Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

^{1}H chemical shift differences of Prelog-Djerassi lactone derivatives: A DFT and NMR conformational studies.

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SUPORTING INFORMATION

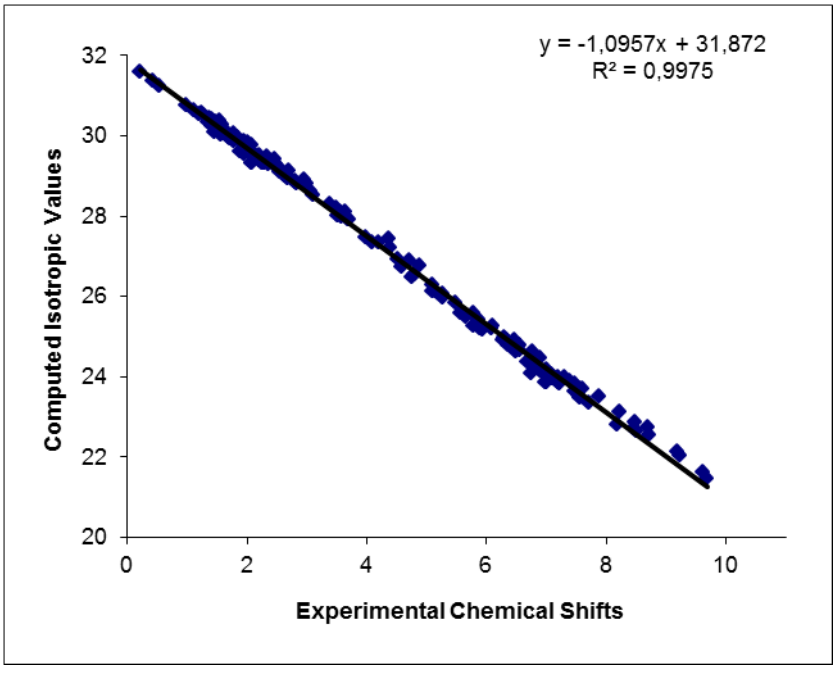
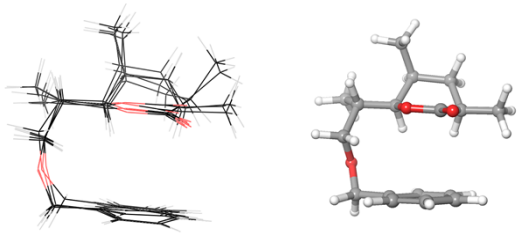
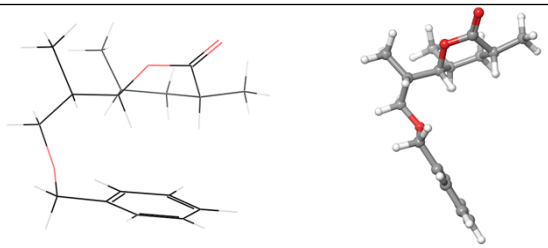


Figure S1. Scaling factor generated and used in this work at *mPW1PW91/6-311+G(2d,p)[SMD=$CHCl_3$]//M062X/6-31+G(d,p)[IEF-PCM-$CHCl_3$] level of theory.*

Table S1. Geometries of clustered-superposed conformers and reoptimized low-energy conformers at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$] of lactone **2'**.

Clusters	Reoptimized low-energy conformer	Clusters	Reoptimized Low-energy conformer
			
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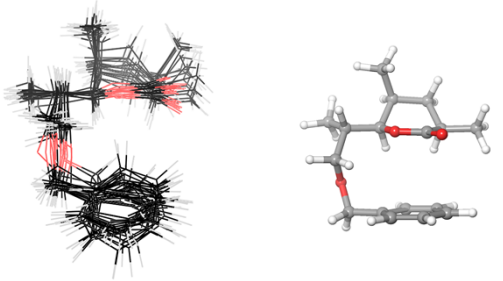		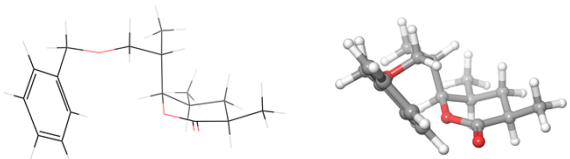	
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		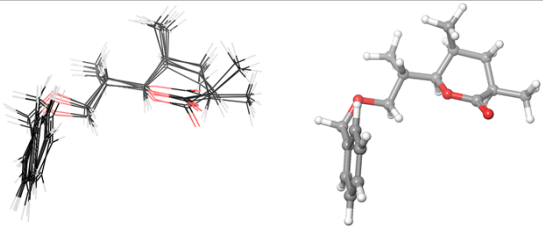	
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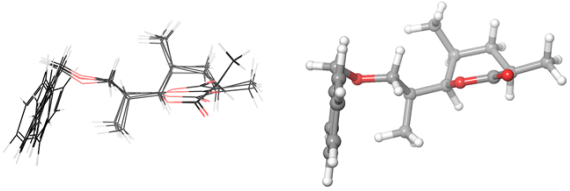		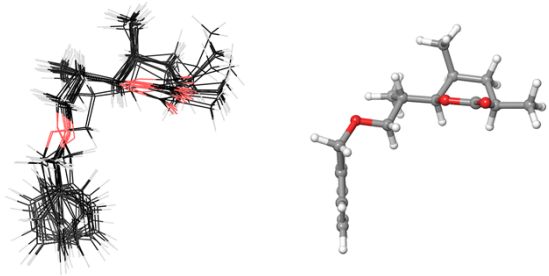	
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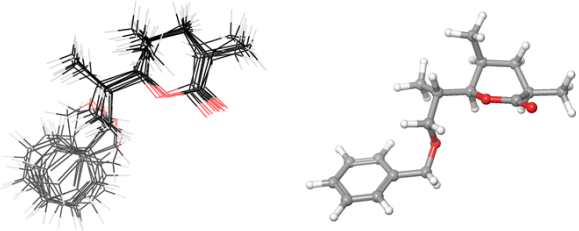		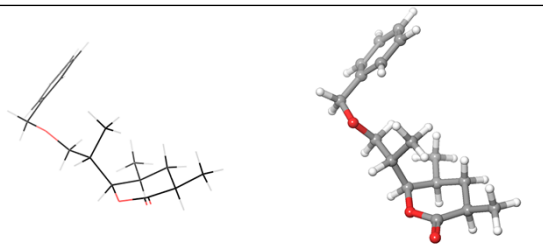	
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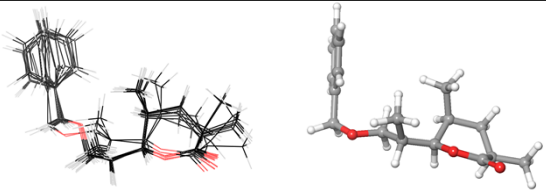		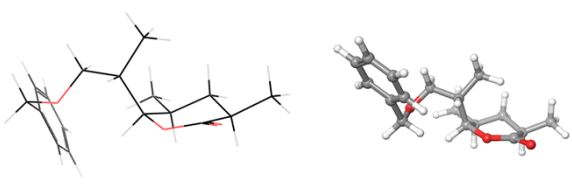	
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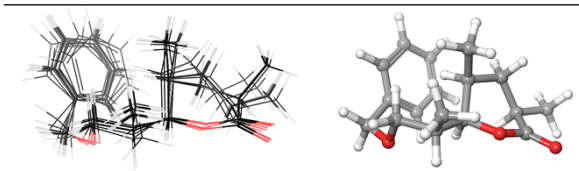

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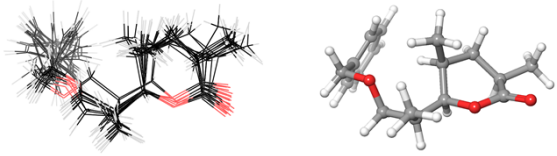

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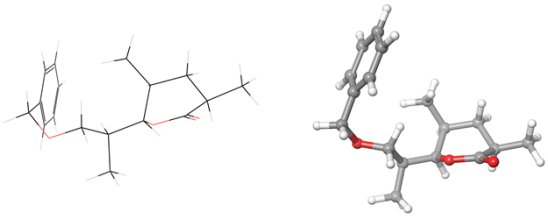

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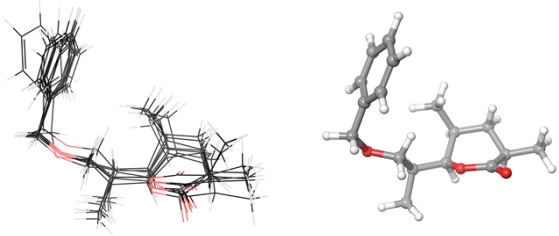

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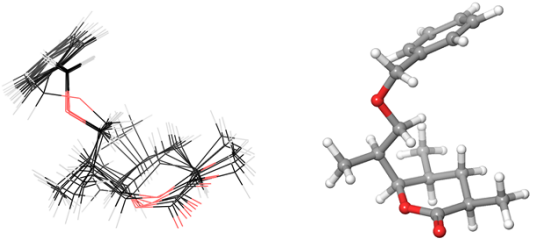

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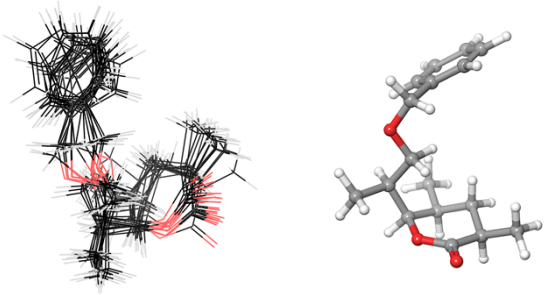

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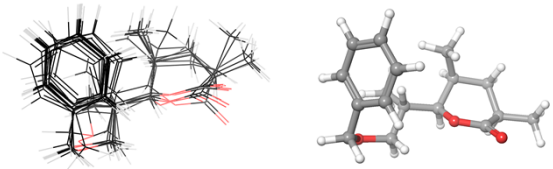

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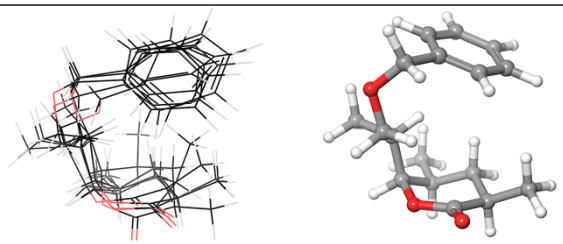

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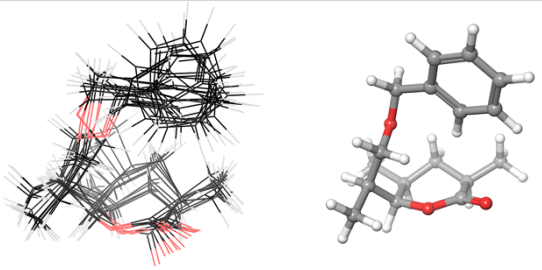

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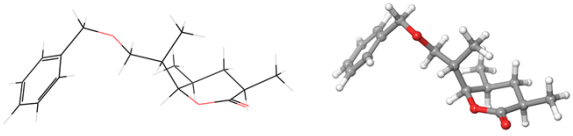

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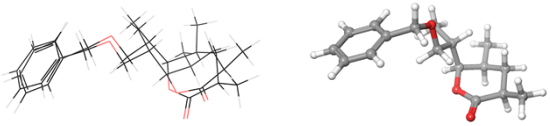

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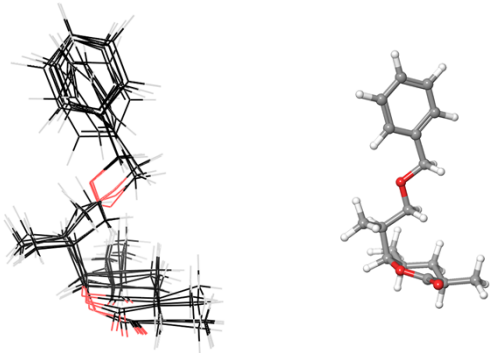

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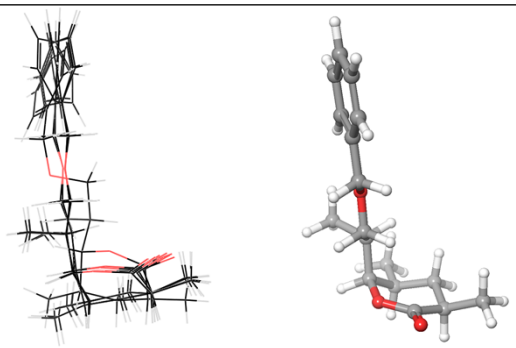

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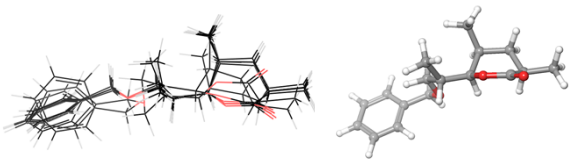

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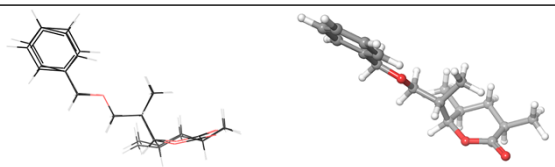

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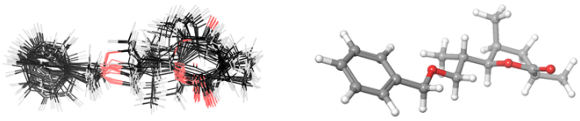


Cluster 28

Table S2. Electronic Energies (*E*), and Gibbs Free Energies (*G*) of low-energy conformers at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$] of lactone **2'**. The highlighted entries correspond to structures considered in the calculation of NMR properties and Boltzmann distribution.

	E (au)	ΔG (au)	ΔΔG (kcal mol^{-1})
2'-c1	-887.6188789	-887.279576	0.76
2'-c2	-887.6092029	-887.273528	4.56
2'-c3	-887.6188760	-887.280044	0.47
2'-c4	-887.6103997	-887.272343	5.30
2'-c5	-887.6133990	-887.275153	3.54
2'-c6	-887.6142475	-887.279493	0.82
2'-c7	-887.6107751	-887.275482	3.33
2'-c8	-887.6152124	-887.280596	0.12
2'-c9	-887.6164266	-887.280795	0.00
2'-c10	-887.6080388	-887.272077	5.47
2'-c11	-887.6099959	-887.274118	4.19
2'-c12	-887.6080291	-887.270454	6.49
2'-c13	-887.6141106	-887.274772	3.78
2'-c14	-887.6106080	-887.273865	4.35
2'-c15	-887.6116358	-887.275056	3.60
2'-c16	-887.6116383	-887.274802	3.76
2'-c17	-887.6103408	-887.275525	3.31
2'-c18	-887.6103325	-887.275028	3.62
2'-c19	-887.6149014	-887.277822	1.87
2'-c20	-887.6112686	-887.273049	4.86
2'-c21	-887.6100508	-887.271307	5.95
2'-c22	-887.6074805	-887.27223	5.37
2'-c23	-887.6099920	-887.274424	4.00
2'-c24	-887.6088462	-887.273472	4.60
2'-c25	-887.6088933	-887.274033	4.24
2'-c26	-887.6110858	-887.276328	2.80
2'-c27	-887.6063731	-887.271221	6.01
2'-c28	-887.6137569	-887.279765	0.65

Table S3. Electronic Energies (*E*), and Gibbs Free Energies (*G*) of low-energy conformers of lactone **3** at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$]. The highlighted entries correspond to structures considered in the calculation of NMR properties and Boltzmann distribution.

	E (au)	ΔG (au)	ΔΔG (kcal mol^{-1})
3-a	-542.161659957	-541.929605	3.93
3-b	-542.158512291	-541.926208	6.06
3-c	-542.162971594	-541.931344	2.84
3-d	-542.160166705	-541.928531	4.60
3-e	-542.167435634	-541.935864	0.00
3-f	-542.163469771	-541.931513	2.73

Table S4. Geometries of low-energy conformers at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$] of lactone **3'**.

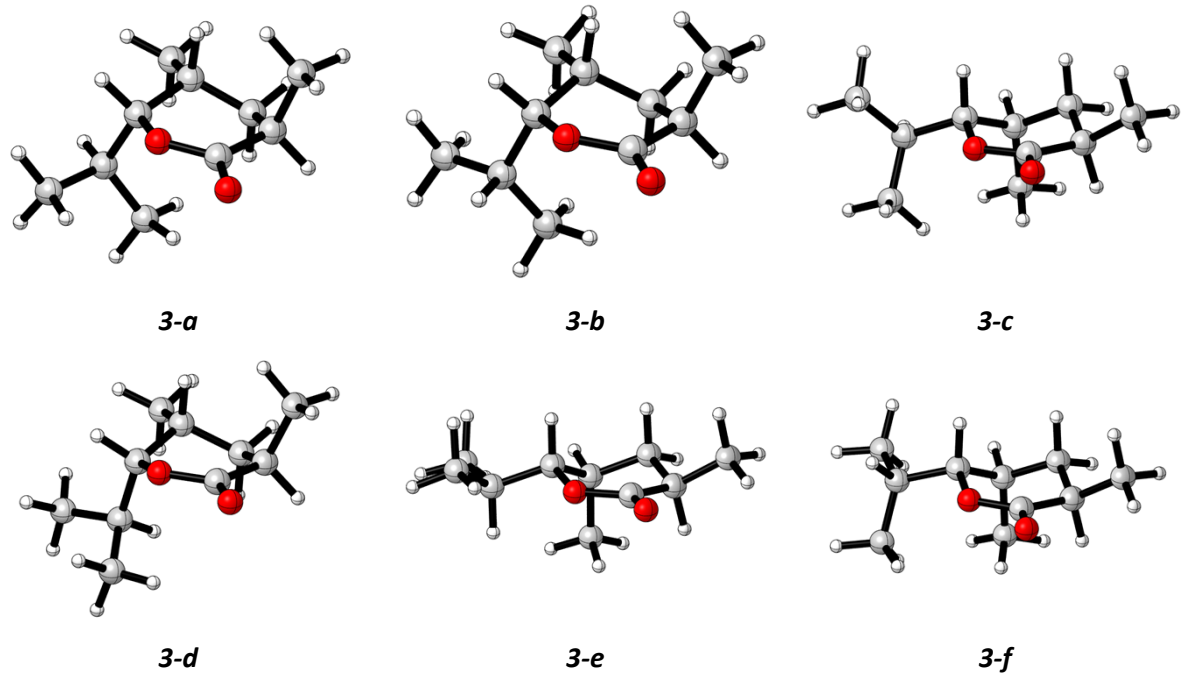
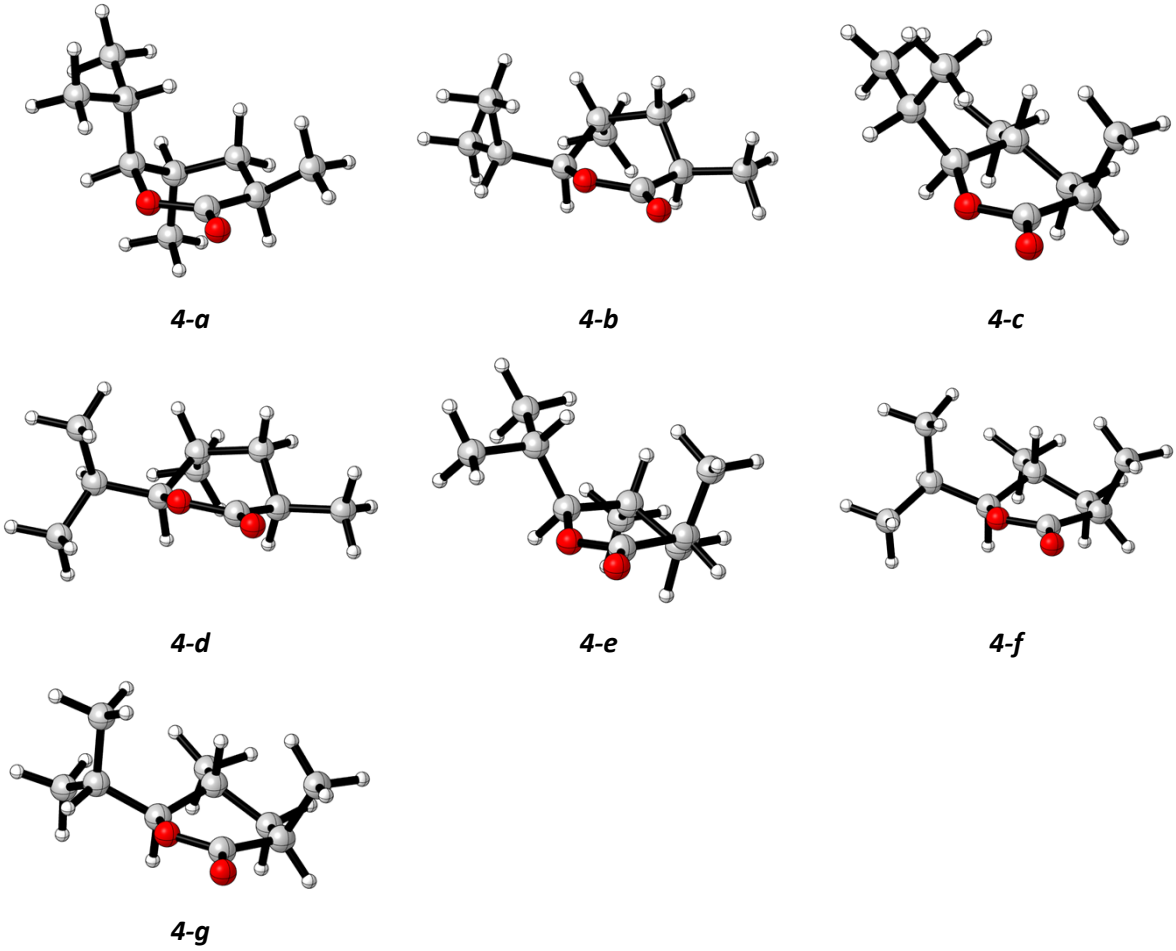


Table S5. Electronic Energies (*E*), and Gibbs Free Energies (*G*) of low-energy conformers of lactone **4** at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$]. The highlighted entries correspond to structures considered in the calculation of NMR properties and Boltzmann distribution.

