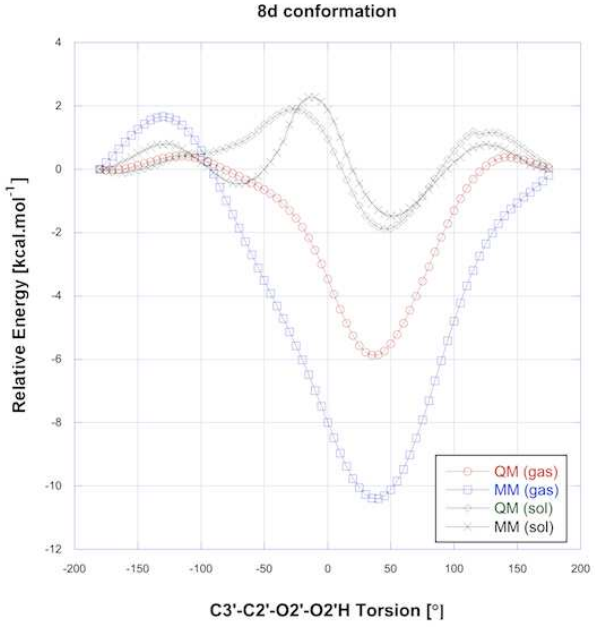

4a conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

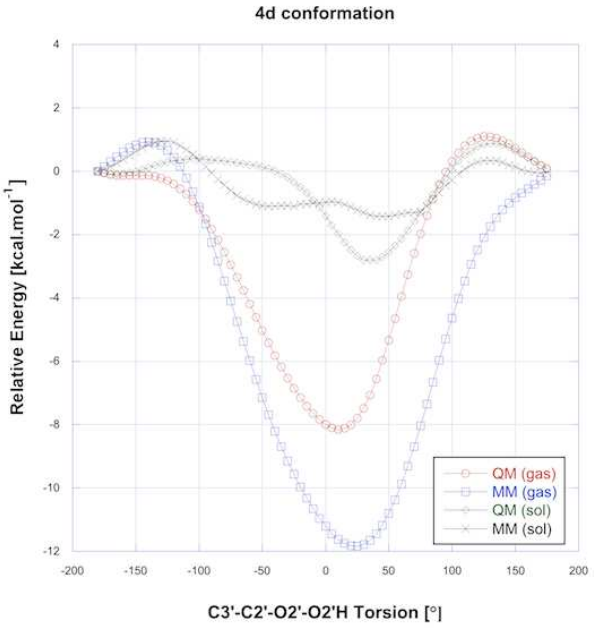

0a conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

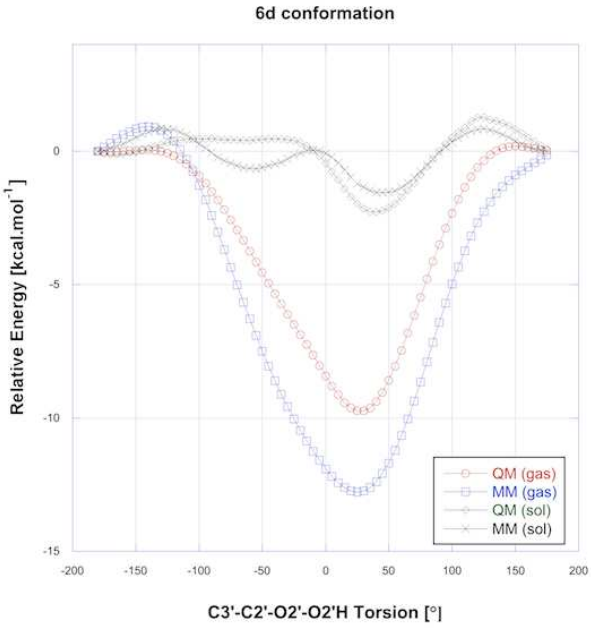

#a conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

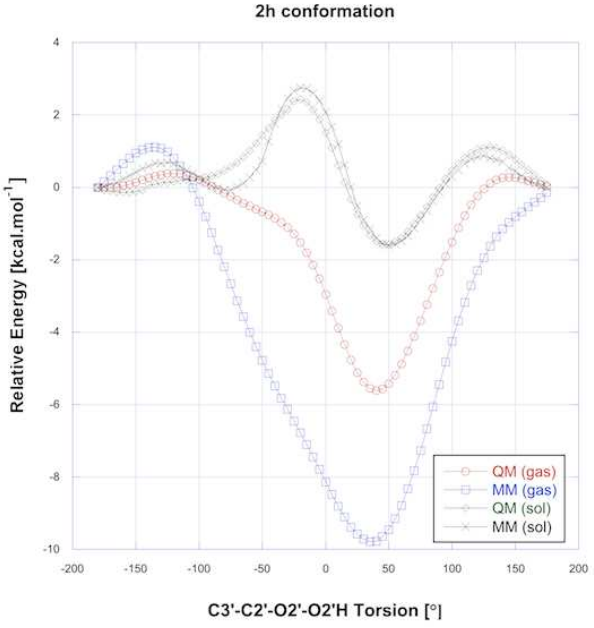

4g conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

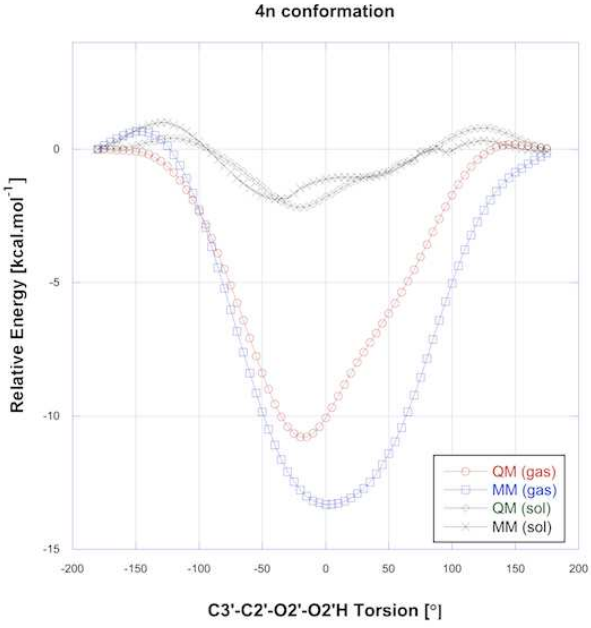

6g conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

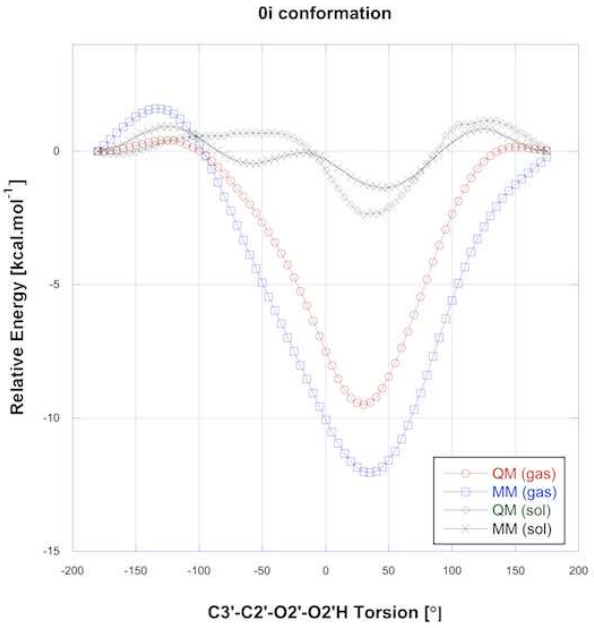

8d conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

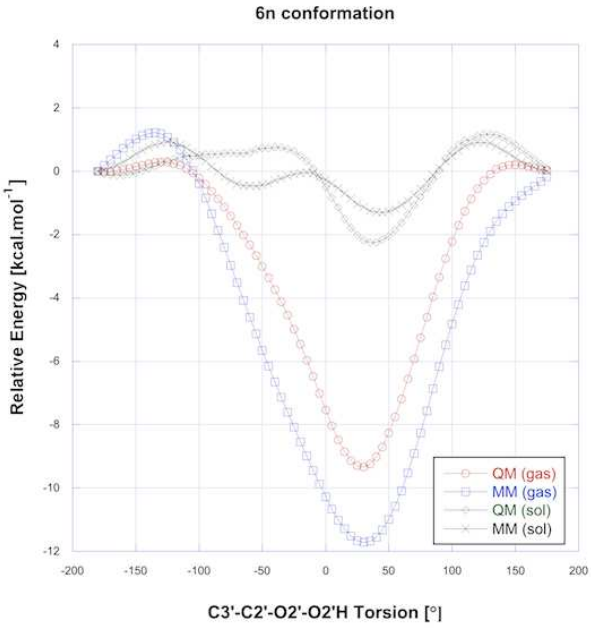

4d conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

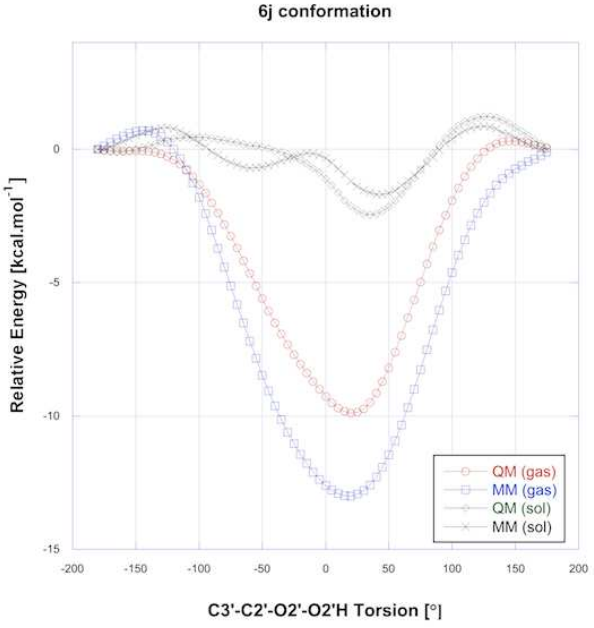

6d conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

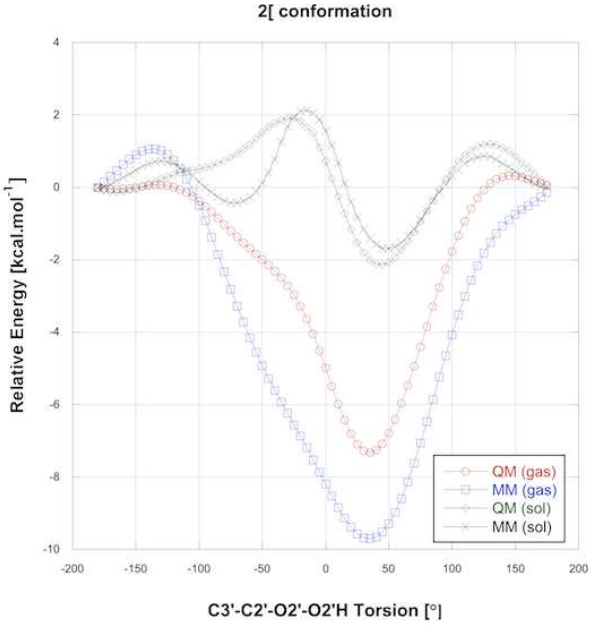

2h conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

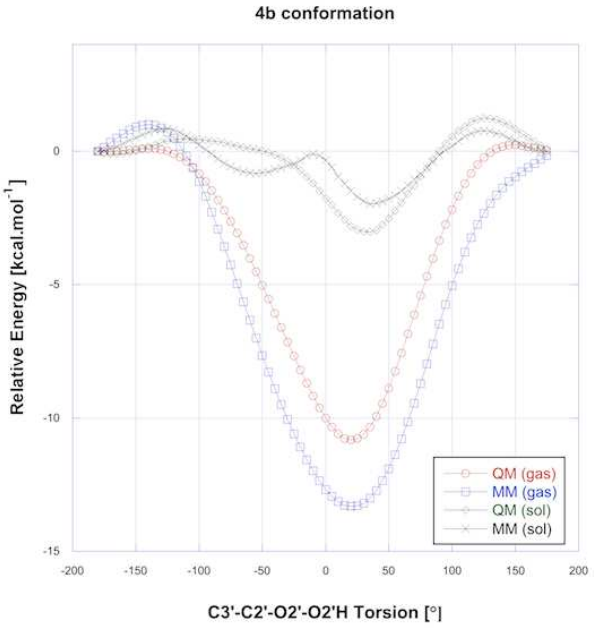

4n conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

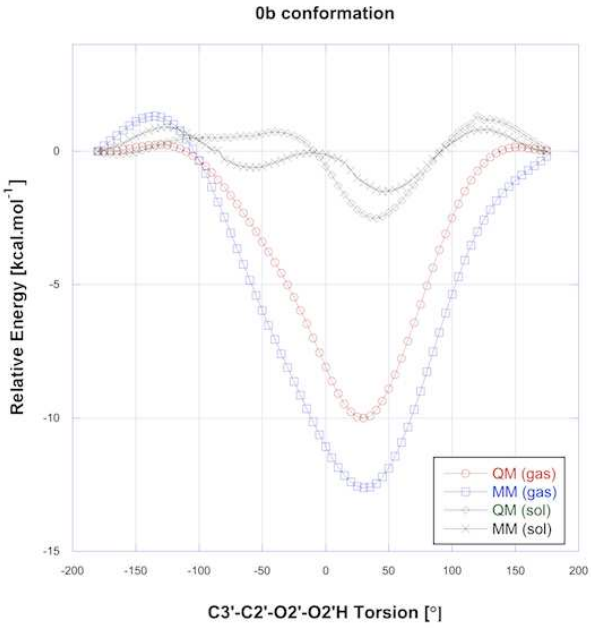

0i conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

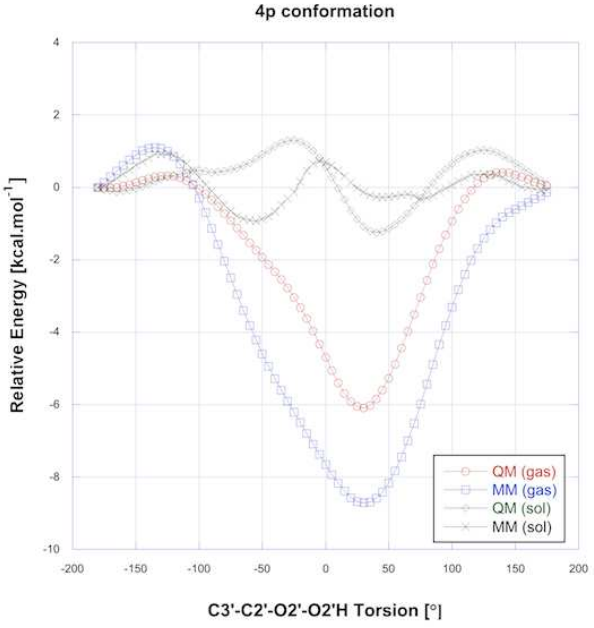

6n conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

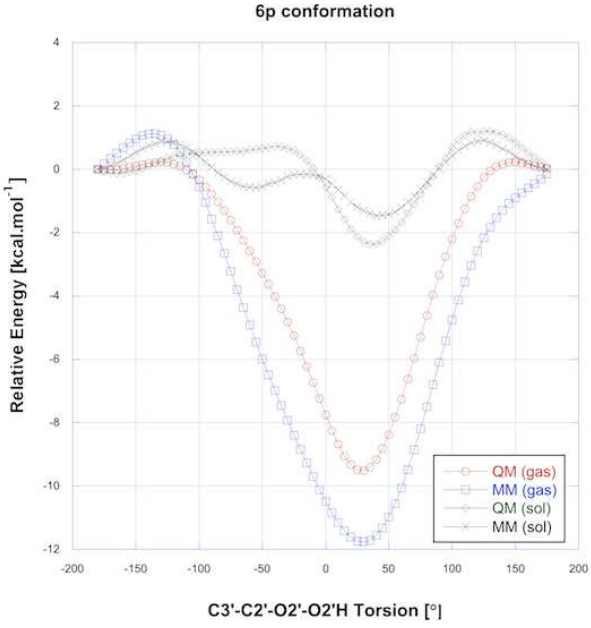

6j conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

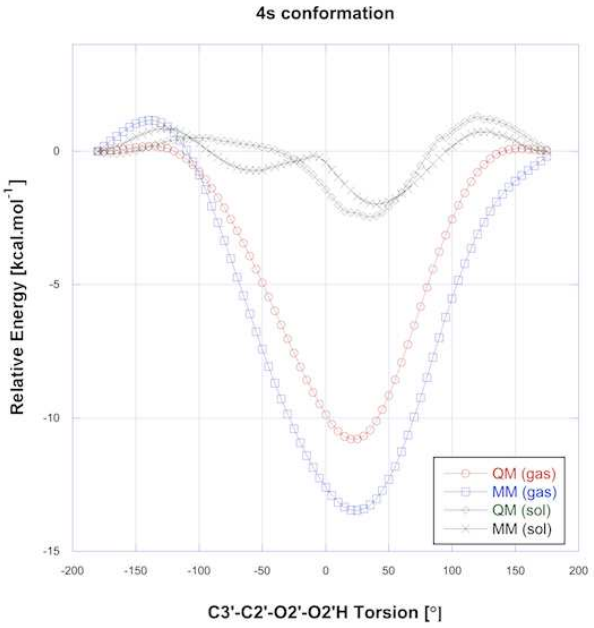

2[conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)

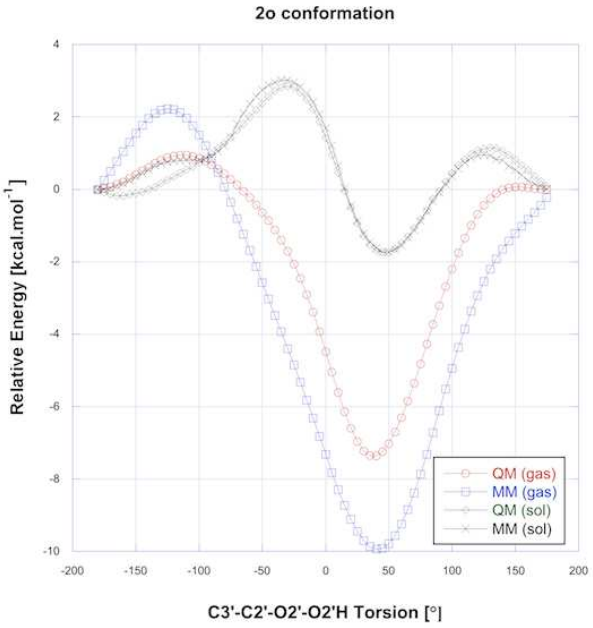

4b conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)


0b conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)


4p conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)


6p conformation
Relative Energy [kcal.mol-1]
C3'-C2'-O2'-O2'H Torsion [°]
QM (gas)
MM (gas)
QM (sol)
MM (sol)


4s conformation
Relative Energy [kcal.mol-1]
0
-5
-10
-15
-200
-150
-100
-50
0
50
100
150
200
QM (gas)
MM (gas)
QM (sol)
MM (sol)
C3'-C2'-O2'-O2'H Torsion [°]


2o conformation
Relative Energy [kcal.mol-1]
4
2
0
-2
-4
-6
-8
-10
-200
-150
-100
-50
0
50
100
150
200
QM (gas)
MM (gas)
QM (sol)
MM (sol)
C3'-C2'-O2'-O2'H Torsion [°]

