Stereostructure Assignment of Medium-sized Rings through an NMR-Computational Combined Approach. Application to the New Germacranes Ketopelenolides C and D.

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Computational details. DFT calculations were performed on a Pentium-4 processor at 3.0 GHz using the Gaussian03 package (Revision B.05).[1] We reported only conformations that are significantly populated. The initial geometries properties were optimized at the hybrid DFT mPW1PW91 level, using the 6-31G(d,p) basis set, and the nuclear shielding were calculated using the same functional and basis set.

[1]Gaussian 03, Revision B.05, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, **2004**.

C1_a

Cartesian coordinates (x, y, z)

C	1.648500	-1.761000	2.024500
C	1.917500	-2.737000	0.880500
O	2.272500	-3.908000	1.020500
C	-3.066500	1.043000	1.687500
C	-0.681500	0.598000	2.039500
C	0.836500	0.723000	2.033500
C	1.617500	-0.402000	1.293500
C	1.160500	-0.807000	-0.133500
O	1.699500	-2.127000	-0.333500
C	1.613500	0.101000	-1.312500
C	-1.362500	2.862000	0.989500
C	-1.015500	2.871000	-0.521500
C	0.386500	2.378000	-0.932500
O	1.371500	3.019000	-0.556500
C	0.578500	1.139000	-1.838500
C	-1.607500	1.467000	1.588500
O	-0.407500	3.626000	1.721500
C	0.941500	1.609000	-3.262500
C	2.682500	-1.844000	3.167500
H	0.648500	-2.006000	2.431500
H	-3.212500	-0.037000	1.492500
H	-3.711500	1.573000	0.961500
H	-3.473500	1.252000	2.694500
H	-1.040500	-0.338000	2.473500
H	1.180500	0.774000	3.082500
H	1.153500	1.692000	1.617500
H	2.665500	-0.049000	1.208500
H	0.057500	-0.910000	-0.162500
H	1.858500	-0.572000	-2.157500
H	2.578500	0.591000	-1.081500
H	-2.307500	3.430000	1.076500
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H	-1.787500	2.309000	-1.079500
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H	0.453500	3.283000	1.471500
H	0.182500	2.302000	-3.674500
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H	1.915500	2.133000	-3.294500
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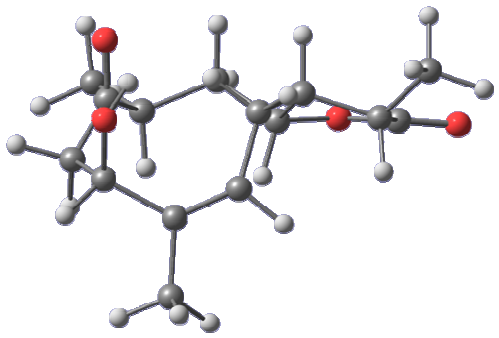
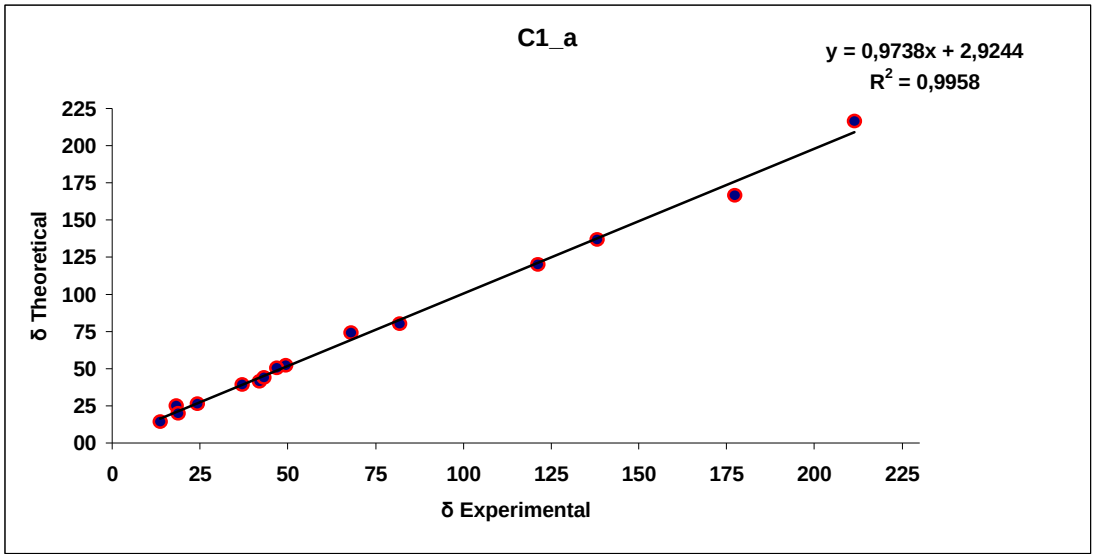


Carbon	δC Theoretical	δC Experimental
1	74.1	68.0
2	43.7	43.2
3	216.6	211.5
4	50.4	46.8
5	39.1	37.0
6	80.0	81.8
7	52.2	49.3
8	26.1	30.2
9	120.2	121.2
10	136.8	138.2
11	41.2	41.9
12	166.6	177.3
13	14.3	13.7
14	25.1	18.2
15	19.9	18.8

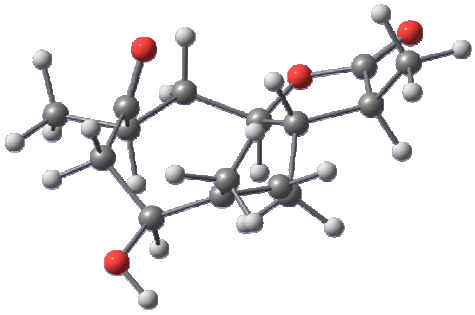
Free Energies = -885.456602 Hartrees



C1_b

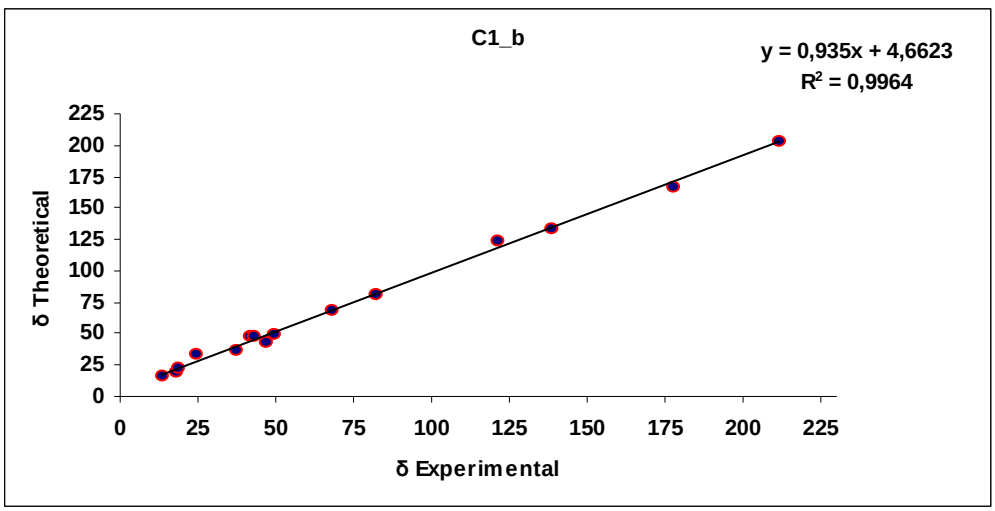
Cartesian coordinates (x, y, z)

