

ADDENDUM III: CONFORMATION ANALYSIS OF FS-2 ***- MONTE CARLO SIMULATION***

Conformation analysis of the two possible configurations proposed for FS-2¹⁹⁷ was conducted using the Monte Carlo simulation package available in MacroModel¹⁹⁸. The simulations were carried out in the gas phase using the MM2 method and the PROCG force field. One thousand interactions were performed for each configuration and those that were not within 50 KJ/mol (~ 12 Kcal/mol) of the lowest energy structure were discarded. The structures with 9-S configuration (α -OH) will be referred as the Tempesta series, and the structures with 9-R configuration (β -OH) will be referred as the Gilbert series.

For the Tempesta series, 303 different structures were found within the limit of 50 KJ/mol and these could be distributed within six main conformations¹⁹⁹. The lowest energy structure for each of the six conformations was examined and they were found to be within 4 Kcal/mol of each other, making it difficult to rule out conformations based on thermodynamic arguments alone.

For the Gilbert series, 346 different structures were found distributed within sixteen main conformations. Again, the lowest energy structure for each conformation

¹⁹⁷ See Chapter 1 “Revised Structure”

¹⁹⁸ MacroModel (version 4.5) was developed by Prof. Clark Still at Columbia University - www.cc.columbia.edu/cu/chemistry/mmod/mmod.html.

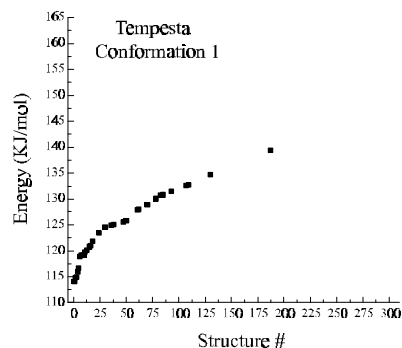
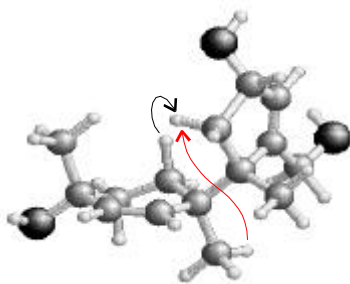
¹⁹⁹ Many structures were found within the same conformation classification due to small variations on angles and/or orientation of OH bonds, etc., which were considered different structures by the computer.

was examined. Of these, nine of the structures lie within 4 Kcal/mol of the overall lowest Gilbert structure energy, only these nine conformations were analyzed further. Four of those conformations contained hydrogen bonds that helped stabilize their structures.

The Nuclear Overhauser Effect data reported for FS-2 by Tempesta²⁰⁰ was used to help decide which of the two configurations best fit the experimental data. The proton-proton distances from the calculated structures (Monte Carlo simulations) were compared to the experimental data. The NOEs reported were assumed to involve atoms within 3Å of each other. It was considered a violation if the distance between two protons was larger than 4Å and there was an observed NOE, or if the distance was less than 3Å and there was no reported NOE. In some instances the chemical shift dispersion of the two nuclei in question was not enough for NOEs to be observed even though it satisfied the distance criteria and these were dismissed.

The results for the analysis of each conformation are presented below. Only one conformation (Tempesta #3) meets the criteria described above for satisfying the experimental NMR data. Shown are a representative model and description for each conformer next to a graph of the distribution of that conformer's energy with respect to all its structures.

²⁰⁰ Corley, D. G.; Rottinghaus, G. E.; Tempesta, M. S. *J. Org. Chem.* **1987**, *52*, 4405.



Tempesta #1

Lowest energy structure: structure #1, $E = 114.06$ KJ/mol (27.26 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, methyl front and primary OH back.

NOE violations: one (4.579 Å) - seen in red.

Expected NOEs not seen: one (2.180 Å) - seen in black.

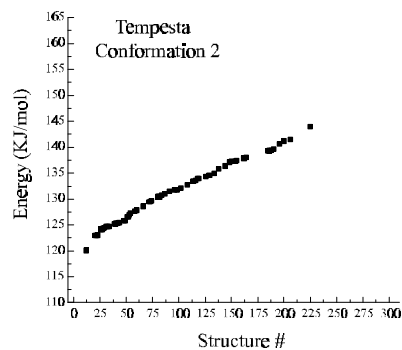
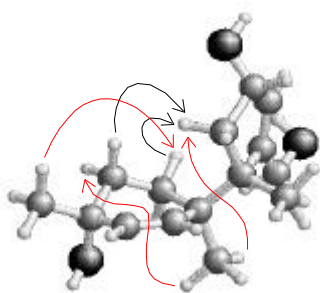
PDB-format file:

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ATOM      6      C           2.500  -0.234  -0.013
ATOM      7      C           1.304   1.422  -1.489
ATOM      8      C           1.083  -1.111  -1.979
ATOM      9      H          -0.966   0.004   1.875
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ATOM     11      O           1.103   0.894   3.271
ATOM     12      C           1.458  -1.421   2.782
ATOM     13      C           2.373  -1.574  -2.648
ATOM     14      C           0.582  -2.442  -1.336
ATOM     15      H           0.376   1.693  -2.041
ATOM     16      H           1.421   2.203  -0.705
ATOM     17      H           2.157   1.542  -2.191
ATOM     18      C           0.102  -0.743  -3.115
ATOM     19      H           3.411   0.122  -0.544
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ATOM     22      C           1.276  -3.601  -2.072
ATOM     23      H           0.390   0.606   3.815
ATOM     24      H           2.374  -1.459   3.414
ATOM     25      H           0.597  -1.722   3.423
ATOM     26      H           1.562  -2.195   1.990
ATOM     27      H          -0.529  -2.546  -1.343
ATOM     28      H           0.886  -2.497  -0.267
ATOM     29      H           2.387   1.559   1.209
ATOM     30      H           3.393   0.273   1.921
ATOM     31      H          -0.048  -1.598  -3.814
ATOM     32      H          -0.904  -0.465  -2.731
ATOM     33      H           0.468   0.105  -3.736
ATOM     34      C           3.341  -0.648  -3.344
ATOM     35      H           0.635  -4.040  -2.875

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ATOM	37	H				3.268	-3.484	-3.164
ATOM	38	O				4.325	-1.325	-4.099
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END								



Tempesta #2

Lowest energy structure: structure #12, E = 120.06 KJ/mol (28.70 Kcal/mol).

Description: Quaternary methyls gauche, twisted chair, methyl front, primary OH back.

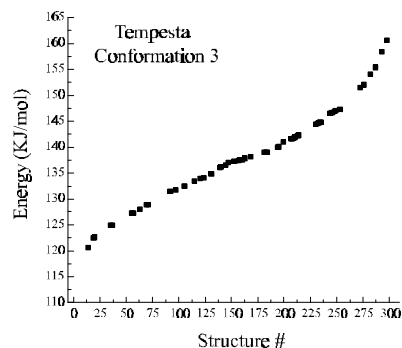
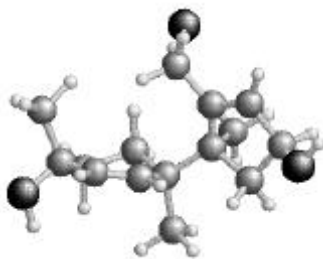
NOE violations: three (4.290 Å, 4.612 Å, 4.844 Å) - seen in red.