	E (au)	ΔG (au)	ΔΔG (kcal mol^{-1})
4-a	-542.166001388	-541.9347860	0.78
4-b	-542.165598461	-541.9335850	1.54
4-c	-542.163255177	-541.9311630	3.06
4-d	-542.167007824	-541.9360330	0.00
4-e	-542.162965562	-541.9318120	2.65
4-f	-542.166957213	-541.9357130	0.20
4-g	-542.163698472	-541.9322580	2,37

Table S6. Geometries of low-energy conformers at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$] of lactone **4**.



4-a ***4-b*** ***4-c***

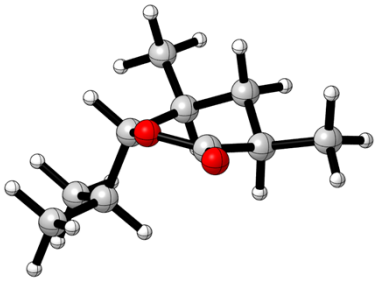
4-d ***4-e*** ***4-f***

4-g

Table S7. Electronic Energies (*E*), and Gibbs Free Energies (*G*) of low-energy conformers of lactone **5** at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$]. The highlighted entries correspond to structures considered in the calculation of NMR properties and Boltzmann distribution.

	E (au)	ΔG (au)	ΔΔG (kcal mol^{-1})
5-a	-542.165111039	-541.934328	2.12
5-b	-542.168231279	-541.937699	0.00
5-c	-542.165455587	-541.933345	2.73
5-d	-542.164560379	-541.932833	3.05
5-e	-542.159527296	-541.927868	6.17
5-f	-542.159870552	-541.927371	6.48
5-g	-542.164556618	-541.932514	3.25
5-h	-542.162398383	-541.930656	4.42
5-i	-542.161005843	-541.928502	5.77
5-j	-542.165102320	-541.934575	1.96
5-k	-542.164969875	-541.934009	2.32

Table S8. Geometries of low-energy conformers at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$] of lactone **5**.



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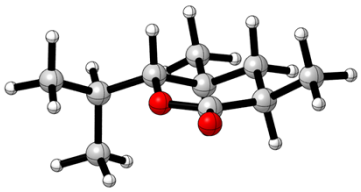

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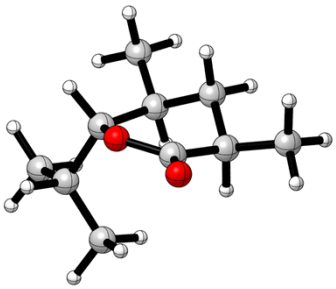

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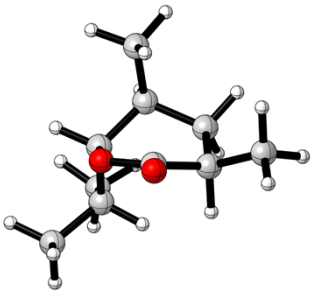

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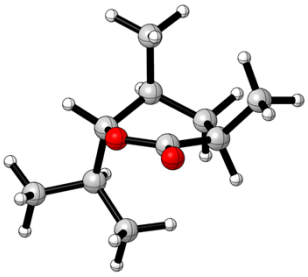

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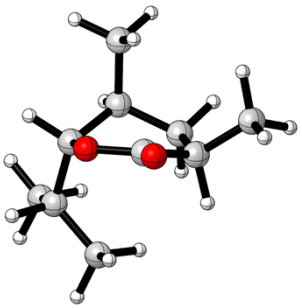

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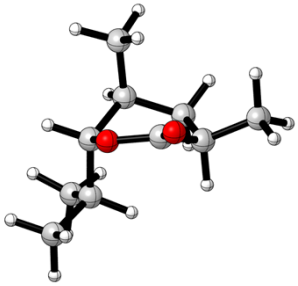

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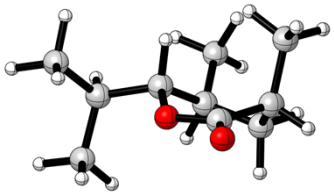

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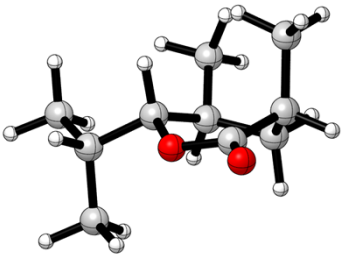

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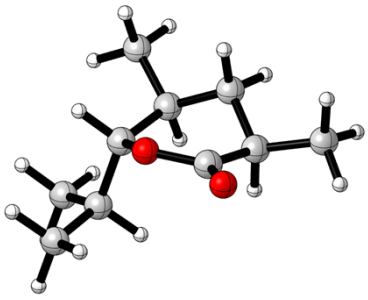

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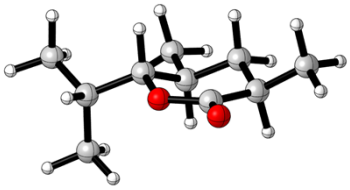
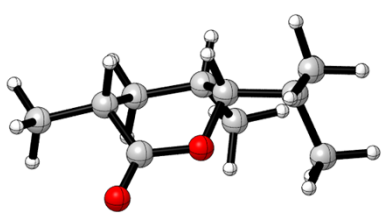


5-k

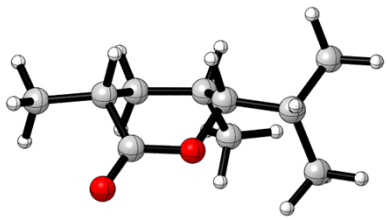
Table S9. Electronic Energies (*E*), and Gibbs Free Energies (*G*) of low-energy conformers of lactone **6** at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$]. The highlighted entries correspond to structures considered in the calculation of NMR properties and Boltzmann distribution.

	E (au)	ΔG (au)	ΔΔG (kcal mol^{-1})
6-a	-542.162896371	-541.9308840	3.20
6-b	-542.162602703	-541.9305000	3.44
6-c	-542.162600647	-541.9304660	3.46
6-d	-542.161745495	-541.9305930	3.38
6-e	-542.163541698	-541.9317730	2.64
6-f	-542.160308237	-541.9280030	5.01
6-g	-542.167572910	-541.9359860	0.00
6-h	-542.162897487	-541.9310290	3.11
6-i	-542.160047400	-541.9296100	4.00

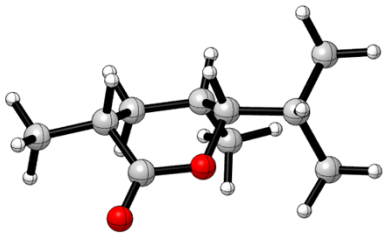
Table S10. Geometries of low-energy conformers at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$] of lactone **6**.



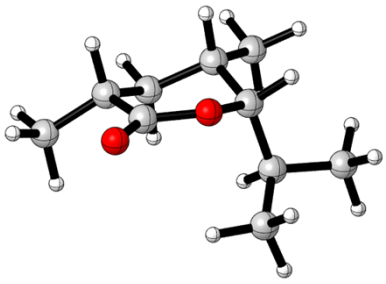
6-a



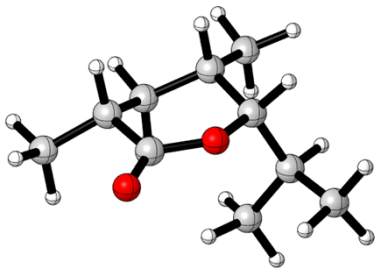
6-b



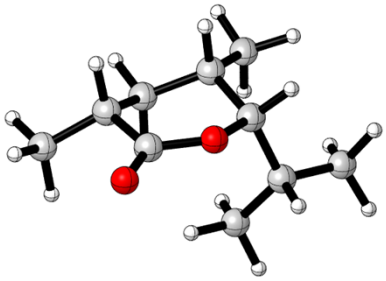
6-c



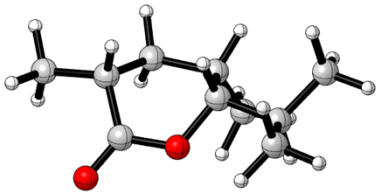
6-d



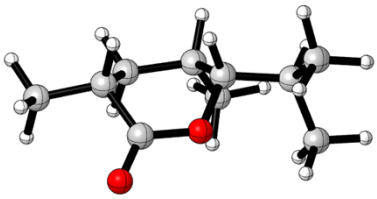
6-e



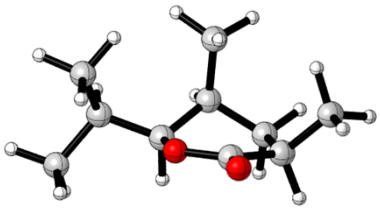
6-f



6-g



6-h



6-i

The Tables S11, S12, S13, and S14 follow the numeration depicted in the figure bellow.

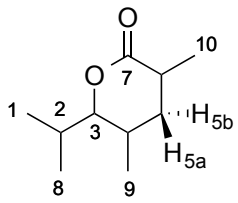


Table S11. Calculated ^{1}H NMR chemical shifts (ppm) of selected low-energy conformer of lactone **3** at mPW1PW91/6-311+G(2d,p)[SMD – $CHCl_3$]//M062X/6-31+G(d,p) [IEF-PCM-$CHCl_3$].

	3-e
1	1.04
2	1.70
3	3.59
4	2.05
5a	1.80
5b	1.62
6	2.52
8	0.88
9	0.99
10	1.19

Table S12. Calculated ^{1}H NMR chemical shifts (ppm) of selected low-energy conformers of lactone **4** at mPW1PW91/6-311+G(2d,p)[SMD – $CHCl_3$]//M062X/6-31+G(d,p) [IEF-PCM-$CHCl_3$].

	4-a	***4-b***	***4-d***	***4-f***	***av***
1	1.08	0.94	1.09	1.05	1.04
2	1.67	2.08	1.76	1.85	1.84
3	3.48	3.71	3.59	3.60	3.60
4	2.05	2.08	2.05	1.93	2.03
5a	1.58	1.45	1.48	1.70	1.55
5b	1.75	1.54	1.58	1.49	1.59
6	2.58	2.44	2.46	2.57	2.51
8	0.84	1.04	0.95	0.88	0.91
9	1.15	1.00	0.94	0.91	1.00
10	1.19	1.08	1.05	1.27	1.15

Table S13. Calculated ^{1}H NMR chemical shifts (ppm) of selected low-energy conformers of lactone **5** at mPW1PW91/6-311+G(2d,p)[SMD – $CHCl_3$]//M062X/6-31+G(d,p) [IEF-PCM-$CHCl_3$].

	5-a	*5-b*	*5-j*	*5-k*	*av*
1	1.04	1.05	1.04	0.99	1.00
2	1.61	1.89	1.64	1.91	1.76
3	3.32	3.65	3.31	3.67	3.48
4	1.94	1.87	1.94	1.90	1.91
5a	1.71	1.78	1.70	1.69	1.72
5b	1.30	1.32	1.34	1.37	1.33
6	2.23	2.46	2.25	2.41	2.34
8	0.95	0.87	0.96	1.07	0.96
9	1.05	0.91	1.06	0.99	1.01
10	1.12	1.21	1.12	1.19	1.16

Table S14. Calculated ^{1}H NMR chemical shifts (ppm) of selected low-energy conformers of lactone **6** at mPW1PW91/6-311+G(2d,p)[SMD – $CHCl_3$]//M062X/6-31+G(d,p) [IEF-PCM-$CHCl_3$].

	6-g
1	1.03
2	1.81
3	3.61
4	2.13
5a	2.27
5b	0.90
6	2.55
8	0.86
9	0.88
10	1.04

Table S15. Calculated ^{1}H NMR chemical shifts (ppm) of selected low-energy conformers of lactone **6'** at mPW1PW91/6-311+G(2d,p)[SMD – $CHCl_3$]//M062X/6-31+G(d,p) [IEF-PCM-$CHCl_3$].

	6'
1	1.06
2	1.65
3	3.62
4a	1.99
4b	1.45
5a	1.97
5b	1.70
6a	2.50
6b	2.27
8	0.87

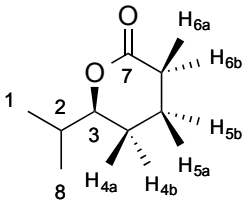
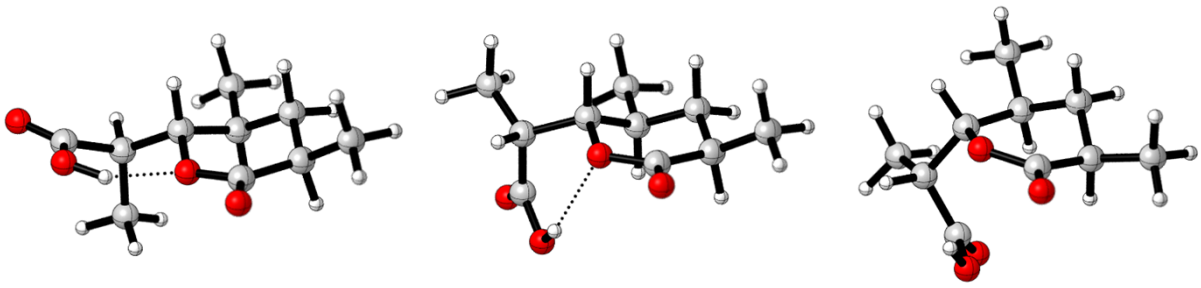


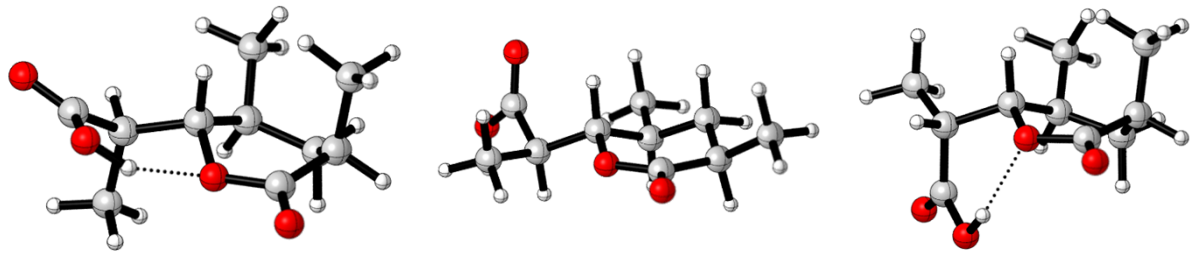
Table S16. Electronic Energies (*E*), and Gibbs Free Energies (*G*) of low-energy conformers of lactone **1** at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$].

	E (au)	ΔG (au)	ΔΔG (kcal mol^{-1})
1-a	-691.3896819	-691.174208	0.00
1-b	-691.3881658	-691.171776	1.53
1-c	-691.3863526	-691.169712	2.82
1-d	-691.3840265	-691.167033	4.50
1-e	-691.3839420	-691.167852	3.99
1-f	-691.3840918	-691.166536	4.81

Table S17. Geometries of low-energy conformers at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$] of lactone **1**.



1-a ***1-b*** ***1-c***

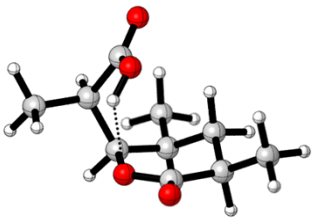


1-d ***1-e*** ***1-f***

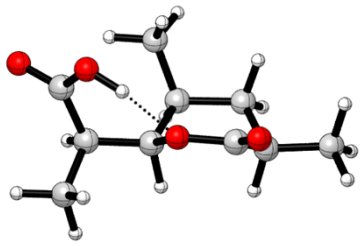
Table S18. Electronic Energies (*E*), and Gibbs Free Energies (*G*) of low-energy conformers of lactone **6''** at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$].

	E (au)	ΔG (au)	ΔΔG (kcal mol^{-1})
6''-a	-691.3856025	-691.168917	2.35
6''-b	-691.3878394	-691.170757	1.20
6''-c	-691.3890941	-691.172665	0.00
6''-d	-691.3856159	-691.169277	2.13
6''-e	-691.3867743	-691.170081	1.62
6''-f	-691.3795075	-691.162771	6.21
6''-g	-691.3778268	-691.16207	6.65
6''-h	-691.3797878	-691.162339	6.48
6''-i	-691.3825572	-691.165091	4.75
6''-j	-691.3827461	-691.165383	4.57

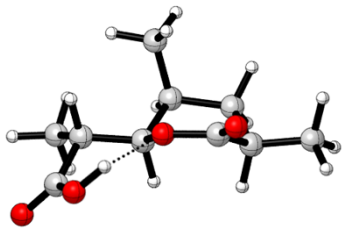
Table S19. Geometries of low-energy conformers at M06-2X/6-31+G(d,p) [IEF-PCM – $CHCl_3$] of lactone **6''**.