C	1.155500	-2.199000	1.572000
C	2.654500	-2.474000	1.596000
O	3.246500	-3.067000	2.499000
C	-2.840500	1.652000	0.051000
C	-1.390500	-0.326000	0.029000
C	-0.322500	-1.328000	-0.380000
C	1.004500	-1.174000	0.427000
C	2.283500	-1.393000	-0.420000
O	3.254500	-1.993000	0.456000
C	2.953500	-0.138000	-1.048000
C	-1.297500	1.197000	-2.025000
C	-0.145500	2.229000	-1.992000
C	1.174500	1.770000	-1.337000
O	1.474500	2.260000	-0.245000
C	2.128500	0.755000	-2.027000
C	-1.806500	0.770000	-0.636000
O	-2.353500	1.747000	-2.806000
C	3.069500	1.530000	-2.974000
C	0.588500	-1.716000	2.923000
H	0.667500	-3.156000	1.308000
H	-2.599500	1.828000	1.117000
H	-3.846500	1.196000	0.011000
H	-2.919500	2.651000	-0.416000
H	-1.840500	-0.534000	1.002000
H	-0.118500	-1.261000	-1.462000
H	-0.735500	-2.348000	-0.271000
H	1.079500	-0.155000	0.858000
H	2.075500	-2.122000	-1.229000
H	3.846500	-0.517000	-1.582000
H	3.378500	0.491000	-0.242000
H	-0.947500	0.316000	-2.591000
H	-0.494500	3.156000	-1.498000
H	0.084500	2.540000	-3.028000
H	1.520500	0.086000	-2.663000
H	-3.050500	1.087000	-2.812000
H	3.730500	2.229000	-2.426000
H	2.508500	2.125000	-3.719000
H	3.721500	0.847000	-3.548000
H	-0.499500	-1.527000	2.861000
H	1.065500	-0.778000	3.265000
H	0.737500	-2.469000	3.719000



Carbon	δC Theoretical	δC Experimental
1	68.0	68.0
2	47.8	43.2
3	202.7	211.5
4	43.2	46.8
5	36.8	37.0
6	81.1	81.8
7	48.6	49.3
8	33.6	30.2
9	124.3	121.2
10	133.9	138.2
11	47.5	41.9
12	166.4	177.3
13	15.7	13.7
14	18.8	18.2
15	21.7	18.8

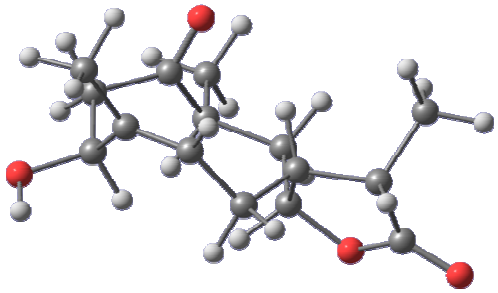
Free Energies = -885.456000 Hartrees



C1_c

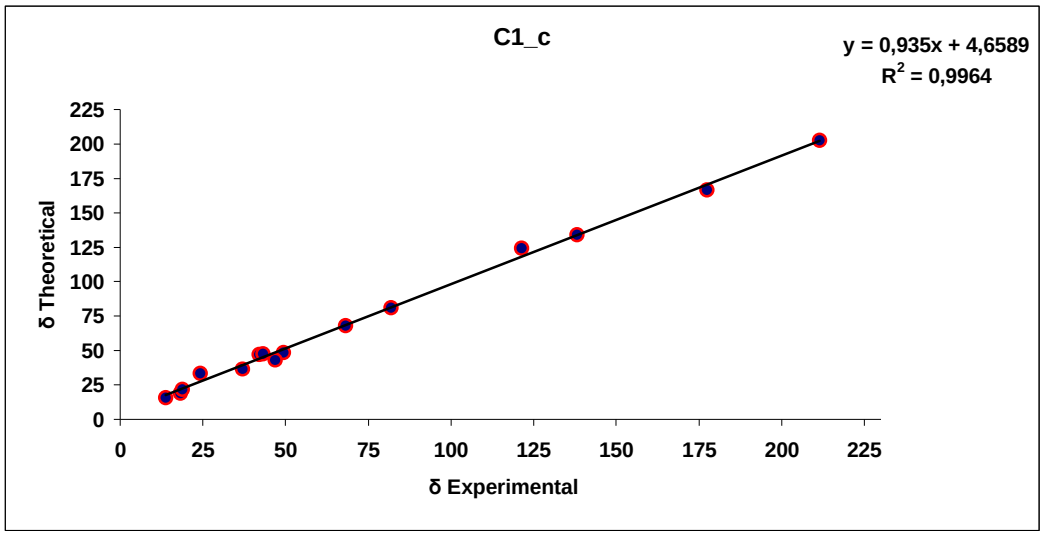
Cartesian coordinates (x, y, z)

C	4.563000	0.750000	-8.200000
C	4.790000	-0.030000	-9.489000
O	5.078000	-1.226000	-9.536000
C	1.332000	5.637000	-6.940000
C	1.942000	3.349000	-7.576000
C	2.357000	2.133000	-8.390000
C	3.895000	2.062000	-8.683000
C	4.240000	2.111000	-10.201000
O	4.619000	0.778000	-10.589000
C	5.373000	3.099000	-10.603000
C	1.792000	5.072000	-9.459000
C	2.991000	6.008000	-9.751000
C	4.376000	5.338000	-9.687000
O	5.035000	5.434000	-8.648000
C	4.946000	4.565000	-10.901000
C	1.696000	4.604000	-7.998000
O	0.597000	5.754000	-9.823000
C	6.111000	5.361000	-11.525000
C	5.882000	0.961000	-7.428000
H	3.890000	0.162000	-7.548000
H	2.177000	5.822000	-6.250000
H	0.470000	5.312000	-6.326000
H	1.058000	6.616000	-7.375000
H	1.864000	3.151000	-6.504000
H	1.755000	2.078000	-9.316000
H	2.019000	1.241000	-7.831000
H	4.386000	2.912000	-8.169000
H	3.349000	2.375000	-10.803000
H	5.844000	2.700000	-11.523000
H	6.185000	3.077000	-9.852000
H	1.868000	4.204000	-10.139000
H	2.972000	6.880000	-9.071000
H	2.870000	6.442000	-10.761000
H	4.154000	4.520000	-11.673000
H	-0.123000	5.150000	-9.625000
H	5.804000	6.385000	-11.809000
H	6.488000	4.879000	-12.446000
H	6.969000	5.455000	-10.832000
H	5.715000	1.539000	-6.500000
H	6.637000	1.509000	-8.023000
H	6.337000	-0.002000	-7.127000



Carbon	δC Theoretical	δC experimental
1	68.0	68.0
2	47.8	43.2
3	202.7	211.5
4	43.2	46.8
5	36.7	37.0
6	81.1	81.8
7	48.6	49.3
8	33.6	30.2
9	124.3	121.2
10	133.9	138.2
11	47.5	41.9
12	166.4	177.3
13	15.6	13.7
14	18.8	18.2
15	21.7	18.8