Expected NOEs not seen: two (2.203 Å, 2.631 Å) - seen in black.

PDB-format file:

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ATOM	6	C	2.511	-0.373	-0.044
ATOM	7	C	1.371	1.480	-1.319
ATOM	8	C	1.037	-0.963	-2.092
ATOM	9	H	-0.959	0.026	1.885
ATOM	10	C	2.263	-0.917	1.372
ATOM	11	O	1.811	1.255	2.281
ATOM	12	C	1.020	-0.615	3.558
ATOM	13	C	2.292	-1.379	-2.853
ATOM	14	C	0.531	-2.352	-1.602
ATOM	15	H	0.457	1.852	-1.832
ATOM	16	H	1.519	2.157	-0.446
ATOM	17	H	2.229	1.651	-2.004
ATOM	18	C	0.046	-0.436	-3.155
ATOM	19	H	3.165	0.524	0.063
ATOM	20	H	3.149	-1.114	-0.575
ATOM	21	C	2.308	-2.695	-3.102
ATOM	22	C	1.100	-3.408	-2.566
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ATOM	25	H	0.307	0.019	4.133
ATOM	26	H	0.596	-1.644	3.507
ATOM	27	H	-0.579	-2.416	-1.507
ATOM	28	H	0.953	-2.563	-0.594
ATOM	29	H	3.229	-0.980	1.929
ATOM	30	H	1.869	-1.959	1.316
ATOM	31	H	-0.149	-1.196	-3.946
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ATOM	33	H	0.432	0.465	-3.682
ATOM	34	C	3.319	-0.401	-3.369
ATOM	35	H	0.397	-3.656	-3.398
ATOM	36	O	1.432	-4.591	-1.875
ATOM	37	H	3.081	-3.228	-3.678

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END							



Tempesta #3

Lowest energy structure: structure #14, E = 120.55 KJ/mol (28.81 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, methyl back and secondary OH front.

NOE violations: **none**.

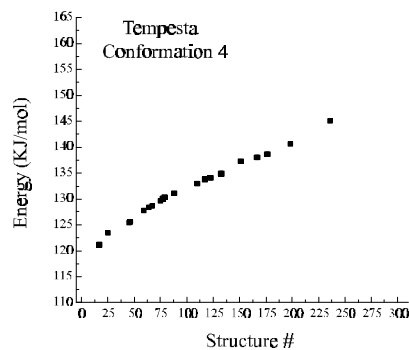
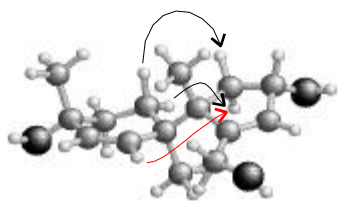
Expected NOEs not seen: **none**.

This is the structure that best fits the experimental data available on the molecule. It is 1.55 Kcal/mol more energetic than the lowest energy overall structure for the Tempesta configuration and 3.9 Kcal/mol more energetic than the lowest energy structure for the Gilbert configuration.

PDB-format file:

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ATOM	6	C	2.458	-0.416	0.001
ATOM	7	C	1.469	1.466	-1.320
ATOM	8	C	1.048	-0.938	-2.111
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ATOM	13	C	0.286	-2.237	-1.857
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ATOM	16	H	1.600	2.162	-0.462
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ATOM	27	H				0.665	0.367	-3.906
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ATOM	33	H				3.024	-1.955	-2.142
ATOM	34	C				0.562	-3.164	-0.701
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ATOM	36	O				-1.873	-1.105	-4.332
ATOM	37	H				-1.196	-3.418	-2.924
ATOM	38	O				-0.186	-4.362	-0.744
ATOM	39	H				1.636	-3.461	-0.706
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END								



Tempesta #4

Lowest energy structure: structure #17, E = 121.18 KJ/mol (28.96 Kcal/mol).

Description: Quaternary methyls anti, pseudo chair, primary OH front, “flat structure”.

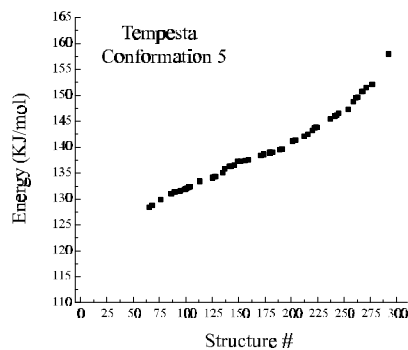
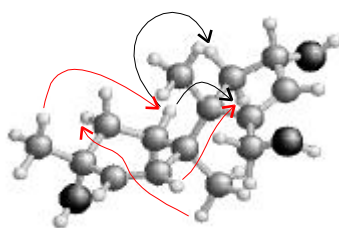
NOE violations: one (4.639 Å) - seen in red.

Expected NOEs not seen: two (2.301 Å, 2.541 Å) - seen in black.

PDB-format file:

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ATOM	6	C	2.487	-0.256	-0.011
ATOM	7	C	1.353	1.423	-1.486
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ATOM	9	H	-0.965	0.010	1.876
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ATOM	11	O	1.110	0.880	3.275
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ATOM	13	C	0.221	-0.776	-3.208
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ATOM	16	H	1.390	2.202	-0.692
ATOM	17	H	2.269	1.553	-2.103
ATOM	18	C	0.606	-2.452	-1.438
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ATOM	20	H	2.617	-1.344	0.178
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ATOM	22	C	2.166	-1.741	-4.170
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ATOM	29	H	2.396	1.543	1.206
ATOM	30	H	3.392	0.249	1.918
ATOM	31	H	0.582	-3.239	-2.226
ATOM	32	H	1.258	-2.840	-0.625
ATOM	33	H	-0.425	-2.386	-1.024
ATOM	34	C	-1.219	-0.327	-3.116
ATOM	35	H	2.108	-2.849	-4.305

ATOM	36	O				3.131	-1.217	-5.053
ATOM	37	H				0.351	-1.063	-5.359
ATOM	38	O				-1.876	-0.275	-4.366
ATOM	39	H				-1.792	-1.052	-2.493
ATOM	40	H				-1.306	0.687	-2.665
ATOM	41	H				2.942	-1.542	-5.918
ATOM	42	H				-1.457	0.391	-4.887
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CONNECT	41	36						
CONNECT	42	38						
END								



Tempesta #5

Lowest energy structure: structure #65, E = 128.41 KJ/mol (30.69 Kcal/mol).

Description: Quaternary methyls anti, twisted chair, primary OH front, “flat structure”.

NOE violations: three (4.631 Å, 4.643 Å, 4.688 Å) - seen in red.

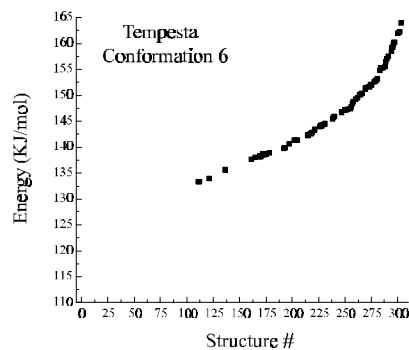
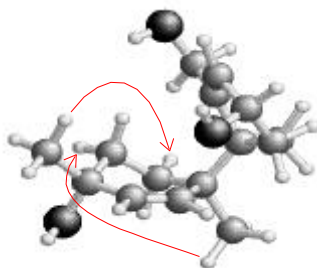
Expected NOEs not seen: two (2.308 Å, 2.346 Å) - seen in black.