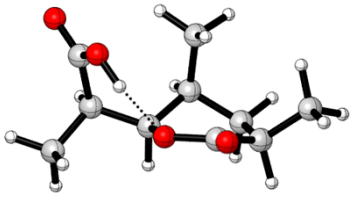
6''-a



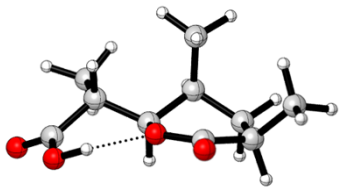
6''-b



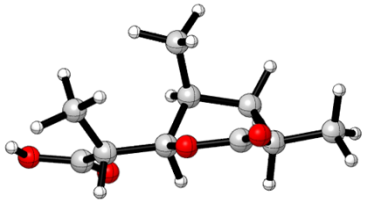
6''-c



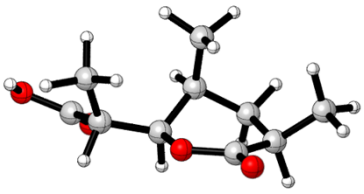
6''-d



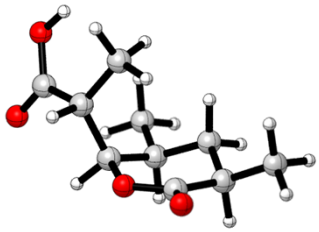
6''-e



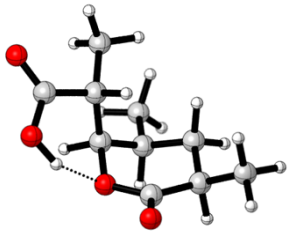
6''-f



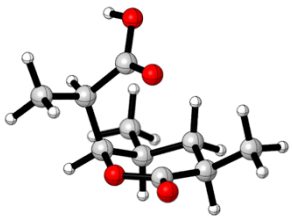
6''-g



6''-h



6''-i



6''-j

CARTESIAN COORDINATES

LACTONE 2'

clust-01

C	-6.73532	0.68006	2.67367
C	-8.06874	2.94202	2.21619
C	-8.21531	2.53712	3.68953
C	-7.37817	1.25651	3.95165
H	-5.96094	1.37912	2.33352
H	-7.02100	3.19681	2.00602
H	-7.80132	3.35860	4.28418
H	-8.02077	0.48101	4.38601
H	-6.58443	1.44912	4.67935
C	-7.78981	0.65105	1.58807
O	-8.11117	-0.32496	0.94888
O	-8.43068	1.81715	1.38162
C	-8.92851	4.11427	1.74730
H	-9.98130	3.80640	1.79145
C	-8.62121	4.42554	0.28474
H	-9.32474	5.18031	-0.09555
H	-8.73073	3.51322	-0.31309
C	-6.65546	4.60715	-1.04162
H	-5.78171	5.26256	-1.09762
H	-7.31382	4.83926	-1.89072
C	-5.47318	0.45684	-1.06621
C	-6.45565	0.90070	-1.94833
C	-6.83010	2.24518	-1.95679
C	-6.23058	3.15624	-1.08552
C	-5.24160	2.70268	-0.20535
C	-4.86226	1.36200	-0.19585
H	-5.18897	-0.59074	-1.04979
H	-6.94045	0.19952	-2.62008
H	-7.60205	2.58811	-2.64176
H	-4.77024	3.40916	0.47500
H	-4.09136	1.02059	0.48974
C	-8.71600	5.35062	2.62369
H	-7.65469	5.61280	2.66975
H	-9.25316	6.20523	2.20214
H	-9.07850	5.19549	3.64315
O	-7.29577	4.92966	0.18428
C	-9.67794	2.32437	4.08863
H	-9.73714	1.98764	5.12752
H	-10.26902	3.24011	3.99954
H	-10.14100	1.55671	3.45885
C	-6.11020	-0.68988	2.88400
H	-5.63758	-1.04662	1.96516
H	-5.35335	-0.63873	3.67173
H	-6.86977	-1.42006	3.17679

clust-02

C	-8.13300	-0.02923	3.08627
C	-8.58513	2.40505	2.08548
C	-7.71554	2.51897	3.34680
C	-7.50477	1.09562	3.93058
H	-7.61869	-0.07457	2.11676
H	-7.98789	1.86678	1.33887
H	-6.75040	2.90722	3.00106
H	-7.95890	1.04467	4.92812
H	-6.43973	0.88407	4.06232
C	-9.57196	0.35308	2.80640
O	-10.53328	-0.35885	2.98797
O	-9.75933	1.60848	2.35480
C	-9.08098	3.67899	1.39014
H	-9.49665	3.33309	0.43396
C	-7.90555	4.61271	1.09440
H	-7.51838	5.03755	2.02647
H	-8.25084	5.44528	0.46285
C	-7.03249	3.56881	-0.84893
H	-7.45764	4.41261	-1.41637
H	-7.76044	2.74497	-0.89492
C	-3.37079	2.32145	-2.75428
C	-4.60858	1.99512	-3.31117
C	-5.78405	2.39070	-2.67758
C	-5.73881	3.12315	-1.48710
C	-4.49955	3.44718	-0.93306
C	-3.32107	3.04509	-1.56438
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H	-4.65819	1.42723	-4.23508
H	-6.74667	2.12739	-3.11028
H	-4.46419	4.00868	-0.00581
H	-2.36204	3.29925	-1.12322
C	-10.20462	4.44651	2.09466
H	-9.84581	5.03505	2.94147
H	-10.67074	5.13760	1.38628
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H	-7.66221	3.33641	5.34258
H	-8.21847	4.50141	4.14359
H	-9.29786	3.19808	4.67980
C	-8.03890	-1.38953	3.76302
H	-8.48535	-2.16969	3.14341
H	-6.99077	-1.64215	3.94402
H	-8.56433	-1.37845	4.72214

clust-03

C	-7.00596	0.65079	2.67509
C	-8.20364	2.98478	2.19717
C	-8.48532	2.53707	3.63806
C	-7.71813	1.21768	3.92024
H	-6.17646	1.32214	2.41940
H	-7.13255	3.20029	2.07966
H	-8.09391	3.32184	4.29427
H	-8.41907	0.45705	4.28511
H	-6.97190	1.35886	4.70759
C	-7.96990	0.70578	1.50912
O	-8.27710	-0.23133	0.80776
O	-8.54362	1.90505	1.29663
C	-8.97537	4.20743	1.70410
H	-10.03901	3.94135	1.64940
C	-8.53535	4.55656	0.28442
H	-9.17312	5.35515	-0.12130
H	-8.63267	3.67263	-0.35652
C	-6.45595	4.68223	-0.86434
H	-5.55641	5.30328	-0.83058
H	-7.03010	4.95808	-1.76007
C	-5.43050	0.49045	-0.89066
C	-6.34378	0.98454	-1.81927
C	-6.66571	2.34233	-1.82683
C	-6.08397	3.21697	-0.90707
C	-5.16657	2.71257	0.02129
C	-4.83813	1.35827	0.02896

H	-5.18638	-0.56723	-0.87667
H	-6.81547	0.31221	-2.52872
H	-7.38202	2.72504	-2.55009
H	-4.71003	3.38984	0.74028
H	-4.12180	0.97737	0.75183
C	-8.79157	5.40328	2.64104
H	-7.72908	5.62056	2.78628
H	-9.25840	6.29287	2.20820
H	-9.24554	5.22828	3.61987
O	-7.18630	5.00464	0.31042
C	-9.98264	2.36588	3.90794
H	-10.13961	1.99937	4.92635
H	-10.53304	3.30484	3.80173
H	-10.41734	1.63569	3.21645
C	-6.46039	-0.75274	2.88687
H	-5.93382	-1.10403	1.99569
H	-5.76541	-0.75979	3.73126
H	-7.27159	-1.45541	3.09744

clust-04

C	-7.85905	0.34314	3.60355
C	-7.66951	3.25735	3.10955
C	-8.26549	2.68609	4.40276
C	-8.90465	1.33219	4.10903
H	-7.20894	0.07857	4.45075
H	-6.99695	4.08657	3.35242
H	-7.41556	2.51433	5.07880
H	-9.70713	1.44070	3.36688
H	-9.37221	0.92958	5.01426
C	-6.89307	0.95375	2.60046
O	-6.15958	0.27174	1.91706
O	-6.77637	2.28808	2.50397
C	-8.69746	3.76662	2.06918
H	-9.63076	3.19771	2.17930
C	-8.24335	3.54419	0.62892
H	-9.03586	3.90004	-0.04870
H	-8.07826	2.47845	0.42388
C	-6.69695	4.38313	-0.95864
H	-5.87682	5.10790	-0.99134
H	-7.53301	4.79769	-1.54350
C	-5.35952	0.67973	-2.72846
C	-5.29709	0.85828	-1.34609
C	-5.73072	2.05222	-0.77116
C	-6.24839	3.07190	-1.57282
C	-6.32383	2.88382	-2.95532
C	-5.87302	1.69741	-3.53349
H	-5.01947	-0.24922	-3.17595
H	-4.91956	0.06804	-0.70434
H	-5.69352	2.18155	0.30679
H	-6.73916	3.66857	-3.58411
H	-5.93339	1.56339	-4.60939
C	-8.99478	5.25693	2.27976
H	-8.09032	5.84459	2.10144
H	-9.75958	5.58889	1.57095
H	-9.35456	5.47606	3.28552
O	-7.05920	4.28453	0.40177
C	-9.23768	3.62971	5.10649
H	-9.53139	3.19575	6.06636
H	-8.78683	4.60688	5.30288
H	-10.14873	3.77886	4.51790
C	-8.47161	-0.94047	3.04527
H	-7.69703	-1.64877	2.74894
H	-9.10609	-1.40565	3.80463
H	-9.09081	-0.72043	2.16981

clust-05

C	-7.46887	0.63251	2.84989
C	-8.47979	3.25254	3.66257
C	-9.42566	2.06336	3.49439
C	-8.86337	1.11634	2.44299
H	-7.59844	-0.10915	3.65249
H	-8.80380	3.82614	4.53684
H	-9.42085	1.53998	4.46156
H	-8.82561	1.61751	1.46503
H	-9.51803	0.24667	2.31732
C	-6.59538	1.69090	3.51999
O	-5.40618	1.52906	3.68228
O	-7.15567	2.80127	4.03916
C	-8.37176	4.22141	2.46014
H	-9.25426	4.08030	1.82445
C	-7.16168	3.92508	1.57751
H	-7.06558	2.84918	1.37525
H	-6.23145	4.25463	2.06582
C	-6.35262	4.27031	-0.60644
H	-5.34407	4.42187	-0.19445
H	-6.48937	4.97401	-1.43322
C	-6.77414	0.22370	-2.05921
C	-7.90532	0.98918	-1.76884
C	-7.76551	2.29283	-1.29745
C	-6.49451	2.84486	-1.10458
C	-5.36802	2.07016	-1.38491
C	-5.50516	0.76711	-1.86722
H	-6.88269	-0.79265	-2.42471
H	-8.89672	0.56880	-1.90916
H	-8.64282	2.89107	-1.06375
H	-4.37656	2.48403	-1.21765
H	-4.62082	0.17418	-2.07910
C	-8.33931	5.67662	2.93151
H	-7.49834	5.83257	3.61686
H	-8.22262	6.35447	2.08244
H	-9.26211	5.93827	3.45830
O	-7.33530	4.61281	0.35208
C	-10.86082	2.49678	3.20280
H	-11.53383	1.64028	3.29736
H	-11.19542	3.26813	3.90431
H	-10.96810	2.88939	2.18728
C	-6.71868	-0.03290	1.69596
H	-5.75945	-0.43377	2.02662
H	-7.32397	-0.84814	1.28903
H	-6.53519	0.68261	0.88603

clust-06

C	-7.77485	0.45772	4.48321
C	-8.14101	2.59429	2.90566
C	-9.34435	2.41464	3.84079
C	-9.06496	1.23745	4.81097
H	-6.91444	1.08942	4.74355
H	-7.25569	2.85226	3.50661
H	-9.43258	3.33785	4.42285
H	-9.90203	0.53013	4.77605
H	-8.99674	1.58993	5.84411
C	-7.69684	0.24084	2.98725

O	-7.50213	-0.82210	2.44371
O	-7.87456	1.34275	2.23278
C	-8.29571	3.65006	1.81335
H	-9.07864	3.31623	1.12040
C	-6.99955	3.75615	1.01509
H	-6.70532	2.77224	0.62958
H	-6.18760	4.13282	1.66159
C	-6.08251	4.80153	-0.89417
H	-5.18693	5.03588	-0.29885
H	-6.29520	5.66631	-1.53106
C	-5.33753	1.37911	-3.42024
C	-6.63864	1.68423	-3.01798
C	-6.87814	2.78201	-2.19346
C	-5.81919	3.58231	-1.75623
C	-4.51841	3.26555	-2.15228
C	-4.27701	2.17320	-2.98605
H	-5.15134	0.52340	-4.06161
H	-7.46775	1.06441	-3.34530
H	-7.88861	3.01927	-1.87185
H	-3.68733	3.87469	-1.80407
H	-3.26086	1.93714	-3.28685
C	-8.67394	5.00802	2.40750
H	-7.95905	5.29923	3.18684
H	-8.65313	5.77035	1.62663
H	-9.67353	4.99901	2.84944
O	-7.20859	4.66298	-0.05355
C	-10.64623	2.19045	3.06691
H	-11.46905	2.01680	3.76591
H	-10.91098	3.04955	2.44468
H	-10.56386	1.31157	2.41809
C	-7.67669	-0.85498	5.24708
H	-6.73585	-1.36644	5.03425
H	-7.73669	-0.66412	6.32203
H	-8.49547	-1.52345	4.96667

clust-07

C	-8.47327	0.29242	4.58735
C	-7.84136	2.46778	3.16352
C	-9.27292	2.58985	3.70685
C	-9.63136	1.30502	4.49648
H	-7.66208	0.73673	5.18013
H	-7.16125	2.47799	4.02494
H	-9.24161	3.44003	4.39930
H	-10.47225	0.79948	4.00542
H	-9.96428	1.54889	5.50943
C	-7.92695	0.07766	3.19043
O	-7.74873	-0.99852	2.66787
O	-7.66093	1.19959	2.49301
C	-7.37493	3.56525	2.19896
H	-7.92309	4.48038	2.45982
C	-7.69510	3.24303	0.73996
H	-8.70136	2.82246	0.61533
H	-6.97639	2.50418	0.35962
C	-7.72180	4.26216	-1.38937
H	-7.81772	5.26585	-1.81491
H	-8.64449	3.70700	-1.61587
C	-4.30958	2.26484	-3.12240
C	-5.59816	1.86217	-3.46658
C	-6.70370	2.50002	-2.90014
C	-6.53147	3.54930	-1.99716
C	-5.23484	3.94864	-1.65613
C	-4.12994	3.30927	-2.21232
H	-3.44841	1.76600	-3.55586
H	-5.74526	1.04541	-4.16646
H	-7.70837	2.17366	-3.15801
H	-5.10054	4.75843	-0.94373
H	-3.12763	3.62441	-1.93851
C	-5.87468	3.82819	2.35102
H	-5.31048	2.90493	2.17690
H	-5.54404	4.57391	1.62381
H	-5.63584	4.19450	3.35388
O	-7.59385	4.45376	0.00683
C	-10.33770	2.87922	2.64747
H	-11.31724	2.95677	3.12886
H	-10.15107	3.81672	2.11597
H	-10.39179	2.06593	1.91583
C	-8.89564	-1.02189	5.22860
H	-8.05765	-1.71914	5.28616
H	-9.26991	-0.83830	6.23927
H	-9.69000	-1.49581	4.64511

clust-08

C	-8.40142	-0.19033	4.03343
C	-7.96776	2.11573	2.73658
C	-8.09751	2.37373	4.24375
C	-8.27419	1.02014	4.98058
H	-7.42396	-0.36742	3.56387
H	-7.05718	1.52617	2.55170
H	-7.15607	2.83073	4.56617
H	-9.18017	1.05745	5.59720
H	-7.43985	0.83479	5.66301
C	-9.35084	0.16676	2.90974
O	-10.29572	-0.49932	2.55340
O	-9.10010	1.33572	2.28936
C	-7.91737	3.35535	1.84639
H	-8.88266	3.87209	1.91848
C	-7.72838	2.93236	0.39259
H	-8.50702	2.21985	0.08935
H	-6.74667	2.44431	0.27407
C	-7.58900	3.81223	-1.79212
H	-7.87072	4.72651	-2.32401
H	-8.25831	3.00627	-2.12835
C	-3.48679	2.84739	-2.73579
C	-4.52621	2.20226	-3.40367
C	-5.85239	2.50048	-3.08591
C	-6.15114	3.45249	-2.11017
C	-5.10393	4.09485	-1.44219
C	-3.77937	3.79274	-1.75057
H	-2.45473	2.61274	-2.97699
H	-4.30673	1.46024	-4.16520
H	-6.66113	1.98564	-3.59915
H	-5.33820	4.82507	-0.67202
H	-2.97372	4.29542	-1.22402
C	-6.79119	4.29786	2.27508
H	-5.83048	3.76816	2.28713
H	-6.71365	5.12396	1.56548
H	-6.96155	4.71843	3.26942
O	-7.79946	4.08894	-0.42259
C	-9.24929	3.32788	4.57019
H	-9.34444	3.43884	5.65395
H	-9.09686	4.32302	4.14394
H	-10.19703	2.93363	4.18727

C	-8.84102	-1.45431	4.75875
H	-8.89352	-2.30406	4.07524
H	-8.13197	-1.68963	5.55708
H	-9.83062	-1.31635	5.20325

clust-09

C	-8.13183	0.11191	4.44098
C	-8.05222	2.16740	2.73133
C	-8.44932	2.66208	4.12868
C	-8.44972	1.46281	5.11296
H	-7.08053	0.12079	4.12266
H	-7.01827	1.80065	2.75383
H	-7.67650	3.37363	4.43910
H	-9.43761	1.37608	5.58165
H	-7.73303	1.62144	5.92381
C	-8.96005	-0.00119	3.17867
O	-9.65909	-0.94401	2.88296
O	-8.90812	1.06302	2.35652
C	-8.15502	3.19119	1.60282
H	-9.20980	3.47224	1.48838
C	-7.72361	2.57388	0.27653
H	-7.82928	3.32284	-0.52191
H	-8.35090	1.70755	0.02639
C	-5.84132	1.67120	-0.82755
H	-6.50369	0.90126	-1.25047
H	-4.89352	1.19032	-0.56495
C	-5.07919	4.76611	-3.74120
C	-5.50688	3.50630	-4.15714
C	-5.77162	2.51179	-3.21434
C	-5.59925	2.76194	-1.85213
C	-5.17138	4.02797	-1.44083
C	-4.91548	5.02565	-2.37912
H	-4.87925	5.54314	-4.47233
H	-5.64452	3.29926	-5.21396
H	-6.11859	1.53437	-3.54134
H	-5.05200	4.22551	-0.37872
H	-4.58717	6.00661	-2.04898
C	-7.32149	4.43734	1.91313
H	-6.28326	4.16367	2.12645
H	-7.32058	5.11055	1.05061
H	-7.71519	4.99023	2.76994
O	-6.36982	2.16334	0.38640
C	-9.80591	3.37118	4.13413
H	-10.07832	3.64779	5.15659
H	-9.79942	4.28399	3.53210
H	-10.58792	2.70999	3.74451
C	-8.36146	-1.07133	5.37038
H	-8.10667	-2.01314	4.88024
H	-7.74479	-0.96443	6.26692
H	-9.41068	-1.12227	5.67472

clust-10

C	-8.60616	0.55924	4.67812
C	-9.16859	2.13810	2.23279
C	-8.96615	0.61807	2.18935
C	-8.06273	0.12986	3.31744
H	-9.53392	-0.00499	4.85978
H	-10.07819	2.36440	1.66464
H	-9.96333	0.19301	2.37503
H	-7.04017	0.49879	3.18880
H	-8.00466	-0.96425	3.28970
C	-9.07170	2.00640	4.70887
O	-9.16737	2.63727	5.73876
O	-9.49708	2.58678	3.57326
C	-8.08243	3.10520	1.72187
H	-8.45445	4.08829	2.03964
C	-8.01674	3.18182	0.19827
H	-9.02783	3.17108	-0.24111
H	-7.45166	2.34178	-0.22477
C	-7.10244	4.51828	-1.51901
H	-6.78836	5.55590	-1.66844
H	-8.01997	4.35544	-2.10436
C	-3.97450	1.86675	-2.87281
C	-5.08817	2.09822	-3.67803
C	-6.10705	2.94358	-3.23483
C	-6.01642	3.57311	-1.99279
C	-4.89628	3.33675	-1.18929
C	-3.88246	2.48640	-1.62463
H	-3.18391	1.20507	-3.21252
H	-5.17005	1.61467	-4.64661
H	-6.98116	3.11191	-3.85949
H	-4.83228	3.81767	-0.21683
H	-3.01829	2.30766	-0.99201
C	-6.68916	2.92260	2.32451
H	-6.18833	2.03420	1.92510
H	-6.07332	3.79067	2.07735
H	-6.72607	2.84359	3.41646
O	-7.37204	4.39987	-0.13592
C	-8.49688	0.11323	0.82622
H	-8.58311	-0.97624	0.79070
H	-9.09835	0.52314	0.00836
H	-7.44769	0.36630	0.64570
C	-7.63135	0.27649	5.81823
H	-8.06772	0.53052	6.78479
H	-7.36327	-0.78357	5.81784
H	-6.71449	0.86129	5.69200

clust-11

C	-9.68985	0.13746	3.92700
C	-8.70331	2.02764	2.31180
C	-7.87983	0.73688	2.16669
C	-8.44913	-0.32848	3.14228
H	-10.51716	0.29800	3.22257
H	-9.71385	1.80701	1.94207
H	-8.04342	0.39282	1.13783
H	-7.67866	-0.58962	3.87828
H	-8.69501	-1.25148	2.60929
C	-9.36703	1.48353	4.54215
O	-9.52789	1.77845	5.70407
O	-8.82477	2.38794	3.70328
C	-8.25043	3.29567	1.57494
H	-9.10427	3.98298	1.64444
C	-8.05714	2.98306	0.09654
H	-8.92466	2.43478	-0.30749
H	-7.16419	2.35602	-0.04768
C	-7.51531	4.02738	-1.94768
H	-7.62440	5.00985	-2.41720
H	-8.19885	3.33187	-2.45765
C	-3.43103	2.68647	-2.35730
C	-4.40851	2.22056	-3.23482
C	-5.73201	2.64176	-3.09385
C	-6.08667	3.53992	-2.08644