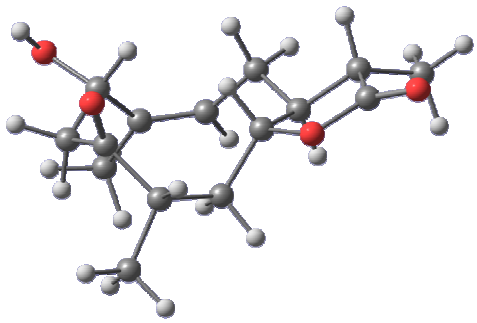
Free Energies = -885.456000 Hartrees



C1_d

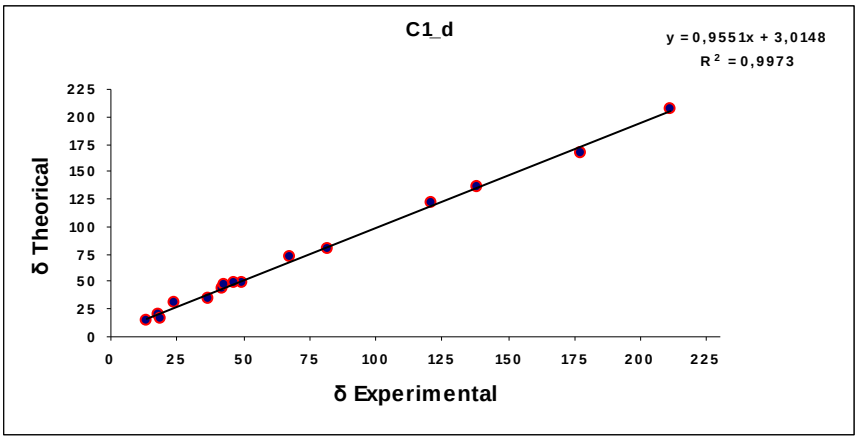
Cartesian coordinates (x, y, z)

C	0.710000	-2.463000	1.247500
C	1.878000	-2.694000	0.286500
O	2.542000	-3.729000	0.221500
C	-1.621000	3.368000	1.379500
C	-1.159000	0.985000	1.666500
C	-0.968000	-0.504000	1.425500
C	0.509000	-0.935000	1.180500
C	1.061000	-0.611000	-0.227500
O	2.074000	-1.589000	-0.509500
C	1.660000	0.814000	-0.392500
C	-1.901000	1.763000	-0.669500
C	-0.942000	2.481000	-1.664500
C	0.114000	1.577000	-2.335500
O	-0.228000	0.947000	-3.336500
C	1.571000	1.401000	-1.825500
C	-1.545000	1.955000	0.813500
O	-3.223000	2.249000	-0.880500
C	2.364000	2.719000	-1.941500
C	0.960000	-3.000000	2.671500
H	-0.167000	-2.987000	0.819500
H	-2.036000	4.095000	0.656500
H	-0.621000	3.743000	1.666500
H	-2.264000	3.419000	2.277500
H	-0.920000	1.283000	2.690500
H	-1.623000	-0.870000	0.613500
H	-1.344000	-1.023000	2.326500
H	1.165000	-0.460000	1.938500
H	0.242000	-0.764000	-0.958500
H	2.715000	0.792000	-0.059500
H	1.182000	1.523000	0.306500
H	-1.935000	0.687000	-0.923500
H	-0.445000	3.349000	-1.192500
H	-1.535000	2.935000	-2.480500
H	2.074000	0.681000	-2.499500
H	-3.428000	2.075000	-1.801500
H	3.428000	2.576000	-1.676500
H	1.966000	3.508000	-1.276500
H	2.346000	3.118000	-2.973500
H	1.851000	-2.541000	3.140500
H	1.117000	-4.095000	2.670500
H	0.099000	-2.800000	3.336500



carbon	δC Theoretical	δC Experimental
1	71.8	68.0
2	47.4	43.2
3	206.7	211.5
4	49.9	46.8
5	34.9	37.0
6	79.2	81.8
7	49.5	49.3
8	30.4	30.2
9	121.5	121.2
10	136.4	138.2
11	42.7	41.9
12	166.5	177.3
13	14.1	13.7
14	19.3	18.2
15	17.1	18.8

Free Energies = -885.455484 Hartrees



C1_e

Cartesian coordinates (x, y, z)

C	1.972000	-1.361500	2.465000
C	2.581000	-2.614500	1.846000
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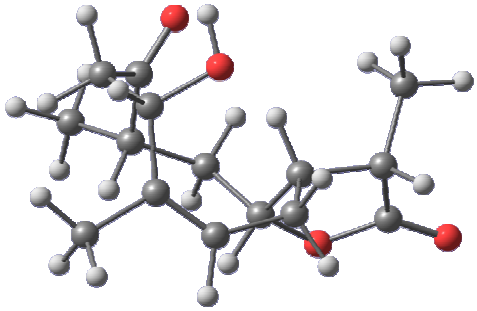
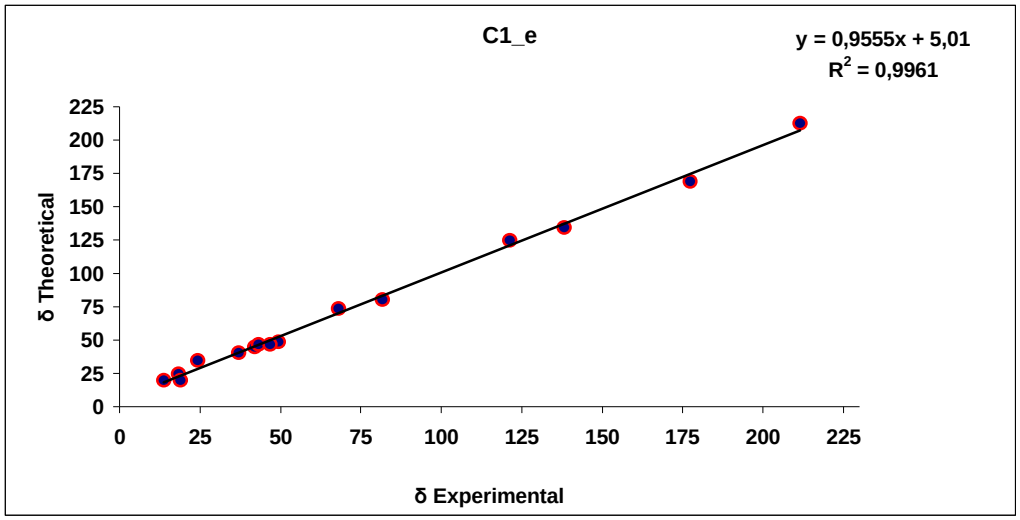
C	-1.437000	-0.577500	0.571000
C	-0.448000	-0.920500	1.679000
C	1.068000	-0.799500	1.344000
C	1.532000	-1.554500	0.065000
O	2.337000	-2.666500	0.493000
C	2.339000	-0.721500	-0.970000
C	-1.058000	1.962500	0.179000
C	-0.063000	2.379500	-0.937000
C	1.312000	1.684500	-0.957000
O	2.236000	2.205500	-0.327000
C	1.563000	0.379500	-1.756000
C	-1.714000	0.590500	-0.044000
O	-0.455000	2.133500	1.459000
C	2.286000	0.730500	-3.073000
C	3.063000	-0.377500	2.939000
H	1.380000	-1.662500	3.350000
H	-3.062000	1.548500	-1.503000
H	-3.721000	0.078500	-0.768000
H	-2.443000	-0.035500	-2.005000
H	-2.001000	-1.452500	0.239000
H	-0.661000	-1.955500	2.006000
H	-0.676000	-0.299500	2.565000
H	1.270000	0.278500	1.244000
H	0.662000	-1.980500	-0.471000
H	2.745000	-1.449500	-1.699000
H	3.239000	-0.291500	-0.489000
H	-1.877000	2.706500	0.145000
H	0.113000	3.468500	-0.850000
H	-0.537000	2.265500	-1.930000
H	0.580000	-0.042500	-2.042000
H	-0.086000	3.019500	1.464000
H	2.415000	-0.159500	-3.716000
H	3.293000	1.154500	-2.896000
H	1.719000	1.469500	-3.671000
H	3.709000	-0.827500	3.716000
H	2.617000	0.532500	3.381000
H	3.721000	-0.049500	2.112000