PDB-format file:

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ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.228	0.000	-0.896
ATOM	4	H	-0.984	0.014	-0.491
ATOM	5	C	1.244	0.037	2.193
ATOM	6	C	2.491	0.182	-0.006
ATOM	7	C	1.126	1.277	-1.773
ATOM	8	C	1.265	-1.292	-1.791
ATOM	9	H	-0.966	0.010	1.874
ATOM	10	C	2.435	-0.485	1.375
ATOM	11	O	1.516	1.375	2.564
ATOM	12	C	1.061	-0.795	3.474
ATOM	13	C	0.288	-1.334	-2.970
ATOM	14	C	2.618	-1.429	-2.556
ATOM	15	H	0.273	1.258	-2.484
ATOM	16	H	0.979	2.188	-1.148
ATOM	17	H	2.043	1.454	-2.378
ATOM	18	C	1.025	-2.598	-1.002
ATOM	19	H	2.645	1.268	0.194
ATOM	20	H	3.419	-0.131	-0.532
ATOM	21	C	0.880	-1.764	-4.094
ATOM	22	C	2.328	-2.105	-3.906
ATOM	23	H	0.796	1.691	3.084
ATOM	24	H	1.986	-0.784	4.095
ATOM	25	H	0.231	-0.398	4.104
ATOM	26	H	0.825	-1.857	3.234
ATOM	27	H	3.403	-1.975	-1.983
ATOM	28	H	3.028	-0.421	-2.788
ATOM	29	H	3.383	-0.296	1.933
ATOM	30	H	2.361	-1.589	1.270
ATOM	31	H	0.975	-3.483	-1.678
ATOM	32	H	1.850	-2.817	-0.292
ATOM	33	H	0.073	-2.580	-0.426
ATOM	34	C	-1.204	-1.124	-2.852
ATOM	35	H	2.460	-3.214	-3.869

ATOM	36	O				3.147	-1.576	-4.925
ATOM	37	H				0.373	-1.946	-5.054
ATOM	38	O				-1.926	-1.548	-3.990
ATOM	39	H				-1.593	-1.729	-2.000
ATOM	40	H				-1.454	-0.051	-2.691
ATOM	41	H				2.982	-2.063	-5.715
ATOM	42	H				-1.696	-0.983	-4.709
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CONNECT	16	7						
CONNECT	17	7						
CONNECT	18	8	31	32	33			
CONNECT	19	6						
CONNECT	20	6						
CONNECT	21	13	22	37				
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CONNECT	24	12						
CONNECT	25	12						
CONNECT	26	12						
CONNECT	27	14						
CONNECT	28	14						
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CONNECT	31	18						
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CONNECT	35	22						
CONNECT	36	22	41					
CONNECT	37	21						
CONNECT	38	34	42					
CONNECT	39	34						
CONNECT	40	34						
CONNECT	41	36						
CONNECT	42	38						

END



Tempesta #6

Lowest energy structure: structure #111, E = 133.38 KJ/mol (31.88 Kcal/mol).

Description: Quaternary methyls gauche, twisted chair, secondary OH front, methyl back.

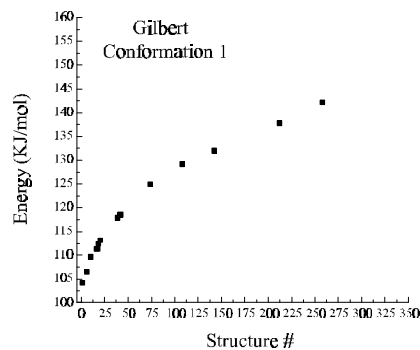
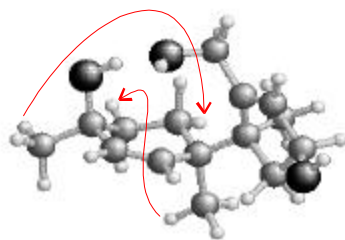
NOE violations: two (4.717 Å, 4.924 Å) - seen in red.

Expected NOEs not seen: **none**.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.232	0.000	-0.893
ATOM	4	H	-0.984	0.045	-0.494
ATOM	5	C	1.244	0.026	2.193
ATOM	6	C	2.466	0.306	-0.010
ATOM	7	C	1.029	1.238	-1.810
ATOM	8	C	1.362	-1.305	-1.770
ATOM	9	H	-0.966	0.024	1.874
ATOM	10	C	2.448	-0.416	1.346
ATOM	11	O	1.481	1.347	2.640
ATOM	12	C	1.084	-0.883	3.425
ATOM	13	C	1.882	-2.548	-1.051
ATOM	14	C	-0.025	-1.849	-2.238
ATOM	15	H	0.197	1.092	-2.535
ATOM	16	H	0.780	2.151	-1.221
ATOM	17	H	1.948	1.490	-2.386
ATOM	18	C	2.249	-1.084	-3.019
ATOM	19	H	2.505	1.396	0.220
ATOM	20	H	3.408	0.113	-0.570
ATOM	21	C	0.905	-3.421	-0.774
ATOM	22	C	-0.438	-2.993	-1.288
ATOM	23	H	0.747	1.617	3.166
ATOM	24	H	2.010	-0.886	4.044
ATOM	25	H	0.246	-0.543	4.076
ATOM	26	H	0.872	-1.935	3.124
ATOM	27	H	0.101	-2.318	-3.243
ATOM	28	H	-0.814	-1.079	-2.393
ATOM	29	H	3.397	-0.226	1.901
ATOM	30	H	2.379	-1.515	1.201
ATOM	31	H	2.422	-2.032	-3.578
ATOM	32	H	1.781	-0.388	-3.750
ATOM	33	H	3.252	-0.681	-2.752
ATOM	34	C	3.349	-2.854	-0.841
ATOM	35	H	-0.958	-3.818	-1.835

ATOM	36	O				-1.280	-2.549	-0.250
ATOM	37	H				1.048	-4.407	-0.303
ATOM	38	O				3.576	-3.884	0.098
ATOM	39	H				3.791	-3.189	-1.807
ATOM	40	H				3.926	-1.967	-0.498
ATOM	41	H				-1.611	-3.306	0.203
ATOM	42	H				3.222	-3.607	0.926
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CONNECT	16	7						
CONNECT	17	7						
CONNECT	18	8	31	32	33			
CONNECT	19	6						
CONNECT	20	6						
CONNECT	21	13	22	37				
CONNECT	22	21	14	35	36			
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CONNECT	24	12						
CONNECT	25	12						
CONNECT	26	12						
CONNECT	27	14						
CONNECT	28	14						
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CONNECT	37	21						
CONNECT	38	34	42					
CONNECT	39	34						
CONNECT	40	34						
CONNECT	41	36						
CONNECT	42	38						
END								



Gilbert #1

Lowest energy structure: structure #1, E = 104.20 KJ/mol (24.91 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, H-bond with primary OH (1.911 Å), six-membered ring donor, secondary OH front, methyl back.