C	-5.10144	4.00445	-1.20925
C	-3.78176	3.57796	-1.34130
H	-2.40266	2.35467	-2.46043
H	-4.14484	1.52191	-4.02287
H	-6.49508	2.26545	-3.77119
H	-5.38179	4.69338	-0.41686
H	-3.02508	3.94147	-0.65266
C	-7.03842	4.02234	2.16687
H	-6.09620	3.52624	1.92332
H	-6.99461	5.03352	1.75563
H	-7.12302	4.09515	3.25345
O	-7.90544	4.20526	-0.60017
C	-6.37361	0.89653	2.38939
H	-5.90491	-0.09167	2.42068
H	-5.89025	1.46389	1.59127
H	-6.17133	1.39603	3.34323
C	-10.12427	-0.86926	4.98299
H	-11.00543	-0.51802	5.52344
H	-10.36106	-1.82554	4.50901
H	-9.32423	-1.03113	5.71090

clust-12

C	-9.95056	1.33997	4.00047
C	-8.22343	1.48365	1.59596
C	-8.26075	0.24210	2.49521
C	-8.62218	0.58903	3.93607
H	-10.74584	0.63368	3.71623
H	-8.33014	1.13656	0.56375
H	-9.08708	-0.36712	2.10063
H	-7.83302	1.18338	4.40784
H	-8.70909	-0.33321	4.52200
C	-10.07134	2.43501	2.95219
O	-10.82829	3.37352	3.07561
O	-9.40011	2.31408	1.79472
C	-7.02411	2.45094	1.61149
H	-7.39467	3.32131	1.05254
C	-5.79432	1.92474	0.85877
H	-5.27292	1.15992	1.43740
H	-5.09729	2.76342	0.71779
C	-6.62683	2.19220	-1.37099
H	-7.61430	2.56596	-1.06494
H	-6.76721	1.56468	-2.25557
C	-4.00824	5.50085	-2.26574
C	-3.56255	4.18583	-2.42333
C	-4.41417	3.12227	-2.13813
C	-5.71856	3.35836	-1.68952
C	-6.15473	4.67391	-1.52892
C	-5.30538	5.74390	-1.81999
H	-3.34491	6.33038	-2.48991
H	-2.55261	3.99286	-2.77183
H	-4.07011	2.09776	-2.25634
H	-7.16531	4.86430	-1.17453
H	-5.65647	6.76321	-1.69296
C	-6.59466	2.96519	2.98610
H	-6.10242	2.18707	3.57795
H	-5.88523	3.78965	2.86743
H	-7.44668	3.34916	3.55672
O	-6.08685	1.31650	-0.38881
C	-6.98958	-0.60134	2.40746
H	-7.16746	-1.57853	2.86506
H	-6.68140	-0.76025	1.36944
H	-6.16157	-0.13192	2.94768
C	-10.25521	1.88354	5.39372
H	-11.23745	2.35615	5.42833
H	-10.22877	1.06712	6.12061
H	-9.50702	2.62700	5.68716

clust-13

C	-8.07034	-0.06925	2.03873
C	-8.41873	2.55797	1.72188
C	-6.97086	2.26281	2.15727
C	-6.85091	0.75442	2.48575
H	-8.19219	0.03950	0.95174
H	-8.54609	2.11670	0.72583
H	-6.35004	2.46607	1.27830
H	-6.74874	0.62481	3.57164
H	-5.94539	0.33903	2.03180
C	-9.27899	0.55972	2.70389
O	-10.11433	-0.03853	3.34355
O	-9.35802	1.90010	2.60498
C	-8.90720	4.00517	1.58983
H	-9.91848	3.91670	1.17110
C	-8.07619	4.74812	0.54944
H	-7.00570	4.67351	0.79269
H	-8.34508	5.81384	0.54547
C	-7.23640	4.23759	-1.62873
H	-6.77309	5.23389	-1.62401
H	-7.65924	4.06069	-2.62143
C	-4.43929	1.16160	-0.48611
C	-4.05624	2.49930	-0.41884
C	-4.94482	3.50146	-0.81893
C	-6.21789	3.17433	-1.28599
C	-6.59051	1.82592	-1.36131
C	-5.70977	0.82466	-0.96281
H	-3.75266	0.38214	-0.17049
H	-3.07068	2.76574	-0.04997
H	-4.64894	4.54601	-0.75490
H	-7.58434	1.56930	-1.72149
H	-6.00972	-0.21789	-1.02066
C	-9.02423	4.80646	2.89074
H	-8.06798	5.21833	3.21986
H	-9.70849	5.64576	2.73732
H	-9.42690	4.18576	3.69484
O	-8.33704	4.19190	-0.73178
C	-6.42853	3.09092	3.32331
H	-5.46119	2.68277	3.63379
H	-6.26981	4.13691	3.05109
H	-7.10203	3.05213	4.18630
C	-7.94681	-1.54605	2.38434
H	-8.83793	-2.09885	2.08031
H	-7.07775	-1.97359	1.87661
H	-7.81904	-1.67931	3.46255

clust-14

C	-8.16615	-0.21364	3.02882
C	-8.73690	2.08912	1.78264
C	-7.26286	2.07997	2.20526
C	-6.92766	0.66685	2.75334
H	-8.54486	-0.58379	2.06579
H	-8.86408	1.29217	1.03593
H	-6.68315	2.25533	1.29295
H	-6.37182	0.76465	3.69292

H	-6.27716	0.12547	2.05929
C	-9.28340	0.63236	3.60091
O	-9.92424	0.36573	4.59266
O	-9.56587	1.75778	2.91880
C	-9.35124	3.35033	1.15448
H	-10.31297	3.00823	0.74839
C	-8.53832	3.80899	-0.05308
H	-9.16170	4.44827	-0.69718
H	-8.22153	2.93850	-0.64997
C	-6.53938	4.90473	-0.68796
H	-5.87908	5.67510	-0.28010
H	-7.11594	5.34556	-1.51452
C	-4.25432	1.49712	-2.02345
C	-4.03523	2.04427	-0.75657
C	-4.76699	3.15410	-0.34250
C	-5.72884	3.72724	-1.18260
C	-5.94058	3.17435	-2.44636
C	-5.20574	2.06435	-2.86866
H	-3.68210	0.63409	-2.34918
H	-3.29068	1.60848	-0.09737
H	-4.59956	3.58308	0.64345
H	-6.68634	3.61415	-3.10456
H	-5.37906	1.64345	-3.85418
C	-9.66104	4.50321	2.11318
H	-8.75981	5.01134	2.45413
H	-10.28257	5.24100	1.59573
H	-10.21321	4.14120	2.98286
O	-7.40807	4.54718	0.37541
C	-6.89489	3.16391	3.22123
H	-6.92523	4.15402	2.76570
H	-7.57036	3.14656	4.08443
H	-5.87832	2.99085	3.58826
C	-7.84678	-1.40303	3.92349
H	-8.72041	-2.04386	4.05809
H	-7.04207	-1.99526	3.47899
H	-7.52168	-1.06242	4.91052

clust-15

C	-8.46702	0.47238	4.18254
C	-8.97599	1.57809	1.79571
C	-8.03090	0.37309	1.63959
C	-7.66303	-0.17513	3.03982
H	-9.53269	0.24763	4.03801
H	-9.94754	1.19129	2.12958
H	-8.63023	-0.37825	1.10995
H	-6.60027	0.01599	3.23632
H	-7.79638	-1.26012	3.08039
C	-8.30659	1.97455	4.05801
O	-7.98372	2.71867	4.95539
O	-8.50438	2.47898	2.82449
C	-9.22092	2.42101	0.54151
H	-9.17272	1.73831	-0.31664
C	-8.13007	3.47182	0.33543
H	-7.15609	3.11245	0.68098
H	-8.36560	4.38232	0.90731
C	-6.95948	4.59299	-1.37893
H	-6.95580	5.50104	-0.75824
H	-7.11010	4.88823	-2.42095
C	-3.28864	2.37712	-0.88952
C	-4.22903	1.98716	-1.84614
C	-5.40118	2.72078	-2.00968
C	-5.65058	3.84902	-1.22074
C	-4.70574	4.23204	-0.26756
C	-3.52705	3.50172	-0.10191
H	-2.37464	1.80572	-0.76052
H	-4.04600	1.11270	-2.46321
H	-6.13973	2.41472	-2.74686
H	-4.89777	5.10165	0.35665
H	-2.80173	3.80755	0.64570
C	-10.60107	3.08042	0.57131
H	-10.70905	3.69068	1.47471
H	-10.72992	3.73037	-0.29836
H	-11.40012	2.33316	0.56298
O	-8.07343	3.77747	-1.04915
C	-6.76407	0.62073	0.81624
H	-6.20315	-0.31549	0.73032
H	-6.98278	0.97289	-0.19630
H	-6.10679	1.35203	1.29999
C	-8.03469	-0.01952	5.55680
H	-8.61382	0.46131	6.34756
H	-8.17638	-1.10131	5.62565
H	-6.97807	0.20418	5.72945

clust-16

C	-8.48935	0.46932	4.25033
C	-8.73970	2.57299	2.60983
C	-9.14542	1.27579	1.88740
C	-8.87956	0.06648	2.81629
H	-9.32223	1.02600	4.70147
H	-9.48115	2.75343	3.39889
H	-10.22756	1.37507	1.73449
H	-8.05498	-0.53119	2.40697
H	-9.75146	-0.59301	2.85570
C	-7.31597	1.42397	4.15119
O	-6.28023	1.32322	4.76792
O	-7.45709	2.42640	3.26215
C	-8.66226	3.83743	1.75065
H	-9.42797	3.74035	0.97026
C	-7.31580	3.96496	1.03782
H	-6.90069	2.98514	0.78314
H	-6.58613	4.47062	1.68894
C	-6.36168	4.77230	-0.96351
H	-5.49846	5.13869	-0.38858
H	-6.58741	5.49997	-1.74790
C	-5.55398	0.87284	-2.62713
C	-4.62722	1.46502	-1.77138
C	-4.87704	2.73315	-1.24274
C	-6.04805	3.41975	-1.56680
C	-6.97179	2.81881	-2.42898
C	-6.72896	1.55301	-2.95615
H	-5.36372	-0.11420	-3.03707
H	-3.71427	0.93965	-1.50866
H	-4.15982	3.18906	-0.56421
H	-7.88955	3.34735	-2.67588
H	-7.45279	1.09572	-3.62391
C	-8.95402	5.09267	2.57528
H	-8.26165	5.15884	3.42173
H	-8.82961	5.98838	1.96068
H	-9.97579	5.08393	2.96627
O	-7.51674	4.73012	-0.14002
C	-8.50246	1.04503	0.51712
H	-8.90793	0.12659	0.08064

H	-8.69961	1.86280	-0.18265
H	-7.41714	0.91665	0.59825
C	-8.15670	-0.72992	5.12690
H	-7.87361	-0.41619	6.13353
H	-9.02445	-1.39125	5.19583
H	-7.32200	-1.29523	4.70261

clust-17

C	-7.67546	0.49724	3.86917
C	-9.38683	2.51170	2.52806
C	-9.36402	1.03773	2.09519
C	-8.02309	0.37034	2.38784
H	-8.43277	-0.06141	4.44021
H	-10.43076	2.77700	2.73067
H	-10.10372	0.53179	2.73179
H	-7.21587	0.79597	1.78126
H	-8.08021	-0.69188	2.12471
C	-7.81806	1.92402	4.37080
O	-7.19272	2.35268	5.31576
O	-8.72676	2.73269	3.80013
C	-8.86806	3.57533	1.54554
H	-9.47454	3.47623	0.63553
C	-7.41049	3.37645	1.14821
H	-7.27707	2.42332	0.62228
H	-6.75967	3.37407	2.04034
C	-5.74360	4.25519	-0.26652
H	-5.00249	4.08832	0.52947
H	-5.49952	5.20156	-0.75910
C	-5.56827	1.05026	-3.15720
C	-4.47252	1.31096	-2.33593
C	-4.53573	2.33649	-1.39123
C	-5.68557	3.11801	-1.26821
C	-6.78190	2.85137	-2.09456
C	-6.72533	1.82147	-3.03139
H	-5.52396	0.24864	-3.88775
H	-3.57186	0.71100	-2.42259
H	-3.68442	2.52779	-0.74207
H	-7.68235	3.45107	-1.98840
H	-7.58367	1.62029	-3.66532
C	-9.09141	4.97766	2.11993
H	-8.45826	5.14052	2.99675
H	-8.85042	5.73589	1.37356
H	-10.13475	5.10711	2.42452
O	-7.03071	4.43648	0.28876
C	-9.80988	0.85760	0.64399
H	-9.93536	-0.20661	0.42683
H	-10.76625	1.35516	0.45411
H	-9.07186	1.25680	-0.05983
C	-6.29515	-0.06046	4.20373
H	-6.09550	-0.00731	5.27461
H	-6.23278	-1.10374	3.88255
H	-5.51717	0.50639	3.68264

clust-18

C	-7.73854	0.46807	3.87476
C	-9.32493	2.65127	2.64888
C	-9.43797	1.19202	2.18063
C	-8.14485	0.41262	2.40408
H	-8.52363	-0.03635	4.45855
H	-10.33456	2.99225	2.90499
H	-10.19101	0.72954	2.83443
H	-7.32764	0.79267	1.78061
H	-8.29508	-0.63332	2.11396
C	-7.73710	1.88934	4.41104
O	-7.04011	2.24143	5.33723
O	-8.59312	2.78631	3.89337
C	-8.76725	3.69646	1.66810
H	-9.41938	3.66920	0.78501
C	-7.34897	3.39592	1.19907
H	-7.31328	2.44789	0.64873
H	-6.66060	3.32363	2.05927
C	-5.69795	4.17005	-0.29367
H	-4.93187	3.90167	0.44917
H	-5.39305	5.11018	-0.76400
C	-5.98172	1.09863	-3.31833
C	-7.07428	1.92572	-3.05194
C	-6.98374	2.91165	-2.07111
C	-5.80306	3.07761	-1.34075
C	-4.71756	2.24010	-1.60398
C	-4.80200	1.25911	-2.59294
H	-6.05179	0.33146	-4.08304
H	-7.99745	1.80288	-3.61030
H	-7.83310	3.55529	-1.85661
H	-3.80043	2.35292	-1.03044
H	-3.95020	0.61512	-2.78894
C	-8.85276	5.09660	2.28349
H	-8.16826	5.18708	3.13170
H	-8.58789	5.85270	1.54311
H	-9.86726	5.29872	2.64124
O	-6.92859	4.44444	0.34392
C	-9.95246	1.08586	0.74493
H	-10.17346	0.04125	0.50937
H	-10.87133	1.66410	0.60516
H	-9.21186	1.44131	0.02062
C	-6.40345	-0.21780	4.14914
H	-6.16393	-0.20677	5.21317
H	-6.44589	-1.25510	3.80622
H	-5.59543	0.28866	3.61204

clust-19

C	-7.68525	0.88128	4.56377
C	-8.01024	2.56108	2.50088
C	-9.15822	1.54167	2.54037
C	-8.97108	0.60246	3.76065
H	-7.78917	1.85558	5.06061
H	-8.07252	3.21087	3.38704
H	-10.08137	2.11594	2.67374
H	-8.92737	-0.43784	3.41596
H	-9.82471	0.66988	4.44109
C	-6.53504	1.01711	3.58889
O	-5.48239	0.42454	3.66152
O	-6.74682	1.85681	2.55817
C	-7.95501	3.44311	1.25819
H	-7.79890	2.78903	0.39442
C	-6.76364	4.40747	1.36530
H	-5.83012	3.84801	1.50349
H	-6.90730	5.05305	2.24212
C	-5.76536	4.82473	-0.76817
H	-4.76499	4.65846	-0.34395
H	-5.70583	5.64975	-1.48321
C	-7.34134	1.20803	-2.49674
C	-7.95601	2.43712	-2.75172

C	-7.41301	3.60779	-2.22930
C	-6.25630	3.56503	-1.44305
C	-5.63840	2.33625	-1.20761
C	-6.17869	1.15940	-1.73003
H	-7.76782	0.29361	-2.89740
H	-8.85782	2.47876	-3.35494
H	-7.89955	4.56379	-2.40849
H	-4.74582	2.29419	-0.58797
H	-5.69768	0.20738	-1.52830
C	-9.25458	4.22619	1.07536
H	-9.49267	4.80323	1.97771
H	-9.14319	4.92775	0.24545
H	-10.10164	3.57059	0.85623
O	-6.65000	5.27765	0.24879
C	-9.25821	0.73462	1.24265
H	-10.02965	-0.03448	1.34108
H	-9.51404	1.35943	0.38237
H	-8.30666	0.23528	1.02688
C	-7.40874	-0.18621	5.61294
H	-6.50978	0.04745	6.18683
H	-8.25525	-0.25798	6.30120
H	-7.26294	-1.16083	5.13887

clust-20

C	-6.93713	0.65373	3.42000
C	-8.53660	3.07639	2.90935
C	-9.18918	1.69231	3.00013
C	-8.18987	0.63203	2.54648
H	-7.22598	0.31451	4.42684
H	-9.14391	3.80402	3.45900
H	-9.40173	1.52225	4.06525
H	-7.91244	0.79378	1.49554
H	-8.64602	-0.36293	2.59938
C	-6.41588	2.06032	3.66276
O	-5.26575	2.29123	3.96479
O	-7.28384	3.08920	3.64459
C	-8.31424	3.60657	1.47399
H	-8.24285	2.75409	0.78807
C	-7.00652	4.41041	1.36724
H	-6.13499	3.79171	1.61454
H	-7.03218	5.24242	2.08098
C	-5.97985	4.24838	-0.78453
H	-4.99242	4.12831	-0.31671
H	-5.86546	4.87214	-1.67539
C	-7.70011	0.40616	-1.72027
C	-8.29342	1.58019	-2.19393
C	-7.71226	2.81420	-1.91726
C	-6.54103	2.89397	-1.15493
C	-5.95095	1.71760	-0.69105
C	-6.52490	0.47566	-0.97565
H	-8.15170	-0.55704	-1.93638
H	-9.20556	1.52895	-2.78053
H	-8.17622	3.73020	-2.27553
H	-5.04083	1.77363	-0.09724
H	-6.05904	-0.43428	-0.60867
C	-9.48319	4.49293	1.03375
H	-9.52396	5.39709	1.65297
H	-9.34595	4.80189	-0.00479
H	-10.44488	3.98314	1.11621
O	-6.83714	4.98202	0.07710
C	-10.50485	1.59073	2.23178
H	-10.95852	0.61262	2.41500
H	-11.21925	2.35761	2.54586
H	-10.34444	1.68622	1.15251
C	-5.83019	-0.25586	2.89474
H	-4.97882	-0.28092	3.57616
H	-6.21614	-1.27160	2.77158
H	-5.47850	0.09685	1.92009

clust-21

C	-8.43937	0.10201	2.17989
C	-8.66897	2.90566	3.07445
C	-9.85180	2.14527	2.43141
C	-9.39808	1.05463	1.46776
H	-8.96364	-0.30587	3.05806
H	-8.96786	3.12353	4.10672
H	-10.34672	1.62540	3.26385
H	-8.92275	1.49697	0.58618
H	-10.27222	0.49015	1.12360
C	-7.26227	0.86425	2.75810
O	-6.14795	0.39717	2.85728
O	-7.46387	2.10996	3.21708
C	-8.21469	4.26036	2.48926
H	-9.11706	4.83704	2.25847
C	-7.36362	4.17728	1.22971
H	-6.44602	3.60869	1.43764
H	-7.06795	5.19631	0.93720
C	-7.45505	3.69303	-1.08750
H	-7.24005	4.74925	-1.30993
H	-8.18939	3.34078	-1.81959
C	-3.85899	1.33284	-1.49371
C	-4.82537	0.97806	-0.55215
C	-5.97934	1.74668	-0.41816
C	-6.18124	2.87930	-1.20797
C	-5.20371	3.23623	-2.13957
C	-4.05209	2.46346	-2.28811
H	-2.95746	0.73809	-1.60149
H	-4.68236	0.11115	0.08632
H	-6.72901	1.47817	0.31914
H	-5.34191	4.12489	-2.75124
H	-3.30023	2.75068	-3.01682
C	-7.41204	5.02356	3.55150
H	-6.51470	4.46410	3.83306
H	-7.10190	6.00368	3.17836
H	-8.01218	5.18085	4.45197
O	-8.09123	3.58262	0.16919
C	-10.88475	3.07812	1.80122
H	-11.76415	2.49876	1.50510
H	-11.21582	3.85065	2.50305
H	-10.47353	3.56417	0.91250
C	-7.97331	-1.06001	1.30814
H	-7.30508	-1.72402	1.85861
H	-8.84098	-1.63253	0.96941
H	-7.43932	-0.69772	0.42391

clust-22

C	-9.35413	0.61510	4.69716
C	-7.89547	1.25271	2.19510
C	-7.26775	1.46099	3.57906
C	-8.32090	1.73771	4.64756
H	-8.84812	-0.28789	5.07216
H	-7.17101	0.70064	1.58544

