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

Conformation analysis of the two possible configurations proposed for FS-2[197] was conducted using the Monte Carlo simulation package available in MacroModel[198]. 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 reffered as the Tempesta series, and the structures with 9-R configuration (β-OH) will be reffered 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 conformations[199]. 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

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[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.

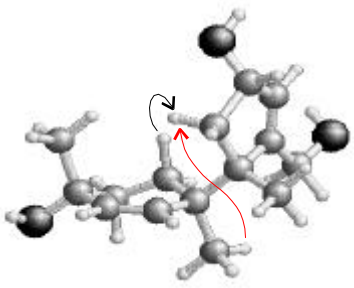
[199] Many structures were found within the same conformation classification due to small variations on angles and/or orientation of OH bonds, etc., which were considered different structures by the computer.

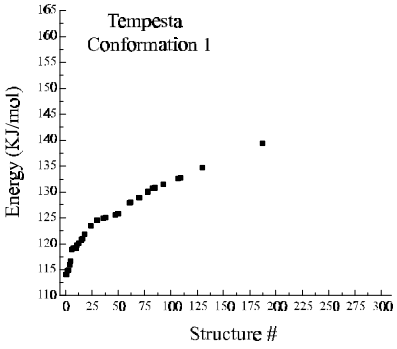
was examined. Of these, nine of the structures lie within 4 Kcal/mol of the overall lowest Gilbert structure energy, only these nine conformations were analyzed further. Four of those conformations contained hydrogen bonds that helped stabilize their structures.

The Nuclear Overhauser Effect data reported for FS-2 by Tempesta[200] 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      5    C                1.245  -0.014   2.194
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
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ATOM     13    C                2.373  -1.574  -2.648
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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     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
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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
ATOM     39    H                    2.787  -0.001  -4.062
ATOM     40    H                    3.878   0.002  -2.617
ATOM     41    H                    2.005  -5.335  -1.669
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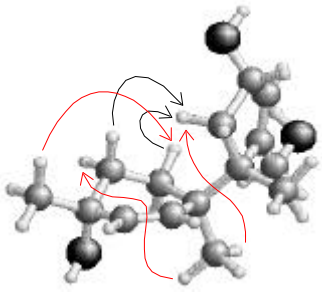
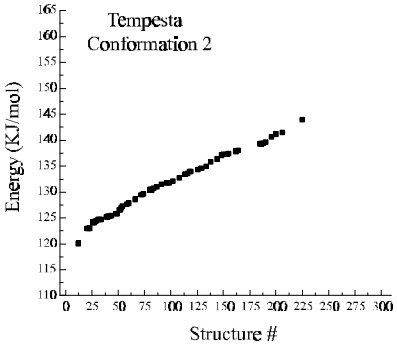
Tempesta #2





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      9    H               -0.959   0.026   1.885
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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     24    H                1.967  -0.667   4.142
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
ATOM     32    H               -0.945  -0.174  -2.722
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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ATOM     38    O                   4.307  -0.999  -4.181
ATOM     39    H                   2.816   0.371  -3.998
ATOM     40    H                   3.846   0.100  -2.524
ATOM     41    H                   1.714  -5.231  -2.508
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END
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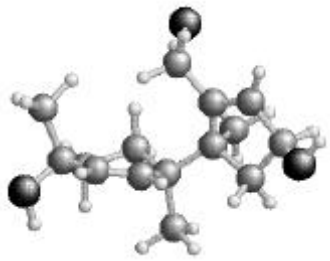

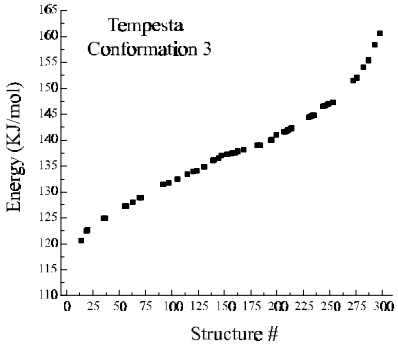

Tempesta #3

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      2    C                0.000   0.000   1.341
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ATOM      4    H               -0.977   0.016  -0.510
ATOM      5    C                1.238  -0.023   2.208
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
ATOM      9    H               -0.968   0.007   1.871
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ATOM     13    C                0.286  -2.237  -1.857
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ATOM     15    H                0.611   1.888  -1.887
ATOM     16    H                1.600   2.162  -0.462
ATOM     17    H                2.372   1.565  -1.962
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ATOM     19    H                3.410  -0.193  -0.535
ATOM     20    H                2.451  -1.513   0.178
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ATOM     22    C               -0.573  -1.471  -3.930
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ATOM     24    H                2.210  -1.410   3.617
ATOM     25    H                0.426  -1.582   3.537
ATOM     26    H                1.452  -2.226   2.211
```