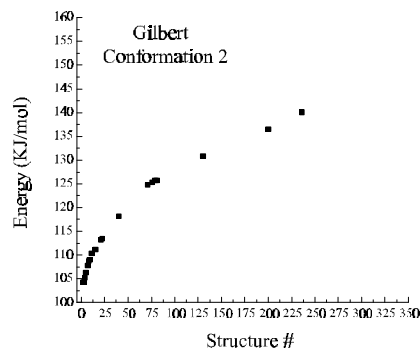
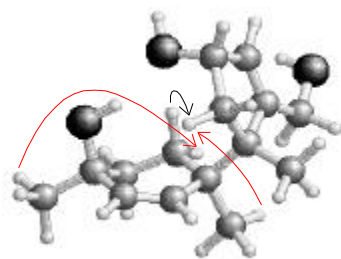
NOE violations: two (3.755 Å, 4.842 Å) - seen in red.

Expected NOEs not seen: **none**.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.244	0.000	-0.873
ATOM	4	H	-0.980	0.036	-0.503
ATOM	5	C	1.245	-0.086	2.192
ATOM	6	C	2.483	-0.353	-0.012
ATOM	7	C	1.421	1.465	-1.353
ATOM	8	C	1.074	-0.965	-2.098
ATOM	9	H	-0.966	0.014	1.874
ATOM	10	C	2.488	0.307	1.374
ATOM	11	C	1.113	0.824	3.427
ATOM	12	O	1.400	-1.412	2.664
ATOM	13	C	0.432	-2.323	-1.819
ATOM	14	C	0.071	-0.408	-3.158
ATOM	15	H	0.549	1.849	-1.927
ATOM	16	H	1.534	2.177	-0.506
ATOM	17	H	2.319	1.587	-1.999
ATOM	18	C	2.410	-1.245	-2.825
ATOM	19	H	3.419	-0.071	-0.548
ATOM	20	H	2.544	-1.450	0.152
ATOM	21	C	-0.470	-2.651	-2.755
ATOM	22	C	-0.612	-1.613	-3.828
ATOM	23	H	0.545	0.274	-3.902
ATOM	24	H	-0.739	0.170	-2.659
ATOM	25	H	2.530	1.414	1.263
ATOM	26	H	3.413	0.026	1.932
ATOM	27	H	2.258	-1.849	-3.749
ATOM	28	H	2.915	-0.305	-3.140
ATOM	29	H	3.125	-1.819	-2.196
ATOM	30	C	0.857	-3.295	-0.748
ATOM	31	H	2.032	0.780	4.056
ATOM	32	H	0.953	1.886	3.131
ATOM	33	H	0.255	0.519	4.069
ATOM	34	H	1.306	-2.011	1.938
ATOM	35	H	-0.089	-1.944	-4.758

ATOM	36	O				-1.959	-1.328	-4.133
ATOM	37	H				-1.010	-3.611	-2.798
ATOM	38	O				0.395	-2.925	0.530
ATOM	39	H				0.446	-4.312	-0.956
ATOM	40	H				1.966	-3.398	-0.717
ATOM	41	H				-2.317	-2.064	-4.599
ATOM	42	H				-0.549	-2.965	0.523
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CONNECT	3	6	1	7	8			
CONNECT	4	1						
CONNECT	5	2	10	11	12			
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CONNECT	9	2						
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CONNECT	12	5	34					
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CONNECT	16	7						
CONNECT	17	7						
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CONNECT	24	14						
CONNECT	25	10						
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CONNECT	27	18						
CONNECT	28	18						
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CONNECT	37	21						
CONNECT	38	30	42					
CONNECT	39	30						
CONNECT	40	30						
CONNECT	41	36						
CONNECT	42	38						
END								



Gilbert #2

Lowest energy structure: structure #2, E = 104.30 KJ/mol (24.93 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, H-bond with secondary OH (1.963 Å), six-membered ring donor, primary OH back, methyl front.

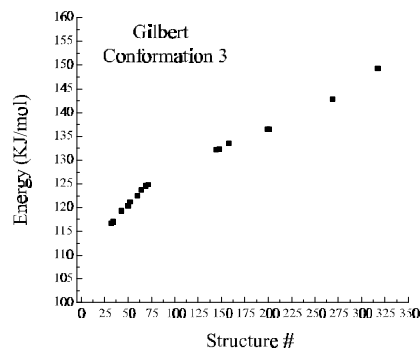
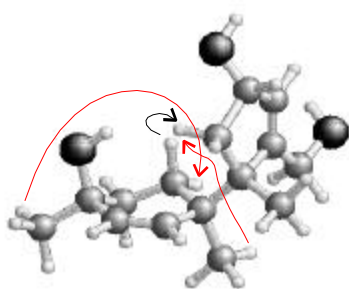
NOE violations: two (4.329 Å, 4.879 Å) - seen in red.

Expected NOEs not seen: one (3.245 Å)* - seen in black.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.340
ATOM	3	C	1.240	0.000	-0.880
ATOM	4	H	-0.975	0.004	-0.516
ATOM	5	C	1.261	-0.002	2.167
ATOM	6	C	2.533	-0.002	-0.024
ATOM	7	C	1.189	1.369	-1.606
ATOM	8	C	1.174	-1.226	-1.863
ATOM	9	H	-0.963	-0.006	1.879
ATOM	10	C	2.384	0.661	1.352
ATOM	11	C	1.043	0.759	3.488
ATOM	12	O	1.620	-1.330	2.501
ATOM	13	C	2.545	-1.722	-2.308
ATOM	14	C	0.624	-2.525	-1.184
ATOM	15	H	0.229	1.540	-2.144
ATOM	16	H	1.282	2.216	-0.888
ATOM	17	H	2.011	1.486	-2.346
ATOM	18	C	0.308	-0.945	-3.113
ATOM	19	H	3.373	0.477	-0.577
ATOM	20	H	2.879	-1.036	0.167
ATOM	21	C	2.871	-2.897	-1.750
ATOM	22	C	1.807	-3.451	-0.847
ATOM	23	H	-0.008	-3.082	-1.914
ATOM	24	H	-0.041	-2.370	-0.306
ATOM	25	H	2.162	1.746	1.219
ATOM	26	H	3.347	0.600	1.914
ATOM	27	H	0.274	-1.822	-3.799
ATOM	28	H	-0.742	-0.704	-2.832
ATOM	29	H	0.698	-0.105	-3.729
ATOM	30	C	3.422	-0.956	-3.268
ATOM	31	H	1.976	0.782	4.096
ATOM	32	H	0.733	1.813	3.302
ATOM	33	H	0.253	0.278	4.110
ATOM	34	H	1.668	-1.865	1.721
ATOM	35	H	1.585	-4.522	-1.074

ATOM	36	O				2.140	-3.345	0.520
ATOM	37	H				3.816	-3.438	-1.916
ATOM	38	O				4.658	-1.589	-3.529
ATOM	39	H				2.903	-0.850	-4.249
ATOM	40	H				3.650	0.058	-2.869
ATOM	41	H				2.772	-4.016	0.725
ATOM	42	H				5.149	-1.609	-2.724
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CONNECT	37	21						
CONNECT	38	30	42					
CONNECT	39	30						
CONNECT	40	30						
CONNECT	41	36						
CONNECT	42	38						
END								



Gilbert #3

Lowest energy structure: structure #12, E = 110.52 KJ/mol (26.42 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, primary OH back, methyl front.