H	-6.80510	0.49603	3.83216
H	-8.81898	2.69623	4.46962
H	-7.83511	1.81508	5.62692
C	-9.84080	0.19454	3.31982
O	-10.90142	-0.36469	3.14609
O	-9.03008	0.34988	2.25889
C	-8.36084	2.44937	1.34234
H	-8.89277	1.96850	0.51059
C	-7.20848	3.20092	0.67777
H	-6.41725	2.50326	0.36261
H	-6.75733	3.94368	1.35172
C	-6.80360	4.70761	-1.09884
H	-6.38444	5.43370	-0.38611
H	-7.37592	5.26124	-1.84944
C	-3.62717	2.51673	-3.03443
C	-3.33053	3.65057	-2.28104
C	-4.35537	4.35260	-1.64304
C	-5.68158	3.93635	-1.76294
C	-5.97243	2.79629	-2.51982
C	-4.95195	2.08867	-3.14990
H	-2.83204	1.96605	-3.52721
H	-2.30257	3.98542	-2.18180
H	-4.12056	5.23058	-1.04591
H	-7.00414	2.46431	-2.60239
H	-5.18777	1.20390	-3.73332
C	-9.33800	3.41134	2.01809
H	-8.84238	4.02672	2.77598
H	-9.75915	4.08375	1.26693
H	-10.17011	2.87804	2.49029
O	-7.74326	3.87177	-0.45117
C	-6.16291	2.51559	3.58071
H	-5.61357	2.46863	4.52500
H	-5.44607	2.35848	2.76831
H	-6.57547	3.52495	3.48953
C	-10.52972	0.93439	5.61668
H	-11.22059	0.09318	5.68307
H	-10.15916	1.16880	6.61836
H	-11.08260	1.80271	5.24428

clust-23

C	-9.65096	0.46747	3.64751
C	-7.13735	1.95114	3.24916
C	-7.90452	2.01955	4.57259
C	-9.39252	1.82547	4.29780
H	-9.45939	-0.30776	4.40499
H	-6.06659	1.84694	3.45468
H	-7.55937	1.16639	5.17369
H	-9.76840	2.62692	3.64743
H	-9.96207	1.88982	5.23135
C	-8.65548	0.13132	2.54762
O	-8.87517	-0.71244	1.70706
O	-7.44503	0.71886	2.54882
C	-7.33291	3.17022	2.31444
H	-8.26267	3.69000	2.58064
C	-7.46505	2.75035	0.85231
H	-8.32192	2.07836	0.70072
H	-6.55942	2.21577	0.52738
C	-7.68878	3.66683	-1.30865
H	-8.05255	4.59058	-1.76973
H	-8.41166	2.86876	-1.53459
C	-3.81839	2.69796	-2.95867
C	-4.95872	2.05000	-3.42990
C	-6.20826	2.34995	-2.88476
C	-6.33045	3.30619	-1.87584
C	-5.18241	3.95124	-1.40524
C	-3.93293	3.64758	-1.94123
H	-2.84480	2.46127	-3.37634
H	-4.87638	1.30318	-4.21357
H	-7.09426	1.83140	-3.24323
H	-5.27743	4.68356	-0.60768
H	-3.04701	4.15139	-1.56663
C	-6.16322	4.14825	2.46782
H	-5.24038	3.68499	2.09838
H	-6.34604	5.05400	1.88647
H	-6.00450	4.43293	3.51059
O	-7.65448	3.92365	0.08110
C	-7.62398	3.29664	5.36143
H	-8.13897	3.25179	6.32507
H	-6.55484	3.42286	5.55699
H	-7.98509	4.18463	4.83247
C	-11.08459	0.31353	3.14466
H	-11.25683	-0.68484	2.74072
H	-11.78331	0.48845	3.96725
H	-11.29410	1.04386	2.35664

clust-24

C	-8.92797	0.17822	4.19307
C	-8.56154	3.04581	3.54328
C	-9.93949	2.37091	3.51250
C	-9.84107	0.88242	3.19215
H	-9.40893	0.23306	5.18164
H	-8.64769	3.93539	4.17734
H	-10.32564	2.44155	4.53934
H	-9.47338	0.71217	2.17419
H	-10.83836	0.43086	3.24023
C	-7.61010	0.90935	4.39062
O	-6.60299	0.35165	4.76756
O	-7.56443	2.24172	4.22131
C	-7.94600	3.53623	2.22054
H	-8.65738	4.25629	1.79634
C	-7.73294	2.42629	1.19518
H	-8.69243	2.02553	0.83835
H	-7.15787	1.59545	1.64151
C	-6.80537	1.99930	-0.91454
H	-7.76787	1.63614	-1.30805
H	-6.27530	1.12976	-0.49291
C	-4.44492	3.63442	-4.13032
C	-4.55989	4.33301	-2.93019
C	-5.32761	3.81755	-1.88405
C	-5.98900	2.59796	-2.03342
C	-5.87447	1.90211	-3.24117
C	-5.10565	2.41405	-4.28326
H	-3.84758	4.03694	-4.94237
H	-4.05078	5.28379	-2.80445
H	-5.42019	4.35935	-0.94887
H	-6.39248	0.95378	-3.36639
H	-5.02536	1.86390	-5.21578
C	-6.63053	4.27056	2.50177
H	-5.86387	3.57037	2.84533
H	-6.26860	4.76325	1.59833
H	-6.77359	5.02785	3.27885
O	-7.02301	2.95677	0.09545

C	-10.91856	3.11017	2.60152
H	-11.92449	2.70192	2.73111
H	-10.95540	4.17851	2.83694
H	-10.64810	3.00404	1.54622
C	-8.68722	-1.28782	3.84388
H	-8.08050	-1.78169	4.60367
H	-9.64531	-1.80822	3.76181
H	-8.16753	-1.37204	2.88411

clust-25

C	-8.47446	0.35069	4.57734
C	-8.73229	3.02490	3.36694
C	-9.95613	2.24962	3.86294
C	-9.68464	0.75373	3.73696
H	-8.75682	0.44620	5.63691
H	-8.81593	4.07266	3.67535
H	-10.05689	2.48411	4.93209
H	-9.51440	0.48349	2.68589
H	-10.55753	0.18074	4.06808
C	-7.30584	1.31441	4.44065
O	-6.17193	1.01035	4.73808
O	-7.53777	2.58526	4.06279
C	-8.50921	2.98906	1.83519
H	-9.02151	2.11595	1.41029
C	-7.02980	2.84470	1.48334
H	-6.61417	1.90867	1.88360
H	-6.44909	3.67659	1.91312
C	-5.58086	2.70157	-0.35414
H	-5.17469	1.73730	-0.01120
H	-4.95836	3.49419	0.09187
C	-5.28488	2.96904	-4.64737
C	-6.45880	3.36168	-4.00739
C	-6.56949	3.27148	-2.61857
C	-5.50520	2.78357	-1.85895
C	-4.33087	2.38577	-2.50600
C	-4.21823	2.47999	-3.89087
H	-5.20071	3.03968	-5.72727
H	-7.29384	3.74008	-4.58931
H	-7.48268	3.57416	-2.11728
H	-3.50034	1.99768	-1.92052
H	-3.30111	2.16706	-4.38044
C	-9.07805	4.25452	1.18488
H	-8.50648	5.13147	1.51069
H	-9.00778	4.18801	0.09762
H	-10.12455	4.41448	1.45394
O	-6.91471	2.84857	0.07474
C	-11.25014	2.66193	3.16499
H	-12.09341	2.13169	3.61611
H	-11.43688	3.73560	3.26249
H	-11.23073	2.41012	2.09967
C	-8.02480	-1.08575	4.32029
H	-7.20192	-1.36623	4.97881
H	-8.86201	-1.76836	4.48926
H	-7.69135	-1.20315	3.28435

clust-26

C	-8.37165	-0.08217	4.25583
C	-8.37557	1.68127	2.25087
C	-7.63404	2.27557	3.45720
C	-7.65658	1.23576	4.61086
H	-7.78919	-0.60394	3.48459
H	-7.78932	0.82310	1.90492
H	-6.59799	2.41479	3.12546
H	-8.17882	1.66670	5.47405
H	-6.64155	1.00342	4.94602
C	-9.70944	0.26304	3.63441
O	-10.77563	-0.20205	3.96857
O	-9.67174	1.18875	2.65794
C	-8.61571	2.55162	1.00933
H	-8.93509	1.84712	0.22977
C	-7.31150	3.17775	0.53604
H	-6.94258	3.91374	1.27005
H	-7.48221	3.71020	-0.41047
C	-5.07706	2.64959	-0.02575
H	-4.39731	1.79444	0.04045
H	-4.73124	3.41415	0.68651
C	-5.00772	4.21274	-4.04884
C	-4.31050	4.86747	-3.03541
C	-4.34642	4.37223	-1.73059
C	-5.06614	3.21502	-1.43117
C	-5.76485	2.56301	-2.45238
C	-5.73875	3.06002	-3.75318
H	-4.98657	4.59935	-5.06290
H	-3.74606	5.76814	-3.25631
H	-3.81180	4.89215	-0.93911
H	-6.33663	1.66954	-2.21573
H	-6.28729	2.54859	-4.53825
C	-9.71057	3.61714	1.13042
H	-9.38388	4.49472	1.69224
H	-9.99934	3.95410	0.13069
H	-10.59706	3.20729	1.61856
O	-6.34398	2.15675	0.36502
C	-8.17678	3.61818	3.95383
H	-7.69469	3.87993	4.90062
H	-7.98437	4.43176	3.25183
H	-9.25670	3.56116	4.13059
C	-8.53547	-0.99888	5.46003
H	-9.03230	-1.93037	5.18166
H	-7.55513	-1.23660	5.88172
H	-9.13767	-0.51338	6.23322

clust-27

C	-9.73488	0.54941	4.77067
C	-7.55417	2.04862	3.43330
C	-8.70590	2.75945	4.15505
C	-9.98234	1.92398	4.15422
H	-9.54112	0.69546	5.84449
H	-6.61838	2.49838	3.78491
H	-8.38032	2.84017	5.20235
H	-10.37895	1.81322	3.13991
H	-10.75490	2.43875	4.73677
C	-8.45631	-0.10610	4.27397
O	-8.27713	-1.30321	4.32176
O	-7.43696	0.66663	3.85968
C	-7.47319	2.01829	1.89402
H	-6.65606	1.31014	1.70319
C	-6.99124	3.33566	1.28882
H	-6.20142	3.78670	1.91180
H	-7.80646	4.06676	1.19180
C	-6.03724	4.19647	-0.67563
H	-5.23532	4.69041	-0.10423
H	-6.86645	4.91711	-0.76341

C	-4.60498	3.23832	-4.62795
C	-5.20811	2.25078	-3.85239
C	-5.67185	2.54558	-2.56843
C	-5.53362	3.83397	-2.05148
C	-4.92431	4.82183	-2.83222
C	-4.46392	4.52864	-4.11292
H	-4.24474	3.00666	-5.62534
H	-5.31908	1.24442	-4.24466
H	-6.13962	1.77798	-1.96159
H	-4.80903	5.82720	-2.43296
H	-3.99243	5.30462	-4.70808
C	-8.71376	1.49643	1.16906
H	-9.53556	2.21909	1.19997
H	-8.46929	1.31616	0.11942
H	-9.06392	0.55039	1.59590
O	-6.47583	3.04408	0.00398
C	-8.95134	4.17553	3.63822
H	-9.62329	4.70315	4.32061
H	-8.02347	4.75261	3.56997
H	-9.42628	4.16343	2.65255
C	-10.92603	-0.39184	4.61235
H	-10.74920	-1.34251	5.11660
H	-11.82042	0.07322	5.03588
H	-11.11499	-0.59569	3.55345

clust-28

C	-8.48241	0.56626	5.29376
C	-8.19127	2.12115	3.13166
C	-9.44373	2.53711	3.91597
C	-9.56820	1.65536	5.18612
H	-7.51632	1.05471	5.48125
H	-7.30102	2.33525	3.74208
H	-9.28922	3.57732	4.22170
H	-10.54305	1.15305	5.18588
H	-9.53308	2.26731	6.09184
C	-8.35843	-0.12329	3.95195
O	-8.38461	-1.31949	3.77444
O	-8.22979	0.69622	2.89013
C	-8.00261	2.78836	1.77148
H	-8.82671	2.47860	1.11679
C	-6.70533	2.29778	1.13435
H	-6.70750	1.20314	1.04946
H	-5.84382	2.59391	1.75852
C	-5.43436	2.45532	-0.83180
H	-5.46451	1.36456	-0.98131
H	-4.53849	2.67725	-0.22928
C	-5.07053	4.42358	-4.65155
C	-6.09177	4.79028	-3.77810
C	-6.22290	4.15821	-2.53968
C	-5.33143	3.15187	-2.16696
C	-4.30885	2.78497	-3.04818
C	-4.17666	3.41626	-4.28199
H	-4.97054	4.91569	-5.61389
H	-6.79221	5.57105	-4.05891
H	-7.01809	4.44024	-1.85820
H	-3.61266	1.99824	-2.76564
H	-3.37891	3.12116	-4.95669
C	-7.99166	4.31254	1.90397
H	-7.22956	4.63115	2.62569
H	-7.75318	4.76521	0.93966
H	-8.95767	4.70211	2.23501
O	-6.58793	2.88203	-0.14727
C	-10.71564	2.45308	3.06839
H	-11.58770	2.69466	3.68249
H	-10.69877	3.14716	2.22393
H	-10.85066	1.43929	2.67554
C	-8.76258	-0.42911	6.41062
H	-7.96825	-1.17461	6.48317
H	-8.83925	0.09660	7.36620
H	-9.70338	-0.95552	6.22709

LACTONE 3

3a

C	-2.31191	-1.73094	0.01001
C	-0.77887	-1.69350	-0.04066
C	-2.40332	0.78347	-0.16802
C	-2.94307	-0.54096	-0.71021
H	-0.41015	-2.29155	0.80100
H	-2.76378	-0.60620	-1.78649
H	-2.57609	-1.64623	1.07266
H	-2.60003	1.58959	-0.88084
H	-4.03038	-0.56818	-0.57196
C	-2.86320	-3.06473	-0.49220
H	-2.38160	-3.91199	0.00652
H	-3.93679	-3.12179	-0.29250
H	-2.71702	-3.17625	-1.57145
C	-3.04517	1.17771	1.17487
H	-2.65155	2.13500	1.52304
H	-4.12694	1.27081	1.04678
H	-2.85548	0.42756	1.94823
C	-0.89791	0.78397	0.02751
O	-0.24930	-0.37152	0.23465
O	-0.26222	1.81520	0.08774
C	-0.06917	-2.23035	-1.29514
H	-0.38555	-3.27658	-1.39398
C	1.44681	-2.22041	-1.06996
H	1.95413	-2.73501	-1.89086
H	1.82264	-1.19426	-1.02400
H	1.71581	-2.72227	-0.13484
C	-0.41181	-1.48928	-2.59036
H	-0.29218	-0.40593	-2.46860
H	0.27026	-1.80285	-3.38620
H	-1.42904	-1.69046	-2.93408

3b

C	-2.42776	-1.75955	0.05965
C	-0.89703	-1.84509	0.11072
C	-2.31290	0.74965	-0.20345
C	-2.90880	-0.55196	-0.74254
H	-0.63305	-2.48373	0.96151
H	-2.65914	-0.67690	-1.79910
H	-2.73734	-1.60423	1.10271
H	-2.34073	1.52591	-0.97417
H	-4.00224	-0.49375	-0.68564
C	-3.09052	-3.04926	-0.42107
H	-2.70172	-3.92793	0.10250
H	-4.16736	-2.99526	-0.23761
H	-2.94486	-3.19561	-1.49555
C	-3.08068	1.27904	1.02187
H	-2.63301	2.20565	1.38682
H	-4.11844	1.47777	0.74174
H	-3.08046	0.55113	1.83890

C	-0.10465	-3.88461	-1.23785
H	-1.03549	-4.23874	-1.68638
H	0.71418	-4.20121	-1.89058
H	0.02392	-4.38827	-0.27415
C	-0.85062	0.63648	0.19280
O	-0.31818	-0.56136	0.47510
O	-0.15780	1.62030	0.34655
C	-0.07082	-2.35956	-1.08526
H	0.95515	-2.09939	-0.79422
C	-0.34768	-1.66666	-2.42043
H	-0.34964	-0.57525	-2.32563
H	0.43421	-1.93079	-3.13871
H	-1.30509	-1.98135	-2.84818

3c

C	-2.05601	-1.25167	-0.04720
C	-0.68313	-1.03288	0.58989
C	-0.13667	0.36004	0.27025
H	0.79412	0.50231	0.83382
H	-0.76816	-1.15049	1.67841
H	0.00325	-1.81031	0.23720
H	-1.92555	-1.34133	-1.13530
C	0.17345	0.53374	-1.21854
H	0.73089	1.45551	-1.40326
H	0.78648	-0.30289	-1.56823
H	-0.73411	0.56306	-1.82980
C	-2.73469	-2.52613	0.45407
H	-2.92287	-2.46365	1.53044
H	-3.68651	-2.69037	-0.05248
H	-2.08338	-3.38505	0.27063
C	-2.98878	-0.05577	0.10088
O	-4.18285	-0.14158	-0.08620
O	-2.47567	1.15683	0.36495
C	-1.12705	1.36690	0.85246
H	-1.16859	1.17811	1.93449
C	-1.37305	3.67937	1.81121
H	-1.15877	4.74346	1.67487
H	-2.46067	3.55813	1.86417
H	-0.94651	3.36597	2.76901
C	-0.80767	2.85714	0.64856
H	0.28829	2.93713	0.66813
C	-1.32313	3.42711	-0.67755
H	-0.96453	4.45397	-0.79501
H	-0.99670	2.85433	-1.54694
H	-2.41625	3.44591	-0.67953

3d

C	1.39488	-2.13187	-1.05975
C	2.91919	-2.03801	-1.04347
C	3.38444	-0.58039	-1.08536
H	4.39925	-0.49474	-0.68494
H	3.30854	-2.53481	-0.14702
H	3.33693	-2.57519	-1.90256
H	1.02473	-1.60503	-1.94979
C	0.92011	-3.58058	-1.14528
H	1.29804	-4.17664	-0.30806
H	-0.17196	-3.64842	-1.15248
H	1.29158	-4.03299	-2.06908
C	3.39769	-0.01575	-2.51753
H	3.72513	1.02574	-2.51845
H	4.08689	-0.60082	-3.13198
H	2.40506	-0.06571	-2.97542
C	2.54025	0.35509	-0.23448
O	1.30924	-0.01184	0.15281
O	2.91730	1.47360	0.04345
C	0.82819	-1.37976	0.14902
H	-0.25224	-1.24917	0.01948
C	1.36745	-1.02899	2.63186
H	1.47253	-1.55111	3.58756
H	2.28752	-0.46911	2.44727
H	0.55092	-0.30559	2.72437
C	-0.14906	-2.88635	1.92397
H	-1.01117	-2.23274	2.10018
H	-0.42911	-3.61272	1.15759
H	0.05201	-3.43433	2.84906
C	1.07088	-2.04653	1.52660
H	1.93684	-2.71666	1.44640

3e

C	-0.46655	-3.82301	-0.22306
C	-2.55006	-2.80571	0.78043
C	-3.08836	-4.21324	1.02680
H	-2.89236	-2.18393	1.61556
H	-2.76058	-4.54254	2.02506
H	-0.57701	-3.33529	-1.20242
C	1.01485	-4.13568	-0.01443
H	1.40261	-4.75976	-0.82059
H	1.58577	-3.20364	0.01725
H	1.16692	-4.66176	0.93319
C	-3.05014	-2.19437	-0.53189
H	-4.11712	-1.96096	-0.48190
H	-2.51324	-1.26517	-0.74590
H	-2.90281	-2.87249	-1.37883
C	-4.60545	-4.37999	0.94038
H	-4.90247	-4.15998	-0.09370
C	-5.30951	-3.40219	1.88447
H	-5.15661	-2.35787	1.59854
H	-6.38616	-3.59329	1.88496
H	-4.94843	-3.53027	2.91218
C	-5.01038	-5.81936	1.26747
H	-6.09367	-5.93920	1.17428
H	-4.52483	-6.53383	0.59995
H	-4.73229	-6.06760	2.29900
C	-1.26935	-5.10789	-0.37788
O	-0.83844	-6.06936	-0.97613
O	-2.53105	-5.16257	0.08086
C	-1.02430	-2.88674	0.84835
H	-0.57766	-1.89417	0.72479
H	-0.72475	-3.25148	1.83998