```
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ATOM     30    H                    3.409  -0.059   1.942
ATOM     31    H                    2.227  -1.892  -3.728
ATOM     32    H                    2.973  -0.411  -3.065
ATOM     33    H                    3.024  -1.955  -2.142
ATOM     34    C                    0.562  -3.164  -0.701
ATOM     35    H                   -0.004  -1.833  -4.821
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
ATOM     40    H                    0.312  -2.659   0.259
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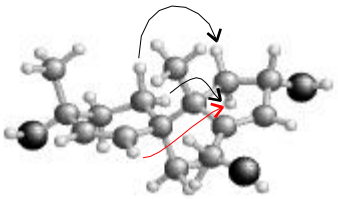

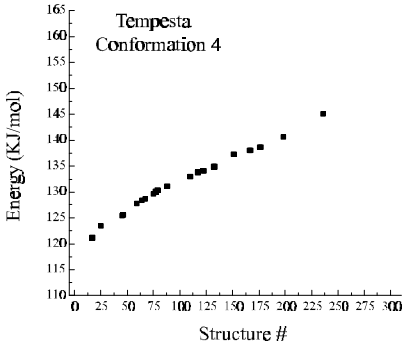

Tempesta #4

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      2    C                0.000   0.000   1.341
ATOM      3    C                1.231   0.000  -0.890
ATOM      4    H               -0.982   0.027  -0.495
ATOM      5    C                1.244  -0.024   2.194
ATOM      6    C                2.487  -0.256  -0.011
ATOM      7    C                1.353   1.423  -1.486
ATOM      8    C                1.103  -1.099  -2.002
ATOM      9    H               -0.965   0.010   1.876
ATOM     10    C                2.447   0.440   1.356
ATOM     11    O                1.110   0.880   3.275
ATOM     12    C                1.440  -1.437   2.773
ATOM     13    C                0.221  -0.776  -3.208
ATOM     14    C                2.468  -1.337  -2.717
ATOM     15    H                0.495   1.698  -2.135
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
ATOM     19    H                3.412   0.064  -0.543
ATOM     20    H                2.617  -1.344   0.178
ATOM     21    C                0.812  -1.125  -4.361
ATOM     22    C                2.166  -1.741  -4.170
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ATOM     24    H                2.367  -1.496   3.389
ATOM     25    H                0.585  -1.725   3.427
ATOM     26    H                1.512  -2.210   1.975
ATOM     27    H                3.121  -2.080  -2.201
ATOM     28    H                3.040  -0.384  -2.769
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
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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
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ATOM     42    H                  -1.457   0.391  -4.887
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END
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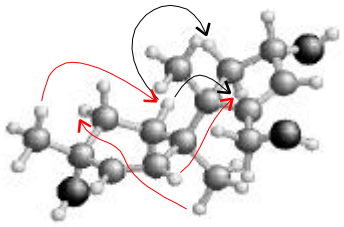
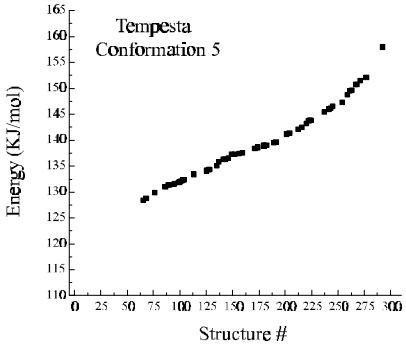
Tempesta #5