Cartesian coordinates (xyz format) of the conformations optimized in gas phase with respective relative CBS(T) energies (kcal.mol^{-1}).

```
37
System: 1a, CBS(T): 0.00
  C      0.0382050      0.1092850     -0.1007310
  C      0.0685840      0.0549230      1.4135750
  O      1.4362850      0.0440110      1.8784280
  C      1.4794110      0.6542190      3.1952000
  C      0.0715230      1.1343670      3.5161190
  O     -0.6307320      0.0985270      4.2288430
  C     -0.5537800      1.2677960      2.1139040
  O     -1.9747500      1.1575670      2.1651480
  P     -2.8639250      2.5887340      2.0998930
  O     -4.2837260      2.1295850      2.0738360
  O     -2.2075830      3.5036500      1.1215320
  O     -2.5555680      3.2679460      3.5852620
  C     -3.0144580      2.6074180      4.7572570
  C     -2.4830170      3.3419630      5.9743960
  O     -1.0479440      3.2721330      6.0779890
  C     -0.5362340      4.5554000      6.4988560
  C     -1.7470150      5.3933860      6.9192720
  C     -2.8133300      4.8420640      5.9841220
  O     -4.1407810      5.1396340      6.4404140
  H     -1.0028950      0.1552800     -0.4350740
  H      0.5125070     -0.7767950     -0.5363090
  H      0.5584550      1.0026240     -0.4607480
  H     -0.4476610     -0.8492150      1.7703150
  H      2.1941080      1.4865150      3.1583400
  H      1.8175710     -0.0847300      3.9308960
  H      0.0481780      2.0639530      4.0937780
  H     -1.5272270      0.1135260      3.8369050
  H     -0.2676210      2.2055640      1.6253050
  H     -2.6760400      1.5652240      4.7827530
  H     -4.1148030      2.6005260      4.7896540
  H     -2.9331150      2.8816240      6.8708210
  H     -0.0078260      5.0161840      5.6527990
  H      0.1790060      4.3897120      7.3123090
  H     -1.5805180      6.4679760      6.8033840
  H     -2.0336470      5.1881890      7.9571540
  H     -2.6687510      5.2326710      4.9697870
  H     -4.7458750      4.8809040      5.7291030

37
System: 1m, CBS(T): -4.09
  C      0.0137930      0.0384510     -0.0692940
  C      0.0658250      0.0634960      1.4451970
  O      1.4442450      0.1025010      1.8778390
  C      1.5153100      0.7841290      3.1548210
  C      0.1261280      1.3339700      3.4627650
  O     -0.5648210      0.4407270      4.3493410
  C     -0.5634160      1.3046730      2.0845950
  O     -1.9744720      1.1478120      2.2204420
  P     -2.9168850      2.5147060      1.9393000
  O     -4.3233940      2.0428940      2.1407570
  O     -2.3915180      3.2112300      0.7307580
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  O     -2.4963180      3.4727610      3.2271750
  C     -2.9213880      3.0156640      4.5158830
  C     -3.4346500      4.1920270      5.3230910
  O     -2.4278300      5.1975000      5.5603960
  C     -2.9560250      6.4880340      5.1866980
  C     -4.4761730      6.3294290      5.1384290
  C     -4.5957900      4.9060040      4.6067080
  O     -5.8744410      4.3196720      4.8789420
  H      0.4910230     -0.8646800     -0.4642590
  H     -1.0312750      0.0605490     -0.3933470
  H      0.5213170      0.9170510     -0.4793190
  H     -0.4282060     -0.8269930      1.8631650
  H      2.2618430      1.5827820      3.0637310
  H      1.8286910      0.0801060      3.9349800
  H      0.1567450      2.3420070      3.8935880
  H     -1.4823160      0.4364060      4.0054930
  H     -0.3399580      2.2038180      1.5005320
  H     -2.0776080      2.5378020      5.0293260
  H     -3.7355070      2.2865070      4.4089160
  H     -3.7966140      3.8170820      6.2940080
  H     -2.5569930      6.7674080      4.2012820
  H     -2.6132750      7.2176020      5.9283000
  H     -4.9626750      7.0710890      4.4983930
  H     -4.9126600      6.3831700      6.1427640
  H     -4.4021250      4.8884750      3.5290260
  H     -5.9656080      3.5791510      4.2570160

37
System: 1L, CBS(T): 2.60
  C      0.0143170      0.0578000     -0.0609760
  C      0.0610080      0.0695160      1.4536770
  O      1.4422820      0.1064770      1.8847950
  C      1.5142860      0.7760730      3.1650960
  C      0.1283540      1.3290380      3.4792430
  O     -0.5514430      0.4349480      4.3732580
  C     -0.5738840      1.3052390      2.1065180
  O     -1.9783820      1.1319360      2.2826610
  P     -3.0455960      2.1174780      1.4380310
  O     -4.2990960      1.3099610      1.3704270
  O     -2.3223930      2.7276680      0.2842800
  O     -3.2962150      3.3716580      2.5039050
  C     -3.7658920      3.0902730      3.8114840
  C     -3.0264540      3.9397520      4.8343460
  O     -1.6078250      3.7504400      4.8164140
  C     -0.9527550      5.0238050      5.0088810
  C     -2.0456500      6.0271370      5.3931220
  C     -3.2363080      5.4495200      4.6431470
  O     -4.4879630      5.9333620      5.1502310
  H     -1.0279170      0.0925480     -0.3916240
  H      0.4910570     -0.8441600     -0.4603410
  H      0.5256720      0.9389080     -0.4602240
  H     -0.4318160     -0.8232340      1.8666540
  H      2.2651180      1.5726200      3.0818700
  H      1.8248030      0.0659460      3.9416920
  H      0.1567710      2.3327130      3.9143810
  H     -1.4832580      0.4785440      4.0784530
  H     -0.3724620      2.2073600      1.5210890
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  H     -3.6496870      2.0258820      4.0467400
  H     -4.8424610      3.3198340      3.8903870
  H     -3.4213630      3.6711020      5.8315070
  H     -0.4624540      5.3075700      4.0677860
  H     -0.1870310      4.9025950      5.7828970
  H     -1.8009850      7.0524420      5.1021600
  H     -2.2496160      6.0021400      6.4696260
  H     -3.1532670      5.6768690      3.5720820
  H     -5.1811840      5.5724730      4.5773610

37
System: &a, CBS(T): -1.95
  C     -0.0602470     -0.0576170      0.0552800
  C     -0.0458780     -0.0131670      1.5720430
  O      1.3340880     -0.0395900      2.0175100
  C      1.4887300      0.8255310      3.1697900
  C      0.1108810      1.3645220      3.5365140
  O     -0.4421950      0.5106480      4.5408030
  C     -0.6158390      1.2696110      2.1750420
  O     -2.0340210      1.2002950      2.2257580
  P     -2.8498310      2.6104550      2.5886300
  O     -4.2026260      2.4772810      1.9704440
  O     -1.9273510      3.7744660      2.4406330
  O     -3.0217630      2.3809690      4.2389040
  C     -3.8253900      1.2628930      4.6198790
  C     -3.9141990      1.2344630      6.1301790
  O     -2.6261110      0.9353520      6.7107960
  C     -2.4349930      1.7435300      7.8951800
  C     -3.7769530      2.4272910      8.1769800
  C     -4.3348690      2.5651530      6.7669710
  O     -5.7516740      2.7868040      6.7612790
  H      0.4048240     -0.9776050     -0.3151330
  H     -1.0946810     -0.0163280     -0.3021240
  H      0.4868250      0.8003140     -0.3492270
  H     -0.5832900     -0.8733620      1.9961890
  H      2.1813540      1.6339460      2.9006250
  H      1.9083720      0.2468400      3.9996720
  H      0.1385770      2.4023920      3.8845920
  H     -1.2511340      0.9326610      4.8821650
  H     -0.3114670      2.1391010      1.5779720
  H     -3.3843060      0.3295280      4.2449010
  H     -4.8311960      1.3559190      4.1857360
  H     -4.6372260      0.4564020      6.4279420
  H     -1.6455130      2.4781680      7.6896590
  H     -2.1034030      1.0887500      8.7084390
  H     -3.6634500      3.3842180      8.6938860
  H     -4.4379480      1.7821960      8.7672750
  H     -3.8256120      3.3758090      6.2333580
  H     -5.9956880      3.0065190      5.8492920

37
System: 7a, CBS(T): 1.20
  C     -0.0122500      0.0061290     -0.0127240
  C     -0.0081450      0.0719900      1.5010190
  O      1.3559990      0.1035050      1.9750740
  C      1.3749150      0.7432370      3.2765170
  C      0.0199380      1.4219970      3.4868340
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  O     -0.7439690      0.6646570      4.4310650
  C     -0.6244880      1.3439890      2.0844330
  O     -2.0355180      1.2401250      2.1585150
  P     -2.9450890      2.6263610      1.8373410
  O     -3.6349140      2.4042300      0.5300260
  O     -2.1287340      3.8274470      2.1800780
  O     -4.0367020      2.4153080      3.0645630
  C     -4.7756130      1.1973850      3.1002740
  C     -5.3330840      1.0071380      4.4973490
  O     -4.2868740      0.7068040      5.4418070
  C     -4.5340820      1.4225630      6.6724970
  C     -5.9550340      1.9856100      6.5687140
  C     -6.0543060      2.2347260      5.0702870
  O     -7.4132070      2.3681340      4.6267330
  H     -1.0454650      0.0578770     -0.3706740
  H      0.4441660     -0.9227600     -0.3711760
  H      0.5428670      0.8544110     -0.4264710
  H     -0.5330650     -0.7960880      1.9293850
  H      2.2079800      1.4549350      3.2721530
  H      1.5388880     -0.0063500      4.0610730
  H      0.1105020      2.4617630      3.8224080
  H     -1.6786150      0.8100990      4.1836310
  H     -0.3297710      2.2213880      1.4982160
  H     -4.1366410      0.3468950      2.8375270
  H     -5.6049340      1.2318230      2.3765550
  H     -6.0479650      0.1661280      4.4696200
  H     -3.7910390      2.2257500      6.7645200
  H     -4.4040930      0.7248720      7.5069410
  H     -6.0988240      2.8885640      7.1686740
  H     -6.7024900      1.2401030      6.8640460
  H     -5.4820850      3.1286100      4.7966680
  H     -7.3780260      2.6732960      3.7079530

37
System: 3a, CBS(T): 0.64
  C     -0.0104820      0.0390720     -0.0682780
  C      0.0085130      0.0799510      1.4468210
  O      1.3801710      0.0821450      1.9007930
  C      1.4430050      0.7374940      3.1923270
  C      0.0946760      1.4122250      3.4428390
  O     -0.6609310      0.6401310      4.3807350
  C     -0.5880700      1.3497890      2.0573500
  O     -1.9987390      1.2410820      2.1867480
  P     -2.8604890      2.6688530      1.9161110
  O     -2.5596540      3.1084160      0.5156890
  O     -2.7324960      3.5411410      3.1180680
  O     -4.3523370      1.9714940      1.9825520
  C     -4.7358910      1.1253770      0.8984630
  C     -5.9303900      0.2861880      1.3182270
  O     -5.5524300     -0.7588980      2.2391350
  C     -6.4980450     -0.8058910      3.3273380
  C     -7.7130710      0.0046320      2.8738940
  C     -7.0402390      1.0781520      2.0298500
  O     -7.9660860      1.7081980      1.1290210
  H      0.5413190      0.8927470     -0.4740270
  H      0.4394010     -0.8861360     -0.4439220
  H     -1.0455410      0.1009120     -0.4185240
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  H     -0.5239140     -0.7868490      1.8677460
  H      2.2700330      1.4558240      3.1506760
  H      1.6417970     -0.0019270      3.9781320
  H      0.1932140      2.4444010      3.8000050
  H     -1.5886510      0.7756140      4.0970030
  H     -0.3247150      2.2232730      1.4485460
  H     -3.9063560      0.4691740      0.6112590
  H     -5.0042430      1.7342890      0.0226900
  H     -6.3579470     -0.1769220      0.4129730
  H     -6.0356260     -0.3630660      4.2205070
  H     -6.7273860     -1.8570000      3.5332970
  H     -8.2914750      0.4117480      3.7080430
  H     -8.3764330     -0.5941270      2.2389970
  H     -6.5728130      1.8312260      2.6734390
  H     -7.5182550      2.4867200      0.7663290

37
System: 9a, CBS(T): 0.56
  C      0.0376820      0.0804890     -0.0829710
  C      0.0698090      0.1000010      1.4314010
  O      1.4471350      0.1197160      1.8684560
  C      1.4845250      0.6403500      3.2201590
  C      0.1427760      1.3243850      3.4935270
  O     -0.6286340      0.5297550      4.3986940
  C     -0.5312850      1.3393740      2.1013960
  O     -1.9410230      1.2336790      2.2160790
  P     -2.8981280      2.6203130      2.1857890
  O     -2.0007860      3.7696710      1.8346380
  O     -3.7973710      2.5489000      3.3685760
  O     -3.8437120      2.2601440      0.8744130
  C     -3.2244600      2.2916260     -0.4065380
  C     -4.0088370      1.4254000     -1.3744260
  O     -3.8675300      0.0219140     -1.0862480
  C     -5.1443350     -0.6314460     -1.2580050
  C     -6.0659430      0.3842880     -1.9402550
  C     -5.5213790      1.6884000     -1.3749720
  O     -5.9120900      2.8263890     -2.1577570
  H     -0.9977890     -0.0003150     -0.4267690
  H      0.5976130     -0.7787790     -0.4674580
  H      0.4810800      0.9968440     -0.4872380
  H     -0.4361920     -0.7910700      1.8347390
  H      2.3329560      1.3311310      3.2735420
  H      1.6330400     -0.1782210      3.9361810
  H      0.2597400      2.3402380      3.8914700
  H     -1.5568240      0.6802970      4.1228550
  H     -0.2640520      2.2549740      1.5628690
  H     -3.1983550      3.3229660     -0.7910980
  H     -2.1889550      1.9401170     -0.3509430
  H     -3.6243930      1.6249890     -2.3904890
  H     -4.9886780     -1.5399120     -1.8504880
  H     -5.5269370     -0.9159190     -0.2686040
  H     -5.9330130      0.3764460     -3.0283570
  H     -7.1225610      0.2200250     -1.7111840
  H     -5.8481550      1.8179510     -0.3366780
  H     -5.6625240      3.6129680     -1.6504070

37
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System: 1g, CBS(T): 0.89

C	0.0544210	0.0459280	-0.0224710
C	0.1040300	0.1230500	1.4878870
O	1.4673400	0.2305830	1.9453890
C	1.4020590	0.6696880	3.3209260
C	0.0947760	1.4661290	3.4922370
O	-0.7334710	0.8607640	4.4849640
C	-0.5651250	1.3582670	2.0930240
O	-1.9741670	1.1880260	2.1756530
P	-2.9317490	2.5155740	1.8296570
O	-4.3410250	2.0551670	1.9441480
O	-2.3688240	3.2430760	0.6461310
O	-2.4726790	3.3548600	3.2015230
C	-2.8074880	4.7338650	3.2680290
C	-2.7699360	5.1856800	4.7185060
O	-3.8350380	4.6136440	5.5011150
C	-3.2905280	4.0793260	6.7256170
C	-1.9182690	4.7321620	6.8995500
C	-1.4680090	4.8115000	5.4483730
O	-0.4065830	5.7619940	5.2569670
H	0.5457650	-0.8612750	-0.3896870
H	0.5438520	0.9201260	-0.4634630
H	-0.9917770	0.0408360	-0.3420380
H	-0.3641370	-0.7719030	1.9309490
H	2.3045720	1.2587130	3.5082490
H	1.3791410	-0.1950900	3.9986710
H	0.2846250	2.5128720	3.7614960
H	-1.6376600	0.9320220	4.1120650
H	-0.3370360	2.2410980	1.4856440
H	-3.8081410	4.9118080	2.8534880
H	-2.0903940	5.3319120	2.6822650
H	-2.8713570	6.2843610	4.7334380
H	-3.1998550	2.9882050	6.6332520
H	-3.9915640	4.3109750	7.5341760
H	-1.2421650	4.1457590	7.5277660
H	-2.0085320	5.7433440	7.3134440
H	-1.1482870	3.8205430	5.1077330
H	-0.0873850	5.6478870	4.3496460

37

System: 7d, CBS(T): -0.17

C	0.1014560	0.0569290	-0.0372330
C	0.1265180	0.1616260	1.4709310
O	1.4708400	0.2911230	1.9777350
C	1.3054160	0.6379240	3.3667440
C	0.0739780	1.5649180	3.4504910
O	-0.8364830	1.1768100	4.4843760
C	-0.5910040	1.3860490	2.0496910
O	-1.9813920	1.1613670	2.1862550
P	-3.1206590	2.1476340	1.3960570
O	-4.2709970	1.2693260	1.0681380
O	-2.3506670	2.9976760	0.4334520
O	-3.5812750	3.0554760	2.7020020
C	-2.6240960	3.9814270	3.2144260
C	-3.2868680	4.8888020	4.2322480
O	-4.2681480	5.7685270	3.6488850
C	-5.4768680	5.7165740	4.4343370

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  C     -5.0869070      5.1011470      5.7798660
  C     -4.0224170      4.1079500      5.3358430
  O     -3.1671350      3.7095600      6.4169470
  H     -0.9406000      0.0288520     -0.3686280
  H      0.6121000     -0.8488010     -0.3809180
  H      0.5795120      0.9312240     -0.4904400
  H     -0.3378160     -0.7360990      1.9151400
  H      2.2394490      1.1002340      3.6965270
  H      1.1056790     -0.2622170      3.9673820
  H      0.3719110      2.6065780      3.6198910
  H     -1.6721620      1.0106980      3.9863460
  H     -0.4239920      2.2601410      1.4129290
  H     -1.8100460      3.4485460      3.7297820
  H     -2.1914360      4.5622010      2.3915210
  H     -2.4990480      5.4990680      4.7044780
  H     -6.2164550      5.0929030      3.9126610
  H     -5.8690940      6.7358080      4.5174470
  H     -5.9296140      4.6315910      6.2952960
  H     -4.6347130      5.8484960      6.4422550
  H     -4.4926750      3.2268770      4.8839930
  H     -2.5699840      3.0239680      6.0751510

37
System: 3d, CBS(T): 1.04
  C      0.0202700      0.0275480     -0.0666990
  C      0.0739960      0.0915470      1.4453820
  O      1.4482190      0.1763820      1.8830030
  C      1.4500160      0.7160150      3.2232960
  C      0.1131910      1.4398570      3.4377770
  O     -0.6819700      0.7486450      4.4109270
  C     -0.5743710      1.3404230      2.0524430
  O     -1.9764630      1.1830390      2.2250850
  P     -2.9826360      2.2135330      1.3171920
  O     -3.3618950      1.5113260      0.0605820
  O     -2.3621380      3.5748460      1.3786150
  O     -4.2776960      2.1184750      2.3293520
  C     -4.1407140      2.6725250      3.6363450
  C     -5.4312520      2.4565950      4.4044710
  O     -6.5403130      3.1866330      3.8417890
  C     -7.6683230      2.2998870      3.7002100
  C     -7.3877900      1.1077230      4.6159620
  C     -5.8782480      0.9843560      4.4617220
  O     -5.2855310      0.2451430      5.5404860
  H      0.5483270      0.8859180     -0.4948530
  H      0.4798750     -0.8931670     -0.4417610
  H     -1.0259770      0.0703630     -0.3874520
  H     -0.4057070     -0.7951670      1.8896340
  H      1.5455850     -0.0916210      3.9617630
  H      2.3160540      1.3821430      3.2981370
  H      0.2469850      2.4823700      3.7510070
  H     -1.5726740      0.7524900      3.9968050
  H     -0.3636110      2.2324170      1.4542650
  H     -3.3239060      2.1788920      4.1863700
  H     -3.8974780      3.7391340      3.5671510
  H     -5.2685330      2.8061390      5.4376450
  H     -8.5704050      2.8579600      3.9718410
  H     -7.7480650      1.9832000      2.6506470
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  H     -7.9268700      0.2032240      4.3203110
  H     -7.6295430      1.3434430      5.6588050
  H     -5.6348840      0.5082160      3.5046390
  H     -4.3646540      0.0691310      5.2970040

37
System: 5d, CBS(T): 0.60
  C      0.0450370      0.0112560     -0.0220610
  C      0.0717360      0.0401870      1.4925580
  O      1.4421360      0.0266800      1.9442260
  C      1.4890830      0.6169260      3.2714000
  C      0.1300220      1.2581720      3.5433660
  O     -0.6339480      0.3928500      4.3931040
  C     -0.5100300      1.2982780      2.1396980
  O     -1.9298390      1.2465430      2.1805150
  P     -2.7272860      2.7307050      2.3150060
  O     -2.0522420      3.5313010      3.3781150
  O     -4.1717310      2.3731390      2.2575050
  O     -2.2458370      3.4308320      0.8840260
  C     -2.7359140      2.8738900     -0.3336330
  C     -3.0094440      3.9812980     -1.3381350
  O     -4.1412780      4.7885720     -0.9713810
  C     -3.8214210      6.1810450     -1.1696700
  C     -2.5483850      6.2146460     -2.0191500
  C     -1.8416170      4.9658120     -1.5132170
  O     -0.8296470      4.5086870     -2.4256740
  H      0.5635390      0.8866940     -0.4291320
  H      0.5316370     -0.8913120     -0.4062500
  H     -0.9940260      0.0218060     -0.3651960
  H     -0.4644920     -0.8315010      1.8984290
  H      2.3041660      1.3492740      3.2710580
  H      1.6965650     -0.1608700      4.0163540
  H      0.1946670      2.2586260      3.9817650
  H     -1.5626350      0.5908040      4.1639930
  H     -0.1715890      2.1941000      1.6020760
  H     -1.9833670      2.1952180     -0.7666090
  H     -3.6517530      2.3032400     -0.1403750
  H     -3.2080450      3.5060910     -2.3151910
  H     -4.6788760      6.6618760     -1.6528620
  H     -3.6586100      6.6502130     -0.1895500
  H     -2.7769740      6.0973030     -3.0848760
  H     -1.9654300      7.1293420     -1.8791050
  H     -1.3984690      5.1555180     -0.5285630
  H     -0.3412980      3.8041690     -1.9747960

37
System: 1e, CBS(T): 1.92
  C     -0.0921400     -0.0704390      0.0820950
  C     -0.0864270     -0.0047960      1.5976760
  O      1.2861540     -0.0502040      2.0633030
  C      1.4275800      0.8167740      3.2166140
  C      0.0438850      1.3509880      3.5615070
  O     -0.5454920      0.4628510      4.5081140
  C     -0.6430050      1.2950500      2.1796390
  O     -2.0617950      1.2589300      2.2035870
  P     -2.8721060      2.7134720      2.2830670
  O     -4.3100790      2.4008610      2.0246400
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  O     -2.0623320      3.7441420      1.5657110
  O     -2.6926790      3.0242130      3.9238920
  C     -3.8624550      2.9582270      4.7306180
  C     -4.1897630      1.5347290      5.1479820
  O     -3.0315240      0.9258690      5.7585370
  C     -3.5172500     -0.2929060      6.3380260
  C     -4.8706540      0.0826740      6.9723390
  C     -5.2548200      1.4000680      6.2451330
  O     -6.5639430      1.3960460      5.6523280
  H     -1.1238610     -0.0075990     -0.2795510
  H      0.3507520     -1.0075240     -0.2731180
  H      0.4761610      0.7681290     -0.3332840
  H     -0.6446220     -0.8484780      2.0281510
  H      2.1202400      1.6283320      2.9555980
  H      1.8400850      0.2387050      4.0508320
  H      0.0712200      2.3750580      3.9526840
  H     -1.4503760      0.7825160      4.7089270
  H     -0.3120190      2.1572560      1.5854540
  H     -3.6526560      3.5590760      5.6266880
  H     -4.7303580      3.3634970      4.2000270
  H     -4.4903900      0.9592190      4.2606450
  H     -3.6450710     -1.0485820      5.5495820
  H     -2.7635430     -0.6401440      7.0474800
  H     -5.6371230     -0.6764590      6.7902690
  H     -4.7801810      0.2353300      8.0523470
  H     -5.1710650      2.2532940      6.9328600
  H     -7.2098760      1.5334720      6.3591240

37
System: 1c, CBS(T): 1.22
  C      0.0121960      0.0408400     -0.0668590
  C      0.0637610      0.0746410      1.4465360
  O      1.4404690      0.1296850      1.8728340
  C      1.4397600      0.5896150      3.2425860
  C      0.1391360      1.3726730      3.4798630
  O     -0.6042780      0.7039230      4.4970740
  C     -0.5597780      1.3142720      2.0890570
  O     -1.9735790      1.1648400      2.1299770
  P     -2.9262900      2.4879200      2.3730140
  O     -4.3372880      2.0171010      2.3403840
  O     -2.4042010      3.6604730      1.5977570
  O     -2.4677380      2.7467230      3.9872890
  C     -2.5609920      4.0817020      4.4557820
  C     -1.8179620      4.2443160      5.7621560
  O     -0.4100670      4.0290740      5.5806540
  C      0.2048300      4.5189010      6.7801530
  C     -0.6193230      5.7539470      7.2124600
  C     -1.8619800      5.6824030      6.3112990
  O     -3.0415930      5.9986990      7.0716020
  H      0.4923830     -0.8619220     -0.4597830
  H     -1.0330750      0.0559320     -0.3905780
  H      0.5192830      0.9190730     -0.4799130
  H     -0.4269010     -0.8151900      1.8723590
  H      2.3435690      1.1918200      3.3752550
  H      1.4645400     -0.2651930      3.9324150
  H      0.3223650      2.4089650      3.7792710
  H     -1.4344080      1.2199590      4.5631830
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  H     -0.3013850      2.2124710      1.5137520
  H     -3.6193390      4.3515950      4.6240350
  H     -2.1491160      4.7616180      3.6985650
  H     -2.2068550      3.5480530      6.5246160
  H      1.2470350      4.7424770      6.5408880
  H      0.1784950      3.7369230      7.5543470
  H     -0.0704460      6.6885700      7.0728610
  H     -0.9328310      5.6916210      8.2586490
  H     -1.7707270      6.3801500      5.4677190
  H     -3.8021440      5.8843700      6.4813290

37
System: 1f, CBS(T): 2.15
  C      0.0149880      0.0148780     -0.0488330
  C      0.0703800      0.0881250      1.4621400
  O      1.4427490      0.1588560      1.9003480
  C      1.3940380      0.5717750      3.2806270
  C      0.1635790      1.4803460      3.4502880
  O     -0.5941670      1.0107610      4.5560040
  C     -0.5654490      1.3366740      2.0752170
  O     -1.9756820      1.1658060      2.1485110
  P     -2.9289770      2.5067400      2.2167420
  O     -4.3427380      2.0538760      2.3412950
  O     -2.4682010      3.5395070      1.2333610
  O     -2.3759340      3.0099790      3.7389980
  C     -2.8325130      4.2924840      4.1408400
  C     -3.2060390      4.2959870      5.6068130
  O     -2.0646130      3.9806600      6.4224150
  C     -2.4535010      4.3227810      7.7605820
  C     -3.3435250      5.5823340      7.6438330
  C     -3.6196000      5.6807200      6.1349860
  O     -4.9950940      6.0248670      5.9008830
  H      0.5205020      0.8813540     -0.4876810
  H      0.4911810     -0.8991040     -0.4198960
  H     -1.0316650      0.0249590     -0.3676420
  H     -0.4148800     -0.7956080      1.9085660
  H      1.2684860     -0.3005420      3.9385140
  H      2.3458120      1.0623640      3.5008830
  H      0.4469190      2.5282110      3.6096850
  H     -1.3804280      1.5958670      4.5861280
  H     -0.3404780      2.2129200      1.4542580
  H     -3.7159410      4.5832000      3.5526880
  H     -2.0437280      5.0374540      3.9603530
  H     -4.0134420      3.5690890      5.7923710
  H     -1.5366480      4.4785330      8.3339760
  H     -3.0134710      3.4872830      8.2078910
  H     -2.8455790      6.4776690      8.0248520
  H     -4.2928800      5.4639060      8.1739030
  H     -2.9694490      6.4378300      5.6731060
  H     -5.1686920      5.9025790      4.9546980

37
System: 5j, CBS(T): 4.75
  C      0.0423400      0.0824760     -0.0860140
  C      0.0671090      0.1049050      1.4294680
  O      1.4459620      0.1221090      1.8617370
  C      1.5181960      0.7413770      3.1694820
```

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  C      0.1708850      1.4077870      3.4459860
  O     -0.5685670      0.6334810      4.3967490
  C     -0.5415310      1.3539890      2.0749020
  O     -1.9471590      1.2279400      2.2659990
  P     -2.9099510      2.5578180      1.8577350
  O     -2.1134350      3.8004170      2.0701930
  O     -4.2349240      2.2359000      2.4644640
  O     -2.9935750      2.3547090      0.2108720
  C     -3.7067150      1.2103750     -0.2518590
  C     -5.0237180      1.5891900     -0.8992120
  O     -4.8118670      2.4397380     -2.0417450
  C     -6.0732890      2.4710850     -2.7157820
  C     -6.6232370      1.0309480     -2.6382460
  C     -5.7829300      0.3953760     -1.5008450
  O     -6.5511990     -0.2625070     -0.4806590
  H     -0.9931110      0.0767340     -0.4368320
  H      0.5505610     -0.8081880     -0.4709230
  H      0.5382180      0.9729940     -0.4845590
  H     -0.4415720     -0.7816180      1.8395920
  H      2.3454690      1.4597500      3.1405060
  H      1.7216320     -0.0188180      3.9342460
  H      0.2727570      2.4403230      3.8009710
  H     -1.4967540      0.7219710      4.0913250
  H     -0.3133010      2.2530630      1.4937280
  H     -3.9201960      0.5162470      0.5687150
  H     -3.0789230      0.7078030     -1.0027090
  H     -5.6593840      2.0973100     -0.1583170
  H     -6.7510820      3.1744570     -2.2066570
  H     -5.8931560      2.8274980     -3.7331460
  H     -7.6833570      1.0060630     -2.3691950
  H     -6.4909520      0.4953420     -3.5834820
  H     -5.0518950     -0.3118700     -1.9167410
  H     -6.7649080     -1.1519600     -0.7939780

37
System: 1b, CBS(T): -0.89
  C      0.0332810      0.1112010     -0.1006660
  C      0.0704960      0.0594500      1.4144150
  O      1.4459240      0.0572150      1.8606820
  C      1.5249130      0.7313790      3.1426220
  C      0.1207170      1.1951960      3.4938510
  O     -0.5384760      0.1708210      4.2627220
  C     -0.5549470      1.2739030      2.1105610
  O     -1.9696730      1.1253110      2.2271760
  P     -2.9015550      2.5245520      2.0856340
  O     -4.3062730      2.0261150      2.1402310
  O     -2.3064260      3.3836140      1.0198360
  O     -2.5531690      3.3192420      3.5001050
  C     -2.8373320      2.7195700      4.7585970
  C     -2.3375370      3.6575020      5.8511610
  O     -0.9089910      3.8494300      5.7603130
  C     -0.6144560      5.2288100      5.4864720
  C     -1.9238510      5.8491470      4.9965560
  C     -2.9726530      5.0476530      5.7722690
  O     -3.1423470      5.5297410      7.1305400
  H      0.5125890     -0.7721790     -0.5361670
  H     -1.0084740      0.1508910     -0.4342210
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  H      0.5474590      1.0074750     -0.4616480
  H     -0.4358220     -0.8463000      1.7800190
  H      2.2163560      1.5783870      3.0405770
  H      1.9099390      0.0362760      3.8973630
  H      0.0998510      2.1441640      4.0405690
  H     -1.4443940      0.1485450      3.8918060
  H     -0.3166900      2.2065770      1.5884000
  H     -2.3233010      1.7570070      4.8564140
  H     -3.9180210      2.5534740      4.8731770
  H     -2.5605760      3.2112310      6.8292470
  H      0.1804180      5.2588430      4.7347170
  H     -0.2588660      5.7128180      6.4085790
  H     -2.0585590      5.6575520      3.9296530
  H     -1.9898520      6.9257540      5.1928010
  H     -3.9415040      5.0175960      5.2625870
  H     -3.4306230      6.4525180      7.0692670