3f

C	-0.45129	-3.77525	-0.23022
C	-2.53134	-2.76628	0.78253
C	-3.09790	-4.17724	0.93936
H	-2.88337	-2.19187	1.64760
H	-2.76342	-4.54397	1.92049
H	-0.53728	-3.22284	-1.17731
C	1.02019	-4.13035	-0.02008
H	1.40665	-4.71458	-0.85610
H	1.60941	-3.21411	0.07405
H	1.14745	-4.71416	0.89691
C	-2.94827	-2.03643	-0.49919

H	-3.96897	-1.65509	-0.42828
H	-2.28713	-1.18146	-0.67391
H	-2.89736	-2.68791	-1.37771
C	-5.31177	-3.46726	1.89885
H	-5.25912	-2.41995	1.58094
H	-6.36876	-3.73372	1.98529
H	-4.86179	-3.54397	2.89452
C	-1.27480	-5.03261	-0.47825
O	-0.85126	-5.96462	-1.12629
O	-2.54344	-5.09123	-0.04023
C	-4.61788	-4.38481	0.89078
H	-4.76307	-5.42150	1.22239
C	-5.25343	-4.27287	-0.49853
H	-6.26288	-4.69389	-0.46559
H	-5.34343	-3.23591	-0.83010
H	-4.67955	-4.82854	-1.24442
C	-1.00973	-2.89980	0.89128
H	-0.53154	-1.91525	0.84861
H	-0.74785	-3.34198	1.86170

LACTONE 4

4a

C	-1.96932	-1.39870	-0.15015
C	-0.47192	-1.27859	0.15540
C	0.02404	0.15254	-0.04536
H	1.06422	0.22371	0.28878
H	-0.28297	-1.59827	1.18771
H	0.07828	-1.97152	-0.49037
H	-2.09465	-1.42259	-1.24244
C	-0.02985	0.59515	-1.51039
H	0.40198	1.59354	-1.62704
H	0.53734	-0.09679	-2.14005
H	-1.05565	0.63399	-1.88915
C	-2.57484	-2.68076	0.42149
H	-2.51926	-2.67620	1.51494
H	-3.62033	-2.78774	0.12991
H	-2.01457	-3.54579	0.05603
C	-2.80796	-0.18707	0.24857
O	-4.01866	-0.22944	0.26784
O	-2.21042	0.99598	0.47653
C	-0.80908	1.07771	0.83955
H	-0.55053	2.12168	0.62180
C	-0.69798	0.85548	2.35534
H	-1.14965	-0.12057	2.58535
C	-1.48883	1.93223	3.10250
H	-1.47359	1.73921	4.17891
H	-1.04193	2.91875	2.93091
H	-2.52941	1.96576	2.77211
C	0.76060	0.84333	2.81727
H	1.28174	1.74578	2.47501
H	0.80670	0.82758	3.90973
H	1.30903	-0.02772	2.44834

4b

C	-2.49070	-1.08680	-0.29423
C	-1.05676	-1.61611	-0.14351
C	-0.09443	-0.47543	0.21812
H	0.75827	-0.89648	0.76139
H	-1.05229	-2.39328	0.63017
H	-0.73751	-2.09199	-1.07693
H	-2.47236	-0.20095	-0.94634
C	0.42799	0.19884	-1.05579
H	1.03966	1.07726	-0.83688
H	1.03677	-0.50278	-1.63287
H	-0.40410	0.52482	-1.69084
C	-3.46462	-2.11128	-0.85921
H	-3.48726	-3.00531	-0.22908
H	-4.47788	-1.70794	-0.90690
H	-3.15343	-2.40356	-1.86544
C	-2.91218	-0.62187	1.08181
O	-3.97343	-0.87287	1.60705
O	-1.98330	0.05672	1.77753
C	-0.79705	0.56738	1.12174
H	-1.12901	1.40606	0.49224
C	0.05834	1.12946	2.26468
H	-0.58005	1.86561	2.76952
C	0.43998	0.05914	3.28990
H	-0.44077	-0.47528	3.65363
H	1.14012	-0.67039	2.86879
H	0.93362	0.52754	4.14647
C	1.29905	1.85499	1.74324
H	1.04269	2.62746	1.01084
H	1.82066	2.33849	2.57394
H	2.00173	1.15604	1.27585

4c

C	-2.28855	-1.69180	-0.30191
C	-2.36116	0.80255	0.08915
C	-2.69182	-0.33317	-0.87257
H	-2.16318	-0.17482	-1.82202
H	-2.88169	-1.88017	0.60189
H	-2.48517	1.76510	-0.41748
H	-3.76382	-0.32931	-1.09920
C	-2.60264	-2.78833	-1.32510
H	-2.32832	-3.78476	-0.97513
H	-3.67341	-2.79343	-1.54940
H	-2.06339	-2.59762	-2.25961
C	-3.23688	0.82489	1.35088
H	-2.96983	1.67507	1.98258
H	-4.28807	0.91942	1.06496
H	-3.12525	-0.08684	1.94370
C	-0.89763	0.76055	0.47663
O	-0.21621	-0.37915	0.30067
O	-0.30819	1.72695	0.91205
C	-0.79395	-1.69457	0.06661
H	-0.22897	-2.06469	-0.79808
C	-0.40110	-2.52803	1.29859
H	0.69006	-2.43394	1.36622
C	-0.73861	-4.01025	1.13352
H	-0.30216	-4.58124	1.95789
H	-1.82116	-4.17640	1.15622
H	-0.34542	-4.41709	0.19624
C	-0.99578	-1.97958	2.59705
H	-2.08184	-2.12030	2.63390
H	-0.57154	-2.51343	3.45241
H	-0.77502	-0.91586	2.72830

4d

C	-0.36877	-4.03034	-0.54898
C	-1.89698	-2.88623	1.12769
H	-1.75594	-2.46490	2.12839
H	-1.26138	-4.14208	-1.18202

C	0.86875	-3.93667	-1.42979
H	0.99272	-4.83783	-2.03332
H	0.78516	-3.07479	-2.09688
H	1.76657	-3.81573	-0.81667
C	-2.99139	-2.08982	0.41200
H	-3.96738	-2.21659	0.89034
H	-2.75158	-1.02329	0.41303
H	-3.08312	-2.41518	-0.63116
C	-0.30729	-5.23421	0.36747
O	0.53815	-6.09904	0.32688
O	-1.24129	-5.27303	1.33525
C	-0.56370	-2.80651	0.36160
H	-0.52774	-1.89379	-0.24259
H	0.28228	-2.76028	1.05709
C	-2.35252	-4.35208	1.26772
H	-2.93012	-4.61901	0.36994
C	-3.22072	-4.63383	2.49738
H	-3.98932	-3.84935	2.50909
C	-3.91581	-5.99114	2.36979
H	-4.56403	-6.17459	3.23156
H	-4.53036	-6.04112	1.46529
H	-3.17445	-6.79542	2.32581
C	-2.42446	-4.56070	3.80301
H	-1.67456	-5.35602	3.83495
H	-1.91105	-3.60323	3.92834
H	-3.09696	-4.69146	4.65552

4e

C	1.47609	-2.39603	-0.85387
C	2.95377	-2.08599	-1.08089
C	3.18261	-0.58787	-1.26055
H	4.25509	-0.37630	-1.30614
H	3.53874	-2.44337	-0.22348
H	3.31222	-2.62856	-1.96265
H	0.93649	-2.15204	-1.77829
C	1.28446	-3.88637	-0.56223
H	1.85801	-4.17375	0.32577
H	0.23712	-4.14131	-0.38302
H	1.64006	-4.48726	-1.40449
C	2.53179	-0.00186	-2.52306
H	2.79073	1.05419	-2.62750
H	2.89289	-0.53751	-3.40555
H	1.44135	-0.08195	-2.50028
C	2.69053	0.14860	-0.03385
O	1.73834	-0.43051	0.71178
O	3.14340	1.21377	0.32675
C	0.89149	-1.53207	0.28451
H	0.81650	-2.14261	1.19423
C	-1.01119	-0.11204	1.15161
H	-0.32673	0.69784	1.40932
H	-1.98643	0.31987	0.90885
H	-1.13691	-0.74897	2.03560
C	-1.50286	-2.02929	-0.38703
H	-1.22148	-2.58747	-1.28395
H	-1.61616	-2.74053	0.43993
H	-2.48137	-1.57695	-0.57068
C	-0.49085	-0.93932	-0.02522
H	-0.36461	-0.27650	-0.89482

4f

C	1.36341	-2.14123	-1.13731
C	2.87910	-2.07786	-0.95715
C	3.39116	-0.64139	-1.08613
H	4.35895	-0.53883	-0.58529
H	3.13169	-2.48606	0.03034
H	3.38122	-2.70784	-1.69994
H	1.10153	-1.69915	-2.10796
C	0.85294	-3.58024	-1.09244
H	0.99554	-4.01212	-0.09482
H	-0.20904	-3.64634	-1.34349
H	1.40557	-4.19665	-1.80697
C	3.57798	-0.22104	-2.55464
H	3.93851	0.80738	-2.61817
H	4.30867	-0.87954	-3.03140
H	2.63896	-0.29231	-3.11226
C	2.49161	0.39099	-0.42163
O	1.23875	0.06733	-0.06987
O	2.85612	1.53512	-0.25467
C	0.73780	-1.29303	-0.03580
H	1.04253	-1.71001	0.93669
C	-1.32555	-0.67943	-1.39150
H	-1.12311	-1.37842	-2.20863
H	-2.40894	-0.53997	-1.33471
H	-0.87406	0.28613	-1.64328
C	-1.28244	-0.31056	1.10368
H	-2.37331	-0.35194	1.17049
H	-0.86930	-0.64596	2.06078
H	-0.98700	0.73132	0.95291
C	-0.78922	-1.18580	-0.05127
H	-1.16079	-2.20444	0.11810

4g

C	1.39651	-2.17161	-1.18977
C	2.91729	-2.09052	-1.05171
C	3.40524	-0.64181	-1.05373
H	4.39470	-0.57495	-0.59076
H	3.21119	-2.59101	-0.11938
H	3.40186	-2.63442	-1.87020
H	1.09153	-1.63474	-2.09819
C	0.94375	-3.62748	-1.30206
H	1.05850	-4.15102	-0.34580
H	-0.09832	-3.71313	-1.61572
H	1.55649	-4.14709	-2.04438
C	3.51324	-0.06395	-2.47594
H	3.86215	0.97006	-2.44558
H	4.22380	-0.65727	-3.05730
H	2.54766	-0.08647	-2.99068
C	2.52191	0.29122	-0.24211
O	1.28624	-0.09255	0.11025
O	2.87719	1.41405	0.04605
C	0.78961	-1.45791	0.01571
H	1.12655	-1.97009	0.92952
C	-0.73754	-1.30213	0.07859
H	-0.88963	-0.48882	0.79892
C	-1.33750	-0.86136	-1.25687
H	-1.28894	-1.66447	-2.00077
H	-2.39012	-0.59389	-1.12758
H	-0.81355	0.01224	-1.65748
C	-1.45148	-2.53254	0.64682
H	-2.49347	-2.28002	0.86396
H	-1.45815	-3.37364	-0.05007
H	-0.98729	-2.86722	1.58018

LACTONE 5

5a

C	-0.39034	-1.81202	-0.02686
C	0.08561	-0.38821	-0.30047
C	-0.49576	0.56175	0.74857
H	1.17978	-0.35396	-0.27400
H	0.10963	-2.13230	0.89733
H	-0.30321	0.13431	1.74450
H	-0.22390	-0.06079	-1.30239
C	-1.99900	0.57952	0.55800
C	0.07938	1.97203	0.68942
H	-0.38463	2.61915	1.43551
H	1.15683	1.93937	0.87056
H	-0.09279	2.41463	-0.29624
C	0.00574	-2.77056	-1.14911
H	1.09074	-2.77401	-1.28993
H	-0.31200	-3.79494	-0.93165
H	-0.46001	-2.46548	-2.09248
O	-2.57011	-0.56388	0.14328
O	-2.69354	1.56300	0.68578
C	-1.91727	-1.85466	0.23447
H	-2.40738	-2.41787	-0.56951
C	-2.29271	-2.50509	1.57243
H	-1.77473	-1.94663	2.36755
C	-1.81739	-3.96056	1.60559
H	-0.73374	-4.05577	1.49398
H	-2.09600	-4.42425	2.55581
H	-2.29445	-4.53450	0.80194
C	-3.79996	-2.43803	1.82221
H	-4.34074	-2.96179	1.02483
H	-4.04740	-2.92359	2.77073
H	-4.16049	-1.40819	1.85530

5b

C	-0.25637	-1.52380	0.27693
C	0.09766	-0.24511	-0.47712
C	-0.19610	0.98780	0.37499
H	1.15670	-0.24180	-0.75737
H	0.29151	-1.52411	1.22970
H	0.53085	1.00348	1.20122
H	-0.48016	-0.20093	-1.41191
C	-1.53628	0.91739	1.09483
C	-0.06838	2.29451	-0.40543
H	-0.22967	3.15708	0.24223
H	0.93022	2.36390	-0.84528
H	-0.80249	2.33083	-1.21625
C	0.11670	-2.77394	-0.51765
H	1.16334	-2.72159	-0.83032
H	-0.01193	-3.68651	0.07046
H	-0.50009	-2.85974	-1.41997
O	-2.11141	-0.27815	1.30259
O	-2.07037	1.89777	1.56517
C	-1.75088	-1.47985	0.57624
H	-2.29174	-1.43397	-0.38186
C	-2.31283	-2.65277	1.38364
H	-2.16315	-3.54265	0.75908
C	-3.81822	-2.48568	1.60545
H	-4.23663	-3.38963	2.05715
H	-4.01987	-1.64338	2.27286
H	-4.34110	-2.30334	0.66072
C	-1.58130	-2.85226	2.71227
H	-1.61383	-1.93384	3.30795
H	-2.06239	-3.64620	3.29073
H	-0.53362	-3.13363	2.56936

5c

C	-0.32772	-1.75657	-0.11431
C	0.05242	-0.32914	-0.49455
C	-0.43673	0.64560	0.57483
H	1.13965	-0.25222	-0.60175
H	0.24586	-2.01030	0.78712
H	-0.07738	0.29126	1.55296
H	-0.38712	-0.06144	-1.46561
C	-1.95061	0.57925	0.62566
C	0.03795	2.07887	0.35964
H	-0.34253	2.74112	1.13867
H	1.13056	2.11073	0.37063
H	-0.30933	2.45713	-0.60664
C	0.05377	-2.74200	-1.22069
H	1.13040	-2.70298	-1.41132
H	-0.20583	-3.77116	-0.95912
H	-0.46589	-2.48794	-2.15104
O	-2.53015	-0.59261	0.32143
O	-2.66219	1.52688	0.87707
C	-1.83286	-1.86170	0.21920
H	-2.34047	-2.34205	-0.62531
C	-2.16749	-2.65706	1.49112
H	-3.26351	-2.68626	1.53611
C	-1.66762	-1.97740	2.76720
H	-2.05488	-0.95832	2.86307
H	-2.00578	-2.53936	3.64261
H	-0.57316	-1.94060	2.80675
C	-1.65668	-4.09570	1.39648
H	-2.00624	-4.67300	2.25693
H	-2.01462	-4.59308	0.48908
H	-0.56143	-4.13138	1.39836

5d

C	-0.38089	-1.53213	-0.34939
C	0.20913	-0.12872	-0.48257
C	-0.66018	0.85850	0.30220
C	-2.17719	0.58093	0.13585
H	1.21683	-0.14924	-0.05531
H	0.21047	-2.23468	-0.95052
H	-0.40659	0.82669	1.36665
H	-0.44453	1.87664	-0.03998
H	-2.55114	0.15611	1.07794
C	0.32829	0.28035	-1.95457
H	0.87561	1.22321	-2.03775
H	0.86130	-0.47929	-2.53450
H	-0.65217	0.42574	-2.42106
C	-1.06956	-3.51053	1.03564
H	-0.40209	-4.18529	0.48655
H	-1.18399	-3.90287	2.05012
H	-2.04642	-3.52624	0.54679
C	-2.97445	1.84989	-0.15527
H	-4.04638	1.64987	-0.18210
H	-2.77170	2.59385	0.61996
H	-2.67961	2.27174	-1.12130
C	-2.50998	-0.50453	-0.88049
O	-1.67789	-1.55419	-0.99390
O	-3.52076	-0.49708	-1.54831

C	-0.48147	-2.09806	1.07261
H	-1.15389	-1.45946	1.66027
C	0.89178	-2.10584	1.74906
H	1.62608	-2.63030	1.12563
H	1.26707	-1.09733	1.94308
H	0.83459	-2.62975	2.70724

5e

C	-0.61926	-1.56422	-0.08172
C	0.07423	-0.21610	-0.26660
C	-0.63943	0.84582	0.56771
C	-2.15452	0.88896	0.28342
H	1.09646	-0.33332	0.11225
H	-0.19004	-2.26682	-0.80452
H	-0.45854	0.64784	1.62853
H	-0.20823	1.83147	0.36121
H	-2.69406	1.01286	1.23053
C	0.15154	0.15030	-1.75197
H	0.60930	1.13515	-1.88314
H	0.75260	-0.58255	-2.29854
H	-0.83846	0.17422	-2.21877
C	-0.43147	-3.73048	1.18685
H	0.44038	-4.02960	0.59726
H	-0.35857	-4.20703	2.16880
H	-1.32855	-4.11625	0.68936
C	-2.55450	2.07392	-0.61018
H	-3.63173	2.08254	-0.78221
H	-2.26731	3.00741	-0.11940
H	-2.04555	2.03022	-1.57733
C	-2.75461	-0.39203	-0.29850
O	-2.00292	-1.48666	-0.49471
O	-3.92619	-0.44833	-0.60603
C	-0.51894	-2.20669	1.32254
H	0.41776	-1.84370	1.76723
C	-1.67611	-1.85138	2.26284
H	-1.50054	-2.30594	3.24189
H	-1.79465	-0.77707	2.42126
H	-2.62057	-2.24685	1.87600

5f

C	-0.39057	-1.50506	-0.21551
C	0.17694	-0.09691	-0.38983
C	-0.61942	0.91119	0.43573
C	-2.14654	0.75114	0.25169
H	1.21288	-0.11563	-0.03493
H	0.11922	-2.15503	-0.93616
H	-0.35623	0.81763	1.49220
H	-0.33070	1.92519	0.13774
H	-2.60634	0.61913	1.24018
C	0.19121	0.28879	-1.87396
H	0.65595	1.26998	-2.00514
H	0.75421	-0.43977	-2.46495
H	-0.81993	0.34144	-2.29253
C	-2.78672	1.98714	-0.38977
H	-3.86727	1.87071	-0.47807
H	-2.57196	2.86613	0.22351
H	-2.37220	2.16034	-1.38833
C	-2.59775	-0.50079	-0.50092
O	-1.76692	-1.54358	-0.65560
O	-3.72300	-0.60467	-0.94067
C	1.16613	-2.14029	1.67033
H	1.88732	-2.43063	0.89882
H	1.41864	-1.12944	2.00952
H	1.29248	-2.81604	2.52060
C	-1.26679	-1.76092	2.23044
H	-2.29878	-1.79257	1.86917
H	-1.20052	-2.44786	3.07943
H	-1.05595	-0.75781	2.61123
C	-0.27250	-2.20514	1.15372
H	-0.50437	-3.25663	0.93908

5g

C	-0.39992	-1.88265	-0.86558
C	0.61789	-0.80080	-0.41856
C	0.05190	0.13166	0.65645
H	1.51510	-1.29447	-0.02935
H	-0.74512	-1.62819	-1.87754
H	0.62286	1.06560	0.66860
H	0.93348	-0.22459	-1.29417
C	-1.69408	-1.89951	-0.06109
O	-2.32844	-2.91006	0.14870
O	-2.19195	-0.73098	0.37915
C	0.21676	-3.27846	-0.91711
H	-0.48708	-4.01158	-1.31341
H	1.10618	-3.26085	-1.55291
H	0.51795	-3.59878	0.08531
C	0.14733	-0.49906	2.04983
H	1.19582	-0.61103	2.33900
H	-0.35218	0.12150	2.80008
H	-0.31209	-1.49304	2.08307
C	-1.39542	0.47684	0.30862
H	-1.82059	1.10515	1.10173
C	-1.62460	1.18875	-1.03034
H	-1.29727	0.52614	-1.84231
C	-3.11441	1.48349	-1.21978
H	-3.46558	2.17623	-0.44574
H	-3.29069	1.94967	-2.19334
H	-3.71472	0.57280	-1.15874
C	-0.80817	2.48178	-1.10160
H	-1.01608	3.11772	-0.23247
H	0.26847	2.29419	-1.13734
H	-1.07775	3.04625	-1.99857