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
```

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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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CONECT    2    1    5    9
CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   29   30
CONECT   11    5   23
CONECT   12    5   24   25   26
CONECT   13    8   21   34
CONECT   14   22    8   27   28
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   31   32   33
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   11
CONECT   24   12
CONECT   25   12
CONECT   26   12
CONECT   27   14
CONECT   28   14
CONECT   29   10
CONECT   30   10
CONECT   31   18
CONECT   32   18
CONECT   33   18
CONECT   34   13   38   39   40
CONECT   35   22
CONECT   36   22   41
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CONECT   39   34
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CONECT   41   36
CONECT   42   38
END
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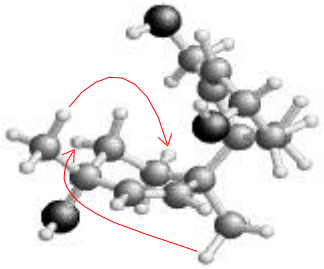

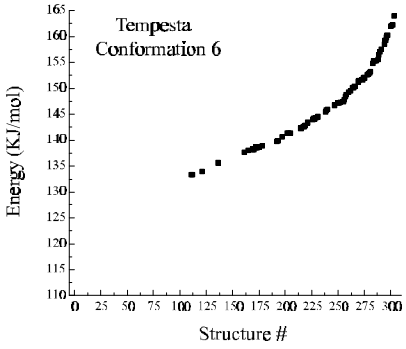

Tempesta #6

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:

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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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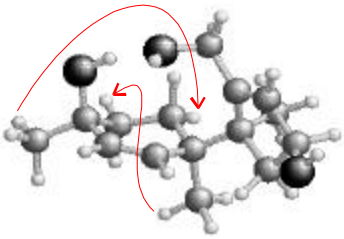
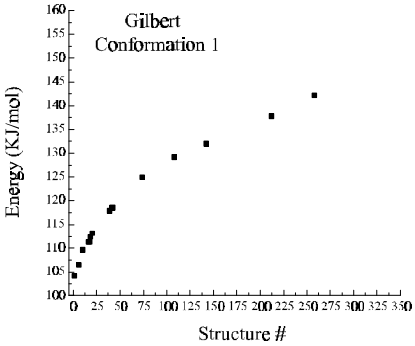
CONECT    2    1    5    9
CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   29   30
CONECT   11    5   23
CONECT   12    5   24   25   26
CONECT   13    8   21   34
CONECT   14   22    8   27   28
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   31   32   33
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   11
CONECT   24   12
CONECT   25   12
CONECT   26   12
CONECT   27   14
CONECT   28   14
CONECT   29   10
CONECT   30   10
CONECT   31   18
CONECT   32   18
CONECT   33   18
CONECT   34   13   38   39   40
CONECT   35   22
CONECT   36   22   41
CONECT   37   21
CONECT   38   34   42
CONECT   39   34
CONECT   40   34
CONECT   41   36
CONECT   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:

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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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CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
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CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
CONECT   12    5   34
CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
CONECT   26   10
CONECT   27   18
CONECT   28   18
CONECT   29   18
CONECT   30   13   38   39   40
CONECT   31   11
CONECT   32   11
CONECT   33   11
CONECT   34   12
CONECT   35   22
CONECT   36   22   41
CONECT   37   21
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CONECT   39   30
CONECT   40   30
CONECT   41   36
CONECT   42   38
END
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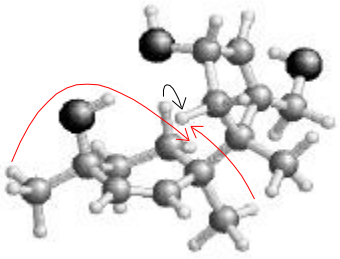

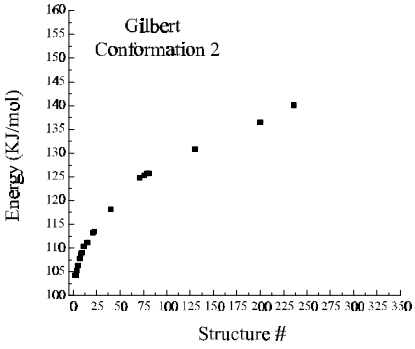

Gilbert #2

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
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```
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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CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
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CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
CONECT   26   10
CONECT   27   18
CONECT   28   18
CONECT   29   18
CONECT   30   13   38   39   40
CONECT   31   11
CONECT   32   11
CONECT   33   11
CONECT   34   12
CONECT   35   22
CONECT   36   22   41
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CONECT   41   36
CONECT   42   38
END
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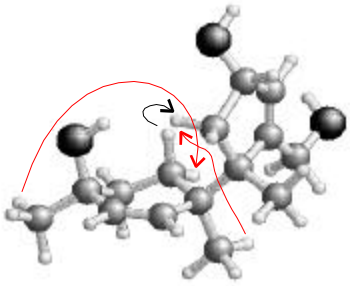

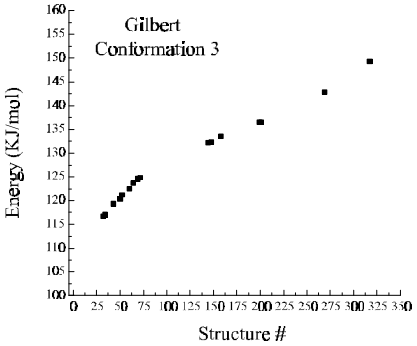

Gilbert #3

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      1    C                0.000   0.000   0.000
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
CONECT    1    2    3    4
CONECT    2    1    5    9
CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
CONECT   12    5   34
CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
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CONECT   29   18
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CONECT   37   21
CONECT   38   30   42
CONECT   39   30
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CONECT   41   36
CONECT   42   38
END
```