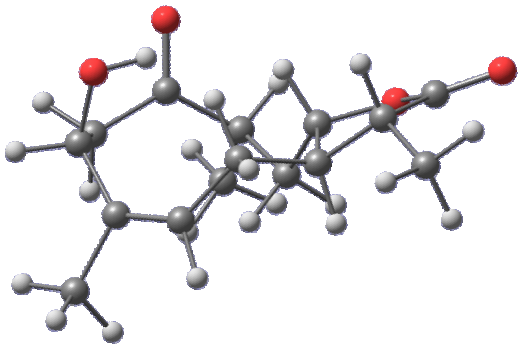


Carbon	δC Theoretical	δC Experimental
1	73.6	68.0
2	46.4	43.2
3	212.3	211.5
4	46.4	46.8
5	40.1	37.0
6	79.9	81.8
7	48.3	49.3
8	34.5	30.2
9	124.8	121.2
10	134.3	138.2
11	44.6	41.9
12	169.0	177.3
13	19.5	13.7
14	24.4	18.2
15	19.7	18.8

Free Energies = -885.453797 Hartrees



C2_a



Cartesian coordinates (x, y, z)

C	3.556000	1.355000	-7.041000
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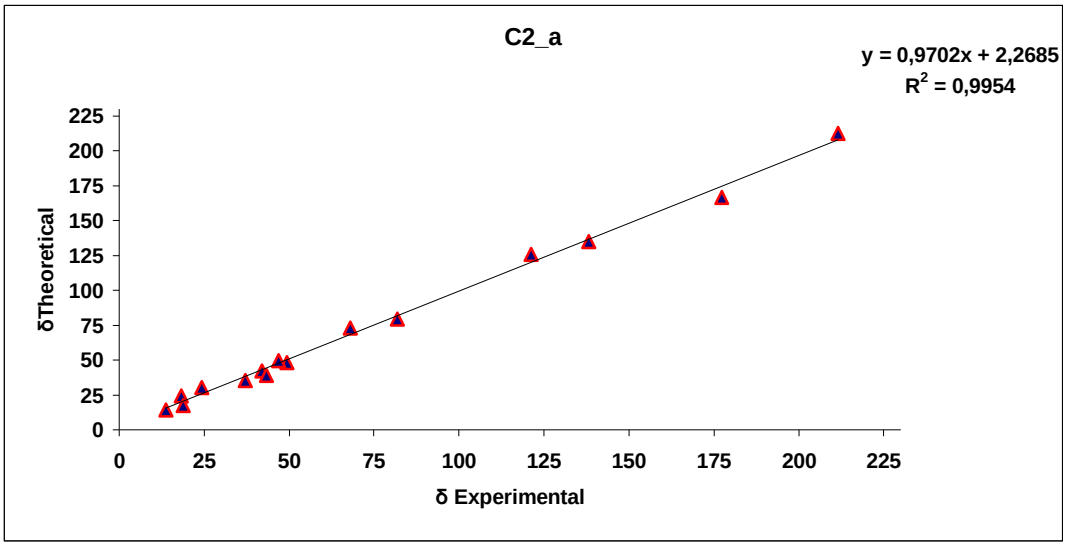
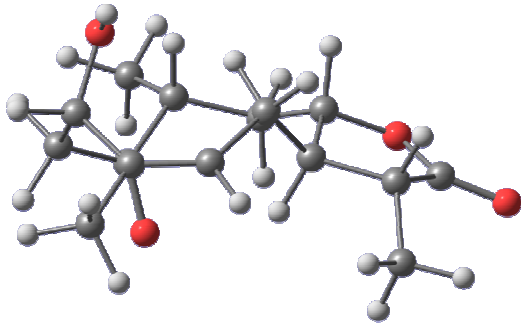
O	5.472000	1.534000	-5.520000
C	1.965000	2.581000	-12.985000
C	2.066000	1.999000	-10.623000
C	2.127000	2.010000	-9.104000
C	3.551000	1.743000	-8.534000
C	4.486000	2.972000	-8.529000
O	5.448000	2.745000	-7.487000
C	5.217000	3.261000	-9.871000
C	1.784000	4.511000	-11.276000
C	3.071000	5.346000	-11.528000
C	4.061000	5.526000	-10.355000
O	3.755000	6.331000	-9.474000
C	5.406000	4.764000	-10.202000
C	1.937000	2.999000	-11.519000
O	1.193000	4.864000	-10.029000
C	6.325000	4.960000	-11.425000
C	3.326000	-0.149000	-6.783000
H	2.788000	1.932000	-6.490000
H	1.852000	3.432000	-13.683000
H	1.150000	1.872000	-13.224000
H	2.919000	2.087000	-13.249000
H	2.167000	0.987000	-11.024000
H	1.446000	1.211000	-8.756000
H	1.700000	2.931000	-8.671000
H	4.037000	0.927000	-9.108000
H	3.884000	3.854000	-8.229000
H	4.693000	2.780000	-10.716000
H	6.200000	2.752000	-9.854000
H	1.057000	4.860000	-12.034000
H	2.757000	6.363000	-11.832000
H	3.607000	4.964000	-12.416000
H	5.945000	5.215000	-9.346000
H	1.874000	4.736000	-9.365000
H	7.323000	4.513000	-11.258000
H	6.491000	6.032000	-11.644000
H	5.913000	4.496000	-12.341000
H	3.360000	-0.384000	-5.703000
H	4.087000	-0.779000	-7.281000
H	2.336000	-0.476000	-7.152000

Carbon	δC Theoretical	δC Experimental
1	73.1	68.0
2	38.8	43.2
3	212.6	211.5
4	49.4	46.8
5	35.6	37.0
6	79.2	81.8
7	48.3	49.3
8	30.2	30.2
9	125.7	121.2
10	135.0	138.2
11	42.2	41.9
12	166.8	177.3
13	14.3	13.7
14	24.4	18.2
15	17.4	18.8

Free Energies = -885.456735 Hartrees



C2_b

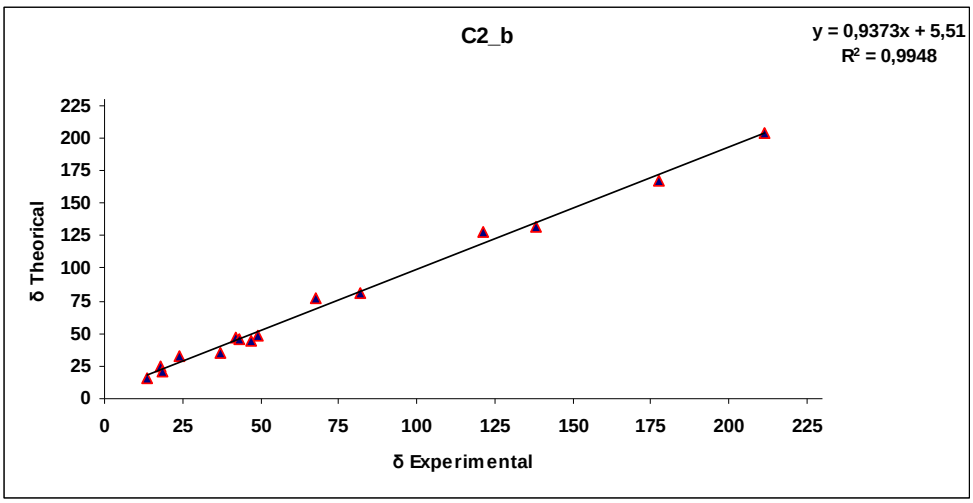


Cartesian coordinates (x, y, z)