37
System: 1[, CBS(T): -3.30
  C      0.0151670      0.0351630     -0.0653240
  C      0.0683960      0.0609830      1.4488410
  O      1.4450850      0.0934050      1.8856310
  C      1.5071630      0.7509130      3.1760560
  C      0.1216180      1.3182440      3.4730860
  O     -0.5901970      0.4318070      4.3493800
  C     -0.5546300      1.3050580      2.0885010
  O     -1.9688100      1.1654570      2.2063110
  P     -2.9008410      2.5297840      1.8730140
  O     -4.3084600      2.0422960      1.9857510
  O     -2.3083090      3.2430350      0.7046220
  O     -2.5578910      3.4857150      3.1850900
  C     -2.9399150      3.0050480      4.4782990
  C     -3.5279140      4.1552750      5.2835910
  O     -2.5239560      5.1648740      5.5446270
  C     -2.9380290      6.4168330      4.9736050
  C     -3.9774340      6.0627270      3.9106590
  C     -4.6707990      4.8477240      4.5347950
  O     -5.6627580      5.2430040      5.5216520
  H      0.4851710     -0.8718170     -0.4603060
  H     -1.0302100      0.0645660     -0.3874930
  H      0.5279250      0.9099670     -0.4770580
  H     -0.4317200     -0.8266530      1.8662460
  H      2.2685310      1.5375850      3.1098310
  H      1.7960830      0.0282290      3.9487590
  H      0.1634910      2.3238610      3.9094150
  H     -1.5044550      0.4426840      3.9974620
  H     -0.3136020      2.2042680      1.5115510
  H     -2.0591250      2.6052900      4.9950040
  H     -3.6975920      2.2168390      4.3778300
  H     -3.8946210      3.7745300      6.2462230
  H     -2.0474900      6.9048170      4.5654370
  H     -3.3715400      7.0543330      5.7597460
  H     -3.4889820      5.7518450      2.9845540
  H     -4.6790500      6.8787800      3.7047410
  H     -5.1159960      4.1820720      3.7885940
  H     -6.3957730      5.6461060      5.0338790
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37
System: 3b, CBS(T): -0.71
  C      0.0015970      0.0480940     -0.0779690
  C      0.0190180      0.0949990      1.4363880
  O      1.3866260      0.1027570      1.8986100
  C      1.4179050      0.7012060      3.2171350
  C      0.0914270      1.4376700      3.4314540
  O     -0.7077870      0.7304890      4.3832490
  C     -0.5804170      1.3677790      2.0390970
  O     -1.9913810      1.2633240      2.1676510
  P     -2.8904490      2.5955320      1.6424950
  O     -2.4849110      2.8593450      0.2242790
  O     -2.9141760      3.6275710      2.7167930
  O     -4.3474910      1.8301970      1.6882890
  C     -4.5827700      0.7678870      0.7634860
  C     -5.9652370      0.1847110      1.0250820
  O     -5.9901380     -0.5407620      2.2762770
  C     -6.8684320      0.1103360      3.2091840
  C     -7.1376820      1.5030750      2.6351760
  C     -7.0582860      1.2499380      1.1276550
  O     -8.2843230      0.6610270      0.6184430
  H      0.5766940      0.8859020     -0.4841490
  H      0.4268580     -0.8900500     -0.4503420
  H     -1.0302800      0.1427280     -0.4293630
  H     -0.5159570     -0.7694230      1.8608980
  H      2.2854400      1.3695890      3.2437250
  H      1.5317800     -0.0764340      3.9835020
  H      0.2334320      2.4744380      3.7612390
  H     -1.6222770      0.8563480      4.0525580
  H     -0.3130640      2.2358920      1.4261670
  H     -3.8287170     -0.0176610      0.8942470
  H     -4.5221390      1.1476090     -0.2657610
  H     -6.2106920     -0.5211960      0.2210660
  H     -6.3656240      0.1391170      4.1808040
  H     -7.7960250     -0.4746860      3.2989150
  H     -6.3431590      2.1963730      2.9178870
  H     -8.1102760      1.9097770      2.9367150
  H     -6.8041160      2.1493640      0.5573700
  H     -8.9986010      1.2856990      0.8129750

37
System: 1z, CBS(T): -0.43
  C      0.0206150      0.0409510     -0.0743800
  C      0.0603400      0.0769790      1.4400870
  O      1.4346820      0.1269950      1.8831870
  C      1.4794300      0.7762600      3.1782810
  C      0.0883260      1.3346720      3.4617310
  O     -0.6236310      0.4403120      4.3274740
  C     -0.5779240      1.3178360      2.0698920
  O     -1.9881170      1.1579290      2.1735060
  P     -2.9374240      2.5354370      2.1894000
  O     -4.3402850      2.0937570      1.9535310
  O     -2.2386570      3.5999600      1.4008060
  O     -2.7379300      2.8741890      3.8189240
  C     -3.6827200      3.8009420      4.3532900
  C     -3.7248050      3.7223000      5.8736310
  O     -4.3020340      2.4712420      6.3098340
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  C     -3.3547930      1.7379930      7.1010280
  C     -1.9894980      2.3558790      6.7962100
  C     -2.3514240      3.8179160      6.5437490
  O     -2.5341370      4.5420790      7.7918700
  H     -1.0226190      0.0431160     -0.4055200
  H      0.5126540     -0.8581380     -0.4602480
  H      0.5204270      0.9229000     -0.4875970
  H     -0.4320180     -0.8136490      1.8590330
  H      2.2387720      1.5658080      3.1248670
  H      1.7628200      0.0497130      3.9497030
  H      0.1122400      2.3412760      3.8969490
  H     -1.5489040      0.4982300      4.0079160
  H     -0.3468150      2.2273800      1.5054380
  H     -4.6791270      3.5751050      3.9548760
  H     -3.4085820      4.8273470      4.0613730
  H     -4.3608820      4.5402530      6.2387270
  H     -3.6134720      1.8373880      8.1665470
  H     -3.4220780      0.6845160      6.8124680
  H     -1.2744660      2.2425720      7.6201120
  H     -1.5601260      1.9170590      5.8937590
  H     -1.6246590      4.3388100      5.9110730
  H     -1.7097210      4.4505830      8.2922560

37
System: 5z, CBS(T): -0.90
  C      0.1772400      0.0020910     -0.0937380
  C      0.1918210      0.0267250      1.4176610
  O      1.5247470     -0.0043820      1.9718710
  C      1.3251880      0.2815070      3.3761500
  C      0.3090630      1.4338450      3.4236810
  O     -0.5299430      1.3702790      4.5562820
  C     -0.4421280      1.2537580      2.0692970
  O     -1.8505850      1.0847940      2.1485870
  P     -2.7686360      2.4518470      2.1831350
  O     -2.2936000      3.2355760      3.3850310
  O     -4.1921880      2.0875490      1.9494880
  O     -2.1528610      3.1902320      0.8213990
  C     -2.9227470      4.2651200      0.2765220
  C     -1.9898010      5.2898240     -0.3601890
  O     -1.1976580      6.0091710      0.5944660
  C     -0.0090580      5.2374100      0.8530240
  C      0.2539310      4.4078160     -0.4248450
  C     -0.9772250      4.6569930     -1.3191420
  O     -0.7100070      5.6220210     -2.3669670
  H     -0.8611760      0.0857890     -0.4275550
  H      0.6032360     -0.9287750     -0.4824680
  H      0.7440740      0.8455820     -0.5041870
  H     -0.3584790     -0.8545230      1.7929400
  H      2.3041420      0.5179520      3.7985070
  H      0.8994180     -0.5950850      3.8882550
  H      0.8395250      2.3974940      3.3969350
  H     -1.2579580      2.0203950      4.3588000
  H     -0.2286840      2.1275180      1.4444880
  H     -3.5079230      4.7558250      1.0626580
  H     -3.6187800      3.8745480     -0.4804710
  H     -2.5972890      6.0348320     -0.8866260
  H      0.7884330      5.9543840      1.0720710
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  H     -0.1718680      4.5891560      1.7201500
  H      1.1648550      4.7297060     -0.9423690
  H      0.3444340      3.3460240     -0.1897230
  H     -1.3593460      3.7297880     -1.7613260
  H      0.0720780      5.3110060     -2.8456710

37
System: 7p, CBS(T): -0.41
  C      0.0196370      0.0326210     -0.0636930
  C      0.0679880      0.0805840      1.4496350
  O      1.4413790      0.1547310      1.8909880
  C      1.4570650      0.7360840      3.2164310
  C      0.0925830      1.3898670      3.4566640
  O     -0.6740430      0.6153910      4.3900540
  C     -0.5801060      1.3241310      2.0666990
  O     -1.9848640      1.1676130      2.2078840
  P     -2.9994440      2.3106030      1.4595760
  O     -3.6958340      1.6328730      0.3327750
  O     -2.2064540      3.5768000      1.3491630
  O     -4.1031680      2.4285970      2.6765590
  C     -3.6964540      3.0255950      3.9080240
  C     -4.6603840      2.5909710      5.0042660
  O     -5.9867880      3.1141000      4.7656030
  C     -6.9120450      2.0332100      4.5609020
  C     -6.0584870      0.7992930      4.2640740
  C     -4.8043160      1.0703730      5.0994790
  O     -5.0016910      0.7406390      6.4980960
  H     -1.0258830      0.0537030     -0.3877210
  H      0.4963090     -0.8758030     -0.4472090
  H      0.5313120      0.9049120     -0.4831120
  H     -0.4144100     -0.8110900      1.8802780
  H      2.2818920      1.4569240      3.2419340
  H      1.6297400     -0.0429010      3.9704270
  H      0.1818870      2.4211260      3.8207080
  H     -1.5704330      0.6129780      3.9910440
  H     -0.3584660      2.2251920      1.4868710
  H     -3.7024560      4.1174970      3.8107570
  H     -2.6806730      2.7082630      4.1806790
  H     -4.3049860      2.9850910      5.9653800
  H     -7.5703250      2.3093790      3.7314250
  H     -7.5146930      1.8947550      5.4713140
  H     -5.7779800      0.7709870      3.2090770
  H     -6.5492600     -0.1396470      4.5447260
  H     -3.9195920      0.5549730      4.7117660
  H     -5.1313850     -0.2179200      6.5470680

37
System: 1t, CBS(T): 2.45
  C     -0.0081450      0.0295790     -0.0818400
  C      0.0574580      0.0676460      1.4310890
  O      1.4399660      0.1174030      1.8410920
  C      1.4647960      0.5984840      3.2040070
  C      0.1707420      1.3880310      3.4518690
  O     -0.5611350      0.7344870      4.4869980
  C     -0.5505990      1.3140090      2.0737350
  O     -1.9656380      1.1744250      2.1536250
  P     -2.8785570      2.5322900      2.3575570
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  O     -4.3099960      2.1178970      2.3487950
  O     -2.3309600      3.6684280      1.5491980
  O     -2.3924400      2.7862270      3.9603980
  C     -2.9636790      3.9212740      4.5858480
  C     -2.1900160      4.2541160      5.8563050
  O     -0.8048040      4.5489730      5.5474430
  C     -0.5003680      5.8984760      5.9156260
  C     -1.8488860      6.6146690      5.9748420
  C     -2.7554140      5.5082850      6.5275350
  O     -2.6017900      5.3588400      7.9581810
  H      0.4984490      0.9048170     -0.5015450
  H      0.4652770     -0.8761690     -0.4761780
  H     -1.0560830      0.0476520     -0.3969440
  H     -0.4322720     -0.8188160      1.8649370
  H      1.5000640     -0.2457660      3.9060830
  H      2.3722460      1.2001920      3.3108860
  H      0.3580420      2.4303260      3.7319570
  H     -1.4000880      1.2384420      4.5412920
  H     -0.3038410      2.2060170      1.4846230
  H     -4.0143550      3.7195300      4.8469470
  H     -2.9308190      4.7749050      3.8928970
  H     -2.2087880      3.4052870      6.5487470
  H     -0.0030610      5.9184680      6.8975140
  H      0.1791530      6.3060930      5.1611200
  H     -1.8456110      7.5096180      6.6070850
  H     -2.1817690      6.8934660      4.9695670
  H     -3.8136820      5.6577440      6.2803630
  H     -2.8894700      6.1882800      8.3679380

37
System: 5q, CBS(T): 3.19
  C      0.0515310      0.0505570     -0.0429510
  C      0.0752040      0.0744890      1.4725120
  O      1.4473850      0.0761650      1.9216720
  C      1.5040830      0.7037550      3.2307770
  C      0.1323040      1.3079970      3.5155630
  O     -0.6030370      0.4273080      4.3761840
  C     -0.5260040      1.3235770      2.1209920
  O     -1.9440810      1.2299070      2.1989460
  P     -2.7789670      2.7008700      2.2592630
  O     -2.0374850      3.6305740      3.1584860
  O     -4.2079590      2.2908730      2.3895410
  O     -2.4898270      3.2437320      0.7140340
  C     -3.0214320      2.4426330     -0.3362100
  C     -4.0979980      3.1902100     -1.1182230
  O     -3.5439850      4.4106420     -1.6874150
  C     -3.6844500      4.3850220     -3.1093780
  C     -3.7628670      2.9037710     -3.4740300
  C     -4.5958700      2.3603740     -2.3066220
  O     -6.0019470      2.6410880     -2.4935250
  H     -0.9865820      0.0363960     -0.3887350
  H      0.5613370     -0.8393160     -0.4272780
  H      0.5452240      0.9409030     -0.4464510
  H     -0.4475910     -0.8062060      1.8765180
  H      2.2929290      1.4640150      3.1937580
  H      1.7552510     -0.0468370      3.9898980
  H      0.1757610      2.3125770      3.9476670
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  H     -1.5351510      0.5651290      4.1146440
  H     -0.2270700      2.2254700      1.5725160
  H     -2.1949640      2.1818140     -1.0136720
  H     -3.4635480      1.5230940      0.0668570
  H     -4.9223080      3.4555330     -0.4504830
  H     -4.6045720      4.9076710     -3.4145820
  H     -2.8210440      4.9018520     -3.5401270
  H     -4.2279060      2.7090730     -4.4468450
  H     -2.7652360      2.4504460     -3.4612790
  H     -4.4508870      1.2860810     -2.1367510
  H     -6.3044200      2.1154770     -3.2490840

37
System: 1o, CBS(T): 0.11
  C      0.0243640      0.0505380     -0.0613660
  C      0.0652480      0.0705780      1.4535410
  O      1.4419240      0.1224230      1.8947720
  C      1.5028240      0.8175640      3.1637660
  C      0.1031100      1.3382430      3.4714190
  O     -0.5712330      0.4306580      4.3544860
  C     -0.5841690      1.3024490      2.0922240
  O     -1.9920140      1.1282230      2.2175790
  P     -2.9563580      2.4961810      1.9583730
  O     -4.3474910      1.9632770      2.0047040
  O     -2.3466340      3.3009880      0.8605810
  O     -2.6454760      3.3547520      3.3492340
  C     -3.0309470      2.7725880      4.5970350
  C     -3.7132430      3.8506250      5.4371500
  O     -4.1653240      3.2454230      6.6823760
  C     -3.4703930      3.8437080      7.7869520
  C     -2.2135420      4.4696510      7.1842160
  C     -2.7442280      4.9622720      5.8311840
  O     -3.4959270      6.1909910      5.9811670
  H     -1.0187780      0.0562380     -0.3924630
  H      0.5186170     -0.8434310     -0.4563320
  H      0.5207360      0.9386550     -0.4646030
  H     -0.4196460     -0.8278270      1.8645820
  H      2.2299030      1.6335990      3.0631530
  H      1.8366100      0.1278980      3.9484440
  H      0.1154400      2.3463670      3.9055260
  H     -1.4864590      0.4032450      4.0045770
  H     -0.3703930      2.2069040      1.5122240
  H     -3.7359430      1.9498500      4.4365430
  H     -2.1443630      2.3910490      5.1208280
  H     -4.5755270      4.2559600      4.9013300
  H     -3.2638090      3.0569530      8.5195730
  H     -4.1038380      4.6133010      8.2526790
  H     -1.4407500      3.7092890      7.0261090
  H     -1.7944440      5.2801930      7.7888170
  H     -1.9704400      5.0852390      5.0674070
  H     -2.8555600      6.9113190      6.0697730

37
System: 7r, CBS(T): 0.77
  C      0.0126920      0.0216710     -0.0655270
  C      0.0790360      0.0768370      1.4471880
  O      1.4605350      0.1622600      1.8591030
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  C      1.5047030      0.7642020      3.1737390
  C      0.1379450      1.4007430      3.4423830
  O     -0.5921530      0.6241930      4.4003460
  C     -0.5701370      1.3191050      2.0694400
  O     -1.9684580      1.1302030      2.2443510
  P     -3.0646550      2.2588550      1.6235310
  O     -4.1832220      1.4910330      1.0191460
  O     -2.2503020      3.3106210      0.9293910
  O     -3.6627180      2.8956060      3.0323400
  C     -2.7637940      3.5844400      3.8967880
  C     -3.5761170      4.1054940      5.0799770
  O     -2.6724820      4.7883680      5.9919310
  C     -3.0442670      6.1738030      6.0812430
  C     -3.8592510      6.4577630      4.8206560
  C     -4.6173200      5.1344870      4.6464220
  O     -5.7436820      5.0534230      5.5545560
  H      0.4913870      0.9069570     -0.4956170
  H      0.5116040     -0.8745360     -0.4494510
  H     -1.0358190      0.0064240     -0.3790720
  H     -0.3891950     -0.8163160      1.8892600
  H      2.3180640      1.4987050      3.1652660
  H      1.7108670      0.0005580      3.9347610
  H      0.2305550      2.4343880      3.8004540
  H     -1.5006170      0.5953370      4.0301110
  H     -0.3902510      2.2135630      1.4657240
  H     -2.2794080      4.4133540      3.3630380
  H     -1.9845840      2.9131750      4.2754690
  H     -4.0576230      3.2777950      5.6092140
  H     -3.6515530      6.3375830      6.9837960
  H     -2.1242300      6.7621070      6.1563050
  H     -4.5335850      7.3139140      4.9197070
  H     -3.2007950      6.6216140      3.9608850
  H     -4.9425050      4.9403990      3.6210310
  H     -6.4743830      5.5405390      5.1482670

37
System: 2a, CBS(T): -0.98
  C     -0.0220910      0.0424910     -0.0302620
  C      0.0082150     -0.0017130      1.4905090
  O      1.4125070     -0.0064600      1.9043370
  C      1.5891090      0.9764920      2.9271040
  C      0.5654300      2.0716010      2.6060920
  O      0.2641500      2.9132930      3.7095660
  C     -0.6480200      1.2217660      2.1495900
  O     -1.3242090      0.8729660      3.3688260
  P     -2.9910910      0.6917800      3.2409520
  O     -3.4302740      0.2406120      4.5949220
  O     -3.2774600      0.0131700      1.9428230
  O     -3.4738820      2.2643810      3.0230780
  C     -3.4036950      3.1472320      4.1390190
  C     -4.1778750      4.4120810      3.8182540
  O     -3.5633310      5.1809530      2.7633660
  C     -4.5776700      5.6037840      1.8288810
  C     -5.9231400      5.3863330      2.5241440
  C     -5.6176060      4.1443530      3.3496320
  O     -6.5489400      3.9694100      4.4277190
  H      0.5784000     -0.7739280     -0.4442660
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  H     -1.0548170     -0.0596890     -0.3784060
  H      0.3873650      0.9905400     -0.3970210
  H     -0.4773550     -0.9075370      1.8651170
  H      2.6286690      1.3158690      2.8894900
  H      1.3745760      0.5635760      3.9248090
  H      0.9230840      2.7070560      1.7894730
  H     -0.4276100      2.4051550      4.1838180
  H     -1.3271320      1.7501610      1.4773720
  H     -2.3594190      3.4074610      4.3575270
  H     -3.8324630      2.6650040      5.0289430
  H     -4.2168800      5.0288130      4.7318140
  H     -4.4995220      4.9932580      0.9181220
  H     -4.3855070      6.6506250      1.5692920
  H     -6.7493440      5.2463940      1.8212430
  H     -6.1633860      6.2192510      3.1951290
  H     -5.6135310      3.2543820      2.7100050
  H     -6.3966070      3.0824530      4.7877520

37
System: 4a, CBS(T): 1.06
  C      0.0208000      0.0268050     -0.0426490
  C      0.0205040     -0.0061600      1.4783330
  O      1.4143070      0.0254990      1.9320720
  C      1.5440810      1.0317790      2.9441720
  C      0.5066370      2.0969280      2.5671810
  O      0.1569870      2.9863780      3.6143100
  C     -0.6712190      1.2022550      2.1253900
  O     -1.3354470      0.8397260      3.3413200
  P     -3.0005110      0.6111250      3.1860130
  O     -3.1862580     -0.4414800      2.1329930
  O     -3.6838580      1.9339640      3.1734470
  O     -3.2256190     -0.0363570      4.6842090
  C     -2.5588170     -1.2607860      4.9869960
  C     -2.6968390     -1.5471340      6.4705410
  O     -1.9436580     -0.6201610      7.2780220
  C     -2.7587040     -0.1782340      8.3832660
  C     -3.9364890     -1.1516730      8.4647200
  C     -4.1417860     -1.4702790      6.9904190
  O     -4.8882980     -2.6822100      6.7982790
  H      0.4058730      0.9843770     -0.4111170
  H      0.6557810     -0.7729850     -0.4372840
  H     -0.9998480     -0.1141960     -0.4124930
  H     -0.4550590     -0.9201860      1.8453960
  H      1.3115570      0.6330660      3.9428560
  H      2.5772430      1.3912340      2.9249790
  H      0.8713570      2.6940690      1.7236650
  H     -0.5974210      2.5393060      4.0532990
  H     -1.3656680      1.7072890      1.4473440
  H     -1.4990190     -1.1932530      4.7155790
  H     -3.0035770     -2.0884070      4.4132610
  H     -2.3175700     -2.5670420      6.6537090
  H     -3.1032950      0.8461360      8.1843350
  H     -2.1351870     -0.1724950      9.2837730
  H     -4.8194650     -0.7150300      8.9398450
  H     -3.6597190     -2.0673380      9.0001870
  H     -4.6472620     -0.6365670      6.4898370
  H     -5.1085560     -2.7294690      5.8560500
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37
System: 0a, CBS(T): 0.52
  C      0.0227790      0.0400180     -0.0715400
  C      0.0471130      0.0104040      1.4511310
  O      1.4479020      0.0668650      1.8754440
  C      1.5950910      1.1247970      2.8392700
  C      0.5235260      2.1531070      2.4512660
  O      0.2194650      3.1153080      3.4430290
  C     -0.6453900      1.2065900      2.1092410
  O     -1.2119960      0.8164320      3.3603910
  P     -2.7447680      1.3503280      3.7582440
  O     -3.4886800      1.6314080      2.4872420
  O     -2.5721840      2.3230370      4.8789710
  O     -3.3149040     -0.0479030      4.4245100
  C     -3.6615600     -1.1015240      3.5297260
  C     -3.6326050     -2.4253730      4.2731090
  O     -2.2882610     -2.8435580      4.5800680
  C     -2.2316380     -3.3096260      5.9442510
  C     -3.6812500     -3.5269760      6.3830710
  C     -4.3776520     -2.4103330      5.6179190
  O     -5.7914860     -2.6365640      5.4971950
  H      0.3850990      1.0040170     -0.4437390
  H      0.6673440     -0.7484240     -0.4733610
  H     -0.9975600     -0.1159540     -0.4397140
  H     -0.3912620     -0.9177880      1.8354710
  H      1.4051880      0.7641040      3.8596680
  H      2.6200680      1.4988620      2.7619510
  H      0.8463420      2.6972490      1.5545970
  H     -0.5119390      2.7599340      3.9969100
  H     -1.4199950      1.6566210      1.4817580
  H     -2.9628100     -1.1388210      2.6853100
  H     -4.6686400     -0.9343310      3.1196260
  H     -4.1023410     -3.1862480      3.6260640
  H     -1.6280170     -4.2232710      5.9660510
  H     -1.7395960     -2.5449080      6.5610580
  H     -4.0599350     -4.4964220      6.0387920
  H     -3.8152190     -3.4570100      7.4662450
  H     -4.1940460     -1.4463450      6.1053270
  H     -6.1790180     -1.8145970      5.1621570

37
System: #a, CBS(T): 0.05
  C      0.0447530      0.1256740     -0.1085390
  C      0.0835020      0.0423900      1.4133770
  O      1.4791070      0.1022500      1.8342530
  C      1.6157120      1.1489530      2.8103300
  C      0.5202810      2.1583290      2.4510600
  O      0.2935990      3.1559790      3.4187360
  C     -0.6507850      1.1892130      2.1198940
  O     -1.1884820      0.6719220      3.3390810
  P     -2.2911330      1.6007290      4.1714460
  O     -3.0918320      2.3869710      3.1804430
  O     -1.5706370      2.2118650      5.3367080
  O     -3.2166840      0.3730440      4.7638330
  C     -4.0345360     -0.3386960      3.8366880
  C     -4.2294340     -1.7684440      4.3173180
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  O     -3.0647010     -2.5799790      4.0556420
  C     -2.7497140     -3.3616570      5.2261680
  C     -3.9915390     -3.3122210      6.1172150
  C     -4.4910220     -1.9037630      5.8266610
  O     -5.8718210     -1.7365690      6.1903390
  H     -0.9736110     -0.0465750     -0.4758280
  H      0.7063570     -0.6313560     -0.5420670
  H      0.3785270      1.1106260     -0.4517030
  H     -0.3379200     -0.9091250      1.7588220
  H      2.6281090      1.5536900      2.7245100
  H      1.4504880      0.7681420      3.8277130
  H      0.8085810      2.6794360      1.5277980
  H     -0.2538660      2.8018700      4.1700730
  H     -1.4437500      1.6543510      1.5273030
  H     -5.0138360      0.1552790      3.7543950
  H     -3.5777610     -0.3453420      2.8411180
  H     -5.0872810     -2.1978690      3.7727270
  H     -1.8803990     -2.9158560      5.7291870
  H     -2.4876540     -4.3732580      4.8981680
  H     -3.7673310     -3.4794060      7.1745250
  H     -4.7434510     -4.0408580      5.7924310
  H     -3.8746400     -1.1670040      6.3523690
  H     -6.0531720     -0.7854860      6.1684250