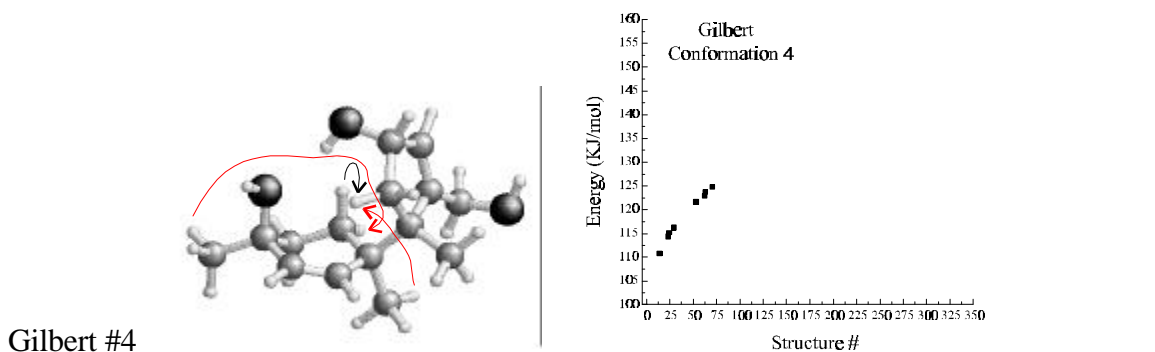
NOE violations: two (4.569 Å, 4.850 Å) - seen in red.

Expected NOEs not seen: one (2.193 Å) - seen in black.

PDB-format file:

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ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.239	0.000	-0.884
ATOM	4	H	-0.978	0.022	-0.508
ATOM	5	C	1.251	-0.031	2.183
ATOM	6	C	2.510	-0.197	-0.017
ATOM	7	C	1.283	1.411	-1.516
ATOM	8	C	1.098	-1.136	-1.954
ATOM	9	H	-0.965	0.004	1.876
ATOM	10	C	2.440	0.487	1.356
ATOM	11	C	1.070	0.825	3.450
ATOM	12	O	1.510	-1.356	2.605
ATOM	13	C	2.395	-1.593	-2.614
ATOM	14	C	0.619	-2.459	-1.277
ATOM	15	H	0.349	1.660	-2.069
ATOM	16	H	1.396	2.206	-0.745
ATOM	17	H	2.131	1.529	-2.226
ATOM	18	C	0.108	-0.810	-3.096
ATOM	19	H	3.409	0.186	-0.550
ATOM	20	H	2.712	-1.278	0.154
ATOM	21	C	2.515	-2.927	-2.601
ATOM	22	C	1.351	-3.625	-1.962
ATOM	23	H	-0.488	-2.589	-1.296
ATOM	24	H	0.907	-2.472	-0.201
ATOM	25	H	2.346	1.589	1.216
ATOM	26	H	3.391	0.324	1.917
ATOM	27	H	-0.026	-1.682	-3.776
ATOM	28	H	-0.902	-0.544	-2.714
ATOM	29	H	0.456	0.033	-3.734
ATOM	30	C	3.342	-0.666	-3.339
ATOM	31	H	1.997	0.825	4.068
ATOM	32	H	0.833	1.883	3.193
ATOM	33	H	0.243	0.438	4.089
ATOM	34	H	1.534	-1.924	1.855
ATOM	35	H	0.726	-4.121	-2.744
ATOM	36	O	1.756	-4.586	-1.014
ATOM	37	H	3.336	-3.496	-3.067

ATOM	38	O			4.330	-1.344	-4.087
ATOM	39	H			2.771	-0.045	-4.068
ATOM	40	H			3.873	0.008	-2.631
ATOM	41	H			2.140	-5.313	-1.477
ATOM	42	H			4.895	-1.796	-3.483
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CONNECT	16	7					
CONNECT	17	7					
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CONNECT	20	6					
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CONNECT	34	12					
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CONNECT	37	21					
CONNECT	38	30	42				
CONNECT	39	30					
CONNECT	40	30					
CONNECT	41	36					
CONNECT	42	38					
END							



Lowest energy structure: structure #14, E = 110.91 KJ/mol (26.51 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, H-bond with secondary OH (2.116 Å)*, five-membered ring donor, primary OH back, methyl front.

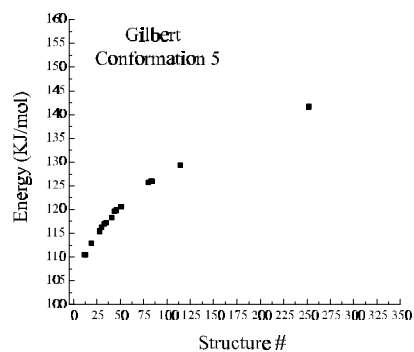
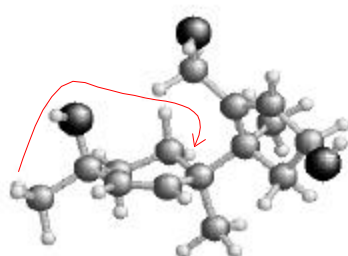
NOE violations: two (4.372 Å, 4.891 Å) - seen in red.

Expected NOEs not seen: one (3.029 Å)* - seen in black.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.340
ATOM	3	C	1.246	0.000	-0.874
ATOM	4	H	-0.974	0.009	-0.518
ATOM	5	C	1.266	-0.030	2.159
ATOM	6	C	2.537	0.023	-0.017
ATOM	7	C	1.163	1.358	-1.617
ATOM	8	C	1.219	-1.252	-1.824
ATOM	9	H	-0.961	-0.001	1.882
ATOM	10	C	2.368	0.684	1.358
ATOM	11	C	1.067	0.640	3.529
ATOM	12	O	1.656	-1.376	2.364
ATOM	13	C	2.602	-1.703	-2.280
ATOM	14	C	0.725	-2.544	-1.086
ATOM	15	H	0.208	1.491	-2.173
ATOM	16	H	1.218	2.213	-0.905
ATOM	17	H	1.990	1.503	-2.345
ATOM	18	C	0.331	-1.035	-3.068
ATOM	19	H	3.370	0.515	-0.573
ATOM	20	H	2.895	-1.010	0.176
ATOM	21	C	2.956	-2.892	-1.776
ATOM	22	C	1.911	-3.511	-0.899
ATOM	23	H	-0.033	-3.068	-1.715
ATOM	24	H	0.204	-2.369	-0.120
ATOM	25	H	2.113	1.762	1.234
ATOM	26	H	3.331	0.644	1.921
ATOM	27	H	0.314	-1.937	-3.723
ATOM	28	H	-0.722	-0.813	-2.784
ATOM	29	H	0.693	-0.201	-3.710
ATOM	30	C	3.483	-0.937	-3.233
ATOM	31	H	2.009	0.624	4.124
ATOM	32	H	0.757	1.704	3.414
ATOM	33	H	0.284	0.121	4.128
ATOM	34	H	1.028	-1.783	2.939
ATOM	35	H	1.673	-4.544	-1.257