C	3.744000	1.025000	-7.678000
C	5.149000	1.045000	-7.084000
O	5.675000	0.103000	-6.491000
C	0.477000	2.791000	-12.085000
C	1.538000	2.655000	-9.882000
C	2.340000	2.994000	-8.635000
C	3.727000	2.285000	-8.569000
C	4.843000	3.167000	-7.957000
O	5.742000	2.271000	-7.280000
C	5.697000	4.027000	-8.931000
C	1.714000	4.886000	-11.185000
C	3.110000	5.069000	-11.833000
C	4.336000	4.442000	-11.136000
O	4.829000	3.436000	-11.651000
C	4.982000	5.057000	-9.862000
C	1.280000	3.425000	-10.959000
O	1.612000	5.705000	-10.025000
C	5.966000	6.166000	-10.294000
C	3.402000	-0.278000	-8.428000
H	3.044000	1.137000	-6.828000
H	0.549000	3.357000	-13.033000
H	-0.597000	2.733000	-11.826000
H	0.815000	1.763000	-12.316000
H	1.146000	1.636000	-9.881000
H	1.729000	2.749000	-7.746000
H	2.473000	4.083000	-8.546000
H	4.063000	2.000000	-9.586000
H	4.408000	3.838000	-7.189000
H	6.336000	3.361000	-9.541000
H	6.420000	4.570000	-8.291000
H	1.000000	5.334000	-11.902000
H	3.302000	6.151000	-11.961000
H	3.065000	4.682000	-12.869000
H	4.187000	5.552000	-9.274000
H	0.713000	5.599000	-9.705000
H	5.471000	6.944000	-10.905000
H	6.809000	5.767000	-10.890000
H	6.401000	6.686000	-9.421000
H	4.093000	-0.468000	-9.272000
H	2.378000	-0.249000	-8.842000
H	3.452000	-1.157000	-7.759000

Carbon	δC Theoretical	δC Experimental
1	76.5	68.0
2	46.0	43.2
3	204.3	211.5
4	44.9	46.8
5	35.9	37.0
6	80.4	81.8
7	48.9	49.3
8	32.4	30.2
9	127.9	121.2
10	132.5	138.2
11	47.2	41.9
12	166.9	177.3
13	15.8	13.7
14	24.2	18.2
15	21.3	18.8

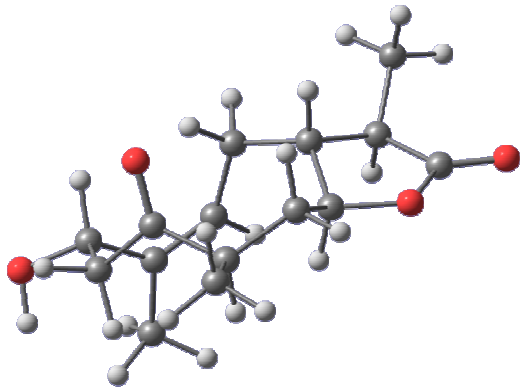
Free Energies = -885.456068 Hartrees



C2_c

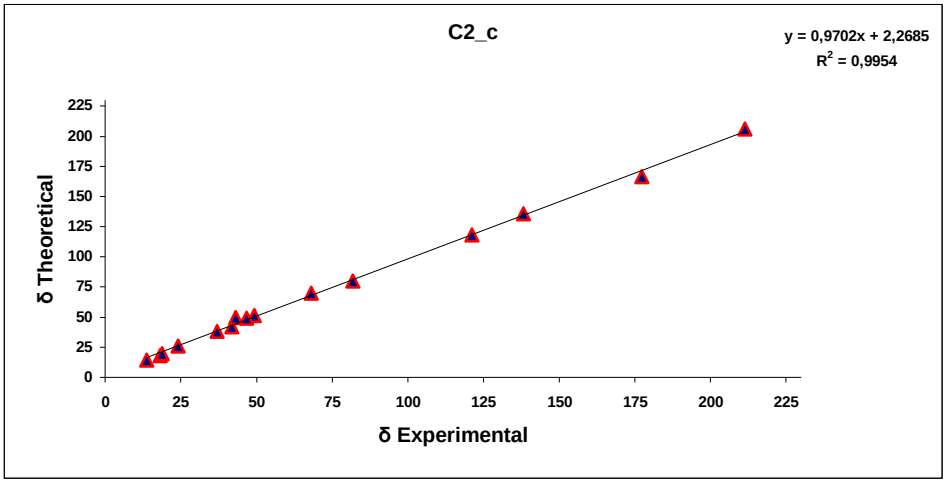
Cartesian coordinates (x, y, z)

C	-1.260500	-1.734500	1.948500
C	-1.038500	-0.929500	3.227500
O	-1.472500	-1.235500	4.339500
C	-2.793500	1.277500	-2.422500
C	-1.630500	-0.428500	-1.096500
C	-0.530500	-1.314500	-0.521500
C	-0.216500	-1.120500	0.991500
C	-0.074500	0.322500	1.547500
O	-0.288500	0.194500	2.965500
C	1.276500	1.057500	1.313500
C	-0.312500	0.650500	-3.003500
C	0.649500	1.748500	-2.486500
C	1.516500	1.353500	-1.274500
O	2.389500	0.496500	-1.430500
C	1.347500	2.036500	0.102500
C	-1.555500	0.441500	-2.121500
O	-0.681500	0.985500	-4.339500
C	2.481500	3.066500	0.289500
C	-1.123500	-3.258500	2.145500
H	-2.286500	-1.511500	1.597500
H	-3.370500	1.537500	-1.514500
H	-3.478500	0.740500	-3.104500
H	-2.538500	2.237500	-2.907500
H	-2.588500	-0.524500	-0.579500
H	0.411500	-1.193500	-1.082500
H	-0.802500	-2.369500	-0.708500
H	0.747500	-1.634500	1.178500
H	-0.896500	0.959500	1.163500
H	2.114500	0.335500	1.287500
H	1.474500	1.652500	2.226500
H	0.248500	-0.299500	-3.086500
H	0.090500	2.679500	-2.272500
H	1.346500	2.025500	-3.299500
H	0.404500	2.615500	0.086500
H	-1.183500	1.800500	-4.279500
H	2.356500	3.644500	1.224500
H	2.508500	3.805500	-0.533500
H	3.478500	2.587500	0.333500
H	-1.871500	-3.643500	2.863500
H	-0.124500	-3.542500	2.527500
H	-1.280500	-3.805500	1.197500



Carbon	δC Theoretical	δC Experimental
1	70.0	68.0
2	49.6	43.2
3	206.3	211.5
4	49.5	46.8
5	38.2	37.0
6	79.9	81.8
7	51.5	49.3
8	25.9	30.2
9	118.1	121.2
10	135.5	138.2
11	41.9	41.9
12	166.3	177.3
13	14.3	13.7
14	18.2	18.2
15	19.4	18.8