37
System: 4g, CBS(T): 3.62
  C      0.0150080      0.0195400     -0.0441750
  C      0.0177820     -0.0083410      1.4773960
  O      1.4145400      0.0198500      1.9248100
  C      1.5650870      1.0558640      2.9035290
  C      0.5244420      2.1132250      2.5136240
  O      0.1945890      3.0356530      3.5391550
  C     -0.6611320      1.2084610      2.1198270
  O     -1.2865880      0.8591300      3.3611010
  P     -2.9520010      0.6978680      3.2673730
  O     -3.2843180     -0.2501180      2.1545340
  O     -3.5698200      2.0548350      3.3823850
  O     -3.0444820     -0.0827860      4.7255710
  C     -4.1601710     -0.9400500      4.9268590
  C     -3.8961350     -1.8351230      6.1243730
  O     -2.8862000     -2.8266270      5.8521830
  C     -1.9848590     -2.9133150      6.9755760
  C     -2.6636780     -2.1750500      8.1316020
  C     -3.4051980     -1.0839690      7.3723650
  O     -4.4634370     -0.5051000      8.1518740
  H      0.4057480      0.9732120     -0.4165460
  H      0.6447230     -0.7855430     -0.4362070
  H     -1.0065700     -0.1163590     -0.4137740
  H     -0.4578190     -0.9182800      1.8535870
  H      2.5988260      1.4113790      2.8552990
  H      1.3483930      0.6871510      3.9169970
  H      0.8756480      2.6834520      1.6460130
  H     -0.5651540      2.6152540      3.9940140
  H     -1.3755820      1.6972760      1.4509700
  H     -4.3390500     -1.5408260      4.0270780
  H     -5.0697680     -0.3497750      5.1320100
  H     -4.8409050     -2.3468440      6.3766700
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  H     -1.0327780     -2.4366460      6.7036570
  H     -1.8012240     -3.9729520      7.1844640
  H     -3.3879830     -2.8183750      8.6447960
  H     -1.9526170     -1.7851320      8.8653720
  H     -2.7066150     -0.3026390      7.0525780
  H     -4.7627610      0.2834780      7.6752500

37
System: 6g, CBS(T): -0.13
  C      0.0306920      0.0332460     -0.0536160
  C      0.0283150      0.0092600      1.4674420
  O      1.4259960      0.0354210      1.9141410
  C      1.5576980      1.0249440      2.9398940
  C      0.5292830      2.1026430      2.5743580
  O      0.1814950      2.9747850      3.6385810
  C     -0.6545020      1.2291570      2.1066450
  O     -1.3483610      0.8796750      3.3157850
  P     -2.9841700      0.5893650      3.2082600
  O     -3.5771150      1.4273090      2.1164000
  O     -3.4937040      0.5443050      4.6082470
  O     -2.8337790     -0.9701440      2.6277250
  C     -3.9309130     -1.4819700      1.8851440
  C     -3.7105390     -2.9667720      1.6651640
  O     -2.5212630     -3.2383090      0.8951160
  C     -1.7621920     -4.2785680      1.5466760
  C     -2.7185930     -4.9521400      2.5323440
  C     -3.5556900     -3.7592820      2.9743220
  O     -4.8066550     -4.1554700      3.5561390
  H     -0.9873080     -0.1093420     -0.4301390
  H      0.6628600     -0.7720320     -0.4408290
  H      0.4179810      0.9877830     -0.4271320
  H     -0.4471620     -0.9018600      1.8406520
  H      1.3168320      0.6137350      3.9318700
  H      2.5934750      1.3774460      2.9312650
  H      0.9028110      2.7154720      1.7466700
  H     -0.5558450      2.5077650      4.0849650
  H     -1.3484990      1.7378380      1.4324640
  H     -4.8796630     -1.3543060      2.4323840
  H     -4.0260650     -0.9473900      0.9318620
  H     -4.5833240     -3.3661910      1.1217240
  H     -0.9083080     -3.8249980      2.0695660
  H     -1.3834880     -4.9547280      0.7730200
  H     -3.3614770     -5.6815790      2.0258340
  H     -2.2014500     -5.4472300      3.3590400
  H     -2.9923400     -3.1447650      3.6861900
  H     -5.1585090     -3.3795700      4.0173280

37
System: 8d, CBS(T): 1.69
  C     -0.0104910      0.0127640     -0.0364510
  C      0.0231960     -0.0190500      1.4855000
  O      1.4306410     -0.0011480      1.8920310
  C      1.6286010      1.0529920      2.8376720
  C      0.5689050      2.1077190      2.4973010
  O      0.2712940      2.9843700      3.5807320
  C     -0.6385470      1.2082350      2.1289990
  O     -1.2373140      0.9128410      3.3920490
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  P     -2.8517120      0.3886140      3.4261080
  O     -2.9153920     -0.8244740      4.2806750
  O     -3.3419800      0.4904900      2.0133020
  O     -3.4876200      1.6192760      4.3319140
  C     -3.4105570      2.9385560      3.7958660
  C     -4.1308890      3.8990620      4.7242170
  O     -5.5526300      3.6577360      4.7768690
  C     -5.9670010      3.5741030      6.1545220
  C     -4.8680880      4.2602560      6.9669910
  C     -3.6357590      3.8364200      6.1809180
  O     -2.5108680      4.6905600      6.4418970
  H     -1.0406370     -0.1051710     -0.3881630
  H      0.6018430     -0.7979470     -0.4434880
  H      0.3858240      0.9634420     -0.4105370
  H     -0.4416340     -0.9301950      1.8739920
  H      2.6583030      1.4085270      2.7320420
  H      1.4659770      0.7022130      3.8679190
  H      0.8813080      2.7214610      1.6470480
  H     -0.3679660      2.4439830      4.0957990
  H     -1.3717510      1.6721030      1.4657610
  H     -3.8584040      2.9615000      2.7944950
  H     -2.3628180      3.2657290      3.7032440
  H     -3.9647460      4.9213810      4.3462810
  H     -6.0680920      2.5169650      6.4386220
  H     -6.9443040      4.0601460      6.2405750
  H     -4.8437380      3.9405230      8.0126590
  H     -4.9695040      5.3510210      6.9279460
  H     -3.3782710      2.7970970      6.4171710
  H     -1.7515910      4.3255840      5.9627380

37
System: 4d, CBS(T): 1.63
  C     -0.0078810     -0.0231770     -0.0307140
  C      0.0142100     -0.0107480      1.4921500
  O      1.4165840      0.0276960      1.9180210
  C      1.5978210      1.1235130      2.8234420
  C      0.5393110      2.1518870      2.4103160
  O      0.2407110      3.1231670      3.4040080
  C     -0.6566430      1.2216260      2.1123620
  O     -1.2227660      0.9132660      3.3876330
  P     -2.9201740      0.8909870      3.4688100
  O     -3.4056350     -0.3807570      2.8651990
  O     -3.3854810      2.2569540      3.0663130
  O     -2.9587670      0.7297090      5.1061000
  C     -2.7643420      1.9140380      5.8777270
  C     -2.3912130      1.5137700      7.2931710
  O     -3.3968380      0.7123920      7.9432040
  C     -2.7889160     -0.5106810      8.4049770
  C     -1.2975050     -0.2059460      8.5464500
  C     -1.0817510      0.6984690      7.3396610
  O      0.0935360      1.5127550      7.4676500
  H     -1.0314610     -0.1720770     -0.3908690
  H      0.6203240     -0.8360370     -0.4084620
  H      0.3744070      0.9214810     -0.4329060
  H     -0.4514470     -0.9126600      1.9001250
  H      1.4200150      0.8158910      3.8649330
  H      2.6279770      1.4766760      2.7174200
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  H      0.8561730      2.6775580      1.5019720
  H     -0.5658430      2.7665230      3.8304550
  H     -1.4075600      1.6824340      1.4632330
  H     -3.6744610      2.5238280      5.8587650
  H     -1.9487420      2.5306330      5.4706850
  H     -2.2465080      2.4336660      7.8818220
  H     -2.9618550     -1.3052120      7.6652330
  H     -3.2745680     -0.7864930      9.3462930
  H     -1.0953320      0.3549200      9.4663790
  H     -0.6712080     -1.1024790      8.5287260
  H     -1.0152350      0.0946860      6.4272690
  H      0.3173490      1.8352720      6.5814560

37
System: 6d, CBS(T): 1.99
  C      0.0361470      0.0167600     -0.0381390
  C      0.0333120      0.0015350      1.4853140
  O      1.4223160      0.0324470      1.9322300
  C      1.5660450      1.0742370      2.9093620
  C      0.5163750      2.1231290      2.5230360
  O      0.1897050      3.0293620      3.5605600
  C     -0.6689770      1.2129610      2.1166140
  O     -1.3141600      0.8613060      3.3456340
  P     -2.9907920      1.0570990      3.4490240
  O     -3.4339960      2.0289950      2.4081180
  O     -3.2484800      1.1497450      4.9143030
  O     -3.4585020     -0.4355120      2.8867580
  C     -3.0013700     -1.5786900      3.6019330
  C     -3.8719290     -2.7736750      3.2581010
  O     -5.2144300     -2.6446450      3.7611990
  C     -6.1485020     -3.0462330      2.7380120
  C     -5.3325340     -3.7845620      1.6739550
  C     -4.0192930     -3.0194410      1.7473600
  O     -2.9298800     -3.7577720      1.1716310
  H     -0.9807880     -0.1232550     -0.4214300
  H      0.6742840     -0.7848600     -0.4238530
  H      0.4203740      0.9717550     -0.4113460
  H     -0.4281910     -0.9190120      1.8639840
  H      2.5974610      1.4345510      2.8578730
  H      1.3540790      0.7034350      3.9226280
  H      0.8634540      2.7093030      1.6647030
  H     -0.5198520      2.5744910      4.0606670
  H     -1.3900530      1.6996840      1.4548840
  H     -3.0290400     -1.3810270      4.6805760
  H     -1.9598340     -1.8151380      3.3273420
  H     -3.4060140     -3.6680620      3.7072820
  H     -6.9182840     -3.6697040      3.2056480
  H     -6.6256200     -2.1485890      2.3205440
  H     -5.1614600     -4.8296290      1.9572410
  H     -5.7965080     -3.7558350      0.6839720
  H     -4.1186420     -2.0489840      1.2468140
  H     -2.1673630     -3.1608140      1.1423650

37
System: 2h, CBS(T): 3.10
  C     -0.0414490      0.0744540     -0.0522030
  C      0.0049460     -0.0123110      1.4671080
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  O      1.4161460     -0.0395010      1.8610320
  C      1.6421650      0.9693210      2.8467090
  C      0.6016310      2.0583420      2.5618660
  O      0.3410200      2.8913580      3.6883180
  C     -0.6284990      1.2010330      2.1620240
  O     -1.2398530      0.8520310      3.4125310
  P     -2.9196330      0.6336760      3.3512920
  O     -3.2807620      0.2091720      4.7340510
  O     -3.2351090     -0.0830300      2.0821910
  O     -3.4148320      2.2020470      3.1095640
  C     -3.1382170      3.1293500      4.1458250
  C     -3.5811620      4.5241510      3.7491220
  O     -5.0000570      4.5600230      3.4708830
  C     -5.5954250      5.7136500      4.0935340
  C     -4.4437420      6.5792790      4.6062720
  C     -3.3813040      5.5269310      4.8967000
  O     -2.0747480      6.1184150      4.9380120
  H     -1.0772240     -0.0155800     -0.3949410
  H      0.3677820      1.0305950     -0.3977940
  H      0.5526770     -0.7320640     -0.4934610
  H     -0.4824000     -0.9232260      1.8245600
  H      2.6776230      1.3102290      2.7487500
  H      1.4813980      0.5796410      3.8637100
  H      0.9199730      2.7039000      1.7378780
  H     -0.2868050      2.3371950      4.2024720
  H     -1.3425760      1.7245540      1.5220410
  H     -3.6541290      2.8209200      5.0654770
  H     -2.0583980      3.1699390      4.3558080
  H     -3.0316490      4.8621620      2.8581160
  H     -6.2193680      6.2259000      3.3519810
  H     -6.2430310      5.3773720      4.9165290
  H     -4.0668290      7.2466430      3.8241340
  H     -4.7122100      7.1773530      5.4817350
  H     -3.5925000      5.0249170      5.8536230
  H     -1.4225670      5.4035010      4.8631660

37
System: 4n, CBS(T): 6.51
  C     -0.0747880     -0.0400920     -0.0717100
  C      0.0066540     -0.0315770      1.4459480
  O      1.4261460      0.0584530      1.8422460
  C      1.5642370      1.1029050      2.8344670
  C      0.4995550      2.1213630      2.4168310
  O      0.1545980      3.1240570      3.3572620
  C     -0.6505930      1.1656820      2.1265730
  O     -1.2541390      0.7461060      3.3535490
  P     -2.8058310      1.2959290      3.5858810
  O     -3.8133740      0.3420100      3.0529820
  O     -2.7347910      2.7589070      3.1839040
  O     -2.8252490      1.2019010      5.2271580
  C     -2.0962160      2.1787620      5.9674030
  C     -1.4599990      1.5467900      7.1917250
  O     -0.3046680      0.7424360      6.8742160
  C      0.7744830      1.0643260      7.7685170
  C      0.1511870      1.8428710      8.9287170
  C     -0.9611080      2.5941860      8.1931320
  O     -2.0544980      3.0664040      8.9937470
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  H     -1.1085140     -0.2174300     -0.3880310
  H      0.5588660     -0.8343370     -0.4802400
  H      0.2611590      0.9165530     -0.4858650
  H     -0.4099330     -0.9523600      1.8664310
  H      1.3499390      0.7289590      3.8446190
  H      2.5939440      1.4664400      2.7737440
  H      0.8226110      2.5845290      1.4694210
  H     -0.8401240      3.1506720      3.3658210
  H     -1.4045180      1.6357780      1.4860280
  H     -1.3126430      2.6340800      5.3537430
  H     -2.7872380      2.9631480      6.3054780
  H     -2.2060020      0.9091470      7.6901770
  H      1.5184140      1.6751080      7.2344850
  H      1.2528880      0.1290580      8.0787340
  H      0.8650530      2.5005370      9.4358810
  H     -0.2995160      1.1677990      9.6641780
  H     -0.5285360      3.4388460      7.6353450
  H     -1.7957610      3.9154100      9.3773430

37
System: 0i, CBS(T): 6.10
  C      0.0348730      0.0103030     -0.0382280
  C      0.0261330     -0.0144230      1.4837000
  O      1.4242640      0.0128860      1.9298930
  C      1.5803440      1.0620640      2.8926960
  C      0.5396510      2.1171310      2.4984360
  O      0.2069560      3.0344480      3.5318460
  C     -0.6492430      1.2150350      2.1079450
  O     -1.2836020      0.9230320      3.3565750
  P     -2.8431590      0.3132900      3.3292360
  O     -3.3563000      0.4384560      1.9322280
  O     -3.4904810      0.8567250      4.5624550
  O     -2.5818730     -1.3142260      3.5541970
  C     -2.3611200     -1.8258370      4.8625880
  C     -0.9458630     -2.3412690      5.0852700
  O      0.0258480     -1.2849800      5.0043820
  C      1.0111890     -1.4200940      6.0427310
  C      0.7387890     -2.7603680      6.7285060
  C     -0.7649200     -2.9283660      6.4904820
  O     -1.2331870     -4.2883480      6.5183100
  H      0.4322390      0.9628300     -0.4066090
  H      0.6655500     -0.7970380     -0.4245390
  H     -0.9842880     -0.1190880     -0.4173610
  H     -0.4445770     -0.9247080      1.8654460
  H      1.3622890      0.7047650      3.9078790
  H      2.6148190      1.4157930      2.8337870
  H      0.8876410      2.6959410      1.6356310
  H     -0.5118840      2.5706090      4.0133010
  H     -1.3690750      1.6778160      1.4288370
  H     -3.0418920     -2.6763380      5.0107730
  H     -2.5970760     -1.0487090      5.6014430
  H     -0.7068630     -3.1142640      4.3379970
  H      2.0075310     -1.3665940      5.5889510
  H      0.9030360     -0.5773190      6.7402370
  H      1.2612230     -3.5798100      6.2237000
  H      1.0170960     -2.7622630      7.7876830
  H     -1.3400880     -2.3244090      7.2074240
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  H     -1.3299230     -4.5490320      7.4447580

37
System: 6n, CBS(T): 3.52
  C      0.0152180      0.0249890     -0.0583370
  C      0.0219010     -0.0045180      1.4640560
  O      1.4229620      0.0195290      1.9122340
  C      1.5977250      1.1023450      2.8331110
  C      0.5324040      2.1377700      2.4485020
  O      0.2179890      3.0648800      3.4772830
  C     -0.6542180      1.2157190      2.0989960
  O     -1.2533270      0.9179180      3.3671070
  P     -2.8728460      0.4516310      3.3984730
  O     -3.5542150      1.0088630      2.1946190
  O     -3.2811770      0.6483660      4.8204340
  O     -2.6863780     -1.1750260      3.1048310
  C     -1.9796270     -1.9002870      4.1047550
  C     -1.6473420     -3.2897950      3.5943920
  O     -0.8439050     -3.2505750      2.3902560
  C      0.3412150     -4.0472160      2.5647480
  C      0.0308660     -5.0010990      3.7166740
  C     -0.8191070     -4.0913440      4.6079510
  O     -1.6906170     -4.7477370      5.5415890
  H     -1.0076250     -0.1062170     -0.4267190
  H      0.6376150     -0.7854120     -0.4511600
  H      0.4081640      0.9761050     -0.4355750
  H     -0.4397050     -0.9244150      1.8284070
  H      2.6254860      1.4659910      2.7322740
  H      1.4246080      0.7782200      3.8705610
  H      0.8525100      2.7076610      1.5693890
  H     -0.4849550      2.6041680      3.9842120
  H     -1.4048450      1.6696990      1.4467010
  H     -1.0455250     -1.3759070      4.3563970
  H     -2.5824870     -1.9857560      5.0188930
  H     -2.5749250     -3.8334020      3.3673720
  H      0.5465430     -4.5542390      1.6166580
  H      1.1935050     -3.3928400      2.8018490
  H     -0.5797790     -5.8452000      3.3785710
  H      0.9282660     -5.3830690      4.2145270
  H     -0.1635070     -3.3966270      5.1537920
  H     -1.1818170     -4.9345610      6.3421780

37
System: 6j, CBS(T): 1.76
  C      0.0378010      0.0115910     -0.0340170
  C      0.0314430      0.0061880      1.4874050
  O      1.4211370      0.0403750      1.9394420
  C      1.5262560      1.0078650      2.9919980
  C      0.5075860      2.0902460      2.6172640
  O      0.1497570      2.9556160      3.6793930
  C     -0.6712760      1.2223920      2.1141120
  O     -1.4136510      0.8472390      3.2843280
  P     -3.0859860      1.0437150      3.2054670
  O     -3.3875340      2.3651240      2.5879720
  O     -3.5678170      0.5537950      4.5326450
  O     -3.4444900     -0.0869550      2.0330290
  C     -3.3322820     -1.4477280      2.4383560
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  C     -4.6357520     -2.1943700      2.2576510
  O     -4.9780410     -2.3276400      0.8662630
  C     -6.0249990     -3.3075100      0.8376170
  C     -5.6659570     -4.3543740      1.9178960
  C     -4.5628290     -3.6556620      2.7313150
  O     -4.7808870     -3.8245880      4.1411380
  H     -0.9806270     -0.1246440     -0.4126920
  H      0.6694640     -0.7981260     -0.4134930
  H      0.4300120      0.9614440     -0.4126970
  H     -0.4333770     -0.9084240      1.8720070
  H      2.5620950      1.3579220      3.0166860
  H      1.2591760      0.5744440      3.9673830
  H      0.9014110      2.7044360      1.7991250
  H     -0.6361350      2.5298070      4.0793440
  H     -1.3256660      1.7547340      1.4192650
  H     -3.0452190     -1.5012740      3.4975500
  H     -2.5589320     -1.9391780      1.8296070
  H     -5.4420600     -1.6701740      2.7950510
  H     -6.9887480     -2.8261860      1.0656910
  H     -6.0647280     -3.7113100     -0.1771440
  H     -6.5122570     -4.5763310      2.5738850
  H     -5.3136560     -5.2916490      1.4792090
  H     -3.5756020     -4.0624980      2.4661720
  H     -4.3033650     -3.1133730      4.5977150

37
System: 2[, CBS(T): -2.27
  C     -0.0117940      0.0301540     -0.0281000
  C      0.0118130     -0.0037060      1.4932310
  O      1.4144560     -0.0017020      1.9142590
  C      1.5906600      1.0047170      2.9146480
  C      0.5610630      2.0881000      2.5734310
  O      0.2580760      2.9546120      3.6576000
  C     -0.6485000      1.2220120      2.1421380
  O     -1.3078880      0.8817280      3.3726750
  P     -2.9779250      0.7081150      3.2686910
  O     -3.3988440      0.3034130      4.6424100
  O     -3.2921880     -0.0104790      1.9982440
  O     -3.4483550      2.2744750      2.9955450
  C     -3.2844460      3.2343050      4.0409820
  C     -4.3692320      4.2966730      3.9130590
  O     -4.2137540      5.0522800      2.6890560
  C     -5.3277990      4.8074600      1.8136770
  C     -6.0453800      3.5755880      2.3700340
  C     -5.7753520      3.6961020      3.8720960
  O     -6.6724500      4.6518450      4.4994090
  H      0.3949660      0.9772590     -0.4001430
  H      0.5945310     -0.7863840     -0.4331510
  H     -1.0420110     -0.0797340     -0.3815350
  H     -0.4723120     -0.9084770      1.8719540
  H      1.3816400      0.6126950      3.9217410
  H      2.6285000      1.3478430      2.8654240
  H      0.9126280      2.7066510      1.7413950
  H     -0.4221150      2.4510420      4.1529930
  H     -1.3403160      1.7345890      1.4701390
  H     -2.3014150      3.7137710      3.9500090
  H     -3.3657070      2.7384280      5.0175850
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```
  H     -4.2873840      4.9957950      4.7552890
  H     -4.9343620      4.6517610      0.8040010
  H     -5.9847050      5.6902460      1.8131070
  H     -7.1177740      3.5673140      2.1427560
  H     -5.5823130      2.6589120      1.9999570
  H     -5.8180230      2.7339280      4.3924700
  H     -7.5691500      4.2983910      4.4041980

37
System: 4b, CBS(T): -0.17
  C      0.0161010      0.0104200     -0.0446160
  C      0.0185120     -0.0054880      1.4765520
  O      1.4100320      0.0346760      1.9309680
  C      1.5269310      1.0385300      2.9514440
  C      0.4962440      2.1029040      2.5539900
  O      0.1453750      3.0200340      3.5748840
  C     -0.6770700      1.2037470      2.1173670
  O     -1.3490040      0.8264150      3.3225310
  P     -3.0264430      0.9617260      3.3091490
  O     -3.5133850      0.2919430      2.0598950
  O     -3.3943640      2.3469900      3.7226100
  O     -3.2898920      0.0030550      4.6216450
  C     -2.9638150     -1.3840850      4.5276260
  C     -3.1034280     -2.0126560      5.9077530
  O     -2.0158190     -1.6005290      6.7689820
  C     -2.5267750     -0.8663000      7.8923860
  C     -3.9420400     -0.4399130      7.5009610
  C     -4.3955810     -1.6077370      6.6217420
  O     -4.8279520     -2.7461460      7.4136240
  H     -1.0057490     -0.1246060     -0.4139090
  H      0.6452700     -0.7972460     -0.4326620
  H      0.4068740      0.9618600     -0.4218210
  H     -0.4482050     -0.9209460      1.8555870
  H      1.2773050      0.6357450      3.9436160
  H      2.5612350      1.3942160      2.9464420
  H      0.8726920      2.6763470      1.6979710
  H     -0.6608310      2.6436440      3.9858520
  H     -1.3715820      1.6939010      1.4297730
  H     -3.6410200     -1.8802340      3.8185060
  H     -1.9325680     -1.5075110      4.1762130
  H     -3.0634350     -3.1053480      5.8089120
  H     -1.8563870     -0.0201430      8.0709090
  H     -2.5342740     -1.5161810      8.7809130
  H     -4.6009270     -0.2889180      8.3641130
  H     -3.9158520      0.4660970      6.8917670
  H     -5.1778390     -1.3230280      5.9109950
  H     -5.5747340     -2.4466030      7.9529510