ATOM	36	O				2.308	-3.606	0.452
ATOM	37	H				3.910	-3.400	-1.989
ATOM	38	O				3.111	-1.155	-4.577
ATOM	39	H				3.460	0.157	-3.036
ATOM	40	H				4.544	-1.266	-3.129
ATOM	41	H				2.229	-2.768	0.879
ATOM	42	H				3.251	-2.067	-4.770
CONNECT	1	2	3	4				
CONNECT	2	1	5	9				
CONNECT	3	6	1	7	8			
CONNECT	4	1						
CONNECT	5	2	10	11	12			
CONNECT	6	10	3	19	20			
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CONNECT	9	2						
CONNECT	10	5	6	25	26			
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CONNECT	12	5	34					
CONNECT	13	8	21	30				
CONNECT	14	22	8	23	24			
CONNECT	15	7						
CONNECT	16	7						
CONNECT	17	7						
CONNECT	18	8	27	28	29			
CONNECT	19	6						
CONNECT	20	6						
CONNECT	21	13	22	37				
CONNECT	22	21	14	35	36			
CONNECT	23	14						
CONNECT	24	14						
CONNECT	25	10						
CONNECT	26	10						
CONNECT	27	18						
CONNECT	28	18						
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CONNECT	37	21						
CONNECT	38	30	42					
CONNECT	39	30						
CONNECT	40	30						
CONNECT	41	36						
CONNECT	42	38						
END								



Gilbert #5

Lowest energy structure: structure #25, E = 115.33 KJ/mol (27.57 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, secondary OH front, methyl back.

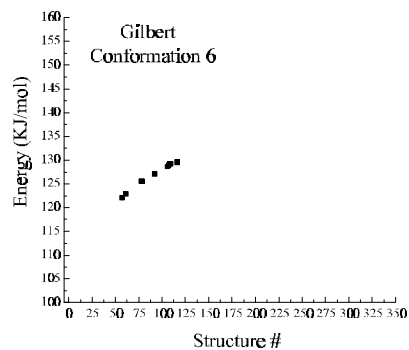
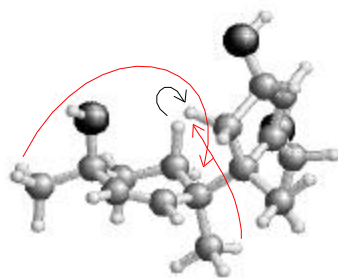
NOE violations: one (4.867 Å) - seen in red.

Expected NOEs not seen: **none**.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.243	0.000	-0.872
ATOM	4	H	-0.978	0.029	-0.508
ATOM	5	C	1.244	-0.060	2.196
ATOM	6	C	2.484	-0.321	0.001
ATOM	7	C	1.411	1.451	-1.395
ATOM	8	C	1.078	-1.004	-2.065
ATOM	9	H	-0.967	0.010	1.873
ATOM	10	C	2.471	0.368	1.374
ATOM	11	C	1.094	0.831	3.442
ATOM	12	O	1.453	-1.391	2.628
ATOM	13	C	0.378	-2.320	-1.735
ATOM	14	C	0.120	-0.471	-3.174
ATOM	15	H	0.527	1.818	-1.962
ATOM	16	H	1.540	2.186	-0.571
ATOM	17	H	2.296	1.550	-2.061
ATOM	18	C	2.424	-1.354	-2.741
ATOM	19	H	3.419	-0.038	-0.537
ATOM	20	H	2.555	-1.414	0.189
ATOM	21	C	-0.480	-2.681	-2.699
ATOM	22	C	-0.540	-1.697	-3.830
ATOM	23	H	0.623	0.188	-3.920
ATOM	24	H	-0.706	0.119	-2.716
ATOM	25	H	2.475	1.475	1.248
ATOM	26	H	3.404	0.123	1.936
ATOM	27	H	2.282	-1.986	-3.647
ATOM	28	H	2.968	-0.440	-3.070
ATOM	29	H	3.101	-1.930	-2.071
ATOM	30	C	0.715	-3.179	-0.542
ATOM	31	H	2.016	0.803	4.069
ATOM	32	H	0.908	1.892	3.158
ATOM	33	H	0.245	0.500	4.083
ATOM	34	H	0.718	-1.652	3.157
ATOM	35	H	0.031	-2.080	-4.711

ATOM	36	O				-1.860	-1.407	-4.229
ATOM	37	H				-1.063	-3.616	-2.720
ATOM	38	O				-0.002	-4.396	-0.503
ATOM	39	H				1.796	-3.448	-0.567
ATOM	40	H				0.484	-2.635	0.401
ATOM	41	H				-2.203	-2.162	-4.677
ATOM	42	H				-0.916	-4.189	-0.404
CONNECT	1	2	3	4				
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CONNECT	9	2						
CONNECT	10	5	6	25	26			
CONNECT	11	5	31	32	33			
CONNECT	12	5	34					
CONNECT	13	8	21	30				
CONNECT	14	22	8	23	24			
CONNECT	15	7						
CONNECT	16	7						
CONNECT	17	7						
CONNECT	18	8	27	28	29			
CONNECT	19	6						
CONNECT	20	6						
CONNECT	21	13	22	37				
CONNECT	22	21	14	35	36			
CONNECT	23	14						
CONNECT	24	14						
CONNECT	25	10						
CONNECT	26	10						
CONNECT	27	18						
CONNECT	28	18						
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CONNECT	34	12						
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CONNECT	37	21						
CONNECT	38	30	42					
CONNECT	39	30						
CONNECT	40	30						
CONNECT	41	36						
CONNECT	42	38						
END								



Gilbert #6

Lowest energy structure: structure #31, E = 116.37 KJ/mol (27.82 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, primary OH back, methyl front.

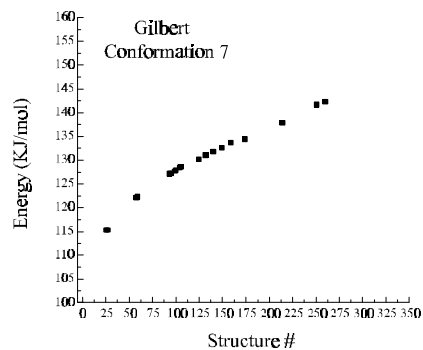
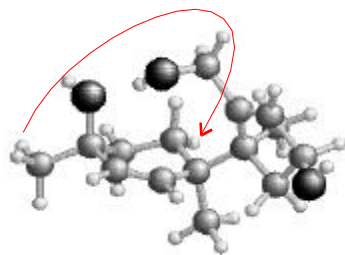
NOE violations: two (4.564 Å, 4.882 Å) - seen in red.