5h

C	-0.05326	-2.61723	-0.74482
C	0.90764	-1.42162	-0.74781
C	0.25214	-0.10246	-0.29366
H	1.77144	-1.65049	-0.11364
H	0.42650	-3.46021	-1.24971
H	0.65762	0.70342	-0.91497
H	1.28916	-1.30493	-1.76754
C	-1.25442	-2.27930	-1.60242
O	-1.79447	-3.06356	-2.35116
O	-1.70543	-1.01479	-1.54793
C	-0.48719	-3.10012	0.64841
H	-1.09780	-4.00235	0.56121
H	0.39971	-3.33969	1.24192
H	-1.06674	-2.35393	1.19671
C	0.57394	0.23202	1.16672
H	1.64910	0.38712	1.29160
H	0.06366	1.14396	1.49275
H	0.27154	-0.58138	1.83439

C	-1.27546	-0.12751	-0.48898
H	-1.74290	-0.49412	0.43528
C	-1.88319	1.24173	-0.81328
H	-1.44202	1.94324	-0.09216
C	-3.39942	1.22501	-0.60871
H	-3.66002	0.94903	0.41806
H	-3.82747	2.21032	-0.81494
H	-3.86610	0.50361	-1.28699
C	-1.53849	1.71119	-2.22912
H	-0.46129	1.71551	-2.41939
H	-2.01183	1.06071	-2.96987
H	-1.90779	2.72902	-2.38318

5i

C	-0.11945	-2.72077	-0.69849
C	0.85906	-1.55445	-0.87458
C	0.32352	-0.21613	-0.33427
H	1.80933	-1.79753	-0.38632
H	0.27254	-3.59720	-1.22183
H	0.74463	0.58018	-0.95792
H	1.07031	-1.45772	-1.94525
C	-1.40815	-2.37380	-1.40622
O	-2.07456	-3.16690	-2.03479
O	-1.80318	-1.09221	-1.35334
C	-0.41093	-3.13164	0.75369
H	-1.00681	-4.04753	0.76909
H	0.52806	-3.32007	1.28192
H	-0.96277	-2.36535	1.30410
C	0.79014	0.03623	1.10591
H	1.88211	0.09355	1.13754
H	0.39387	0.97283	1.50534
H	0.47846	-0.77073	1.77498
C	-1.21738	-0.13463	-0.43392
H	-1.64859	-0.35358	0.55320
C	-1.77175	1.21711	-0.90702
H	-2.86307	1.10411	-0.88388
C	-1.39285	2.35473	0.04154
H	-0.31684	2.55894	0.00902
H	-1.90951	3.27114	-0.25709
H	-1.67077	2.13326	1.07720
C	-1.36637	1.54602	-2.34565
H	-1.88549	2.45005	-2.67747
H	-0.29129	1.73897	-2.42783
H	-1.62656	0.73356	-3.02820

5j

C	0.20861	0.46338	-0.24158
C	-1.25730	0.08596	-0.04898
C	-1.41071	-1.43522	-0.10524
H	0.73523	0.12744	0.66205
H	-1.61171	0.46443	0.91554
H	-1.88214	0.54633	-0.82637
H	-0.66856	-1.88082	0.57468
C	3.18096	-0.14772	-0.56558
H	2.87883	0.39605	0.33375
H	4.08158	-0.71811	-0.32250
H	3.44885	0.58721	-1.33432
C	0.39422	1.97402	-0.37781
H	1.45009	2.23976	-0.48742
H	-0.14073	2.34516	-1.25873
H	0.00290	2.49269	0.50246
C	-2.80064	-1.92973	0.27822
H	-2.86830	-3.01578	0.19752
H	-3.02613	-1.63688	1.30688
H	-3.55782	-1.49333	-0.38003
C	-1.04493	-1.87594	-1.50846
O	-1.59617	-2.77003	-2.11085
O	-0.09558	-1.16378	-2.13832
C	2.08960	-1.08708	-1.08687
H	1.81700	-1.79070	-0.28502
C	0.82933	-0.28884	-1.44577
H	1.09306	0.43363	-2.22815
C	2.60744	-1.88104	-2.28692
H	3.51523	-2.42754	-2.01503
H	1.86696	-2.59656	-2.64935
H	2.85681	-1.20298	-3.11193

5k

C	0.85121	-0.64260	-1.03717
C	0.24842	0.03544	0.19106
C	-1.26987	0.02171	0.02353
C	-1.80555	-1.40540	-0.04109
H	0.50270	-0.56344	1.07714
H	-1.75020	0.54560	0.85705
H	-1.54032	0.56635	-0.89305
H	-1.67788	-1.85621	0.95484
H	0.56183	-0.06524	-1.92820
C	3.15378	0.35628	-1.56152
H	3.18040	1.15959	-0.82183
H	4.18855	0.06704	-1.76710
H	2.72944	0.75936	-2.48677
C	0.76315	1.46127	0.38818
H	1.79988	1.48237	0.72955
H	0.69639	2.03681	-0.54235
H	0.15635	1.97097	1.14216
C	-3.28458	-1.47158	-0.41651
H	-3.64964	-2.49927	-0.39918
H	-3.87030	-0.87626	0.28919
H	-3.44433	-1.06675	-1.42064
C	-0.97782	-2.30831	-0.94241
O	-1.39395	-3.36664	-1.36054
O	0.29284	-1.97426	-1.21961
C	2.37068	-0.86704	-1.07493
H	2.50255	-1.64796	-1.83401
C	2.91799	-1.40350	0.24790
H	2.34786	-2.27317	0.58922
H	3.96130	-1.70928	0.12812
H	2.88481	-0.63925	1.03250

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6a

C	-0.23909	-0.23272	-0.45636
C	-2.39867	1.06895	0.10458
H	0.37282	-0.49552	0.41582
H	-2.53568	0.50225	1.03573
C	0.68008	-0.17146	-1.67651
H	1.40620	0.63648	-1.54262
H	1.23710	-1.10076	-1.82263
H	0.10922	0.04259	-2.58620
C	-3.04049	2.44092	0.25618
H	-4.10796	2.35545	0.46853
H	-2.56199	2.98652	1.07382

H	-2.92522	3.02196	-0.66326
C	-3.05342	0.27043	-1.00543
O	-2.44151	-0.88423	-1.32907
O	-4.03377	0.61448	-1.62595
C	-1.33306	-1.31243	-0.50702
H	-1.72011	-1.42302	0.51451
C	-0.91555	-2.71060	-0.98597
H	0.11543	-2.85758	-0.63579
C	-0.89416	1.14912	-0.21258
H	-0.38625	1.68326	0.59581
H	-0.78174	1.76700	-1.11280
C	-0.95432	-2.88130	-2.50875
H	-0.38473	-2.11853	-3.04120
H	-0.54369	-3.85971	-2.77501
H	-1.98699	-2.83697	-2.86476
C	-1.80309	-3.77443	-0.33150
H	-1.52579	-4.77559	-0.67426
H	-1.71871	-3.75257	0.75938
H	-2.85245	-3.60578	-0.59807

6b

C	-0.17647	-0.21082	-0.68348
C	-0.82568	1.13349	-0.25815
C	-2.29110	1.00517	0.19665
H	0.57703	-0.48908	0.06289
H	-0.24753	1.60908	0.53948
H	-0.80974	1.82575	-1.10940
H	-2.32904	0.39315	1.10795
C	0.52010	-0.04761	-2.03611
H	1.14160	0.85297	-2.01967
H	1.16951	-0.89237	-2.27319
H	-0.21372	0.06416	-2.84194
C	-2.93705	2.35481	0.47660
H	-3.97394	2.23645	0.79727
H	-2.38381	2.87543	1.26286
H	-2.93111	2.97736	-0.42261
C	-3.03796	0.24471	-0.88014
O	-2.44366	-0.88488	-1.30823
O	-4.07946	0.59478	-1.38722
C	-1.24382	-1.31573	-0.62737
H	-1.50422	-1.45475	0.43077
C	-0.91540	-2.71574	-1.16191
H	-1.75563	-3.33574	-0.82176
C	-0.86468	-2.85290	-2.68757
H	0.06028	-2.45805	-3.11269
H	-0.91874	-3.91356	-2.95130
H	-1.70851	-2.34362	-3.15940
C	0.35478	-3.25414	-0.50035
H	0.30365	-3.18114	0.59138
H	0.49693	-4.30658	-0.76103
H	1.24193	-2.70663	-0.83602

6c

C	-1.81991	-1.98203	-0.10129
C	-0.28553	-1.96778	-0.19526
C	0.22877	-0.56590	0.22904
C	-0.87799	0.38534	0.72008
H	0.99355	-0.65153	1.00652
H	0.06251	-2.70629	0.53673
H	-2.07537	-1.90435	0.96439
H	-1.31801	-0.02412	1.63938
H	0.71156	-0.08488	-0.63099
C	-1.97033	0.39387	-0.32970
C	-0.36160	1.78998	0.99809
H	-1.16521	2.44405	1.34217
H	0.41595	1.75499	1.76585
H	0.06477	2.22816	0.09129
C	0.28629	-2.33804	-1.56556
H	1.36428	-2.14961	-1.57349
H	0.13383	-3.39118	-1.80910
H	-0.16776	-1.72898	-2.35500
C	-2.60113	-3.19250	-0.62877
C	-2.07597	-4.48282	0.00390
H	-2.73417	-5.31920	-0.24721
H	-1.07373	-4.72766	-0.36355
H	-2.02838	-4.40720	1.09557
O	-2.37061	-0.81815	-0.75754
O	-2.46234	1.38626	-0.81703
C	-2.70403	-3.30751	-2.15354
H	-1.78284	-3.67713	-2.60837
H	-3.49933	-4.01635	-2.40357
H	-2.95334	-2.34546	-2.60772
H	-3.62305	-3.03316	-0.25947

6d

C	0.21997	0.07216	-0.00448
C	-1.30445	0.03256	-0.05630
C	-1.81400	-1.40406	0.03889
H	0.53819	-0.44727	0.91072
H	-1.72708	0.61814	0.76762
H	-1.66646	0.49454	-0.98472
H	-1.62234	-1.75891	1.06299
C	0.75526	1.50089	0.05469
H	1.84857	1.52093	0.09363
H	0.42976	2.08845	-0.80997
H	0.37771	1.99608	0.95373
C	-3.30960	-1.52317	-0.24501
H	-3.65750	-2.54750	-0.10673
H	-3.86562	-0.86610	0.42932
H	-3.52894	-1.22174	-1.27422
C	-1.02163	-2.38071	-0.81761
O	-1.45407	-3.46973	-1.12664
O	0.24040	-2.08000	-1.16639
C	0.78367	-0.73616	-1.17789
H	1.85330	-0.91199	-1.01660
C	0.60559	-0.08684	-2.57429
H	-0.21785	0.63757	-2.52218
C	1.88142	0.66803	-2.96591
H	1.73029	1.21087	-3.90346
H	2.19321	1.38928	-2.20662
H	2.70402	-0.04075	-3.11553
C	0.26119	-1.10590	-3.66373
H	1.02978	-1.88263	-3.72879
H	-0.69631	-1.60099	-3.48296
H	0.20394	-0.59803	-4.63111

6e

C	0.21252	-0.11529	-0.01261
C	-1.29236	-0.01488	0.21802
C	-1.93072	-1.40215	0.22742
H	0.61517	-0.72459	0.80941
H	-1.48275	0.47014	1.18223

H	-1.77151	0.60731	-0.54473
H	-1.54491	-1.94182	1.10602
C	0.90306	1.24667	0.03852
H	1.97686	1.16004	-0.15599
H	0.47829	1.93786	-0.69637
H	0.77466	1.69129	1.02923
C	-3.45350	-1.35201	0.31134
H	-3.87997	-2.35375	0.37631
H	-3.75457	-0.78057	1.19360
H	-3.86912	-0.86049	-0.57405
C	-1.48108	-2.26060	-0.94360
O	-2.14972	-3.17187	-1.38107
O	-0.25619	-2.07272	-1.46126
C	0.55018	-0.87910	-1.29998
H	1.56726	-1.27322	-1.18950
C	0.52470	-0.11423	-2.63434
H	1.24777	0.70418	-2.52535
C	1.02148	-1.02884	-3.75928
H	0.30324	-1.83168	-3.94877
H	1.14844	-0.45715	-4.68295
H	1.98335	-1.48675	-3.50676
C	-0.83711	0.48032	-3.00391
H	-1.62971	-0.27495	-2.93570
H	-1.11088	1.32957	-2.37348
H	-0.81625	0.83476	-4.03873

6f

C	0.24145	-0.01743	0.02698
C	-1.27690	-0.01237	0.17836
C	-1.83655	-1.43239	0.14369
H	0.63860	-0.62633	0.85251
H	-1.54507	0.44910	1.13572
H	-1.74759	0.59462	-0.60162
H	-1.51375	-1.94036	1.06552
C	0.82908	1.38552	0.16834
H	1.90989	1.39493	-0.00209
H	0.36374	2.08475	-0.53267
H	0.64302	1.75790	1.17968
C	-3.36114	-1.46394	0.07690
H	-3.73862	-2.48616	0.11936
H	-3.77752	-0.89687	0.91399
H	-3.71298	-1.00750	-0.85393
C	-1.22716	-2.29069	-0.95361
O	-1.78151	-3.27619	-1.39053
O	0.01448	-2.02035	-1.38774
C	0.69040	-0.74016	-1.24983
H	1.73904	-1.02806	-1.11301
C	0.60535	-0.06541	-2.63393
H	0.79837	-0.90191	-3.31785
C	1.71553	0.96235	-2.88170
H	1.78147	1.17222	-3.95333
H	1.52758	1.91101	-2.37413
H	2.69097	0.58710	-2.55519
C	-0.76542	0.50628	-2.99945
H	-1.57354	-0.21034	-2.81473
H	-0.98087	1.42541	-2.44491
H	-0.78672	0.75391	-4.06494

6g

C	-0.41555	-1.99063	-0.86987
C	0.63801	-1.16244	-0.10819
C	0.03669	0.01964	0.69645
C	-1.47824	0.08305	0.45449
H	1.16066	-1.84095	0.57700
H	-0.82494	-1.37274	-1.68064
H	0.45307	0.95648	0.31095
H	-1.66320	0.31630	-0.60505
H	1.38399	-0.80861	-0.82560
C	-1.56575	-2.28000	0.07133
O	-2.04032	-3.37394	0.27875
O	-2.05734	-1.21373	0.72874
C	0.16169	-3.26902	-1.46050
H	-0.59864	-3.82820	-2.00929
H	0.98023	-3.02619	-2.14353
H	0.55043	-3.91581	-0.66892
C	0.38498	-0.10254	2.18214
H	1.46675	-0.20880	2.30343
H	0.06809	0.77231	2.75604
H	-0.09133	-0.98809	2.61736
C	-2.25923	1.09179	1.29438
H	-2.16599	0.79322	2.34628
C	-1.68474	2.49941	1.11669
H	-2.30153	3.22542	1.65348
H	-0.66192	2.58665	1.49336
H	-1.68219	2.78376	0.05740
C	-3.74167	1.06939	0.91428
H	-4.30424	1.76888	1.53935
H	-3.87257	1.37336	-0.13138
H	-4.17155	0.07332	1.03883

6h

C	-0.39183	-2.05667	-0.89619
C	0.60826	-1.15985	-0.14362
C	-0.05531	0.04448	0.56897
C	-1.58448	-0.09005	0.47793
H	1.11445	-1.78742	0.60113
H	-0.86898	-1.46763	-1.69134
H	0.17850	0.96082	0.01240
H	-1.85833	0.08242	-0.57132
H	1.38029	-0.82241	-0.84136
C	-1.48040	-2.44544	0.08459
O	-1.86725	-3.57465	0.28410
O	-2.00304	-1.43424	0.80321
C	0.26724	-3.28327	-1.51112
H	-0.46526	-3.90618	-2.02802
H	1.03324	-2.97381	-2.22715
H	0.74154	-3.89308	-0.73686
C	0.50697	0.19513	1.98283
H	1.59799	0.26644	1.93297
H	0.13561	1.09380	2.48252
H	0.25892	-0.67645	2.59777
C	-3.76913	1.14014	0.64690
H	-4.38347	1.81498	1.25015
H	-3.63665	1.59194	-0.34103
H	-4.32104	0.20155	0.52402
C	-2.42318	0.87452	1.32923
H	-1.86119	1.81796	1.36371
C	-2.66548	0.38616	2.76180
H	-1.74634	0.12339	3.28702
H	-3.17066	1.17104	3.33238
H	-3.30974	-0.49698	2.75312

6i

C	1.35943	-2.08283	-1.15232
C	2.86852	-1.94756	-0.93581
C	3.36639	-0.50157	-1.12438
H	4.11928	-0.28330	-0.35670
H	3.10149	-2.28560	0.07981
H	3.41275	-2.60719	-1.62050
C	4.03463	-0.27130	-2.48758
H	4.37938	0.75959	-2.58123
H	4.89233	-0.94156	-2.58741
H	3.34205	-0.48304	-3.30739
C	2.30808	0.57515	-0.89798
O	1.08995	0.24907	-0.44320
O	2.54148	1.74622	-1.10887
C	0.69193	-1.11585	-0.17640
H	1.07036	-1.35966	0.82662
C	-1.51764	-0.21963	-1.14943
H	-1.17464	-0.40073	-2.16944
H	-2.59982	-0.37813	-1.12239
H	-1.32027	0.82933	-0.91266
C	-1.32010	-0.74823	1.28829
H	-2.41273	-0.75279	1.34433
H	-0.93745	-1.44145	2.04377
H	-0.97387	0.26014	1.54156
C	-0.84519	-1.13106	-0.11704
H	-1.14458	-2.17039	-0.31265
H	1.06252	-3.08972	-0.83266
C	0.94760	-1.89951	-2.61493
H	1.57482	-2.52331	-3.25900
H	-0.09248	-2.19558	-2.77354
H	1.05402	-0.86076	-2.94659

LACTONE 6'

C	-0.41782514	-1.98983188	-0.87957499
C	0.63573486	-1.16164188	-0.11789499
C	0.03441486	0.02043812	0.68674501
C	-1.48051514	0.08384812	0.44478501
H	1.15838486	-1.84015188	0.56729501
H	-0.82721514	-1.37194188	-1.69034499
H	0.45079486	0.95727812	0.30124501
H	-1.66547514	0.31709812	-0.61475499
H	1.38171486	-0.80781188	-0.83530499
C	-1.56802514	-2.27920188	0.06162501
O	-2.04259514	-3.37314188	0.26904501
O	-2.05961514	-1.21293188	0.71903501
C	-2.26150514	1.09258812	1.28467501
H	-2.16826514	0.79401812	2.33657501
C	-1.68701514	2.50020812	1.10698501
H	-2.30380514	3.22621812	1.64377501
H	-0.66419514	2.58744812	1.48365501
H	-1.68446514	2.78455812	0.04769501
C	-3.74394514	1.07018812	0.90457501
H	-4.30651514	1.76967812	1.52964501
H	-3.87484514	1.37415812	-0.14108499
H	-4.17382514	0.07411812	1.02912501
H	0.28240489	-0.06655669	1.74458850
H	-0.00441357	-2.90539770	-1.30257629

conf-1.log Energy: -433853.5721436

C	0.69239	2.36726	0.68544
C	1.21084	1.79685	-0.63470
C	-1.41732	1.12919	0.47034
C	-0.82741	2.52096	0.66756
H	1.16979	3.33646	0.86249
H	0.98365	1.71118	1.51812
H	1.04575	2.55654	-1.41410
H	-1.10839	0.49823	1.31647
H	-1.10164	3.14318	-0.19510
C	0.40229	0.61235	-1.13161
O	0.80703	-0.18966	-1.93516
O	-0.89036	0.50105	-0.72767
C	-2.94450	1.07656	0.34107
H	-3.36154	1.51797	1.24939
C	2.69879	1.45542	-0.59391
H	3.04946	1.10528	-1.56553
H	3.27007	2.34336	-0.31152
H	2.89323	0.67266	0.14535
C	-1.34528	3.17235	1.94901
H	-2.40758	3.42134	1.88499
H	-1.19893	2.51003	2.80970
H	-0.79858	4.09910	2.14143
C	-3.47382	1.84027	-0.88285
H	-3.26142	2.90780	-0.78861
H	-3.01473	1.47535	-1.80541
H	-4.55657	1.71917	-0.96016
C	-3.50635	-0.34452	0.32587
O	-4.48943	-0.65346	0.95867
O	-2.90897	-1.24598	-0.46343
H	-2.11097	-0.87227	-0.88193