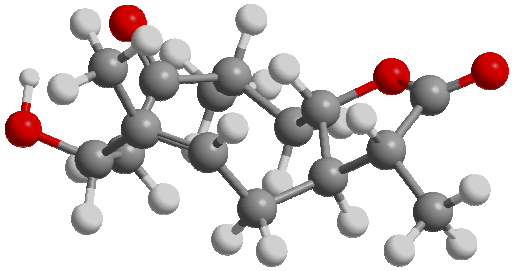
Free Energies = -885.455399 Hartrees



C2_d

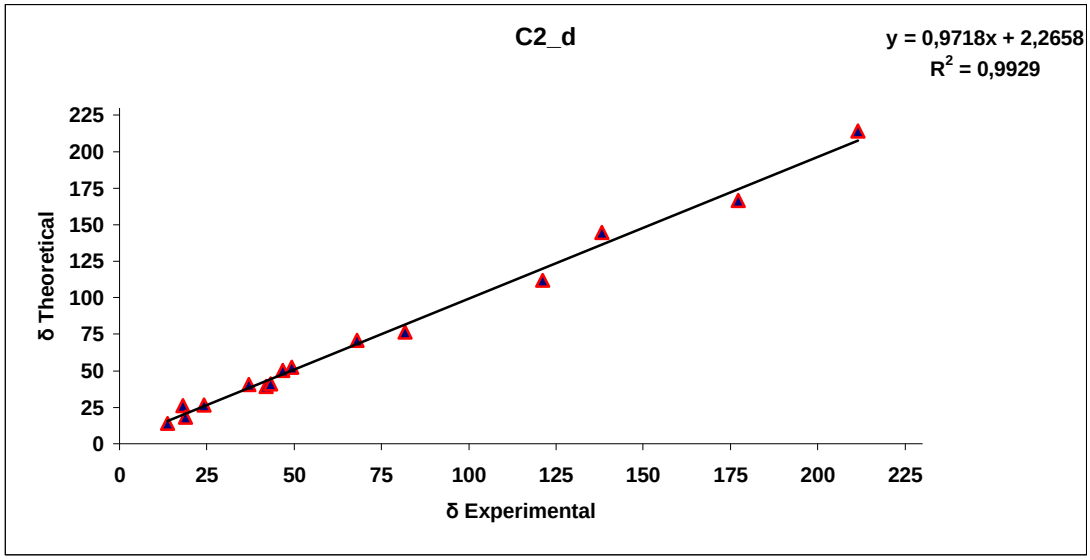
Cartesian coordinates (x, y, z)

C	1.183000	-2.059000	1.585000
C	2.579000	-1.570000	1.980000
O	3.325000	-2.139000	2.778000
C	-2.589000	1.793000	1.855000
C	-1.399000	-0.122000	0.896000
C	-0.613000	-1.028000	-0.041000
C	0.894000	-1.228000	0.317000
C	1.740000	0.044000	0.576000
O	2.885000	-0.396000	1.325000
C	2.193000	0.817000	-0.694000
C	-1.998000	1.818000	-0.700000
C	-0.657000	2.174000	-1.401000
C	0.471000	2.799000	-0.549000
O	0.183000	3.701000	0.240000
C	1.956000	2.356000	-0.663000
C	-1.941000	1.091000	0.665000
O	-2.764000	3.021000	-0.653000
C	2.609000	3.034000	-1.884000
C	1.092000	-3.584000	1.374000
H	0.495000	-1.772000	2.402000
H	-3.690000	1.804000	1.755000
H	-2.259000	2.846000	1.927000
H	-2.360000	1.334000	2.837000
H	-1.495000	-0.536000	1.902000
H	-0.695000	-0.681000	-1.085000
H	-1.110000	-2.016000	-0.061000
H	1.354000	-1.759000	-0.540000
H	1.171000	0.725000	1.240000
H	1.717000	0.389000	-1.596000
H	3.270000	0.620000	-0.859000
H	-2.542000	1.144000	-1.389000
H	-0.863000	2.866000	-2.239000
H	-0.274000	1.278000	-1.914000
H	2.484000	2.742000	0.231000
H	-2.264000	3.627000	-0.101000
H	2.154000	2.705000	-2.837000
H	3.690000	2.810000	-1.945000
H	2.518000	4.136000	-1.839000
H	1.335000	-4.136000	2.301000
H	1.786000	-3.940000	0.589000
H	0.073000	-3.892000	1.077000



Carbon	δC Theoretical	δC Experimental
1	70.8	68.0
2	41.0	43.2
3	214.4	211.5
4	50.5	46.8
5	40.5	37.0
6	76.6	81.8
7	52.5	49.3
8	26.8	30.2
9	112.0	121.2
10	144.7	138.2
11	39.3	41.9
12	166.7	177.3
13	14.2	13.7
14	26.0	18.2
15	18.3	18.8

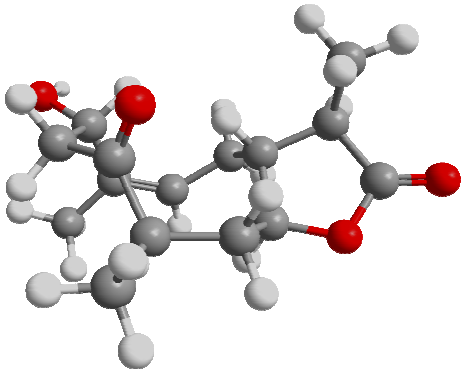
Free Energies = -885.454988 Hartrees



C2_e

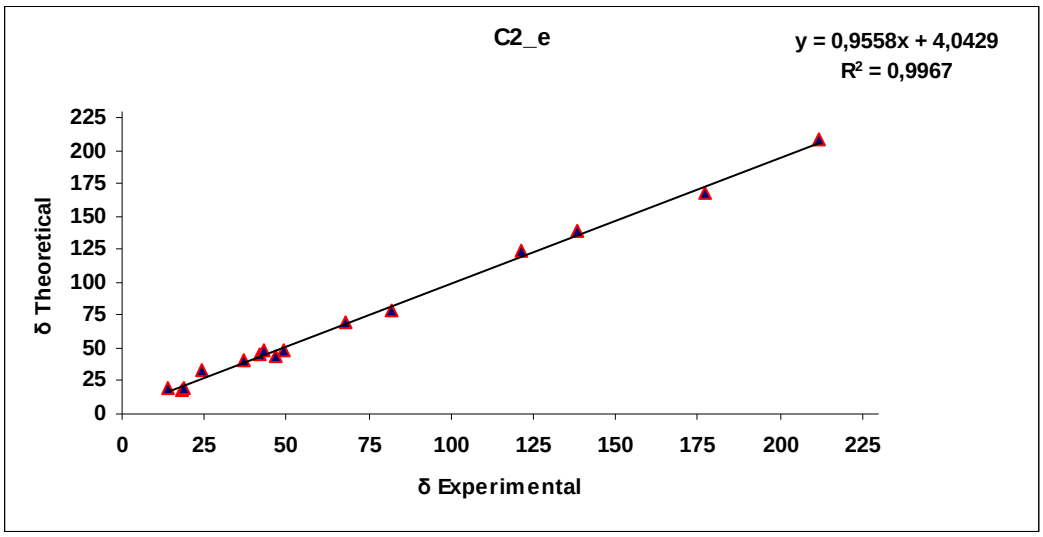
Cartesian coordinates (x, y, z)