Expected NOEs not seen: one (2.272 Å) - seen in black.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.244	0.000	-0.877
ATOM	4	H	-0.975	0.025	-0.516
ATOM	5	C	1.253	-0.040	2.181
ATOM	6	C	2.514	-0.180	-0.010
ATOM	7	C	1.262	1.419	-1.497
ATOM	8	C	1.121	-1.153	-1.932
ATOM	9	H	-0.965	0.007	1.876
ATOM	10	C	2.432	0.510	1.360
ATOM	11	C	1.074	0.770	3.477
ATOM	12	O	1.543	-1.380	2.530
ATOM	13	C	2.423	-1.724	-2.479
ATOM	14	C	0.524	-2.434	-1.268
ATOM	15	H	0.337	1.646	-2.075
ATOM	16	H	1.325	2.209	-0.716
ATOM	17	H	2.124	1.584	-2.176
ATOM	18	C	0.252	-0.785	-3.153
ATOM	19	H	3.407	0.204	-0.555
ATOM	20	H	2.711	-1.261	0.175
ATOM	21	C	2.419	-3.064	-2.499
ATOM	22	C	1.143	-3.653	-1.975
ATOM	23	H	-0.591	-2.464	-1.282
ATOM	24	H	0.834	-2.485	-0.199
ATOM	25	H	2.318	1.610	1.223
ATOM	26	H	3.385	0.360	1.922
ATOM	27	H	0.092	-1.661	-3.823
ATOM	28	H	-0.757	-0.426	-2.851
ATOM	29	H	0.729	0.004	-3.778
ATOM	30	C	3.528	-0.926	-3.118
ATOM	31	H	2.004	0.757	4.090
ATOM	32	H	0.828	1.834	3.256
ATOM	33	H	0.253	0.357	4.107
ATOM	34	H	0.821	-1.719	3.031
ATOM	35	H	0.514	-4.023	-2.822
ATOM	36	O	1.361	-4.709	-1.068
ATOM	37	H	3.224	-3.687	-2.921

ATOM	38	O			4.770	-1.145	-2.484
ATOM	39	H			3.628	-1.223	-4.189
ATOM	40	H			3.326	0.166	-3.094
ATOM	41	H			1.674	-5.454	-1.554
ATOM	42	H			5.001	-2.052	-2.594
CONNECT	1	2	3	4			
CONNECT	2	1	5	9			
CONNECT	3	6	1	7	8		
CONNECT	4	1					
CONNECT	5	2	10	11	12		
CONNECT	6	10	3	19	20		
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CONNECT	8	3	13	14	18		
CONNECT	9	2					
CONNECT	10	5	6	25	26		
CONNECT	11	5	31	32	33		
CONNECT	12	5	34				
CONNECT	13	8	21	30			
CONNECT	14	22	8	23	24		
CONNECT	15	7					
CONNECT	16	7					
CONNECT	17	7					
CONNECT	18	8	27	28	29		
CONNECT	19	6					
CONNECT	20	6					
CONNECT	21	13	22	37			
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CONNECT	23	14					
CONNECT	24	14					
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CONNECT	26	10					
CONNECT	27	18					
CONNECT	28	18					
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CONNECT	31	11					
CONNECT	32	11					
CONNECT	33	11					
CONNECT	34	12					
CONNECT	35	22					
CONNECT	36	22	41				
CONNECT	37	21					
CONNECT	38	30	42				
CONNECT	39	30					
CONNECT	40	30					
CONNECT	41	36					
CONNECT	42	38					
END							



Gilbert #7

Lowest energy structure: structure #32, E = 116.81 KJ/mol (27.92 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, H-bond with primary OH (1.908 Å), five-membered ring donor, secondary OH front, methyl back.

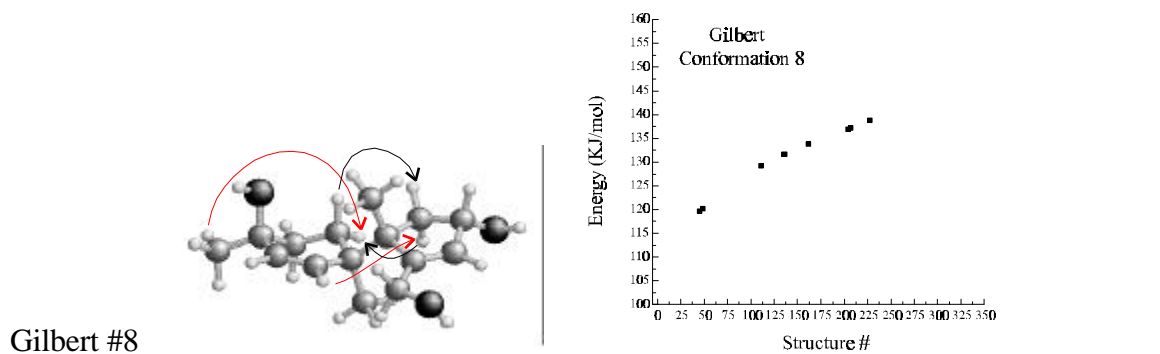
NOE violations: one (4.894 Å) - seen in red.

Expected NOEs not seen: **none**.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.242	0.000	-0.873
ATOM	4	H	-0.979	0.042	-0.504
ATOM	5	C	1.249	-0.096	2.184
ATOM	6	C	2.499	-0.269	-0.008
ATOM	7	C	1.379	1.447	-1.417
ATOM	8	C	1.093	-1.028	-2.048
ATOM	9	H	-0.965	0.018	1.875
ATOM	10	C	2.459	0.398	1.375
ATOM	11	C	1.088	0.708	3.486
ATOM	12	O	1.453	-1.457	2.519
ATOM	13	C	0.446	-2.370	-1.710
ATOM	14	C	0.103	-0.525	-3.146
ATOM	15	H	0.483	1.795	-1.977
ATOM	16	H	1.510	2.193	-0.602
ATOM	17	H	2.253	1.555	-2.097
ATOM	18	C	2.438	-1.338	-2.743
ATOM	19	H	3.420	0.058	-0.546
ATOM	20	H	2.621	-1.358	0.165
ATOM	21	C	-0.436	-2.745	-2.648
ATOM	22	C	-0.556	-1.764	-3.776
ATOM	23	H	0.582	0.133	-3.909
ATOM	24	H	-0.723	0.061	-2.683
ATOM	25	H	2.417	1.506	1.270
ATOM	26	H	3.400	0.176	1.935
ATOM	27	H	2.300	-1.980	-3.643
ATOM	28	H	2.949	-0.411	-3.087
ATOM	29	H	3.144	-1.887	-2.080
ATOM	30	C	0.838	-3.297	-0.585
ATOM	31	H	2.014	0.663	4.103
ATOM	32	H	0.877	1.781	3.271
ATOM	33	H	0.251	0.314	4.108
ATOM	34	H	2.106	-1.515	3.198
ATOM	35	H	-0.006	-2.138	-4.674

ATOM	36	O				-1.894	-1.502	-4.132
ATOM	37	H				-0.977	-3.705	-2.653
ATOM	38	O				0.110	-3.074	0.603
ATOM	39	H				0.612	-4.347	-0.890
ATOM	40	H				1.929	-3.273	-0.371
ATOM	41	H				-2.248	-2.280	-4.528
ATOM	42	H				0.584	-2.467	1.150
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CONNECT	3	6	1	7	8			
CONNECT	4	1						
CONNECT	5	2	10	11	12			
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CONNECT	12	5	34					
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CONNECT	17	7						
CONNECT	18	8	27	28	29			
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CONNECT	20	6						
CONNECT	21	13	22	37				
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CONNECT	23	14						
CONNECT	24	14						
CONNECT	25	10						
CONNECT	26	10						
CONNECT	27	18						
CONNECT	28	18						
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CONNECT	37	21						
CONNECT	38	30	42					
CONNECT	39	30						
CONNECT	40	30						
CONNECT	41	36						
CONNECT	42	38						
END								



Gilbert #8

Lowest energy structure: structure #36, E = 117.43 KJ/mol (28.07 Kcal/mol).

Description: Quaternary methyls anti, pseudo chair, primary OH front, “flat structure”.