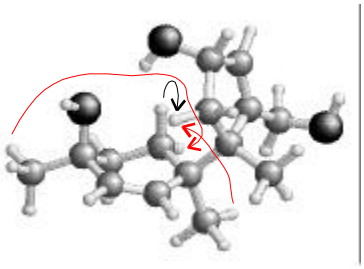

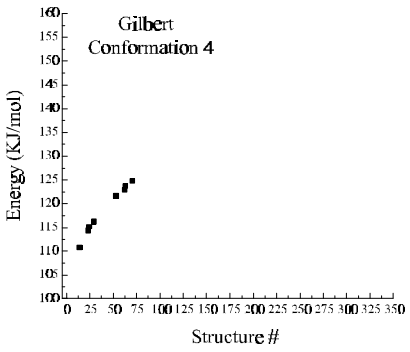

Gilbert #4

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:

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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
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CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
CONECT   12    5   34
CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
CONECT   26   10
CONECT   27   18
CONECT   28   18
CONECT   29   18
CONECT   30   13   38   39   40
CONECT   31   11
CONECT   32   11
CONECT   33   11
CONECT   34   12
CONECT   35   22
CONECT   36   22   41
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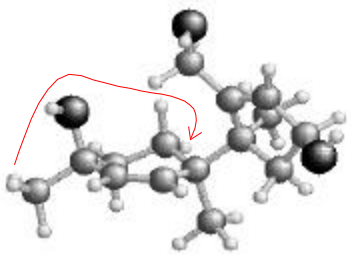
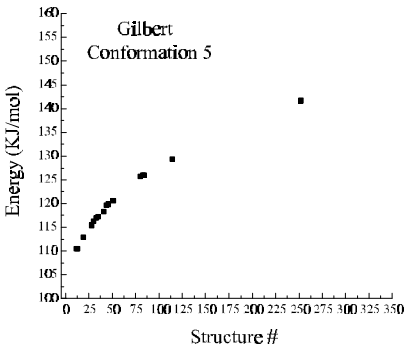
CONECT   41   36
CONECT   42   38
END
```





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
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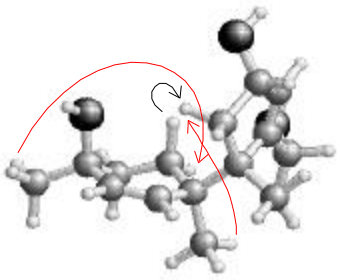
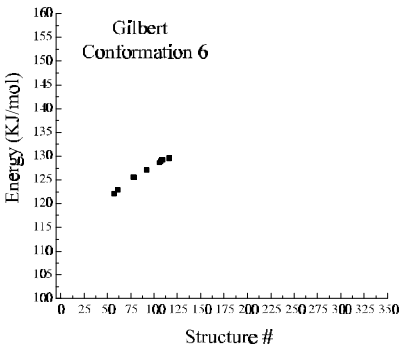
CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
CONECT   12    5   34
CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
CONECT   26   10
CONECT   27   18
CONECT   28   18
CONECT   29   18
CONECT   30   13   38   39   40
CONECT   31   11
CONECT   32   11
CONECT   33   11
CONECT   34   12
CONECT   35   22
CONECT   36   22   41
CONECT   37   21
CONECT   38   30   42
CONECT   39   30
CONECT   40   30
CONECT   41   36
CONECT   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
CONECT    1    2    3    4
CONECT    2    1    5    9
CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
CONECT   12    5   34
CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
CONECT   26   10
CONECT   27   18
CONECT   28   18
CONECT   29   18
CONECT   30   13   38   39   40
CONECT   31   11
CONECT   32   11
CONECT   33   11
CONECT   34   12
CONECT   35   22
CONECT   36   22   41
CONECT   37   21
CONECT   38   30   42
CONECT   39   30
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CONECT   41   36
CONECT   42   38
END
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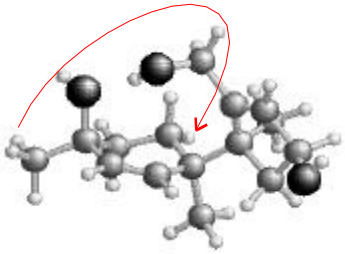

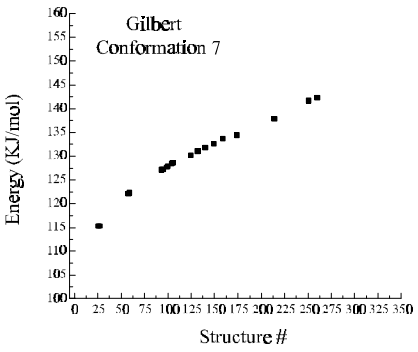

Gilbert #7

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
CONECT    1    2    3    4
CONECT    2    1    5    9
CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
CONECT   12    5   34
CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
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CONECT   32   11
CONECT   33   11
CONECT   34   12
CONECT   35   22
CONECT   36   22   41
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CONECT   39   30
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CONECT   41   36
CONECT   42   38
END
```
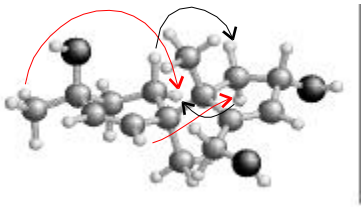
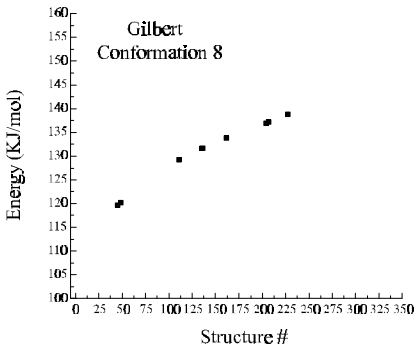