37
System: 0b, CBS(T): 0.88
  C      0.0269910      0.0212500     -0.0508530
  C      0.0282100     -0.0019870      1.4717660
  O      1.4273690      0.0281840      1.9064120
  C      1.5836650      1.0683840      2.8809500
  C      0.5403940      2.1245330      2.4955660
  O      0.2187160      3.0439100      3.5250750
  C     -0.6515150      1.2205390      2.1060720
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  O     -1.2843430      0.8968990      3.3459140
  P     -2.9592370      0.9267870      3.4870900
  O     -3.5178930      1.3574160      2.1638210
  O     -3.2409990      1.5542600      4.8067660
  O     -3.2611560     -0.6896630      3.6880910
  C     -3.3854190     -1.5121390      2.5329040
  C     -3.2835740     -2.9714580      2.9608040
  O     -1.9944440     -3.2684500      3.5285900
  C     -2.1262440     -3.5735590      4.9275750
  C     -3.5543230     -3.1824140      5.3207560
  C     -4.3261700     -3.3591160      4.0100140
  O     -4.7039620     -4.7383130      3.7654480
  H      0.4158310      0.9761450     -0.4201520
  H      0.6592040     -0.7829020     -0.4403140
  H     -0.9914200     -0.1119310     -0.4326670
  H     -0.4261500     -0.9204980      1.8577080
  H      2.6176650      1.4215560      2.8246490
  H      1.3729870      0.7018070      3.8962620
  H      0.8873270      2.7000730      1.6300230
  H     -0.4939840      2.5966850      4.0296890
  H     -1.3800560      1.6939880      1.4429460
  H     -2.5906070     -1.2934140      1.8098710
  H     -4.3485200     -1.3345750      2.0344870
  H     -3.4144230     -3.6035190      2.0718500
  H     -1.3680010     -3.0021770      5.4716770
  H     -1.9446760     -4.6486050      5.0738660
  H     -3.5944380     -2.1292120      5.6066390
  H     -3.9590940     -3.8009160      6.1306800
  H     -5.2114830     -2.7160880      3.9555730
  H     -5.2273320     -5.0276450      4.5274920

37
System: 4p, CBS(T): 1.00
  C     -0.0414650     -0.0265900     -0.0451640
  C      0.0146960     -0.0278980      1.4773820
  O      1.4279830     -0.0156280      1.8663620
  C      1.6540210      1.0782560      2.7611110
  C      0.5915380      2.1202990      2.3940020
  O      0.3391950      3.0751360      3.4156520
  C     -0.6277430      1.2129850      2.1152200
  O     -1.1788970      0.9162770      3.4036280
  P     -2.8608210      0.6605780      3.4734420
  O     -3.0970870     -0.8024790      3.6099920
  O     -3.4679420      1.5353980      2.4189770
  O     -3.1041340      1.3109440      4.9662670
  C     -3.0107520      2.7259450      5.1250020
  C     -2.5773240      3.0375670      6.5532080
  O     -3.5566610      2.5734220      7.5068430
  C     -3.0116560      1.4983950      8.2934440
  C     -1.7140640      1.0726330      7.6017890
  C     -1.2542970      2.3739530      6.9386750
  O     -0.5866520      3.2548180      7.8770190
  H     -1.0747400     -0.1545170     -0.3853750
  H      0.5659300     -0.8451360     -0.4441100
  H      0.3463020      0.9162570     -0.4464470
  H     -0.4511790     -0.9279820      1.8901950
  H      2.6827370      1.4227960      2.6163660
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  H      1.5135780      0.7730350      3.8091440
  H      0.8824040      2.6664240      1.4905170
  H     -0.3377970      2.6243610      3.9622820
  H     -1.3974610      1.6741540      1.4907670
  H     -2.2941750      3.1619550      4.4161110
  H     -3.9898960      3.1794620      4.9291140
  H     -2.4868440      4.1260810      6.6640380
  H     -3.7549820      0.6958130      8.3294220
  H     -2.8243510      1.8655930      9.3132090
  H     -1.9169830      0.3333800      6.8244740
  H     -0.9673250      0.6798700      8.3010330
  H     -0.6139510      2.1957190      6.0685470
  H      0.2373480      2.8174580      8.1371710

37
System: 6p, CBS(T): -1.04
  C      0.0357860      0.0324390     -0.0516750
  C      0.0335700      0.0071200      1.4703420
  O      1.4251850      0.0347150      1.9194600
  C      1.5618140      1.0484750      2.9248890
  C      0.5177390      2.1102220      2.5562020
  O      0.1695140      2.9857580      3.6155970
  C     -0.6625410      1.2169590      2.1122270
  O     -1.3291840      0.8632250      3.3289800
  P     -3.0038710      0.6605680      3.2890700
  O     -3.5377490      1.3496960      2.0776700
  O     -3.4387730      0.8748850      4.6984800
  O     -3.0625460     -0.9592390      2.9318920
  C     -2.6105450     -1.8803070      3.9225270
  C     -2.9159700     -3.2982910      3.4530440
  O     -4.3336950     -3.5267600      3.3291040
  C     -4.6963060     -3.6698200      1.9450350
  C     -3.4572530     -3.2856030      1.1291220
  C     -2.3109460     -3.6208570      2.0862260
  O     -1.9812690     -5.0332670      2.0762210
  H      0.4272950      0.9864420     -0.4206250
  H      0.6665310     -0.7725560     -0.4427930
  H     -0.9837040     -0.0980690     -0.4302630
  H     -0.4347100     -0.9108160      1.8419270
  H      2.5945550      1.4078240      2.8933290
  H      1.3395910      0.6525160      3.9267610
  H      0.8763440      2.7200620      1.7195390
  H     -0.5584490      2.5124760      4.0728540
  H     -1.3741010      1.7070220      1.4430290
  H     -3.1176040     -1.6775530      4.8726080
  H     -1.5248380     -1.7784950      4.0768840
  H     -2.5272450     -4.0029700      4.1998600
  H     -4.9925630     -4.7136960      1.7652260
  H     -5.5492110     -3.0133450      1.7459340
  H     -3.4481370     -2.2111220      0.9351390
  H     -3.3828500     -3.8337940      0.1825420
  H     -1.4101260     -3.0281950      1.8912070
  H     -1.7353690     -5.2603180      1.1672270

37
System: 4s, CBS(T): 5.56
  C      0.0055480      0.0174100     -0.0475240
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  C      0.0113740     -0.0114790      1.4751380
  O      1.4054240      0.0090810      1.9225190
  C      1.5721400      1.0760210      2.8702750
  C      0.5307280      2.1242150      2.4578070
  O      0.2250390      3.0912860      3.4466720
  C     -0.6613750      1.2066880      2.1191500
  O     -1.2444620      0.8682070      3.3820750
  P     -2.9292560      0.9104410      3.4283700
  O     -3.4182380     -0.0163330      2.3530270
  O     -3.3519330      2.3329000      3.5663930
  O     -3.1030330      0.2015190      4.9076370
  C     -3.0422670     -1.2190480      4.9804690
  C     -1.6181340     -1.7733360      5.0623880
  O     -0.9478360     -1.2440130      6.2421960
  C     -0.5754260     -2.3184930      7.1071890
  C     -1.5294010     -3.4602860      6.7589590
  C     -1.6342350     -3.2943870      5.2375230
  O     -0.4641700     -3.8325820      4.5804730
  H     -1.0160730     -0.1140940     -0.4196280
  H      0.6331820     -0.7888480     -0.4406350
  H      0.3984640      0.9703620     -0.4187770
  H     -0.4630470     -0.9249800      1.8464140
  H      1.3659000      0.7367660      3.8951080
  H      2.6065910      1.4247580      2.7967720
  H      0.8714000      2.6558640      1.5611850
  H     -0.5341590      2.7106940      3.9354160
  H     -1.4005370      1.6764480      1.4641520
  H     -3.5335060     -1.6491000      4.0971180
  H     -3.5932060     -1.5017650      5.8871880
  H     -1.0437740     -1.4814660      4.1812900
  H     -0.6671370     -1.9654250      8.1394000
  H      0.4680400     -2.6165790      6.9210390
  H     -2.5102190     -3.2995360      7.2208470
  H     -1.1607090     -4.4509160      7.0478590
  H     -2.5415170     -3.7422840      4.8129890
  H     -0.4718980     -4.7923400      4.7127670