C	3.371000	0.745000	-8.139000
C	3.470000	1.149000	-6.672000
O	3.436000	0.356000	-5.731000
C	1.229000	5.618000	-11.401000
C	1.340000	3.576000	-10.056000
C	1.728000	2.217000	-9.485000
C	3.157000	2.088000	-8.875000
C	3.534000	3.167000	-7.820000
O	3.594000	2.512000	-6.541000
C	4.870000	3.928000	-8.055000
C	2.970000	3.762000	-12.023000
C	4.289000	4.565000	-11.874000
C	5.143000	4.221000	-10.639000
O	6.030000	3.373000	-10.763000
C	4.928000	4.911000	-9.266000
C	1.834000	4.249000	-11.113000
O	2.550000	3.845000	-13.381000
C	6.027000	5.975000	-9.062000
C	4.626000	-0.027000	-8.598000
H	2.498000	0.075000	-8.257000
H	0.131000	5.566000	-11.522000
H	1.626000	6.074000	-12.327000
H	1.438000	6.332000	-10.582000
H	0.539000	4.058000	-9.491000
H	1.596000	1.449000	-10.271000
H	0.981000	1.954000	-8.712000
H	3.854000	2.129000	-9.728000
H	2.738000	3.932000	-7.747000
H	5.710000	3.208000	-8.100000
H	5.059000	4.505000	-7.129000
H	3.186000	2.693000	-11.837000
H	4.093000	5.653000	-11.897000
H	4.916000	4.384000	-12.768000
H	3.967000	5.458000	-9.302000
H	1.739000	3.333000	-13.439000
H	7.036000	5.526000	-9.001000
H	5.869000	6.549000	-8.131000
H	6.044000	6.712000	-9.887000
H	4.553000	-0.312000	-9.664000
H	4.763000	-0.962000	-8.024000
H	5.551000	0.570000	-8.483000



Carbon	δC Theoretical	δC Experimental
1	69.1	68.0
2	47.8	43.2
3	208.2	211.5
4	43.8	46.8
5	40.7	37.0
6	79.2	81.8
7	47.9	49.3
8	33.3	30.2
9	123.5	121.2
10	139.3	138.2
11	44.7	41.9
12	168.3	177.3
13	19.1	13.7
14	18.4	18.2
15	20.3	18.8

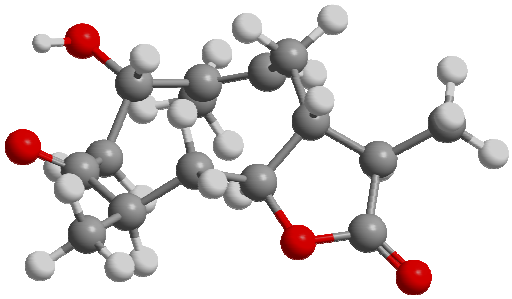
Free Energies = -885.454142 Hartrees



C2_f

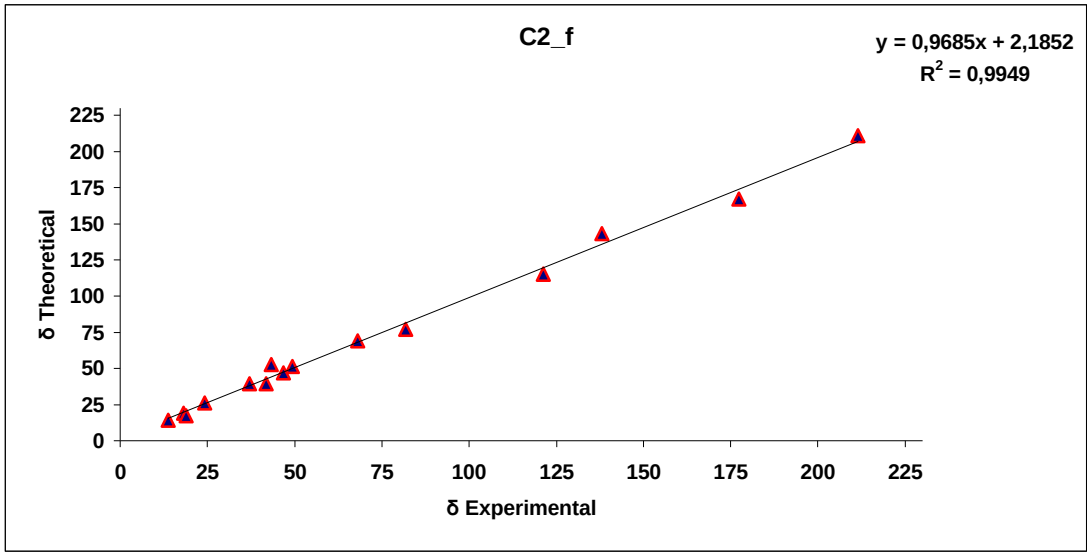
Cartesian coordinates (x, y, z)

C	-0.093000	-2.454000	1.968500
C	-1.149000	-1.949000	2.957500
O	-1.777000	-2.662000	3.741500
C	-0.910000	-0.802000	-3.030500
C	0.475000	-1.309000	-1.069500
C	1.342000	-1.159000	0.180500
C	0.616000	-1.146000	1.560500
C	-0.511000	-0.108000	1.745500
O	-1.307000	-0.584000	2.842500
C	-0.047000	1.350000	2.012500
C	0.136000	1.160000	-1.651500
C	-1.136000	1.868000	-1.103500
C	-0.835000	2.847000	0.046500
O	-0.389000	3.957000	-0.256500
C	-1.050000	2.448000	1.541500
C	-0.048000	-0.351000	-1.860500
O	0.535000	1.797000	-2.861500
C	-1.017000	3.663000	2.495500
C	0.850000	-3.527000	2.551500
H	-0.633000	-2.885000	1.104500
H	-1.778000	-1.399000	-2.691500
H	-0.337000	-1.427000	-3.741500
H	-1.319000	0.046000	-3.611500
H	0.247000	-2.349000	-1.316500
H	1.979000	-0.260000	0.101500
H	2.076000	-1.985000	0.181500
H	1.390000	-0.929000	2.324500
H	-1.157000	-0.135000	0.849500
H	0.941000	1.533000	1.546500
H	0.159000	1.439000	3.097500
H	0.973000	1.321000	-0.948500
H	-1.897000	1.144000	-0.760500
H	-1.650000	2.415000	-1.917500
H	-2.076000	2.042000	1.622500
H	0.647000	2.727000	-2.646500
H	-0.024000	4.151000	2.513500
H	-1.259000	3.373000	3.535500
H	-1.756000	4.432000	2.201500
H	1.397000	-3.164000	3.441500
H	1.604000	-3.848000	1.809500
H	0.293000	-4.432000	2.854500



Carbon	δC Theoretical	δC Experimental
1	69.3	68.0
2	52.9	43.2
3	210.8	211.5
4	46.8	46.8
5	39.4	37.0
6	77.2	81.8
7	51.4	49.3
8	26.3	30.2
9	115.1	121.2
10	143.0	138.2
11	39.6	41.9
12	166.9	177.3
13	14.2	13.7
14	19.2	18.2
15	17.4	18.8