LACTONE 1

1a

C	0.28254	2.62318	0.11896
C	0.96009	1.78066	-0.95942
C	-1.17744	0.75697	0.76304
C	-1.17734	2.21608	0.31316
H	0.34550	3.67832	-0.16588
H	0.81978	2.51799	1.07256

H	0.51650	2.06056	-1.92733
H	-0.62204	0.67118	1.70672
H	-1.68734	2.27668	-0.66010
C	0.63931	0.30043	-0.85609
O	1.28637	-0.55957	-1.40095
O	-0.49313	-0.08106	-0.20893
C	-2.54075	0.06272	0.96185
H	-2.32240	-1.01021	0.88840
C	2.46905	2.00464	-1.03416
H	2.91121	1.43608	-1.85319
H	2.67396	3.06676	-1.19094
H	2.94991	1.69668	-0.10084
C	-1.88810	3.14162	1.30045
H	-2.97068	3.00181	1.27949
H	-1.53168	2.97898	2.32395
H	-1.68317	4.18223	1.03480
C	-3.19182	0.31738	2.31844
H	-2.48335	0.08905	3.11894
H	-3.53311	1.34532	2.43148
H	-4.06052	-0.33379	2.43456
C	-3.47117	0.40491	-0.19346
O	-4.50764	1.01200	-0.07870
O	-3.06049	0.00059	-1.40924
H	-2.19744	-0.44302	-1.35039

1b

C	0.27257	2.57750	0.13904
C	0.48236	1.61933	-1.03016
C	-1.33329	0.89959	1.13008
C	-1.11151	2.37771	0.74980
H	0.37193	3.61141	-0.20671
H	1.05179	2.41445	0.89646
H	-0.36514	1.73099	-1.72495
H	-1.15920	0.77738	2.20461
H	-1.85025	2.65607	-0.01468
C	0.40535	0.19933	-0.51928
O	1.02165	-0.73351	-0.97615
O	-0.41181	-0.04767	0.53248
C	-2.75136	0.36045	0.83041
H	-2.75954	-0.68126	1.17337
C	1.78392	1.85409	-1.78984
H	1.89520	1.14205	-2.60874
H	1.79167	2.86733	-2.19894
H	2.64334	1.74370	-1.12167
C	-1.29693	3.28541	1.96863
H	-2.27867	3.16763	2.43190
H	-0.53593	3.06309	2.72450
H	-1.18733	4.33289	1.67444
C	-3.84540	1.13939	1.55267
H	-3.64500	1.16851	2.62690
H	-3.91836	2.16037	1.17224
H	-4.81217	0.65702	1.39540
C	-2.99876	0.35863	-0.67434
O	-3.68650	1.16870	-1.24724
O	-2.37726	-0.60128	-1.38364
H	-1.83567	-1.16739	-0.81130

1c

C	0.44736	2.90501	-0.17979
C	1.24905	1.63553	-0.49719
C	-1.38030	1.20942	0.32092
C	-0.87227	2.63978	0.57294
H	0.22828	3.40632	-1.12791
H	1.07510	3.58981	0.40023
H	2.06654	1.89298	-1.17604
H	-0.99129	0.54812	1.10617
H	-1.62127	3.33877	0.18629
C	0.37618	0.68462	-1.28287
O	0.74729	-0.01002	-2.19571
O	-0.93931	0.65748	-0.94367
C	-2.91229	1.10534	0.30847
H	-3.28195	1.62469	1.19714
C	1.86537	0.92915	0.72191
H	2.48840	0.09241	0.39713
H	2.49435	1.63683	1.26866
H	1.11630	0.54051	1.41568
C	-0.74646	2.87853	2.08117
H	-1.67532	2.63817	2.60791
H	0.05456	2.27029	2.51281
H	-0.51451	3.92860	2.27608
C	-3.55309	1.72095	-0.94601
H	-3.27911	2.77357	-1.04531
H	-3.23543	1.19973	-1.85169
H	-4.64104	1.66051	-0.87208
C	-3.39253	-0.33403	0.45496
O	-4.26357	-0.66398	1.22457
O	-2.82859	-1.24675	-0.35082
H	-2.12953	-0.84924	-0.90107

1d

C	0.57739	2.12361	0.90231
C	1.41840	2.06361	-0.36997
C	-1.15080	0.68725	-0.09884
C	-0.91289	2.03186	0.58400
H	0.79852	3.05560	1.43313
H	0.85443	1.29984	1.57571
H	1.25452	2.99997	-0.92478
H	-0.89171	-0.12802	0.59028
H	-1.16791	2.82195	-0.13868
C	0.94943	0.99642	-1.34641
O	1.63835	0.59518	-2.25591
O	-0.31633	0.53938	-1.26735
C	-2.58757	0.45880	-0.58738
H	-2.94711	1.38085	-1.06296
C	2.91330	1.92210	-0.08981
H	3.49076	1.94222	-1.01486
H	3.24553	2.74228	0.55214
H	3.11988	0.97908	0.42532
C	-1.75804	2.21870	1.84398
H	-2.82739	2.29368	1.62655
H	-1.60966	1.39027	2.54379
H	-1.46503	3.14611	2.34355
C	-2.69237	-0.70353	-1.59216
H	-2.14740	-0.46235	-2.50388
H	-2.26519	-1.61175	-1.15824
H	-3.73788	-0.89760	-1.84596
C	-3.48240	0.09255	0.58743
O	-3.15027	-0.65855	1.47102
O	-4.73160	0.59399	0.57832
H	-4.87588	1.18277	-0.17546

1e

C	-0.26552	2.63554	-0.88751
C	1.00582	1.77765	-0.91099
C	-1.10895	0.80930	0.67988
C	-1.21939	2.29644	0.27350
H	-0.78379	2.48992	-1.84126
H	0.01172	3.69367	-0.83778
H	1.56328	1.99384	-1.82623
H	-0.47693	0.71357	1.57123
H	-2.24401	2.47510	-0.07733
C	0.59638	0.33131	-1.02890
O	1.14593	-0.49882	-1.70964
O	-0.51310	-0.03867	-0.33757
C	-2.45547	0.13393	1.00186
H	-2.23285	-0.93122	1.14795
C	1.96212	1.96648	0.27795
H	2.88618	1.40977	0.10519
H	2.21057	3.02594	0.38448
H	1.53608	1.62162	1.22340
C	-0.98069	3.21020	1.48320
H	-1.62423	2.95311	2.32736
H	0.05712	3.15600	1.82317
H	-1.18923	4.24717	1.20681
C	-3.10455	0.68893	2.26579
H	-2.39479	0.67323	3.09715
H	-3.45764	1.71111	2.11371
H	-3.96972	0.08162	2.53616
C	-3.42956	0.22369	-0.17512
O	-4.52907	0.71644	-0.09528
O	-3.01477	-0.29349	-1.34139
H	-2.09654	-0.60728	-1.27101

LACTONE 6''

6''-a

C	-0.15917	-0.94716	2.68721
C	0.41472	0.45274	2.47747
C	-1.18380	-0.90155	0.38230
C	-1.44048	-1.11976	1.87801
H	-0.37582	-1.08823	3.75142
H	0.58667	-1.70671	2.42128
H	-0.31516	1.17803	2.86808
H	-2.13082	-0.62899	-0.09629
H	-2.12525	-0.31658	2.18349
C	0.53491	0.79663	1.00633
O	1.33678	1.58618	0.56569
O	-0.31379	0.22449	0.11657
C	-0.63760	-2.10157	-0.42132
H	-1.30957	-2.94515	-0.25043
C	-0.61202	-1.78915	-1.92481
H	-1.63201	-1.61356	-2.27583
H	-0.02767	-0.89343	-2.15195
H	-0.19721	-2.62833	-2.48793
C	0.72519	-2.56345	0.06822
O	0.91959	-3.61695	0.62564
O	1.75898	-1.72526	-0.13990
H	1.48152	-0.92641	-0.61645
C	-2.12789	-2.45693	2.15297
H	-3.00999	-2.59553	1.51942
H	-1.44386	-3.29460	1.98520
H	-2.45506	-2.49247	3.19522
C	1.75107	0.66247	3.18487
H	2.11041	1.68418	3.05648
H	1.63493	0.45930	4.25253
H	2.50590	-0.02056	2.78350

6''-b

C	-0.61020	-0.21944	2.99557
C	-0.31544	1.12099	2.29459
C	-0.72178	-0.90096	0.57684
C	-0.93745	-1.37818	2.02007
H	-1.42609	-0.07166	3.70827
H	0.27623	-0.48380	3.58533
H	-1.21243	1.44189	1.74750
H	-1.51510	-0.18625	0.32616
H	-2.00655	-1.61180	2.08684
C	0.76445	0.86675	1.26742
O	1.79164	1.48283	1.14062
O	0.53676	-0.19815	0.45172
C	-0.75374	-1.97000	-0.52030
H	-1.65310	-2.57062	-0.35420
C	-0.83233	-1.32117	-1.91403
H	-1.73510	-0.70941	-1.98716
H	0.03382	-0.68008	-2.09871
H	-0.87152	-2.08682	-2.69191
C	0.40049	-2.97083	-0.53929
O	0.22560	-4.15216	-0.72717
O	1.64516	-2.48761	-0.43504
H	1.63469	-1.53310	-0.23851
C	-0.14597	-2.63315	2.39149
H	-0.45503	-3.50645	1.81130
H	0.92940	-2.47927	2.24797
H	-0.30731	-2.86566	3.44786
C	0.09663	2.21564	3.26909
H	0.30720	3.15022	2.74574
H	-0.70623	2.38998	3.98972
H	0.99740	1.92317	3.81581

6''-c

C	-1.36700	0.33835	2.40359
C	-0.16689	1.19248	1.93878
C	-0.42481	-1.13031	0.60460
C	-1.41534	-1.07745	1.77337
H	-2.28020	0.89516	2.17724
H	-1.31590	0.24632	3.49424
H	-0.37309	1.54599	0.91872
H	-0.69500	-0.37005	-0.14121
H	-2.41343	-1.24212	1.35675
C	1.06631	0.32909	1.81973
O	2.15385	0.56673	2.28096
O	0.89528	-0.81940	1.11187
C	-0.30463	-2.49048	-0.10053
H	0.18524	-3.18123	0.59929
C	-1.66857	-3.04114	-0.50967
H	-2.27276	-3.27980	0.36737
H	-2.21239	-2.31789	-1.12458
H	-1.54099	-3.94827	-1.10063
C	0.60871	-2.39968	-1.32855
O	0.26520	-2.73469	-2.43683
O	1.85431	-1.94684	-1.12851
H	1.96973	-1.63295	-0.21445
C	-1.12423	-2.15731	2.81937
H	-1.21263	-3.16796	2.41130

H	-0.11511	-2.04273	3.22939
H	-1.83403	-2.06998	3.64592
C	0.07774	2.39434	2.84038
H	0.88898	3.01674	2.45803
H	-0.83011	3.00014	2.90149
H	0.34557	2.06762	3.84886

6''-d

C	-1.24388	-0.03228	2.70231
C	-0.10290	0.98554	2.47371
C	-0.88237	-0.93924	0.46189
C	-1.03367	-1.33597	1.92782
H	-2.19786	0.40724	2.39424
H	-1.32364	-0.24361	3.77323
H	-0.54559	1.96730	2.26023
H	-1.74740	-0.32466	0.17936
H	-1.95258	-1.92992	1.99778
C	0.75449	0.71757	1.24492
O	1.82513	1.24235	1.05750
O	0.29784	-0.11963	0.27935
C	-0.79500	-2.07150	-0.56828
H	-1.64698	-2.73266	-0.38554
C	-0.88484	-1.51897	-2.00163
H	-1.83273	-0.99111	-2.13379
H	-0.07087	-0.81951	-2.20920
H	-0.83894	-2.33161	-2.73004
C	0.43824	-2.96482	-0.47330
O	0.37080	-4.17197	-0.48157
O	1.63510	-2.36217	-0.45899
H	1.53453	-1.39522	-0.39222
C	0.13155	-2.16347	2.47944
H	0.18372	-3.15320	2.01917
H	1.10059	-1.67418	2.32952
H	-0.00070	-2.30825	3.55517
C	0.80528	1.14487	3.69889
H	1.59238	1.87625	3.51210
H	0.20705	1.47755	4.55050
H	1.27186	0.19048	3.96195

6''-e

C	-1.54842	0.44683	2.05511
C	-0.21316	1.18772	2.26478
C	-0.48024	-1.12781	0.50909
C	-1.36636	-1.04217	1.74851
H	-2.09694	0.90329	1.22467
H	-2.16909	0.56909	2.94858
H	-0.26721	2.16324	1.76599
H	-0.93607	-0.54070	-0.30016
H	-2.34747	-1.44430	1.47489
C	0.99121	0.52565	1.61202
O	2.12242	0.91134	1.78058
O	0.81412	-0.53932	0.79301
C	-0.18940	-2.55047	0.00117
H	0.46959	-3.03023	0.73812
C	-1.46898	-3.36665	-0.16412
H	-1.94009	-3.55590	0.80216
H	-2.18388	-2.84437	-0.80685
H	-1.24088	-4.32438	-0.63208
C	0.58571	-2.52851	-1.32210
O	0.21460	-3.10737	-2.31532
O	1.74132	-1.85098	-1.34169
H	1.87366	-1.36092	-0.51059
C	-0.80887	-1.84044	2.93010
H	-0.81831	-2.91552	2.72975
H	0.22346	-1.56114	3.16609
H	-1.41588	-1.66198	3.82183
C	0.10016	1.45278	3.74467
H	1.05046	1.97730	3.85321
H	-0.69387	2.06780	4.17490
H	0.14989	0.51783	4.31017

6''-f

C	-0.48759	-0.65882	3.06187
C	-0.60374	0.82705	2.63862
C	-0.09203	-0.87848	0.63526
C	0.17274	-1.55419	1.98745
H	-1.49320	-1.01984	3.29596
H	0.09461	-0.71285	3.98797
H	-1.54155	0.94125	2.07621
H	-1.16685	-0.67244	0.56951
H	-0.33424	-2.52336	1.97191
C	0.47264	1.21023	1.64429
O	1.16153	2.20152	1.70432
O	0.62025	0.37349	0.59376
C	0.28290	-1.59705	-0.66740
H	-0.05314	-0.91764	-1.46440
C	1.77939	-1.85847	-0.89599
H	2.36157	-1.02894	-0.48992
H	2.12097	-2.78319	-0.42624
H	2.00827	-1.90901	-1.96525
C	-0.58759	-2.83570	-0.82777
O	-1.59819	-3.03678	-0.19845
O	-0.20699	-3.72443	-1.76171
H	0.62056	-3.46520	-2.19062
C	1.65670	-1.76786	2.30701
H	2.13006	-2.48963	1.64088
H	2.22238	-0.83119	2.25111
H	1.75129	-2.15202	3.32627
C	-0.62786	1.77417	3.83035
H	-0.79966	2.80525	3.51541
H	-1.42447	1.47975	4.51907
H	0.32463	1.73607	4.36643

6''-g

C	-0.90845	-0.61566	2.87954
C	-0.51360	0.87663	2.80187
C	-0.22640	-0.88480	0.56332
C	-0.05749	-1.49424	1.95657
H	-1.96032	-0.73609	2.60201
H	-0.81259	-0.95790	3.91504
H	-1.42657	1.47922	2.71098
H	-1.30125	-0.77322	0.38130
H	-0.50431	-2.49308	1.92791
C	0.28924	1.26939	1.56418
O	0.85045	2.33791	1.47202
O	0.36726	0.42821	0.51597
C	0.34987	-1.61261	-0.65905
H	0.05540	-0.99285	-1.51865
C	1.87906	-1.74929	-0.69844
H	2.33550	-0.84813	-0.28384
H	2.23958	-2.61094	-0.13298
H	2.23971	-1.83630	-1.72818

C	-0.39071	-2.92731	-0.86042
O	-1.44448	-3.19623	-0.33590
O	0.16460	-3.80980	-1.70909
H	1.00883	-3.49212	-2.05871
C	1.38948	-1.60004	2.45289
H	1.94070	-2.39384	1.94721
H	1.94817	-0.66752	2.31509
H	1.39061	-1.83114	3.52215
C	0.22999	1.35659	4.05483
H	0.48534	2.41410	3.97745
H	-0.40425	1.20757	4.93218
H	1.15211	0.78521	4.20066

6''-h

C	0.16984	-0.61662	2.86599
C	0.05731	0.90220	2.75323
C	-0.72641	-0.85010	0.50189
C	-0.84841	-1.30585	1.96210
H	-0.01529	-0.90774	3.90586
H	1.19209	-0.93419	2.63418
H	-0.92129	1.19511	3.16344
H	-1.67816	-1.04395	0.00225
H	-1.84068	-0.96463	2.28879
C	-0.00334	1.38101	1.31294
O	0.33850	2.49096	0.97325
O	-0.54264	0.57690	0.37554
C	0.36138	-1.48854	-0.39116
H	0.29971	-0.91245	-1.32435
C	1.79664	-1.37358	0.12395
H	1.99938	-0.34736	0.44329
H	2.00051	-2.03343	0.97249
H	2.51723	-1.58848	-0.67158
C	-0.07523	-2.88897	-0.81723
O	-1.21505	-3.15481	-1.11304
O	0.86505	-3.84458	-0.90487
H	1.74110	-3.51966	-0.65563
C	-0.81397	-2.82687	2.10643
H	-1.57553	-3.31047	1.48995
H	0.16364	-3.23849	1.82972
H	-0.99538	-3.09860	3.14973
C	1.15307	1.63490	3.52213
H	1.01505	2.71561	3.47451
H	1.13941	1.32134	4.56935
H	2.13706	1.39715	3.10535

6''-i

C	-0.71144	-0.52000	2.86547
C	0.18493	0.68895	2.57462
C	-0.74125	-1.10079	0.45043
C	-1.61581	-0.81544	1.67446
H	-1.30978	-0.30805	3.75759
H	-0.09657	-1.39814	3.10497
H	-0.45063	1.58637	2.62379
H	-1.38380	-1.21677	-0.42897
H	-2.12646	0.12070	1.40656
C	0.71833	0.74275	1.15124
O	1.67164	1.40236	0.82075
O	0.02794	0.10270	0.16214
C	0.27464	-2.26798	0.50328
H	1.10903	-1.94741	1.14671
C	-0.27841	-3.58391	1.04367
H	-0.47031	-3.51459	2.11443
H	-1.20412	-3.86656	0.53462
H	0.44987	-4.37704	0.87485
C	0.89560	-2.51036	-0.88509
O	1.02238	-3.61345	-1.36101
O	1.32871	-1.44368	-1.56753
H	1.11838	-0.61232	-1.10168
C	-2.71569	-1.83723	1.96877
H	-3.21321	-2.16501	1.05076
H	-2.34601	-2.71992	2.49146
H	-3.46951	-1.36942	2.60756
C	1.32392	0.84132	3.58041
H	1.89221	1.75459	3.40039
H	0.91397	0.87380	4.59311
H	2.00904	-0.00977	3.51516

6''-j

C	-0.25121	-1.00063	2.71119
C	0.30658	0.42158	2.63118
C	-1.19634	-0.72820	0.39099
C	-1.48508	-1.16295	1.83036
H	-0.51400	-1.21897	3.75231
H	0.52439	-1.72549	2.43735
H	-0.36912	1.07277	3.20728
H	-2.15593	-0.61689	-0.12670
H	-2.24771	-0.46060	2.19490
C	0.26029	1.04983	1.24564
O	0.88498	2.04513	0.96440
O	-0.62138	0.58423	0.33098
C	-0.37456	-1.69367	-0.48921
H	-0.92898	-2.63839	-0.51467
C	-0.25672	-1.15060	-1.92285
H	-1.25409	-0.99185	-2.34097
H	0.27925	-0.19989	-1.91865
H	0.27806	-1.85527	-2.56478
C	1.03329	-1.93287	0.02960
O	1.79384	-1.04212	0.32414
O	1.45131	-3.20906	0.12229
H	0.77427	-3.83380	-0.17155
C	-2.06799	-2.57326	1.90027
H	-2.89804	-2.70330	1.19809
H	-1.30935	-3.33248	1.68132
H	-2.44414	-2.77123	2.90724
C	1.70919	0.53008	3.22585
H	2.05264	1.56531	3.23877
H	1.70342	0.14699	4.25030
H	2.41141	-0.06327	2.63349