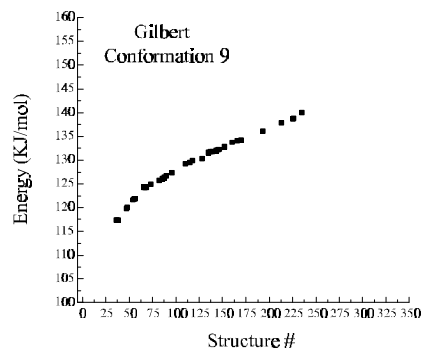
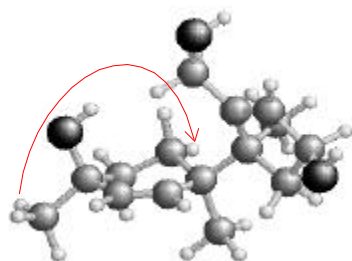
NOE violations: two (4.642 Å, 4.878 Å) - seen in red.

Expected NOEs not seen: two (2.309 Å, 2.512 Å) - seen in black.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.233	0.000	-0.888
ATOM	4	H	-0.981	0.031	-0.497
ATOM	5	C	1.250	-0.037	2.184
ATOM	6	C	2.497	-0.194	-0.005
ATOM	7	C	1.322	1.406	-1.530
ATOM	8	C	1.131	-1.139	-1.962
ATOM	9	H	-0.965	0.010	1.876
ATOM	10	C	2.424	0.510	1.357
ATOM	11	C	1.071	0.780	3.477
ATOM	12	O	1.538	-1.376	2.538
ATOM	13	C	0.244	-0.877	-3.180
ATOM	14	C	2.502	-1.372	-2.667
ATOM	15	H	0.450	1.647	-2.173
ATOM	16	H	1.359	2.208	-0.759
ATOM	17	H	2.226	1.532	-2.165
ATOM	18	C	0.661	-2.480	-1.350
ATOM	19	H	3.411	0.158	-0.540
ATOM	20	H	2.669	-1.274	0.198
ATOM	21	C	0.844	-1.251	-4.319
ATOM	22	C	2.211	-1.830	-4.105
ATOM	23	H	3.168	-2.085	-2.126
ATOM	24	H	3.054	-0.410	-2.749
ATOM	25	H	2.309	1.609	1.211
ATOM	26	H	3.378	0.365	1.918
ATOM	27	H	0.661	-3.297	-2.107
ATOM	28	H	1.314	-2.820	-0.517
ATOM	29	H	-0.375	-2.422	-0.946
ATOM	30	C	-1.206	-0.455	-3.105
ATOM	31	H	2.001	0.767	4.090
ATOM	32	H	0.828	1.843	3.250
ATOM	33	H	0.249	0.371	4.108
ATOM	34	H	0.831	-1.701	3.070
ATOM	35	H	2.177	-2.943	-4.204

ATOM	36	O				3.166	-1.316	-5.005
ATOM	37	H				0.384	-1.233	-5.319
ATOM	38	O				-1.865	-0.472	-4.354
ATOM	39	H				-1.762	-1.165	-2.450
ATOM	40	H				-1.315	0.575	-2.698
ATOM	41	H				2.987	-1.674	-5.858
ATOM	42	H				-1.462	0.179	-4.904
CONNECT	1	2	3	4				
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CONNECT	3	6	1	7	8			
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CONNECT	20	6						
CONNECT	21	13	22	37				
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CONNECT	39	30						
CONNECT	40	30						
CONNECT	41	36						
CONNECT	42	38						
END								



Gilbert #9

Lowest energy structure: structure #45, E = 119.69 KJ/mol (28.61 Kcal/mol).

Description: Quaternary methyls gauche, pseudo chair, secondary OH front, methyl back.

NOE violations: one (4.816 Å) - seen in red.

Expected NOEs not seen: **none**.

PDB-format file:

ATOM	1	C	0.000	0.000	0.000
ATOM	2	C	0.000	0.000	1.341
ATOM	3	C	1.244	0.000	-0.871
ATOM	4	H	-0.978	0.033	-0.509
ATOM	5	C	1.240	-0.064	2.202
ATOM	6	C	2.458	-0.427	-0.009
ATOM	7	C	1.478	1.472	-1.304
ATOM	8	C	1.037	-0.926	-2.122
ATOM	9	H	-0.967	0.013	1.872
ATOM	10	C	2.504	0.238	1.375
ATOM	11	C	1.128	0.924	3.378
ATOM	12	O	1.353	-1.360	2.763
ATOM	13	C	0.303	-2.241	-1.865
ATOM	14	C	0.085	-0.295	-3.186
ATOM	15	H	0.627	1.903	-1.875
ATOM	16	H	1.605	2.158	-0.438
ATOM	17	H	2.388	1.576	-1.937
ATOM	18	C	2.366	-1.276	-2.831
ATOM	19	H	3.408	-0.200	-0.545
ATOM	20	H	2.448	-1.525	0.158
ATOM	21	C	-0.601	-2.504	-2.820
ATOM	22	C	-0.666	-1.446	-3.881
ATOM	23	H	0.612	0.364	-3.916
ATOM	24	H	-0.693	0.325	-2.685
ATOM	25	H	2.618	1.338	1.256
ATOM	26	H	3.412	-0.097	1.933
ATOM	27	H	2.194	-1.875	-3.755
ATOM	28	H	2.923	-0.361	-3.136
ATOM	29	H	3.043	-1.886	-2.193
ATOM	30	C	0.645	-3.197	-0.751
ATOM	31	H	2.045	0.897	4.011
ATOM	32	H	0.996	1.969	3.015
ATOM	33	H	0.262	0.681	4.034
ATOM	34	H	1.395	-1.994	2.069
ATOM	35	H	-0.159	-1.797	-4.813

ATOM	36	O				-1.988	-1.067	-4.191
ATOM	37	H				-1.219	-3.413	-2.879
ATOM	38	O				-0.043	-4.430	-0.829
ATOM	39	H				1.734	-3.433	-0.776
ATOM	40	H				0.379	-2.742	0.231
ATOM	41	H				-2.405	-1.782	-4.642
ATOM	42	H				0.207	-4.854	-1.632
CONNECT	1	2	3	4				
CONNECT	2	1	5	9				
CONNECT	3	6	1	7	8			
CONNECT	4	1						
CONNECT	5	2	10	11	12			
CONNECT	6	10	3	19	20			
CONNECT	7	3	15	16	17			
CONNECT	8	3	13	14	18			
CONNECT	9	2						
CONNECT	10	5	6	25	26			
CONNECT	11	5	31	32	33			
CONNECT	12	5	34					
CONNECT	13	8	21	30				
CONNECT	14	22	8	23	24			
CONNECT	15	7						
CONNECT	16	7						
CONNECT	17	7						
CONNECT	18	8	27	28	29			
CONNECT	19	6						
CONNECT	20	6						
CONNECT	21	13	22	37				
CONNECT	22	21	14	35	36			
CONNECT	23	14						
CONNECT	24	14						
CONNECT	25	10						
CONNECT	26	10						
CONNECT	27	18						
CONNECT	28	18						
CONNECT	29	18						
CONNECT	30	13	38	39	40			
CONNECT	31	11						
CONNECT	32	11						
CONNECT	33	11						
CONNECT	34	12						
CONNECT	35	22						
CONNECT	36	22	41					
CONNECT	37	21						
CONNECT	38	30	42					
CONNECT	39	30						
CONNECT	40	30						
CONNECT	41	36						
CONNECT	42	38						
END								