37
System: 2o, CBS(T): -0.66
  C     -0.0217950      0.0616000     -0.0286230
  C      0.0090550     -0.0009060      1.4920210
  O      1.4148270     -0.0026270      1.9052570
  C      1.6034540      1.0069000      2.9001050
  C      0.5620700      2.0841940      2.5771050
  O      0.2700020      2.9462880      3.6692980
  C     -0.6495500      1.2112690      2.1666730
  O     -1.2832480      0.8531640      3.4031030
  P     -2.9708000      0.7468040      3.3298460
  O     -3.3876990      0.4237610      4.7236130
  O     -3.3155590     -0.0126480      2.0924220
  O     -3.3474460      2.3277310      2.9811090
  C     -3.2072820      3.2960130      4.0218780
  C     -3.9523930      4.5532890      3.5830810
  O     -3.8817130      5.5292330      4.6591220
  C     -3.1472950      6.6815160      4.2136190
  C     -2.3295320      6.2048270      3.0143580
  C     -3.2946660      5.2033290      2.3678970
```

O	-4.3239430	5.8715800	1.5980910
H	0.3789630	1.0175370	-0.3847380
H	0.5869310	-0.7437750	-0.4518720
H	-1.0526210	-0.0467700	-0.3809790
H	-0.4699560	-0.9136420	1.8571870
H	2.6384670	1.3557060	2.8322040
H	1.4144490	0.6155770	3.9113160
H	0.8963700	2.7081390	1.7417700
H	-0.3812780	2.4214320	4.1835030
H	-1.3577570	1.7221910	1.5104580
H	-3.6253050	2.9122470	4.9577230
H	-2.1489370	3.5416300	4.1831580
H	-5.0020290	4.3250610	3.3756670
H	-2.5373030	7.0338660	5.0514450
H	-3.8489510	7.4762020	3.9190620
H	-1.4237750	5.6822370	3.3400850
H	-2.0466740	7.0119330	2.3309130
H	-2.7971320	4.4479310	1.7528690
H	-3.9150960	6.1736200	0.7743090

Cartesian coordinates (xyz format) of the conformations optimized in COSMO solvent with respective relative CBS(T)/COSMO energies (kcal.mol^{-1}).

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37
System: 1a, CBS(T): 0.00
  C      0.0123320      0.0576650     -0.0571130
  C      0.0345650      0.0351770      1.4581100
  O      1.4026040      0.0518040      1.9316500
  C      1.4645850      0.7695410      3.2012130
  C      0.0442810      1.1929000      3.5329030
  O     -0.5877050      0.1473660      4.2999160
  C     -0.5901760      1.2565370      2.1365360
  O     -2.0231570      1.1410050      2.1842380
  P     -2.9289010      2.5218210      2.0971050
  O     -4.3431800      2.0251710      2.0000760
  O     -2.3425680      3.4524330      1.0759950
  O     -2.6749120      3.2514890      3.5310400
  C     -3.1256630      2.6335220      4.7532620
  C     -2.6320480      3.4459760      5.9328500
  O     -1.1956590      3.3932980      6.0367110
  C     -0.6833190      4.7238220      6.3395730
  C     -1.8927750      5.5460840      6.7754820
  C     -2.9904890      4.9339920      5.9017840
  O     -4.3385280      5.0966000      6.3634540
  H     -1.0256410      0.0566200     -0.4054180
  H      0.5118200     -0.8251670     -0.4670340
  H      0.5098690      0.9563500     -0.4359000
  H     -0.4698960     -0.8673490      1.8323470
  H      2.1215730      1.6360890      3.0730080
  H      1.8760450      0.1085900      3.9697010
  H     -0.0114040      2.1391250      4.0794340
  H     -1.5190090      0.1277690      4.0132310
  H     -0.3085880      2.1795170      1.6206040
  H     -2.7419000      1.6111540      4.8225370
  H     -4.2205200      2.6002870      4.7689490
  H     -3.0782470      3.0013880      6.8367790
  H     -0.2216950      5.1331360      5.4324660
  H      0.0802640      4.6213480      7.1144130
  H     -1.7563800      6.6172780      6.6084030
  H     -2.1271490      5.3720520      7.8310290
  H     -2.9067990      5.3094820      4.8756580
  H     -4.6209260      5.9978770      6.1448860

37
System: 1m, CBS(T): 0.23
  C     -0.0010190      0.0301350     -0.0460160
  C      0.0362340      0.0557290      1.4687990
  O      1.4121980      0.1150050      1.9109330
  C      1.4839720      0.8248080      3.1820690
  C      0.0831160      1.3347960      3.4908090
  O     -0.5758140      0.4179050      4.3844260
  C     -0.5997630      1.2896310      2.1138740
  O     -2.0223600      1.1217000      2.2396080
  P     -3.0044760      2.4291560      1.9785960
  O     -4.3922490      1.8697600      2.0936600
  O     -2.5436920      3.1746210      0.7607940
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  O     -2.6626280      3.4093980      3.2354170
  C     -3.0444610      3.0173680      4.5734060
  C     -3.6060070      4.2144790      5.3159430
  O     -2.6119300      5.2521220      5.4598160
  C     -3.1791740      6.5242200      5.0329990
  C     -4.6902580      6.3340870      5.0884580
  C     -4.8169810      4.8736060      4.6461080
  O     -6.0069500      4.1906270      5.0672710
  H      0.5101570     -0.8563490     -0.4327710
  H     -1.0414360      0.0017750     -0.3859880
  H      0.4780760      0.9254070     -0.4546540
  H     -0.4467860     -0.8415100      1.8828160
  H      2.1999320      1.6439430      3.0663590
  H      1.8318020      0.1432430      3.9647690
  H      0.0926770      2.3397690      3.9260380
  H     -1.5155830      0.4245240      4.1210890
  H     -0.3781900      2.1902730      1.5340880
  H     -2.1585460      2.6345330      5.0898620
  H     -3.8097950      2.2349810      4.5329660
  H     -3.9049570      3.8685630      6.3172230
  H     -2.8379720      6.7398900      4.0124460
  H     -2.8038420      7.2964420      5.7081260
  H     -5.2287150      7.0277550      4.4380930
  H     -5.0604800      6.4383700      6.1139060
  H     -4.7193280      4.7983630      3.5578090
  H     -6.6989980      4.3679740      4.4126710

37
System: 1L, CBS(T): 1.80
  C     -0.0042720      0.0220460     -0.0398530
  C      0.0349290      0.0497350      1.4750950
  O      1.4149060      0.0936320      1.9116120
  C      1.5076090      0.8359270      3.1616120
  C      0.1137010      1.3495690      3.4875560
  O     -0.5215310      0.4434260      4.4092910
  C     -0.5934250      1.2873530      2.1252360
  O     -2.0094260      1.1192530      2.3029260
  P     -3.0829130      2.0697270      1.4916770
  O     -4.3208630      1.2207460      1.3873050
  O     -2.4405530      2.6773960      0.2802920
  O     -3.3544740      3.3120900      2.5119410
  C     -3.8207500      3.0644120      3.8553770
  C     -3.0937530      3.9622160      4.8387230
  O     -1.6749910      3.7559120      4.8236460
  C     -1.0012650      5.0470030      4.8855810
  C     -2.0680900      6.0558250      5.3052810
  C     -3.3068480      5.4637360      4.6282160
  O     -4.5794260      5.8336160      5.1738180
  H     -1.0440340      0.0010400     -0.3806100
  H      0.5044360     -0.8671590     -0.4242920
  H      0.4774730      0.9153480     -0.4495110
  H     -0.4534510     -0.8433590      1.8916700
  H      2.2160320      1.6565500      3.0120230
  H      1.8768260      0.1755520      3.9528750
  H      0.1160170      2.3584060      3.9061790
  H     -1.4785610      0.5483690      4.2571260
  H     -0.3913690      2.1852210      1.5352510
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  H     -3.6598340      2.0140590      4.1177820
  H     -4.8939600      3.2773120      3.9104080
  H     -3.4893710      3.7087220      5.8372020
  H     -0.5969350      5.2753270      3.8915650
  H     -0.1757890      4.9607250      5.5962040
  H     -1.8386630      7.0722230      4.9763350
  H     -2.2082250      6.0503720      6.3914650
  H     -3.2892220      5.6917270      3.5551990
  H     -4.7902460      6.7261020      4.8593740

37
System: &a, CBS(T): -0.72
  C     -0.0240310     -0.0440000      0.0625890
  C     -0.0422200      0.0082680      1.5776960
  O      1.3250400      0.0364070      2.0610630
  C      1.4127640      0.8721780      3.2506610
  C      0.0073460      1.3720650      3.5629970
  O     -0.5868140      0.4960510      4.5320060
  C     -0.6615670      1.2714930      2.1716250
  O     -2.0878570      1.1513340      2.1948810
  P     -2.9911720      2.4830670      2.5334520
  O     -4.2962390      2.2901050      1.8137460
  O     -2.1801220      3.7357080      2.3780160
  O     -3.2092840      2.2785530      4.1413390
  C     -3.9574090      1.1254950      4.5819400
  C     -4.0643730      1.1834270      6.0876900
  O     -2.7442250      0.9903170      6.6528660
  C     -2.5628860      1.8961560      7.7852510
  C     -3.9469170      2.4650330      8.0860030
  C     -4.5665110      2.4967150      6.6855490
  O     -5.9988240      2.5198270      6.6221230
  H      0.4873670     -0.9447210     -0.2898630
  H     -1.0506180     -0.0616450     -0.3183040
  H      0.4866490      0.8365120     -0.3406720
  H     -0.5587450     -0.8690200      1.9933640
  H      2.0960860      1.6996060      3.0340780
  H      1.8090860      0.2791410      4.0799290
  H      0.0080800      2.4000790      3.9358600
  H     -1.3547640      0.9415210      4.9368370
  H     -0.3743960      2.1498470      1.5837350
  H     -3.4410040      0.2102410      4.2715730
  H     -4.9567980      1.1399750      4.1344950
  H     -4.7251080      0.3666000      6.4152640
  H     -1.8569320      2.6797450      7.4872430
  H     -2.1356270      1.3218270      8.6105810
  H     -3.9015800      3.4492560      8.5583020
  H     -4.5222000      1.7853520      8.7232660
  H     -4.1594590      3.3362680      6.1120270
  H     -6.2902670      3.4244820      6.8130740

37
System: 7a, CBS(T): 2.52
  C      0.0006650     -0.0016330     -0.0168420
  C     -0.0101640      0.0697200      1.4961740
  O      1.3482510      0.1450090      1.9799130
  C      1.3340950      0.7353980      3.3119010
  C     -0.0281870      1.4053190      3.4972500
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  O     -0.8103730      0.6368190      4.4282120
  C     -0.6463510      1.3292930      2.0843040
  O     -2.0673880      1.2058170      2.1526100
  P     -3.0487870      2.5016140      1.8573570
  O     -3.7031800      2.2937690      0.5187100
  O     -2.3327170      3.7838900      2.1663650
  O     -4.1169080      2.2524560      3.0579310
  C     -4.8221440      0.9937370      3.1305790
  C     -5.3688320      0.8183170      4.5309670
  O     -4.2833490      0.5718570      5.4524540
  C     -4.5086900      1.3253050      6.6800200
  C     -5.9592080      1.7963210      6.6180370
  C     -6.1370340      2.0065330      5.1115720
  O     -7.4845470      1.9744520      4.6201470
  H     -1.0283200     -0.0221330     -0.3894570
  H      0.5094790     -0.9064130     -0.3620660
  H      0.5077770      0.8744890     -0.4341330
  H     -0.5126770     -0.8107600      1.9247840
  H      2.1644540      1.4433810      3.3563380
  H      1.4737730     -0.0448160      4.0686440
  H      0.0556390      2.4383900      3.8496130
  H     -1.7460780      0.8153790      4.2139490
  H     -0.3600070      2.2109450      1.5030290
  H     -4.1425770      0.1695750      2.8948670
  H     -5.6473150      0.9952140      2.4095380
  H     -6.0378500     -0.0567000      4.5153390
  H     -3.8085830      2.1692590      6.7013130
  H     -4.2988920      0.6646470      7.5248490
  H     -6.1329120      2.7032040      7.2023230
  H     -6.6427750      1.0114030      6.9586510
  H     -5.6560970      2.9410000      4.8026760
  H     -7.8949640      2.8290860      4.8226310

37
System: 3a, CBS(T): 2.50
  C      0.0113640      0.0344700     -0.0554040
  C      0.0193960      0.0678580      1.4597830
  O      1.3859820      0.1099060      1.9304500
  C      1.4385490      0.8143190      3.2049920
  C      0.0483260      1.3804590      3.4707470
  O     -0.6653410      0.5261480      4.3823570
  C     -0.6170030      1.3117260      2.0832390
  O     -2.0345770      1.1405410      2.2000420
  P     -3.0054930      2.4582200      1.9607470
  O     -2.7252600      3.0255050      0.5961350
  O     -2.9638760      3.3469040      3.1722000
  O     -4.4277900      1.6813220      2.0106920
  C     -4.7864340      0.8148520      0.9090620
  C     -5.9272670     -0.0941650      1.3244520
  O     -5.4544340     -1.1272510      2.2177010
  C     -6.3493980     -1.2317630      3.3600920
  C     -7.6392370     -0.5425070      2.9308410
  C     -7.0883080      0.5877270      2.0574580
  O     -7.9955440      1.1269690      1.0834250
  H      0.5143510      0.9192430     -0.4585630
  H      0.5141370     -0.8627400     -0.4282950
  H     -1.0226330      0.0243710     -0.4147650
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  H     -0.4863920     -0.8192080      1.8691130
  H      2.1897350      1.6043490      3.1145070
  H      1.7328480      0.1190380      3.9979720
  H      0.0832160      2.4001440      3.8680530
  H     -1.5951490      0.5608450      4.0812840
  H     -0.3836640      2.2029420      1.4917290
  H     -3.9220260      0.2100930      0.6181790
  H     -5.0982400      1.4283290      0.0570060
  H     -6.3170480     -0.5666690      0.4099470
  H     -5.8876610     -0.7262700      4.2178740
  H     -6.4716040     -2.2922920      3.5926960
  H     -8.2293380     -0.1812780      3.7767410
  H     -8.2551240     -1.2096900      2.3185080
  H     -6.7031280      1.3967420      2.6864540
  H     -8.5997970      1.7300450      1.5428960

37
System: 9a, CBS(T): 1.77
  C      0.0331800      0.0575200     -0.0630650
  C      0.0518730      0.0803320      1.4515460
  O      1.4242510      0.1314940      1.9048580
  C      1.4700740      0.7486370      3.2247130
  C      0.0833400      1.3171390      3.5045150
  O     -0.6356190      0.4311000      4.3817810
  C     -0.5727430      1.3125000      2.1110050
  O     -1.9955710      1.1722190      2.2072370
  P     -3.0017450      2.4840130      2.1650860
  O     -2.1813010      3.7193400      1.9168000
  O     -3.9200450      2.3722410      3.3475740
  O     -3.9243070      2.1290930      0.8721290
  C     -3.3229990      2.2009380     -0.4395980
  C     -4.0937480      1.3320890     -1.4123070
  O     -3.8772160     -0.0651920     -1.1332500
  C     -5.1365660     -0.7881140     -1.2636000
  C     -6.0999840      0.1722780     -1.9551900
  C     -5.6131390      1.5193110     -1.4145370
  O     -5.9395640      2.6719930     -2.2042130
  H     -0.9994150     -0.0292670     -0.4153180
  H      0.5928330     -0.8035840     -0.4402310
  H      0.4741820      0.9732530     -0.4696710
  H     -0.4387340     -0.8181360      1.8546600
  H      2.2375190      1.5264260      3.1942450
  H      1.7380550     -0.0015220      3.9762670
  H      0.1232920      2.3207000      3.9417250
  H     -1.5731700      0.5140800      4.1221120
  H     -0.3217000      2.2266300      1.5667710
  H     -3.3431990      3.2393320     -0.7873300
  H     -2.2829370      1.8663940     -0.3940890
  H     -3.7138230      1.5647640     -2.4202950
  H     -4.9447480     -1.7007160     -1.8335010
  H     -5.4854690     -1.0588490     -0.2595680
  H     -5.9675720      0.1484620     -3.0420790
  H     -7.1457780     -0.0349680     -1.7156750
  H     -5.9667800      1.6650370     -0.3880050
  H     -6.8642210      2.9021800     -2.0259120

37
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System: 1g, CBS(T): 1.54
  C      0.0377580      0.0434120     -0.0327790
  C      0.0684390      0.0827690      1.4804140
  O      1.4329710      0.1912610      1.9383910
  C      1.4125810      0.6998680      3.3014830
  C      0.0489470      1.3651620      3.5200960
  O     -0.7186860      0.5921940      4.4564850
  C     -0.5911790      1.3052130      2.1186450
  O     -2.0174430      1.1498140      2.1852180
  P     -2.9660420      2.4571160      1.8849560
  O     -4.3787160      1.9505000      1.9502120
  O     -2.4888240      3.2021840      0.6678930
  O     -2.5732550      3.2928350      3.2313300
  C     -2.9406000      4.6827520      3.3210750
  C     -2.9344580      5.1032090      4.7780930
  O     -4.0148860      4.4775140      5.5026870
  C     -3.4971860      3.8882470      6.7283560
  C     -2.1647120      4.5843130      6.9809620
  C     -1.6551110      4.7536730      5.5476130
  O     -0.6896860      5.7938720      5.3345970
  H      0.5623000     -0.8391440     -0.4105000
  H      0.5055620      0.9421160     -0.4475380
  H     -1.0007190     -0.0005980     -0.3751510
  H     -0.3932930     -0.8250640      1.8993260
  H      2.2467980      1.3983110      3.3940910
  H      1.5406830     -0.1247300      4.0123050
  H      0.1412720      2.3945190      3.8809650
  H     -1.6519940      0.7527680      4.2217710
  H     -0.3446770      2.2043650      1.5454680
  H     -3.9382580      4.8418330      2.8968660
  H     -2.2180430      5.2891600      2.7626240
  H     -3.0730920      6.1948050      4.8056080
  H     -3.3655730      2.8094000      6.5750050
  H     -4.2381550      4.0511570      7.5142770
  H     -1.4910790      3.9961950      7.6091630
  H     -2.3169490      5.5688430      7.4356110
  H     -1.2570310      3.8019830      5.1791720
  H      0.1661860      5.4775130      5.6616740

37
System: 7d, CBS(T): 1.24
  C      0.0098390      0.0124930     -0.0260580
  C      0.0378100      0.0549800      1.4882180
  O      1.4079150      0.1133940      1.9460560
  C      1.4600730      0.8163580      3.2211310
  C      0.0614660      1.3542820      3.5012530
  O     -0.6255990      0.4763880      4.4107250
  C     -0.6035030      1.2961910      2.1167760
  O     -2.0241900      1.1392980      2.2416110
  P     -3.0902600      2.1760200      1.5201690
  O     -4.2883170      1.3510600      1.1556020
  O     -2.3541280      3.0050560      0.5062560
  O     -3.5781710      3.1030330      2.7706720
  C     -2.6541230      4.0381570      3.3614910
  C     -3.3967980      4.9445080      4.3225420
  O     -4.3138120      5.8062920      3.6150230
  C     -5.6082840      5.7926320      4.2845020
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  C     -5.3427950      5.2340230      5.6776700
  C     -4.2322980      4.2210100      5.3845750
  O     -3.3808060      3.8899640      6.4913820
  H     -1.0287690     -0.0145520     -0.3710570
  H      0.5191070     -0.8807180     -0.3997830
  H      0.4940020      0.9011520     -0.4430790
  H     -0.4523470     -0.8367000      1.9068180
  H      2.1933940      1.6222730      3.1254740
  H      1.7753300      0.1258420      4.0100170
  H      0.0899060      2.3687970      3.9140910
  H     -1.5686100      0.5296050      4.1647080
  H     -0.3779010      2.1909620      1.5310450
  H     -1.8867980      3.4944700      3.9258550
  H     -2.1695170      4.6246660      2.5746760
  H     -2.6437970      5.5642250      4.8329400
  H     -6.2921980      5.1507900      3.7151010
  H     -5.9931560      6.8150030      4.2847140
  H     -6.2294290      4.7808670      6.1276450
  H     -4.9567490      6.0120630      6.3447580
  H     -4.6561340      3.3047820      4.9604380
  H     -3.8275120      3.2094630      7.0173770

37
System: 3d, CBS(T): 1.81
  C      0.0063760      0.0129740     -0.0367700
  C      0.0284490      0.0543450      1.4779220
  O      1.3989790      0.1141050      1.9372180
  C      1.4504580      0.8107210      3.2158180
  C      0.0541180      1.3569170      3.4897390
  O     -0.6426640      0.4791280      4.3949320
  C     -0.6087480      1.2984560      2.1040460
  O     -2.0285910      1.1631720      2.2526760
  P     -3.0443740      2.1661490      1.4140190
  O     -3.4552080      1.5109620      0.1275870
  O     -2.4584000      3.5515260      1.4102390
  O     -4.3293150      2.0561080      2.4016610
  C     -4.2281530      2.5927380      3.7393780
  C     -5.5311900      2.3531300      4.4741150
  O     -6.6104070      3.0985060      3.8708320
  C     -7.7534050      2.2179740      3.6684520
  C     -7.5161590      1.0249180      4.5866090
  C     -5.9922570      0.8911030      4.5122490
  O     -5.3671120      0.2431510      5.6301230
  H      0.5027600      0.8978990     -0.4484600
  H      0.5098820     -0.8836680     -0.4099870
  H     -1.0315880      0.0002770     -0.3840980
  H     -0.4629380     -0.8364710      1.8963320
  H      1.7558190      0.1146290      4.0037920
  H      2.1913530      1.6104950      3.1272980
  H      0.0754730      2.3716580      3.9009450
  H     -1.5765180      0.5070860      4.1117380
  H     -0.3708260      2.1987700      1.5302080
  H     -3.4190330      2.0901760      4.2821640
  H     -4.0057290      3.6629800      3.6864720
  H     -5.3904890      2.7017400      5.5083370
  H     -8.6554960      2.7862460      3.9059550
  H     -7.7847340      1.9163930      2.6138690
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  H     -8.0424910      0.1258050      4.2570780
  H     -7.8093920      1.2588590      5.6154580
  H     -5.6999410      0.3868130      3.5851780
  H     -5.4340140     -0.7142980      5.4947960

37
System: 5d, CBS(T): 0.19
  C      0.0385970      0.0211070     -0.0264590
  C      0.0567260      0.0436620      1.4880490
  O      1.4222020      0.0768130      1.9566690
  C      1.4566800      0.7096830      3.2713320
  C      0.0631750      1.2660000      3.5418120
  O     -0.6584640      0.3516230      4.3882740
  C     -0.5636380      1.2817210      2.1374440
  O     -1.9958110      1.1686720      2.1607890
  P     -2.8862670      2.5604730      2.2889540
  O     -2.3523480      3.4090170      3.4056880
  O     -4.3103120      2.0864040      2.2671870
  O     -2.4955120      3.3483750      0.9201690
  C     -2.9248520      2.8266310     -0.3564470
  C     -3.2936710      3.9686160     -1.2825410
  O     -4.5079000      4.6133930     -0.8455600
  C     -4.3413800      6.0601560     -0.9096900
  C     -3.1055110      6.2958880     -1.7714010
  C     -2.2496630      5.0839800     -1.3940040
  O     -1.2546240      4.6925160     -2.3510010
  H      0.5168900      0.9188670     -0.4319430
  H      0.5605460     -0.8616430     -0.4072360
  H     -0.9972130     -0.0182230     -0.3778380
  H     -0.4514130     -0.8466550      1.8885750
  H      2.2141500      1.4972380      3.2361520
  H      1.7317430     -0.0306760      4.0295830
  H      0.0851480      2.2590150      3.9984530
  H     -1.5989120      0.4642290      4.1567590
  H     -0.2659710      2.1881310      1.5982950
  H     -2.0999930      2.2595250     -0.8014410
  H     -3.7840550      2.1645520     -0.2149380
  H     -3.4531280      3.5377530     -2.2835890
  H     -5.2572120      6.4844690     -1.3279790
  H     -4.2018920      6.4410170      0.1097510
  H     -3.3541770      6.2482690     -2.8369240
  H     -2.6175670      7.2499600     -1.5575700
  H     -1.7779530      5.2434610     -0.4185840
  H     -0.4867770      5.2726800     -2.2355070

37
System: 1e, CBS(T): -1.18
  C     -0.0726580     -0.0805130      0.1035150
  C     -0.0985640     -0.0111730      1.6180200
  O      1.2585600     -0.0377310      2.1317620
  C      1.3662950      0.8651960      3.2709740
  C     -0.0430780      1.3347550      3.5955600
  O     -0.6352180      0.3990830      4.5006190
  C     -0.6841320      1.2774750      2.1949600
  O     -2.1128430      1.2147830      2.1919200
  P     -2.9919380      2.5991970      2.2589830
  O     -4.3963100      2.2169380      1.8913740
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  O     -2.2549230      3.6879050      1.5281860
  O     -2.9023690      2.9562490      3.8571590
  C     -4.0711290      2.8602750      4.6975510
  C     -4.2960210      1.4327160      5.1633070
  O     -3.0675460      0.9144400      5.7268930
  C     -3.3405450      0.2252710      6.9850440
  C     -4.8528470      0.0470830      7.0274540
  C     -5.3335030      1.2974990      6.2819370
  O     -6.6393910      1.2018650      5.6984690
  H     -1.0976450     -0.0504830     -0.2810740
  H      0.3933400     -1.0100830     -0.2372220
  H      0.4831120      0.7678950     -0.3090790
  H     -0.6546400     -0.8637520      2.0326050
  H      2.0102630      1.7059180      2.9897630
  H      1.8144170      0.3254800      4.1096160
  H     -0.0571950      2.3450760      4.0178890
  H     -1.5316040      0.7100400      4.7641550
  H     -0.3567030      2.1451590      1.6109830
  H     -3.8667350      3.5065740      5.5558890
  H     -4.9562260      3.2179840      4.1644670
  H     -4.5884870      0.8055300      4.3115600
  H     -2.7859920     -0.7155780      6.9793430
  H     -2.9779360      0.8531650      7.8065620
  H     -5.1601280     -0.8415790      6.4669330
  H     -5.2401240     -0.0176220      8.0469030
  H     -5.2876530      2.1739280      6.9421260
  H     -7.2908860      1.2685920      6.4137310

37
System: 1c, CBS(T): -0.14
  C      0.0091220      0.0604540     -0.0875220
  C      0.0691080      0.0777840      1.4248540
  O      1.4430260      0.1657610      1.8564290
  C      1.4147310      0.5308260      3.2574090
  C      0.1334480      1.3479290      3.4877460
  O     -0.6367690      0.7112530      4.5121950
  C     -0.5649390      1.2960120      2.0972100
  O     -1.9898150      1.1289160      2.1519780
  P     -2.9654400      2.4067910      2.4265290
  O     -4.3640810      1.8639080      2.3535400
  O     -2.5610970      3.5935720      1.5968900
  O     -2.5582570      2.6949000      3.9994380
  C     -2.6927800      4.0373350      4.5241790
  C     -1.9523700      4.1330350      5.8395530
  O     -0.5487790      3.8721070      5.6412110
  C      0.2435380      4.8505770      6.3773730
  C     -0.7359570      5.5825530      7.2886070
  C     -2.0214920      5.5341890      6.4574390
  O     -3.2439140      5.6636510      7.1952070
  H      0.5141270     -0.8225800     -0.4900090
  H     -1.0365020      0.0355740     -0.4098340
  H      0.4803950      0.9595750     -0.4979580
  H     -0.3916620     -0.8315090      1.8425540
  H      2.3324340      1.0836200      3.4638160
  H      1.3780610     -0.3718060      3.8812790
  H      0.3392280      2.3791750      3.7848180
  H     -1.4095890      1.2992850      4.6393460
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  H     -0.3291530      2.2029050      1.5300010
  H     -3.7535490      4.2626150      4.6854410
  H     -2.2743780      4.7413330      3.7988110
  H     -2.3614950      3.4034570      6.5541310
  H      0.7126350      5.5291930      5.6549840
  H      1.0250700      4.3124810      6.9196750
  H     -0.4158090      6.6007040      7.5218960
  H     -0.8941290      5.0317580      8.2214990
  H     -1.9887570      6.2924560      5.6637970
  H     -3.3473070      6.5960790      7.4405110

37
System: 1f, CBS(T): 0.61
  C      0.0380030      0.0121310     -0.0316200
  C      0.0750660      0.0998380      1.4782550
  O      1.4349240      0.2233390      1.9448000
  C      1.3372450      0.5928390      3.3390130
  C      0.1085810      1.5088360      3.4668960
  O     -0.6809120      1.0785590      4.5761840
  C     -0.5981600      1.3310270      2.0863860
  O     -2.0174970      1.1240030      2.1532820
  P     -3.0187000      2.4101400      2.2154640
  O     -4.4109680      1.8512960      2.2814980
  O     -2.6679080      3.4388230      1.1759840
  O     -2.5434870      2.9596490      3.6939550
  C     -3.0328130      4.2372020      4.1620070
  C     -3.3744080      4.1269090      5.6321490
  O     -2.2121570      3.7155540      6.3813590
  C     -2.1022910      4.5193230      7.5953290
  C     -3.4256080      5.2661010      7.7240790
  C     -3.8140610      5.4559420      6.2543190
  O     -5.2108790      5.6529710      6.0001790
  H      0.5003860      0.8983630     -0.4789010
  H      0.5617060     -0.8804570     -0.3860690
  H     -1.0028790     -0.0446740     -0.3643550
  H     -0.3799680     -0.7990740      1.9253110
  H      1.1754710     -0.3017690      3.9558850
  H      2.2789600      1.0679310      3.6156470
  H      0.3963830      2.5555950      3.6059550
  H     -1.4328130      1.7070430      4.6134000
  H     -0.3975820      2.2065530      1.4596390
  H     -3.9274790      4.5306890      3.6027820
  H     -2.2471130      4.9838810      4.0047600
  H     -4.1734590      3.3833550      5.7664410
  H     -1.2566010      5.2072930      7.4785170
  H     -1.8994960      3.8429010      8.4292640
  H     -3.3262300      6.2096560      8.2657120
  H     -4.1824430      4.6462060      8.2156820
  H     -3.2394240      6.2820310      5.8143160
  H     -5.4338840      6.5636260      6.2475910

37
System: 5j, CBS(T): 0.92
  C      0.0193660      0.0407720     -0.0520360
  C      0.0323470      0.0572260      1.4637990
  O      1.4050470      0.0760560      1.9287650
  C      1.5092760      0.8821920      3.1372520
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  C      0.1092750      1.3682650      3.4726670
  O     -0.5163690      0.4534920      4.3892760
  C     -0.5951830      1.2959580      2.1099140
  O     -2.0123570      1.1309830      2.2819730
  P     -3.0301820      2.3732870      1.8960400
  O     -2.3564430      3.6912180      2.1451170
  O     -4.3302380      2.0040760      2.5492690
  O     -3.1493810      2.2488610      0.2717190
  C     -3.8135930      1.0895340     -0.2862480
  C     -5.1532320      1.4656190     -0.8849280
  O     -4.9772850      2.4616950     -1.9163290
  C     -5.7930030      2.1180670     -3.0771830
  C     -6.7183830      0.9951880     -2.6216270
  C     -5.8512310      0.2892360     -1.5748930