Gilbert #8

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".

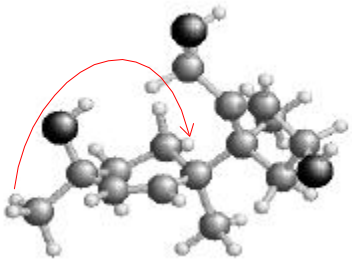
NOE violations: two (4.642 Å, 4.878 Å) - seen in red.

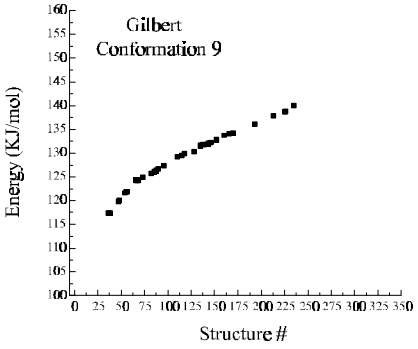
Expected NOEs not seen: two (2.309 Å, 2.512 Å) - seen in black.

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
CONECT    1    2    3    4
CONECT    2    1    5    9
CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
CONECT   12    5   34
CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
CONECT   26   10
CONECT   27   18
CONECT   28   18
CONECT   29   18
CONECT   30   13   38   39   40
CONECT   31   11
CONECT   32   11
CONECT   33   11
CONECT   34   12
CONECT   35   22
CONECT   36   22   41
CONECT   37   21
CONECT   38   30   42
CONECT   39   30
CONECT   40   30
CONECT   41   36
CONECT   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
CONECT    1    2    3    4
CONECT    2    1    5    9
CONECT    3    6    1    7    8
CONECT    4    1
CONECT    5    2   10   11   12
CONECT    6   10    3   19   20
CONECT    7    3   15   16   17
CONECT    8    3   13   14   18
CONECT    9    2
CONECT   10    5    6   25   26
CONECT   11    5   31   32   33
CONECT   12    5   34
CONECT   13    8   21   30
CONECT   14   22    8   23   24
CONECT   15    7
CONECT   16    7
CONECT   17    7
CONECT   18    8   27   28   29
CONECT   19    6
CONECT   20    6
CONECT   21   13   22   37
CONECT   22   21   14   35   36
CONECT   23   14
CONECT   24   14
CONECT   25   10
CONECT   26   10
CONECT   27   18
CONECT   28   18
CONECT   29   18
CONECT   30   13   38   39   40
CONECT   31   11
CONECT   32   11
CONECT   33   11
CONECT   34   12
CONECT   35   22
CONECT   36   22   41
CONECT   37   21
CONECT   38   30   42
CONECT   39   30
CONECT   40   30
CONECT   41   36
CONECT   42   38
END
```