  O     -6.5632720     -0.4753350     -0.5932130
  H     -1.0128130     -0.0112410     -0.4103160
  H      0.5564020     -0.8326380     -0.4334780
  H      0.4852610      0.9477280     -0.4504040
  H     -0.4719230     -0.8352230      1.8615050
  H      2.1827050      1.7208250      2.9313510
  H      1.9241340      0.2711370      3.9444260
  H      0.1063300      2.3810840      3.8896590
  H     -1.4706970      0.4968660      4.1878330
  H     -0.3838270      2.1969150      1.5268480
  H     -3.9595720      0.3237470      0.4817270
  H     -3.1567450      0.6982140     -1.0694580
  H     -5.8075600      1.8671260     -0.0985880
  H     -6.3238090      3.0189390     -3.3950650
  H     -5.1253830      1.7928400     -3.8837670
  H     -7.6126790      1.3946420     -2.1324280
  H     -7.0198220      0.3385810     -3.4412120
  H     -5.1053890     -0.3486730     -2.0685500
  H     -6.8671860     -1.2935850     -1.0156520

37
System: 1b, CBS(T): -0.35
  C      0.0154950      0.0571860     -0.0592910
  C      0.0384010      0.0366350      1.4567480
  O      1.4107280      0.0599960      1.9225220
  C      1.4999570      0.8535850      3.1423610
  C      0.0815120      1.2505920      3.5053060
  O     -0.5024150      0.2154100      4.3237660
  C     -0.5980730      1.2563480      2.1291970
  O     -2.0247360      1.0956060      2.2373010
  P     -2.9734700      2.4429920      2.0743000
  O     -4.3739070      1.8970720      2.0690320
  O     -2.4591750      3.3026110      0.9582690
  O     -2.6912830      3.2851340      3.4374650
  C     -2.9828180      2.7102640      4.7252180
  C     -2.5542180      3.6822610      5.8129460
  O     -1.1263610      3.9042840      5.7549500
  C     -0.8574070      5.3107970      5.5306630
  C     -2.1630250      5.8988620      5.0011480
  C     -3.2169340      5.0593220      5.7299830
  O     -3.4161610      5.5129860      7.0891830
  H      0.5260740     -0.8200430     -0.4675360
  H     -1.0217030      0.0441440     -0.4099540
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  H      0.5035190      0.9612600     -0.4373660
  H     -0.4567870     -0.8690590      1.8349310
  H      2.1199250      1.7338930      2.9396660
  H      1.9656640      0.2516930      3.9278300
  H      0.0193190      2.2143740      4.0208040
  H     -1.4320120      0.1395770      4.0390400
  H     -0.3673410      2.1754700      1.5827060
  H     -2.4320410      1.7732030      4.8470970
  H     -4.0562550      2.5057420      4.8108130
  H     -2.7973730      3.2199950      6.7781560
  H     -0.0286500      5.3796030      4.8216360
  H     -0.5615400      5.7748100      6.4800310
  H     -2.2504550      5.7286160      3.9254620
  H     -2.2689470      6.9670660      5.2096830
  H     -4.1759410      5.0253720      5.2031430
  H     -3.7414580      6.4263820      7.0465190

37
System: 1[, CBS(T): -1.24
  C      0.0087920      0.0177240     -0.0400060
  C      0.0419120      0.0468290      1.4747450
  O      1.4135780      0.0977350      1.9310890
  C      1.4792380      0.8314680      3.1894920
  C      0.0701750      1.3159080      3.4985950
  O     -0.5827260      0.3760700      4.3724630
  C     -0.5955880      1.2821680      2.1151900
  O     -2.0206720      1.1242840      2.2171460
  P     -2.9951800      2.4228500      1.8986650
  O     -4.3830330      1.8507880      1.9380800
  O     -2.4780480      3.1765760      0.7097730
  O     -2.7393210      3.4052150      3.1755740
  C     -3.1038720      2.9529210      4.4985320
  C     -3.7663740      4.0821240      5.2695330
  O     -2.8079300      5.1474590      5.4946290
  C     -3.3284710      6.3893050      4.9583310
  C     -4.3547460      5.9706650      3.9105950
  C     -4.9596370      4.7151380      4.5454160
  O     -5.9328810      5.0584850      5.5607270
  H      0.5181840     -0.8714760     -0.4229640
  H     -1.0310820     -0.0089310     -0.3812610
  H      0.4910250      0.9103060     -0.4511700
  H     -0.4483150     -0.8480050      1.8859120
  H      2.1725310      1.6675170      3.0561010
  H      1.8501400      0.1703060      3.9787310
  H      0.0639970      2.3140360      3.9498700
  H     -1.5222760      0.3791160      4.1091410
  H     -0.3583040      2.1840950      1.5433400
  H     -2.1951570      2.6369220      5.0204150
  H     -3.7978090      2.1082400      4.4290430
  H     -4.0900820      3.6866710      6.2404770
  H     -2.4838940      6.9503320      4.5516210
  H     -3.7938870      6.9682220      5.7663570
  H     -3.8608780      5.7018980      2.9736710
  H     -5.1100720      6.7368940      3.7152090
  H     -5.4021930      4.0334660      3.8125130
  H     -6.6624010      5.5211120      5.1183990
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37
System: 3b, CBS(T): 1.05
  C      0.0112910      0.0299570     -0.0547600
  C      0.0209840      0.0639460      1.4601530
  O      1.3867210      0.0994820      1.9347850
  C      1.4451060      0.8266600      3.1970040
  C      0.0517460      1.3795800      3.4684240
  O     -0.6496270      0.5142190      4.3793510
  C     -0.6121300      1.3099010      2.0832020
  O     -2.0317200      1.1520270      2.2046870
  P     -3.0097950      2.3974620      1.7263990
  O     -2.6263580      2.8007870      0.3293800
  O     -3.0951030      3.4303800      2.8139040
  O     -4.4140990      1.5860630      1.7559040
  C     -4.6220470      0.5233040      0.7998050
  C     -5.9745210     -0.1264860      1.0398580
  O     -5.9452180     -0.8844380      2.2773710
  C     -6.9175430     -0.3484430      3.2101670
  C     -7.2632260      1.0434740      2.6872520
  C     -7.1422550      0.8536790      1.1729580
  O     -8.3097540      0.1827560      0.6405690
  H      0.5228080      0.9091710     -0.4591120
  H      0.5033200     -0.8729560     -0.4281410
  H     -1.0236790      0.0337210     -0.4113410
  H     -0.4878070     -0.8218390      1.8688400
  H      2.1840790      1.6256250      3.0855540
  H      1.7579450      0.1483140      3.9972250
  H      0.0794790      2.3984850      3.8691880
  H     -1.5872930      0.5693560      4.1099820
  H     -0.3737810      2.1985500      1.4903760
  H     -3.8329230     -0.2270930      0.9121050
  H     -4.5831010      0.9351930     -0.2149960
  H     -6.1622430     -0.8219900      0.2131190
  H     -6.4572720     -0.3407640      4.2012990
  H     -7.7979390     -1.0028900      3.2246650
  H     -6.5270720      1.7776730      3.0211750
  H     -8.2637590      1.3741430      2.9795000
  H     -6.9647910      1.7885860      0.6323900
  H     -9.0754640      0.7549370      0.8083520

37
System: 1z, CBS(T): -0.01
  C      0.0133850      0.0258150     -0.0565790
  C      0.0383000      0.0529740      1.4585370
  O      1.4091310      0.1107410      1.9178470
  C      1.4683020      0.8419850      3.1776560
  C      0.0550460      1.3106750      3.4855860
  O     -0.5877970      0.3468520      4.3380090
  C     -0.6043620      1.2863700      2.0967560
  O     -2.0284250      1.1169360      2.1862960
  P     -3.0134660      2.4297710      2.2121470
  O     -4.3943400      1.9170190      1.9169500
  O     -2.4201340      3.5382720      1.3860210
  O     -2.8816560      2.7940490      3.8061450
  C     -3.8766540      3.6905660      4.3471030
  C     -3.9181600      3.6013760      5.8628110
  O     -4.4461490      2.3090000      6.2591590
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  C     -3.4955490      1.6333320      7.1196600
  C     -2.1520120      2.2965870      6.8331020
  C     -2.5644650      3.7442420      6.5662450
  O     -2.8172200      4.4473630      7.8076670
  H     -1.0242830     -0.0078320     -0.4042780
  H      0.5309370     -0.8591700     -0.4382850
  H      0.4927390      0.9219860     -0.4636250
  H     -0.4488130     -0.8437860      1.8679140
  H      2.1537410      1.6848560      3.0464290
  H      1.8457410      0.1827270      3.9654050
  H      0.0305370      2.3018170      3.9509080
  H     -1.5381700      0.4015130      4.1253300
  H     -0.3734670      2.1958520      1.5348290
  H     -4.8595130      3.4238890      3.9456260
  H     -3.6374410      4.7205770      4.0533870
  H     -4.5995600      4.3841100      6.2184750
  H     -3.7955570      1.7669670      8.1667540
  H     -3.5237980      0.5698880      6.8697790
  H     -1.4483060      2.2191170      7.6667160
  H     -1.6914870      1.8725240      5.9389960
  H     -1.8381400      4.2974640      5.9626680
  H     -1.9856250      4.4607120      8.3078890

37
System: 5z, CBS(T): 2.19
  C      0.0378220      0.0055570     -0.0261590
  C      0.0559430      0.0245720      1.4893510
  O      1.4254330      0.0602110      1.9540170
  C      1.4912140      0.7739650      3.2226830
  C      0.0958900      1.3124650      3.5140220
  O     -0.5828260      0.4189280      4.4129860
  C     -0.5701820      1.2644590      2.1280570
  O     -1.9955950      1.1187160      2.2087000
  P     -2.9519490      2.4558760      2.2335810
  O     -2.6410080      3.2895480      3.4448860
  O     -4.3525320      1.9590760      2.0059090
  O     -2.3641020      3.1818980      0.8913020
  C     -3.1471190      4.2428390      0.3065520
  C     -2.2420440      5.2792340     -0.3422230
  O     -1.5145420      6.0087230      0.6762700
  C     -0.0895000      5.7869130      0.5287700
  C      0.0496520      4.5805900     -0.3966160
  C     -1.1847300      4.7099350     -1.2910010
  O     -0.9752290      5.7030040     -2.3227360
  H     -0.9981190      0.0010330     -0.3800790
  H      0.5364190     -0.8888830     -0.4104560
  H      0.5421170      0.8915830     -0.4251210
  H     -0.4466840     -0.8664750      1.8926920
  H      2.2236850      1.5790920      3.1127780
  H      1.8169760      0.0898990      4.0129300
  H      0.1118540      2.3238040      3.9317370
  H     -1.5328840      0.5171050      4.2173090
  H     -0.3161090      2.1603580      1.5551260
  H     -3.7494190      4.7383640      1.0757040
  H     -3.8189370      3.8159290     -0.4472930
  H     -2.8837690      5.9858410     -0.8823670
  H      0.3667020      6.6838270      0.0924020
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  H      0.3274190      5.6197060      1.5253520
  H      0.9783880      4.5868250     -0.9732190
  H     -0.0137620      3.6490560      0.1683920
  H     -1.4936010      3.7600830     -1.7389480
  H     -0.2272990      5.4056630     -2.8650140

37
System: 7p, CBS(T): 0.68
  C      0.0094500      0.0168940     -0.0448310
  C      0.0401570      0.0528470      1.4698020
  O      1.4106950      0.1206710      1.9253050
  C      1.4584870      0.8105540      3.2092870
  C      0.0562080      1.3362700      3.4906720
  O     -0.6348270      0.4368610      4.3800980
  C     -0.6033490      1.2894340      2.1033060
  O     -2.0236250      1.1410040      2.2345370
  P     -3.0620980      2.2339640      1.5468290
  O     -3.7721300      1.5736240      0.4025470
  O     -2.3369550      3.5379170      1.3592370
  O     -4.1547740      2.3249100      2.7479080
  C     -3.7587540      2.9330560      3.9958850
  C     -4.7016830      2.4884960      5.1011860
  O     -6.0342060      3.0001720      4.8450200
  C     -6.9718500      1.8975730      4.7446270
  C     -6.1189350      0.6683230      4.4454500
  C     -4.8440830      0.9695010      5.2379680
  O     -5.0254350      0.6919260      6.6450700
  H     -1.0302840     -0.0088430     -0.3875430
  H      0.5186890     -0.8735180     -0.4249060
  H      0.4936020      0.9078770     -0.4574940
  H     -0.4428650     -0.8436250      1.8857750
  H      2.1884160      1.6203920      3.1223680
  H      1.7762640      0.1132640      3.9911810
  H      0.0667560      2.3443920      3.9185930
  H     -1.5629120      0.4400100      4.0775090
  H     -0.3714750      2.1949220      1.5369120
  H     -3.7914880      4.0220490      3.8920830
  H     -2.7354230      2.6353930      4.2538550
  H     -4.3374270      2.9125470      6.0448000
  H     -7.6843140      2.1422820      3.9533870
  H     -7.5074870      1.7927580      5.6963210
  H     -5.8795750      0.6125040      3.3811880
  H     -6.5875580     -0.2675350      4.7621500
  H     -3.9678970      0.4336340      4.8575290
  H     -5.2106730     -0.2566750      6.7336120

37
System: 1t, CBS(T): -0.82
  C      0.0149100      0.0391590     -0.0733790
  C      0.0700660      0.0835620      1.4388770
  O      1.4432440      0.1960530      1.8688080
  C      1.4118800      0.5901950      3.2616930
  C      0.1335590      1.4182610      3.4670980
  O     -0.6264800      0.8312750      4.5287840
  C     -0.5761280      1.3091130      2.0852570
  O     -1.9999120      1.1278950      2.1629780
  P     -2.9733440      2.4198330      2.3679960
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  O     -4.3806070      1.8990070      2.2965180
  O     -2.5482960      3.5767100      1.5082150
  O     -2.5608980      2.7333420      3.9336600
  C     -3.1880310      3.8461450      4.6020060
  C     -2.3957020      4.1560770      5.8622880
  O     -1.0301830      4.4946740      5.5178590
  C     -0.7470990      5.8531600      5.9405590
  C     -2.1108760      6.5185590      6.0834770
  C     -2.9710020      5.3636010      6.6073800
  O     -2.7578600      5.1349460      8.0170670
  H      0.4763110      0.9371150     -0.4972160
  H      0.5334310     -0.8441130     -0.4577240
  H     -1.0287310     -0.0053640     -0.3997580
  H     -0.3797010     -0.8235570      1.8725370
  H      1.3656330     -0.2988630      3.9040680
  H      2.3320640      1.1412950      3.4600480
  H      0.3466470      2.4636520      3.7088050
  H     -1.4311640      1.3876330      4.5965330
  H     -0.3608010      2.2020860      1.4892130
  H     -4.2179590      3.5784550      4.8646840
  H     -3.1941300      4.7119200      3.9302690
  H     -2.3796750      3.2764080      6.5158050
  H     -0.2106290      5.8314500      6.8975760
  H     -0.1095630      6.3090600      5.1796940
  H     -2.1098400      7.3736020      6.7644510
  H     -2.4889190      6.8466030      5.1096700
  H     -4.0393560      5.5033140      6.4098590
  H     -3.0578440      5.9274990      8.4902740

37
System: 5q, CBS(T): -0.89
  C      0.0426830      0.0366480     -0.0324280
  C      0.0541620      0.0543310      1.4827320
  O      1.4207340      0.0857220      1.9547630
  C      1.4714920      0.7725840      3.2399340
  C      0.0708520      1.2978310      3.5268770
  O     -0.6206040      0.3732560      4.3866440
  C     -0.5729570      1.2899410      2.1307970
  O     -2.0021550      1.1515450      2.1881800
  P     -2.9221310      2.5242810      2.2441480
  O     -2.3154260      3.5217330      3.1862370
  O     -4.3247350      2.0175970      2.4150000
  O     -2.7052310      3.1526200      0.7523580
  C     -3.1617600      2.3928310     -0.3910490
  C     -4.2874460      3.1334380     -1.0965510
  O     -3.8249130      4.4469980     -1.5082640
  C     -3.9417480      4.5700730     -2.9491040
  C     -3.9460600      3.1368220     -3.4660080
  C     -4.7364060      2.4121320     -2.3712240
  O     -6.1575770      2.6300880     -2.5061770
  H     -0.9903790     -0.0113470     -0.3900970
  H      0.5752750     -0.8398880     -0.4127890
  H      0.5135630      0.9407620     -0.4317530
  H     -0.4516020     -0.8383500      1.8796820
  H      2.1995380      1.5845610      3.1545600
  H      1.7933310      0.0724280      4.0174190
  H      0.0765160      2.2947970      3.9760730
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  H     -1.5633590      0.4429360      4.1466850
  H     -0.2993930      2.1964200      1.5800420
  H     -2.3034660      2.2726470     -1.0592320
  H     -3.5159330      1.4072580     -0.0730530
  H     -5.1313990      3.2608250     -0.4103880
  H     -4.8773820      5.0872460     -3.1964760
  H     -3.0955830      5.1661590     -3.2975820
  H     -4.4099460      3.0281160     -4.4497570
  H     -2.9276100      2.7369120     -3.5119810
  H     -4.5269120      1.3374530     -2.3346160
  H     -6.4376140      2.2228420     -3.3415580

37
System: 1o, CBS(T): -1.08
  C      0.0170930      0.0339730     -0.0399170
  C      0.0396190      0.0498100      1.4754260
  O      1.4100830      0.0999230      1.9402120
  C      1.4828590      0.8802260      3.1687020
  C      0.0654150      1.3184850      3.4986930
  O     -0.5486510      0.3475750      4.3658050
  C     -0.6084500      1.2781500      2.1193620
  O     -2.0317760      1.1010290      2.2286680
  P     -3.0223180      2.4025220      1.9892670
  O     -4.4017820      1.8115690      1.9686070
  O     -2.5014900      3.2558160      0.8716020
  O     -2.7980090      3.2907830      3.3441770
  C     -3.1718370      2.7380760      4.6261030
  C     -3.9239230      3.8062410      5.4147450
  O     -4.3562740      3.2054320      6.6620480
  C     -3.7117050      3.8828320      7.7756380
  C     -2.5110590      4.5974720      7.1656680
  C     -3.0494850      5.0014260      5.7883310
  O     -3.9136530      6.1553290      5.8731070
  H     -1.0205980      0.0067050     -0.3880840
  H      0.5320970     -0.8498920     -0.4275580
  H      0.4992250      0.9315970     -0.4401640
  H     -0.4488150     -0.8503290      1.8759820
  H      2.1356700      1.7405700      2.9882030
  H      1.9045940      0.2621880      3.9667970
  H      0.0333260      2.3116240      3.9602870
  H     -1.4886580      0.3136860      4.1068570
  H     -0.3884300      2.1847520      1.5485410
  H     -3.8165670      1.8648800      4.4917780
  H     -2.2626740      2.4383390      5.1587470
  H     -4.8047200      4.1328440      4.8519650
  H     -3.4473110      3.1240040      8.5151370
  H     -4.4192560      4.5938130      8.2186500
  H     -1.6666650      3.9101810      7.0477890
  H     -2.1771100      5.4600250      7.7478260
  H     -2.2605840      5.1761850      5.0502530
  H     -3.3736430      6.9043710      6.1716540

37
System: 7r, CBS(T):
  C      0.0068020      0.0181750     -0.0442240
  C      0.0478740      0.0566700      1.4704820
  O      1.4231980      0.1370060      1.9085580
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C	1.4874820	0.8528280	3.1751460
C	0.0853120	1.3689770	3.4760330
O	-0.5732310	0.4878690	4.4045450
C	-0.6050270	1.2893740	2.1042630
O	-2.0197070	1.0953000	2.2563420
P	-3.1246380	2.1768820	1.6723840
O	-4.2359760	1.3803260	1.0576030
O	-2.3980010	3.2471360	0.9081390
O	-3.7593810	2.7903780	3.0474430
C	-2.9121190	3.5207490	3.9556000
C	-3.7541350	3.9258360	5.1613820
O	-2.8827830	4.6233460	6.0854080
C	-3.3531260	5.9893010	6.2539230
C	-4.2377610	6.2579950	5.0416960
C	-4.8874740	4.8882630	4.8120750
O	-5.9597320	4.6419420	5.7481760
H	0.4708610	0.9176580	-0.4611290
H	0.5310460	-0.8630800	-0.4253320
H	-1.0335500	-0.0300940	-0.3821460
H	-0.4226070	-0.8433530	1.8931120
H	2.2049160	1.6702660	3.0582630
H	1.8286250	0.1760140	3.9651020
H	0.1043980	2.3869550	3.8803400
H	-1.5095780	0.4663730	4.1285650
H	-0.4165900	2.1892620	1.5142110
H	-2.5028030	4.4045760	3.4537440
H	-2.0843380	2.8889960	4.2923200
H	-4.1534210	3.0329730	5.6548880
H	-3.9216540	6.0578980	7.1890820
H	-2.4743860	6.6348430	6.3144370
H	-4.9782250	7.0438960	5.2108380
H	-3.6330560	6.5303510	4.1704250
H	-5.2422470	4.7452920	3.7874200
H	-6.6593630	5.2899740	5.5683960

37
System: a2, CBS(T):

C	-0.0260500	0.0227930	-0.0208190
C	-0.0010590	0.0029490	1.4993430
O	1.3984760	0.0082110	1.9358480
C	1.5729290	1.0204020	2.9406150
C	0.5451060	2.0948780	2.5744780
O	0.2417400	3.0006760	3.6312240
C	-0.6571410	1.2296830	2.1461600
O	-1.3350310	0.8745520	3.3781160
P	-2.9712750	0.6722960	3.3212900
O	-3.3342870	0.1510990	4.6829970
O	-3.3412360	-0.0584950	2.0634310
O	-3.5277490	2.1896580	3.1181170
C	-3.4668600	3.1263480	4.2128490
C	-4.3191530	4.3366750	3.8875320
O	-3.7553320	5.0932820	2.7949430
C	-4.8030970	5.4142090	1.8364850
C	-6.1170280	5.2156720	2.5842710
C	-5.7636390	4.0266550	3.4813800
O	-6.5543500	3.8738980	4.6695820
H	0.5749020	-0.8007590	-0.4172590

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  H     -1.0542790     -0.0928380     -0.3777990
  H      0.3770260      0.9656360     -0.4045990
  H     -0.4789950     -0.9037170      1.8838280
  H      2.6077250      1.3653060      2.8934340
  H      1.3612340      0.6248980      3.9449950
  H      0.8992670      2.6911450      1.7304110
  H     -0.3655570      2.5085600      4.2157540
  H     -1.3488520      1.7457590      1.4783810
  H     -2.4289850      3.4394460      4.3702460
  H     -3.8418170      2.6517420      5.1257830
  H     -4.3375590      4.9704140      4.7877240
  H     -4.7187920      4.7322650      0.9807160
  H     -4.6402240      6.4391420      1.4950180
  H     -6.9581730      5.0148400      1.9161840
  H     -6.3492150      6.0864560      3.2066110
  H     -5.7896110      3.0967780      2.9029020
  H     -7.3942980      3.4615810      4.4160570

37
System: a4, CBS(T):
  C      0.0041260      0.0151750     -0.0317300
  C      0.0090080     -0.0040760      1.4883200
  O      1.4024740      0.0222820      1.9476440
  C      1.5489920      1.0434560      2.9500170
  C      0.5138470      2.1024710      2.5581980
  O      0.1697480      3.0140990      3.5977810
  C     -0.6674100      1.2136680      2.1291680
  O     -1.3327230      0.8534890      3.3615480
  P     -2.9637250      0.6202480      3.3106010
  O     -3.2695710     -0.3859980      2.2340810
  O     -3.6782320      1.9426690      3.3247150
  O     -3.1472890     -0.0092390      4.7952150
  C     -2.4833180     -1.2526660      5.1157710
  C     -2.5921380     -1.5148050      6.6041530
  O     -1.7929050     -0.5739200      7.3527890
  C     -2.5696980     -0.0576620      8.4705340
  C     -3.7330290     -1.0278170      8.6443330
  C     -4.0050510     -1.4208950      7.1900600
  O     -4.6696620     -2.6778470      6.9913890
  H      0.4000370      0.9624450     -0.4120460
  H      0.6204590     -0.8011270     -0.4195000
  H     -1.0175130     -0.1147160     -0.4028840
  H     -0.4629050     -0.9155940      1.8677140
  H      1.3246440      0.6515190      3.9526500
  H      2.5803420      1.3999550      2.9162130
  H      0.8726060      2.6920690      1.7111850
  H     -0.4849760      2.5327950      4.1415060
  H     -1.3651040      1.7167120      1.4555140
  H     -1.4308120     -1.1894120      4.8237110
  H     -2.9594120     -2.0731220      4.5669050
  H     -2.2081710     -2.5313700      6.7818390
  H     -2.9196200      0.9516910      8.2194820
  H     -1.9093090     -0.0018050      9.3391430
  H     -4.5961610     -0.5705180      9.1342590
  H     -3.4238710     -1.9136260      9.2094570
  H     -4.5637340     -0.6265520      6.6830380
  H     -5.6052650     -2.5574350      7.2158650
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37
System: a0, CBS(T):
  C      0.0111350      0.0323770     -0.0608710
  C      0.0283520      0.0069350      1.4599750
  O      1.4260810      0.0464630      1.9111930
  C      1.5975370      1.1297950      2.8460750
  C      0.5250600      2.1490730      2.4468610
  O      0.2073460      3.1148200      3.4463260
  C     -0.6474840      1.2137490      2.1086390
  O     -1.2286510      0.8224880      3.3706040
  P     -2.7265590      1.3277140      3.8223190
  O     -3.5168740      1.7266650      2.6073870
  O     -2.5385960      2.2842730      4.9713770
  O     -3.2943240     -0.0449840      4.4766490
  C     -3.6932470     -1.1113690      3.5854610
  C     -3.6673600     -2.4343830      4.3250200
  O     -2.3078640     -2.8533090      4.5714320
  C     -2.1810420     -3.3103020      5.9482010
  C     -3.6058880     -3.5526070      6.4331330
  C     -4.3592850     -2.4446450      5.6924020
  O     -5.7647130     -2.6634920      5.4966710
  H      0.3945020      0.9851170     -0.4396070
  H      0.6337260     -0.7759210     -0.4549840
  H     -1.0108100     -0.1071840     -0.4290120
  H     -0.4245180     -0.9142320      1.8417340
  H      1.4282670      0.7906110      3.8776990
  H      2.6193690      1.5004530      2.7429140
  H      0.8384640      2.7016290      1.5571900
  H     -0.4254880      2.6921720      4.0638940
  H     -1.4157240      1.6679920      1.4806430
  H     -3.0110930     -1.1574400      2.7301770
  H     -4.7066640     -0.9139600      3.2207890
  H     -4.1595310     -3.1771020      3.6780540
  H     -1.5575010     -4.2075550      5.9467940
  H     -1.6826850     -2.5273040      6.5336140
  H     -3.9733450     -4.5287870      6.0992510
  H     -3.7010530     -3.4837600      7.5195910
  H     -4.2038680     -1.4829590      6.1924810
  H     -6.2162310     -2.4562140      6.3291900

37
System: ahash, CBS(T):
  C      0.0377290      0.1099490     -0.0995920
  C      0.0659450      0.0380870      1.4202710
  O      1.4600430      0.0890490      1.8709470
  C      1.6145710      1.1648100      2.8143630
  C      0.5153770      2.1600490      2.4376270
  O      0.2565300      3.1565070      3.4174580
  C     -0.6522760      1.1999190      2.1110620
  O     -1.2104270      0.6953570      3.3422440
  P     -2.2919840      1.5756520      4.2039340
  O     -3.0817340      2.4611170      3.2810260
  O     -1.5633800      2.1688280      5.3880860
  O     -3.2121550      0.3756630      4.7883200
  C     -4.0754170     -0.3350450      3.8694990
  C     -4.2831290     -1.7618620      4.3449480
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  O     -3.1260200     -2.5698620      4.0314970
  C     -2.7465080     -3.3521340      5.1971040
  C     -3.9700600     -3.3468720      6.1058180
  C     -4.5133690     -1.9387170      5.8502100
  O     -5.9083730     -1.7430260      6.1317120
  H     -0.9833100     -0.0420160     -0.4651540
  H      0.6760190     -0.6715560     -0.5218340
  H      0.3967290      1.0817930     -0.4532590
  H     -0.3658350     -0.9058260      1.7698270
  H      2.6240280      1.5667080      2.7052700
  H      1.4671450      0.8096440      3.8442540
  H      0.7983480      2.6934770      1.5249100
  H     -0.2137770      2.7540950      4.1886920
  H     -1.4401140      1.6549450      1.5079870
  H     -5.0392500      0.1828140      3.8260630
  H     -3.6313010     -0.3461360      2.8697730
  H     -5.1531140     -2.1634240      3.8034130
  H     -1.8839370     -2.8736940      5.6785970
  H     -2.4568120     -4.3475590      4.8520490
  H     -3.7215650     -3.5256070      7.1548960
  H     -4.7061020     -4.0880250      5.7766440
  H     -3.9221820     -1.2011410      6.4017690
  H     -6.0025230     -1.6122270      7.0876390

37
System: g4, CBS(T):
  C      0.0020050      0.0165610     -0.0314690
  C      0.0057930     -0.0074580      1.4891790
  O      1.3997460      0.0096200      1.9497560
  C      1.5682080      1.0606110      2.9179330
  C      0.5269350      2.1111480      2.5193490
  O      0.2005340      3.0464410      3.5439530
  C     -0.6608650      1.2131220      2.1317790
  O     -1.2893410      0.8577920      3.3840990
  P     -2.9256770      0.6886210      3.3826690
  O     -3.3541160     -0.2147310      2.2573710
  O     -3.5646450      2.0495500      3.4999030
  O     -2.9691520     -0.0798210      4.8146750
  C     -4.0720890     -0.9565230      5.1099260
  C     -3.7171940     -1.8232760      6.3023430
  O     -2.7192340     -2.8053780      5.9496530
  C     -1.6856630     -2.8367520      6.9747770
  C     -2.2968270     -2.1507530      8.1919100
  C     -3.1518190     -1.0769270      7.5147330
  O     -4.2428770     -0.5514470      8.2854730
  H      0.4034530      0.9628680     -0.4083310
  H      0.6149710     -0.8015830     -0.4205450
  H     -1.0195980     -0.1066640     -0.4053250
  H     -0.4698770     -0.9171180      1.8677000
  H      2.5992200      1.4140380      2.8525610
  H      1.3641980      0.6980850      3.9356710
  H      0.8699170      2.6818800      1.6530840
  H     -0.4497310      2.5806300      4.1059660
  H     -1.3768530      1.7049460      1.4691900
  H     -4.2896350     -1.5819700      4.2384420
  H     -4.9632890     -0.3650920      5.3560880
  H     -4.6376440     -2.3444060      6.6089510
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  H     -0.8071570     -2.2934120      6.6044740
  H     -1.4162140     -3.8816890      7.1455510
  H     -2.9430630     -2.8387490      8.7473730
  H     -1.5437110     -1.7374770      8.8673740
  H     -2.5160920     -0.2538560      7.1711760
  H     -3.8794900      0.0890380      8.9160100

37
System: g6, CBS(T):
  C      0.0026330      0.0123320     -0.0387640
  C      0.0046320      0.0015590      1.4813010
  O      1.3986960      0.0157700      1.9431350
  C      1.5500070      1.0302610      2.9505860
  C      0.5280920      2.1009320      2.5562770
  O      0.1933860      3.0201730      3.5924190
  C     -0.6606410      1.2314560      2.1139930
  O     -1.3558530      0.8833120      3.3377100
  P     -2.9708020      0.6006260      3.2814120
  O     -3.6380990      1.4904480      2.2680390
  O     -3.4277110      0.6056350      4.7130820
  O     -2.8950280     -0.9294220      2.7167900
  C     -4.0170400     -1.4811570      2.0030830
  C     -3.7855110     -2.9672670      1.8138080
  O     -2.6152890     -3.2168650      1.0073510
  C     -1.7743980     -4.1980060      1.6743420
  C     -2.6910060     -4.9158710      2.6595850
  C     -3.5873440     -3.7594790      3.1106980
  O     -4.8752010     -4.1149350      3.6347160
  H     -1.0190410     -0.1145710     -0.4111500
  H      0.6133610     -0.8111010     -0.4203910
  H      0.4046730      0.9545130     -0.4251280
  H     -0.4784480     -0.9032260      1.8614170
  H      1.3177350      0.6355930      3.9506180
  H      2.5849370      1.3769410      2.9241780
  H      0.8985560      2.6864250      1.7113250
  H     -0.4583570      2.5505390      4.1480470
  H     -1.3546630      1.7404640      1.4429840
  H     -4.9459390     -1.3417460      2.5702200
  H     -4.1144220     -0.9779910      1.0357620
  H     -4.6681350     -3.3700890      1.2930810
  H     -0.9588680     -3.6752660      2.1911880
  H     -1.3516360     -4.8500190      0.9066180
  H     -3.2962930     -5.6728500      2.1493650
  H     -2.1458710     -5.3837370      3.4830930
  H     -3.0564690     -3.1381870      3.8409390
  H     -4.7500880     -4.4248280      4.5447700

37
System: d8, CBS(T):
  C     -0.0102860      0.0091760     -0.0163380
  C      0.0085460     -0.0066210      1.5049610
  O      1.4046680      0.0068110      1.9537430
  C      1.6011280      1.0929040      2.8758400
  C      0.5426370      2.1276640      2.4831540
  O      0.2542170      3.0855100      3.4995260
  C     -0.6539500      1.2215680      2.1383030
  O     -1.2615810      0.9076550      3.4119310
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  P     -2.8249050      0.3846270      3.4974330
  O     -2.8554870     -0.8396150      4.3650370
  O     -3.4032190      0.3769070      2.1098770
  O     -3.4977940      1.5617250      4.4041760
  C     -3.5004500      2.9125030      3.8948480
  C     -4.2588510      3.8071750      4.8544120
  O     -5.6591320      3.4545190      4.8920750
  C     -6.0834370      3.3046360      6.2771010
  C     -5.0428920      4.0511540      7.1026880
  C     -3.7673360      3.7584470      6.3069060
  O     -2.7034370      4.7098550      6.4626360
  H     -1.0360880     -0.1112190     -0.3792510
  H      0.5958290     -0.8133320     -0.4065750
  H      0.3915830      0.9518170     -0.4018420
  H     -0.4614180     -0.9183330      1.8882970
  H      2.6271570      1.4489420      2.7628560
  H      1.4369070      0.7648340      3.9125500
  H      0.8575130      2.6867160      1.5993260
  H     -0.2881940      2.6043130      4.1523370
  H     -1.3927360      1.6842250      1.4835860
  H     -3.9700520      2.9296500      2.9055990
  H     -2.4715490      3.2796040      3.8026860
  H     -4.1623090      4.8393580      4.4861830
  H     -6.1070230      2.2363630      6.5274990
  H     -7.0923750      3.7147880      6.3600590
  H     -4.9923140      3.7023250      8.1370050
  H     -5.2368500      5.1289680      7.0936440
  H     -3.3977230      2.7541530      6.5387440
  H     -2.2117270      4.4776320      7.2648680

37
System: d4, CBS(T):
  C     -0.0249350      0.0007020     -0.0281570
  C      0.0114520     -0.0108500      1.4931770
  O      1.4127030      0.0196060      1.9281820
  C      1.6137420      1.1280330      2.8237800
  C      0.5354700      2.1414840      2.4293700
  O      0.2480720      3.1160990      3.4282900
  C     -0.6535040      1.2095010      2.1357940
  O     -1.2124760      0.8691200      3.4266640
  P     -2.8596950      0.8255980      3.5764680
  O     -3.3829690     -0.4460970      2.9724390
  O     -3.4251180      2.1551500      3.1579020
  O     -2.9094910      0.6328070      5.1873730
  C     -2.7321610      1.7845880      6.0409540
  C     -2.3764160      1.3063480      7.4352170
  O     -3.4111670      0.4657010      7.9868290
  C     -2.8240650     -0.7988360      8.4046750
  C     -1.3480150     -0.4977070      8.6343000
  C     -1.0735100      0.4964450      7.5020210
  O      0.0169470      1.4062580      7.7127340
  H     -1.0552850     -0.1125990     -0.3811710
  H      0.5696010     -0.8282520     -0.4225840
  H      0.3796300      0.9387210     -0.4217490
  H     -0.4454780     -0.9244740      1.8860240
  H      1.4728950      0.8191820      3.8697790
  H      2.6330540      1.4936790      2.6842000
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  H      0.8256310      2.6818200      1.5253510
  H     -0.3418390      2.6586060      4.0572610
  H     -1.4174890      1.6695110      1.5055090
  H     -3.6566100      2.3692280      6.0490020
  H     -1.9197430      2.4214200      5.6715700
  H     -2.2685360      2.1961970      8.0722450
  H     -2.9647940     -1.5401170      7.6074170
  H     -3.3560590     -1.1272420      9.2999340
  H     -1.1976120     -0.0027240      9.5995080
  H     -0.7190920     -1.3899140      8.5831070
  H     -0.9235410     -0.0396600      6.5582680
  H      0.8412400      0.9312560      7.5270440

37
System: d6, CBS(T):
  C      0.0039620      0.0078350     -0.0319410
  C      0.0074330     -0.0007560      1.4893070
  O      1.4002770      0.0167930      1.9461590
  C      1.5683970      1.0702900      2.9111540
  C      0.5309260      2.1213250      2.5060170
  O      0.2163330      3.0655870      3.5248710
  C     -0.6620340      1.2265510      2.1169620
  O     -1.3118220      0.8739130      3.3621750
  P     -2.9393040      1.0687870      3.5377890
  O     -3.4608800      2.0967910      2.5768170
  O     -3.1472810      1.1966800      5.0204310
  O     -3.5139480     -0.3618080      3.0048620
  C     -3.0926980     -1.5735520      3.6636740
  C     -4.0654290     -2.6895230      3.3424970
  O     -5.3501290     -2.4474010      3.9526310
  C     -6.4075250     -2.7288080      2.9886710
  C     -5.7448840     -3.5239600      1.8686200
  C     -4.3465430     -2.9007200      1.8513700
  O     -3.3028110     -3.7135050      1.2952780
  H     -1.0170550     -0.1189990     -0.4071450
  H      0.6170440     -0.8141050     -0.4124140
  H      0.4048860      0.9506740     -0.4173920
  H     -0.4642280     -0.9115990      1.8733660
  H      2.6004870      1.4205520      2.8479650
  H      1.3615330      0.7110890      3.9296810
  H      0.8773110      2.6881630      1.6386340
  H     -0.3760700      2.5912150      4.1391960
  H     -1.3821720      1.7149540      1.4591930
  H     -3.0503890     -1.4094540      4.7455400
  H     -2.0953230     -1.8560480      3.3072840
  H     -3.6404590     -3.6194330      3.7517360
  H     -7.1977490     -3.2757070      3.5084800
  H     -6.8100310     -1.7755690      2.6243320
  H     -5.6661180     -4.5839420      2.1324140
  H     -6.2705720     -3.4280440      0.9155230
  H     -4.3689110     -1.9318180      1.3410050
  H     -3.3471120     -3.6364330      0.3302250

37
System: h2, CBS(T):
  C     -0.0277190      0.0260700     -0.0270910
  C      0.0010260     -0.0072430      1.4938720
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  O      1.4008160     -0.0225180      1.9308360
  C      1.6159450      1.0376760      2.8764350
  C      0.5779860      2.0998340      2.5043760
  O      0.3214330      3.0499300      3.5338470
  C     -0.6382680      1.2228360      2.1475160
  O     -1.2600850      0.8826310      3.4143100
  P     -2.8901680      0.6396930      3.4263770
  O     -3.1879850      0.1735350      4.8233900
  O     -3.2994140     -0.1521540      2.2192030
  O     -3.5019730      2.1347830      3.1806910
  C     -3.2705730      3.1609750      4.1694120
  C     -3.8691630      4.4621500      3.6779700
  O     -5.2840480      4.3037690      3.4268380
  C     -6.0226790      5.3793570      4.0770450
  C     -4.9880480      6.4479200      4.4031400
  C     -3.7568530      5.5906760      4.7116650
  O     -2.4908110      6.2442820      4.5506070
  H     -1.0571400     -0.0793490     -0.3841040
  H      0.3818820      0.9684660     -0.4050620
  H      0.5667530     -0.7986380     -0.4305990
  H     -0.4849130     -0.9121400      1.8707940
  H      2.6484230      1.3778270      2.7738910
  H      1.4435120      0.6903630      3.9059200
  H      0.9013610      2.6636160      1.6265540
  H     -0.1968350      2.5684300      4.2047500
  H     -1.3608720      1.7222940      1.4999580
  H     -3.7346370      2.8589400      5.1146350
  H     -2.1952000      3.3013120      4.3216480
  H     -3.3762080      4.7710050      2.7457870
  H     -6.7994350      5.7142900      3.3857630
  H     -6.4962510      4.9836820      4.9840870
  H     -4.7796410      7.0733360      3.5289170
  H     -5.2848650      7.0844630      5.2400450
  H     -3.8296940      5.1764580      5.7261210
  H     -2.3762200      6.8576880      5.2929950

37
System: n4, CBS(T):
  C     -0.0767300     -0.0342420     -0.0682330
  C      0.0081980     -0.0253620      1.4479250
  O      1.4252980      0.0586220      1.8565650
  C      1.5763700      1.1135340      2.8376700
  C      0.5065710      2.1211230      2.4171550
  O      0.1823590      3.1257060      3.3766760
  C     -0.6488810      1.1753110      2.1233070
  O     -1.2586010      0.7528350      3.3654500
  P     -2.7869210      1.2529240      3.6666580
  O     -3.7970610      0.2572220      3.1790290
  O     -2.8555540      2.7031890      3.2312930
  O     -2.7740390      1.1470500      5.2879640
  C     -2.0512540      2.1345290      6.0646270
  C     -1.4054490      1.4661430      7.2590600
  O     -0.2506280      0.6943180      6.8827060
  C      0.8330300      0.9590630      7.8213280
  C      0.1943820      1.6762700      9.0078540
  C     -0.9142280      2.4677660      8.3092140
  O     -2.0213440      2.8759930      9.1206490
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  H     -1.1127340     -0.2007250     -0.3811050
  H      0.5400560     -0.8413650     -0.4740780
  H      0.2693910      0.9159210     -0.4873920
  H     -0.4087590     -0.9474310      1.8652090
  H      1.3770720      0.7478730      3.8536280
  H      2.6007170      1.4830260      2.7635980
  H      0.8167420      2.5937330      1.4754580
  H     -0.7983960      3.1568880      3.4273380
  H     -1.4063000      1.6408280      1.4873500
  H     -1.2815710      2.6090840      5.4506720
  H     -2.7667950      2.8872970      6.4107270
  H     -2.1441300      0.8024690      7.7352600
  H      1.5787520      1.5895370      7.3213100
  H      1.2930410      0.0032670      8.0839010
  H      0.9013390      2.3103420      9.5481390
  H     -0.2559440      0.9613870      9.7043930
  H     -0.4846920      3.3480100      7.8106310
  H     -1.7378340      3.6350860      9.6531180

37
System: i0, CBS(T):
  C     -0.0186090      0.0109800     -0.0507590
  C     -0.0029850     -0.0134530      1.4706590
  O      1.3984990     -0.0077040      1.9043890
  C      1.5888760      1.0330460      2.8767590
  C      0.5633660      2.1017570      2.4856360
  O      0.2626990      3.0409280      3.5176370
  C     -0.6447680      1.2239270      2.1110320
  O     -1.2638270      0.9249820      3.3809680
  P     -2.7963980      0.3463510      3.4550280
  O     -3.4459580      0.4937410      2.1079370
  O     -3.3956230      0.9495350      4.6955650
  O     -2.6059030     -1.2610160      3.6709730
  C     -2.3284690     -1.8382990      4.9671050
  C     -0.9322390     -2.4256670      5.0530860
  O      0.0653140     -1.3992970      4.9259890
  C      1.1351480     -1.6232130      5.8868730
  C      0.8638900     -2.9854540      6.5194950
  C     -0.6612520     -3.0802680      6.4137070
  O     -1.1937520     -4.4130490      6.4146020
  H      0.3642720      0.9647660     -0.4281670
  H      0.6055680     -0.7957710     -0.4458360
  H     -1.0403580     -0.1278610     -0.4198040
  H     -0.4768440     -0.9193440      1.8604780
  H      1.3738030      0.6673060      3.8890650
  H      2.6258580      1.3684960      2.8074430
  H      0.9052800      2.6698450      1.6172160
  H     -0.3918560      2.5810100      4.0803700
  H     -1.3684880      1.7107420      1.4560260
  H     -3.0571410     -2.6411090      5.1209230
  H     -2.4660000     -1.0747420      5.7392110
  H     -0.7945390     -3.1762140      4.2593000
  H      2.0894750     -1.5779400      5.3545570
  H      1.1034820     -0.8156280      6.6278660
  H      1.3089920     -3.7913020      5.9270200
  H      1.2276380     -3.0548440      7.5474850
  H     -1.1381820     -2.4929650      7.2096810
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  H     -1.1581930     -4.7481010      7.3238140

37
System: n6, CBS(T):
  C     -0.0032400      0.0075190     -0.0389290
  C      0.0007080     -0.0086320      1.4826460
  O      1.3953930     -0.0014330      1.9474890
  C      1.5930370      1.0961160      2.8556760
  C      0.5434580      2.1316700      2.4407350
  O      0.2482710      3.1111090      3.4335570
  C     -0.6524760      1.2272850      2.1087230
  O     -1.2576010      0.9288140      3.3892420
  P     -2.8383180      0.4880740      3.4879290
  O     -3.6148860      1.0634720      2.3396730
  O     -3.2229080      0.7486320      4.9166220
  O     -2.7648380     -1.1209110      3.2107590
  C     -2.0547750     -1.9401910      4.1651880
  C     -1.8784770     -3.3270920      3.5838450
  O     -1.1455350     -3.2699910      2.3401450
  C     -0.0459800     -4.2234310      2.3781490
  C     -0.3863020     -5.1931540      3.5032240
  C     -1.0673750     -4.2519370      4.5004600
  O     -1.9514610     -4.8635970      5.4488930
  H     -1.0260840     -0.1065710     -0.4133680
  H      0.5985770     -0.8218720     -0.4218640
  H      0.4092250      0.9452090     -0.4255690
  H     -0.4731200     -0.9195510      1.8580120
  H      2.6215260      1.4464960      2.7444760
  H      1.4208800      0.7822210      3.8955280
  H      0.8670540      2.6680110      1.5454810
  H     -0.3598970      2.6671960      4.0556500
  H     -1.3967090      1.6934290      1.4608270
  H     -1.0728340     -1.4944660      4.3642320
  H     -2.6219440     -1.9961920      5.1007560
  H     -2.8627120     -3.7774760      3.3925940
  H      0.0203320     -4.6929980      1.3942020
  H      0.8869230     -3.6815120      2.5797130
  H     -1.1045170     -5.9481090      3.1668750
  H      0.4942390     -5.6897640      3.9178310
  H     -0.3071170     -3.6674400      5.0366680
  H     -1.4091880     -5.3214290      6.1098720

37
System: j6, CBS(T):
  C      0.0070280      0.0074870     -0.0293440
  C      0.0077700      0.0012810      1.4905410
  O      1.3991360      0.0198980      1.9494790
  C      1.5267580      0.9904470      3.0021340
  C      0.5181790      2.0775790      2.6202740
  O      0.1689710      2.9667120      3.6763000
  C     -0.6674770      1.2263340      2.1244290
  O     -1.4122060      0.8413500      3.3071090
  P     -3.0513990      1.0300040      3.3071750
  O     -3.4161770      2.3768730      2.7528300
  O     -3.4760060      0.5937320      4.6790890
  O     -3.5309910     -0.0386300      2.1689540
  C     -3.4661170     -1.4559850      2.4544090
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  C     -4.8347040     -2.0866180      2.3112830
  O     -5.3013880     -1.9932490      0.9482340
  C     -5.8561490     -3.2774690      0.5315140
  C     -6.0160800     -4.0958380      1.8077260
  C     -4.8430720     -3.5815870      2.6479890
  O     -4.9762980     -3.7396520      4.0660660
  H     -1.0146710     -0.1130300     -0.4041460
  H      0.6149740     -0.8187060     -0.4090780
  H      0.4136800      0.9481260     -0.4140830
  H     -0.4655270     -0.9078310      1.8768470
  H      2.5631380      1.3326040      3.0169210
  H      1.2656940      0.5569090      3.9787900
  H      0.9103890      2.6853370      1.8011440
  H     -0.5007950      2.4886140      4.2017080
  H     -1.3238190      1.7629280      1.4375060
  H     -3.1041350     -1.6175950      3.4746250
  H     -2.7693970     -1.9068520      1.7399650
  H     -5.5437880     -1.5675940      2.9722210
  H     -6.7989260     -3.0843060      0.0140010
  H     -5.1542430     -3.7484010     -0.1672040
  H     -6.9538590     -3.8518850      2.3173370
  H     -5.9740510     -5.1724400      1.6264350
  H     -3.9055160     -4.0456930      2.3125700
  H     -4.8218710     -4.6733270      4.2775840

37
System: par2, CBS(T):
  C     -0.0122690      0.0128070     -0.0209780
  C      0.0075750     -0.0018730      1.4997100
  O      1.4053580      0.0066940      1.9432460
  C      1.5824110      1.0399070      2.9263540
  C      0.5499200      2.1040430      2.5438980
  O      0.2477730      3.0323990      3.5819280
  C     -0.6505510      1.2266130      2.1394800
  O     -1.3117150      0.8791100      3.3828410
  P     -2.9504050      0.6865110      3.3548920
  O     -3.2948040      0.2201820      4.7407320
  O     -3.3485470     -0.0867980      2.1325190
  O     -3.4985330      2.2012890      3.1022440
  C     -3.3355010      3.1978170      4.1327210
  C     -4.4666210      4.2110750      4.0594910
  O     -4.3851980      4.9519540      2.8142070
  C     -5.5868530      4.7332960      2.0309260
  C     -6.2360010      3.4823010      2.6172110
  C     -5.8689120      3.5997870      4.0988530
  O     -6.7223710      4.5597020      4.7668510
  H      0.3927910      0.9539050     -0.4069380
  H      0.5899960     -0.8123940     -0.4118430
  H     -1.0390010     -0.1038660     -0.3821170
  H     -0.4700010     -0.9079700      1.8855660
  H      1.3767200      0.6639430      3.9394310
  H      2.6159240      1.3867290      2.8671160
  H      0.8969680      2.6840170      1.6857710
  H     -0.3408530      2.5464380      4.1902280
  H     -1.3529670      1.7298980      1.4728470
  H     -2.3805650      3.7114800      3.9793410
  H     -3.3368620      2.7167970      5.1171010
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  H     -4.3422060      4.9148600      4.8913280
  H     -5.2855480      4.6216510      0.9864410
  H     -6.2409140      5.6086650      2.1278260
  H     -7.3183920      3.4503980      2.4647180
  H     -5.7842180      2.5791970      2.2012890
  H     -5.8893700      2.6416840      4.6277260
  H     -7.6310600      4.2222110      4.7194700

37
System: b4, CBS(T):
  C      0.0063830      0.0154610     -0.0367650
  C      0.0122690     -0.0024460      1.4832580
  O      1.4045470      0.0252440      1.9446600
  C      1.5444080      1.0387950      2.9571720
  C      0.5110790      2.0987770      2.5634900
  O      0.1637230      3.0157660      3.5976160
  C     -0.6670920      1.2116460      2.1275560
  O     -1.3445250      0.8262960      3.3457970
  P     -2.9875640      0.9456170      3.4114810
  O     -3.5680590      0.3481730      2.1588240
  O     -3.3788230      2.3323860      3.8393840
  O     -3.2300520     -0.0077830      4.7027490
  C     -2.9188990     -1.4143470      4.5908240
  C     -3.0294100     -2.0734730      5.9551690
  O     -1.9027090     -1.6766700      6.7808700
  C     -2.3803020     -1.0362610      7.9893920
  C     -3.8003690     -0.5813320      7.6680460
  C     -4.2881470     -1.7010380      6.7450690
  O     -4.6660410     -2.8749950      7.5039990
  H     -1.0151960     -0.1144920     -0.4081890
  H      0.6226350     -0.8010480     -0.4241330
  H      0.4018160      0.9627530     -0.4173180
  H     -0.4559980     -0.9168210      1.8631220
  H      1.3142510      0.6375040      3.9545790
  H      2.5759990      1.3950990      2.9318930
  H      0.8751860      2.6848870      1.7158300
  H     -0.5242480      2.5597940      4.1219310
  H     -1.3621730      1.7111750      1.4500680
  H     -3.6205890     -1.8857760      3.8932580
  H     -1.8991020     -1.5342990      4.2116790
  H     -2.9889730     -3.1596380      5.8092570
  H     -1.6966170     -0.2157070      8.2200220
  H     -2.3681280     -1.7607690      8.8137440
  H     -4.4312240     -0.4771730      8.5551230
  H     -3.7889090      0.3624880      7.1180900
  H     -5.1115500     -1.3941630      6.0929650
  H     -5.4123510     -2.6255960      8.0720810

37
System: b0, CBS(T):
  C      0.0075000      0.0148570     -0.0392320
  C      0.0115320     -0.0021900      1.4818020
  O      1.4068410      0.0148570      1.9378260
  C      1.5845390      1.0800360      2.8889110
  C      0.5389690      2.1251310      2.4878060
  O      0.2211200      3.0697640      3.5065110
  C     -0.6528200      1.2249300      2.1144700
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  O     -1.2858760      0.8878280      3.3683490
  P     -2.9229890      0.9072320      3.5633560
  O     -3.5676370      1.4355920      2.3118010
  O     -3.1693750      1.5321340      4.9063420
  O     -3.2529450     -0.6762060      3.7585180
  C     -3.4366020     -1.5002120      2.5895650
  C     -3.3617590     -2.9676490      2.9808640
  O     -2.0489210     -3.2860490      3.4952320
  C     -2.1550520     -3.7465710      4.8659370
  C     -3.5403290     -3.3140280      5.3416340
  C     -4.3658050     -3.3937060      4.0542310
  O     -4.7490760     -4.7560380      3.7522700
  H      0.4070290      0.9607930     -0.4181960
  H      0.6214460     -0.8039930     -0.4247460
  H     -1.0131490     -0.1105210     -0.4164550
  H     -0.4542390     -0.9147630      1.8681280
  H      2.6149750      1.4318010      2.8079360
  H      1.3919570      0.7313290      3.9137500
  H      0.8747950      2.6905880      1.6154200
  H     -0.3942010      2.5996610      4.1028990
  H     -1.3841740      1.7015300      1.4604380
  H     -2.6541840     -1.2877710      1.8536800
  H     -4.4093260     -1.2851860      2.1340430
  H     -3.5319010     -3.5560330      2.0702460
  H     -1.3385920     -3.2919970      5.4326520
  H     -2.0450890     -4.8381700      4.8850860
  H     -3.5221320     -2.2796870      5.6926910
  H     -3.9423860     -3.9564170      6.1299750
  H     -5.2520540     -2.7512710      4.0720960
  H     -5.3018960     -5.0720580      4.4847010

37
System: p4, CBS(T):
  C     -0.0515060     -0.0296800     -0.0385270
  C      0.0099030     -0.0256340      1.4824600
  O      1.4169230     -0.0127090      1.8961180
  C      1.6551070      1.1118010      2.7611730
  C      0.5771270      2.1300890      2.3797120
  O      0.3235520      3.1163480      3.3781620
  C     -0.6304870      1.2121260      2.1179030
  O     -1.1801360      0.9095540      3.4227830
  P     -2.8063840      0.6421490      3.5825450
  O     -3.0478050     -0.8310790      3.7382570
  O     -3.5307040      1.4341780      2.5288360
  O     -3.0272420      1.2797970      5.0618850
  C     -2.9679500      2.7121270      5.2275040
  C     -2.5111400      3.0480430      6.6390580
  O     -3.4716280      2.5455520      7.5999290
  C     -2.8410400      1.5630550      8.4633290
  C     -1.5557280      1.1511810      7.7498690
  C     -1.1605220      2.4459770      7.0350040
  O     -0.5407270      3.3772310      7.9481590
  H     -1.0852700     -0.1652680     -0.3733580
  H      0.5509180     -0.8524280     -0.4338860
  H      0.3306440      0.9106370     -0.4488570
  H     -0.4518800     -0.9304470      1.8907550
  H      2.6735960      1.4636980      2.5845760
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  H      1.5420440      0.8256610      3.8170110
  H      0.8500150      2.6623920      1.4660290
  H     -0.2130390      2.6499240      4.0462660
  H     -1.4056650      1.6655620      1.4986880
  H     -2.2801070      3.1578410      4.4993590
  H     -3.9653160      3.1282940      5.0546320
  H     -2.4690550      4.1405240      6.7257750
  H     -3.5468700      0.7402950      8.6000360
  H     -2.6315140      2.0270380      9.4346970
  H     -1.7537130      0.3728100      7.0098920
  H     -0.7765320      0.8090500      8.4362330
  H     -0.5071460      2.2712210      6.1728170
  H      0.2811960      2.9710170      8.2666520

37
System: p6, CBS(T):
  C      0.0066670      0.0126650     -0.0391530
  C      0.0102930      0.0001030      1.4812960
  O      1.4030800      0.0178290      1.9388350
  C      1.5588060      1.0428210      2.9361410
  C      0.5274130      2.1049650      2.5433190
  O      0.1943670      3.0250580      3.5793050
  C     -0.6605150      1.2234270      2.1198170
  O     -1.3286970      0.8685530      3.3532980
  P     -2.9663670      0.6766520      3.3839860
  O     -3.5970730      1.4131820      2.2396560
  O     -3.3623410      0.9373400      4.8097760
  O     -3.1227840     -0.9096770      3.0404990
  C     -2.6692610     -1.8821920      4.0012890
  C     -3.0750200     -3.2732980      3.5398330
  O     -4.5186120     -3.3846670      3.4966540
  C     -4.9536820     -3.6432340      2.1358840
  C     -3.7656700     -3.2814940      1.2475290
  C     -2.5779320     -3.6466350      2.1413500
  O     -2.3462060     -5.0745560      2.1472120
  H      0.3907820      0.9633770     -0.4222520
  H      0.6334140     -0.7977070     -0.4224760
  H     -1.0123470     -0.1304830     -0.4137480
  H     -0.4622310     -0.9111380      1.8632870
  H      2.5921030      1.3928550      2.8967160
  H      1.3369390      0.6559050      3.9412220
  H      0.8859510      2.6892160      1.6925390
  H     -0.4446330      2.5475280      4.1437520
  H     -1.3709620      1.7200690      1.4577150
  H     -3.1198140     -1.6677870      4.9755450
  H     -1.5769760     -1.8328450      4.0964060
  H     -2.6916450     -3.9926820      4.2734910
  H     -5.2179770     -4.7037410      2.0434990
  H     -5.8400910     -3.0322000      1.9486780
  H     -3.7479380     -2.2086940      1.0438900
  H     -3.7542970     -3.8325460      0.3030600
  H     -1.6567130     -3.1184740      1.8736180
  H     -2.1367440     -5.3392700      1.2372670

37
System: s4, CBS(T):
  C      0.0018220      0.0139150     -0.0392310
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  C      0.0086490     -0.0069500      1.4823210
  O      1.4013070      0.0105850      1.9402740
  C      1.5821310      1.0890580      2.8759120
  C      0.5352050      2.1287600      2.4626850
  O      0.2227320      3.0901650      3.4672710
  C     -0.6558320      1.2157060      2.1211930
  O     -1.2413640      0.8690440      3.3984950
  P     -2.8849450      0.8882280      3.5322260
  O     -3.4745740      0.0270710      2.4488390
  O     -3.3498640      2.3065800      3.7124340
  O     -3.0101670      0.1817050      4.9926400
  C     -2.9488270     -1.2600780      5.1058190
  C     -1.5166120     -1.7799590      5.1594240
  O     -0.8269530     -1.1877270      6.2911190
  C     -0.4146210     -2.2327970      7.2054470
  C     -1.3308600     -3.4114360      6.8986610
  C     -1.4816170     -3.2949380      5.3781170
  O     -0.3133000     -3.7991090      4.6941250
  H     -1.0195460     -0.1113320     -0.4135210
  H      0.6153740     -0.8046970     -0.4262520
  H      0.4025540      0.9594850     -0.4182660
  H     -0.4643420     -0.9185930      1.8606380
  H      1.3896920      0.7545780      3.9052320
  H      2.6121200      1.4403740      2.7871450
  H      0.8638040      2.6760440      1.5758270
  H     -0.4131860      2.6371960      4.0556940
  H     -1.3974440      1.6857200      1.4720030
  H     -3.4729510     -1.7079390      4.2551620
  H     -3.4759620     -1.5030290      6.0320360
  H     -0.9781110     -1.5078570      4.2485130
  H     -0.5175820     -1.8432050      8.2209400
  H      0.6368460     -2.4872340      7.0197510
  H     -2.3064710     -3.2822120      7.3791100
  H     -0.9175140     -4.3776460      7.1997850
  H     -2.3806320     -3.7915050      4.9968580
  H     -0.2541310     -4.7493310      4.8835300

37
System: o2, CBS(T):
  C     -0.0202170      0.0300870     -0.0249510
  C      0.0024140     -0.0036050      1.4958870
  O      1.4008690     -0.0144960      1.9366640
  C      1.6023520      1.0294510      2.9037200
  C      0.5688960      2.0970810      2.5338840
  O      0.2913190      3.0293540      3.5742480
  C     -0.6418960      1.2243320      2.1484390
  O     -1.2871800      0.8758150      3.4006960
  P     -2.9323380      0.7652610      3.4039300
  O     -3.2878830      0.3958820      4.8149620
  O     -3.3854810     -0.0480820      2.2272170
  O     -3.3983000      2.2949070      3.0653250
  C     -3.2657460      3.3228530      4.0703470
  C     -4.1035490      4.5157350      3.6238250
  O     -4.0344010      5.5154740      4.6718580
  C     -3.4012890      6.7170810      4.1529600
  C     -2.6426070      6.2623620      2.9113980
  C     -3.5684970      5.1752880      2.3537720
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O	-4.6982930	5.7387820	1.6522020
H	0.3939190	0.9715390	-0.4002170
H	0.5730080	-0.7963620	-0.4267310
H	-1.0485030	-0.0716420	-0.3865210
H	-0.4825210	-0.9099430	1.8717310
H	2.6362920	1.3702930	2.8207350
H	1.4155270	0.6651090	3.9247020
H	0.9040900	2.6744330	1.6692930
H	-0.2637150	2.5401190	4.2101490
H	-1.3522660	1.7322150	1.4942480
H	-3.6216150	2.9509880	5.0348400
H	-2.2139820	3.6164800	4.1613230
H	-5.1472670	4.2122310	3.4889180
H	-2.7618230	7.1193230	4.9415850
H	-4.1774100	7.4503600	3.9026550
H	-1.6783770	5.8202560	3.1833650
H	-2.4667380	7.0656810	2.1915170
H	-3.0499820	4.4563950	1.7122380
H	-4.3556150	6.2091700	0.8756310