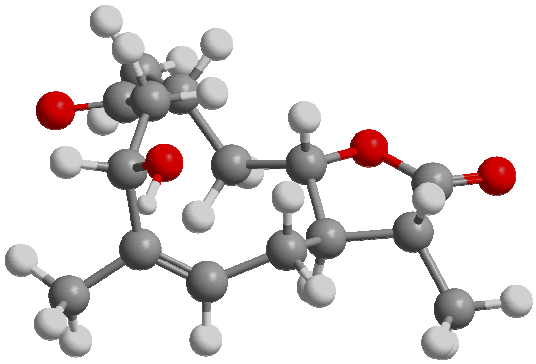
Free Energies = -885.453944 Hartrees



C2_g

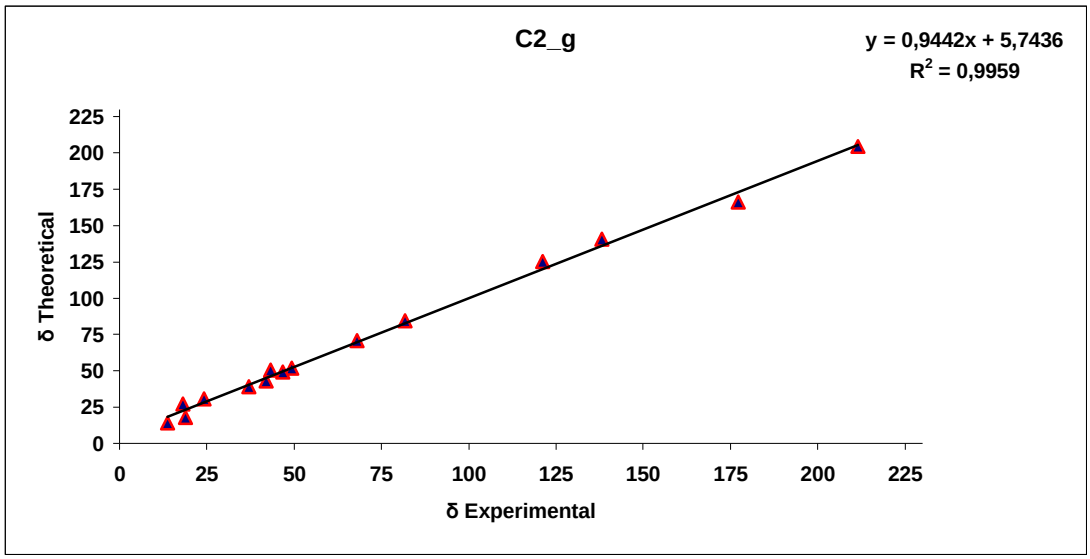
Cartesian coordinates (x, y, z)

C	2.644000	1.557000	-7.058000
C	3.184000	2.568000	-6.045000
O	3.015000	2.506000	-4.827000
C	4.781000	1.821000	-12.987000
C	3.647000	1.413000	-10.845000
C	2.722000	1.533000	-9.647000
C	3.465000	1.883000	-8.323000
C	3.769000	3.385000	-8.109000
O	3.878000	3.568000	-6.687000
C	5.051000	3.934000	-8.804000
C	2.871000	3.413000	-12.292000
C	2.983000	4.651000	-11.363000
C	4.408000	5.130000	-11.014000
O	5.178000	5.367000	-11.949000
C	4.875000	5.300000	-9.535000
C	3.737000	2.189000	-11.943000
O	1.502000	3.030000	-12.366000
C	6.154000	6.160000	-9.410000
C	2.760000	0.090000	-6.595000
H	1.575000	1.797000	-7.220000
H	5.632000	1.245000	-12.576000
H	5.224000	2.717000	-13.462000
H	4.336000	1.212000	-13.795000
H	4.336000	0.568000	-10.769000
H	2.221000	0.553000	-9.535000
H	1.895000	2.242000	-9.833000
H	4.419000	1.318000	-8.269000
H	2.885000	3.968000	-8.429000
H	5.470000	3.189000	-9.508000
H	5.843000	4.009000	-8.033000
H	3.146000	3.768000	-13.303000
H	2.407000	4.473000	-10.441000
H	2.454000	5.496000	-11.842000
H	4.089000	5.878000	-9.015000
H	1.466000	2.292000	-12.979000
H	6.418000	6.348000	-8.352000
H	6.029000	7.150000	-9.886000
H	7.028000	5.675000	-9.885000
H	3.806000	-0.199000	-6.381000
H	2.375000	-0.608000	-7.360000
H	2.175000	-0.090000	-5.673000



Carbon	δC Theoretical	δC Experimental
1	70.6	68.0
2	50.6	43.2
3	204.7	211.5
4	49.4	46.8
5	39.1	37.0
6	84.2	81.8
7	51.9	49.3
8	30.8	30.2
9	125.4	121.2
10	140.8	138.2
11	43.2	41.9
12	166.4	177.3
13	14.2	13.7
14	27.1	18.2
15	17.8	18.8

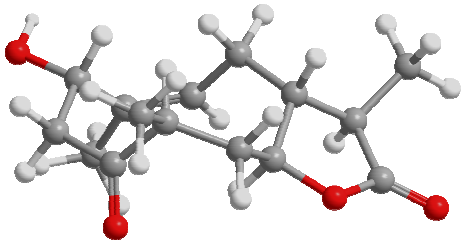
Free Energies = -885.453737 Hartrees



C3_a

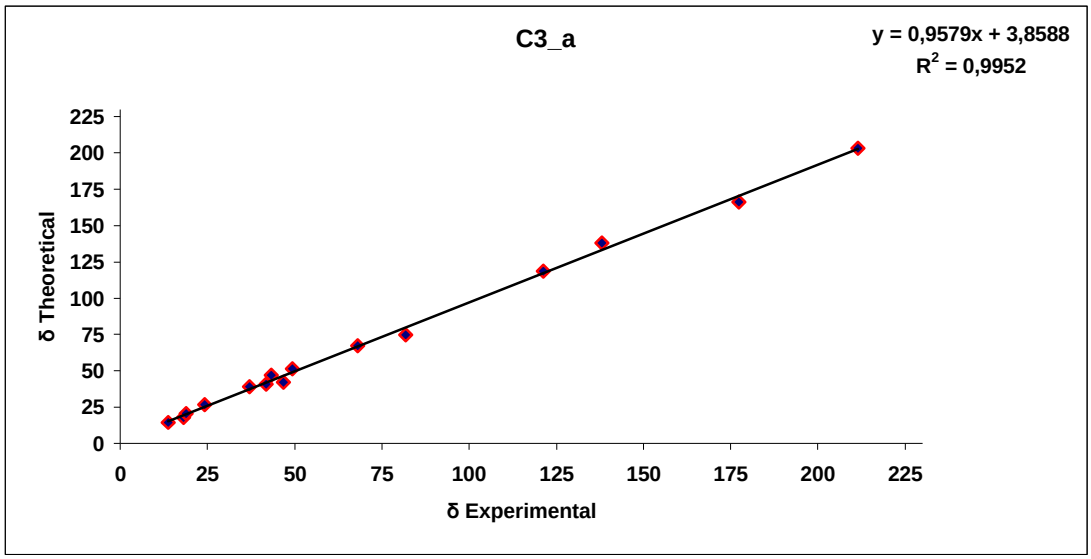
Cartesian coordinates (x, y, z)

C	4.398000	0.328000	-8.685000
C	5.909000	0.558000	-8.656000
O	6.735000	-0.238000	-8.208000
C	1.447000	4.483000	-6.755000
C	2.078000	2.654000	-8.256000
C	2.428000	1.845000	-9.501000
C	3.919000	1.423000	-9.663000
C	5.014000	2.508000	-9.493000
O	6.221000	1.786000	-9.194000
C	5.291000	3.442000	-10.702000
C	1.379000	4.867000	-9.346000
C	2.454000	5.960000	-9.572000
C	3.894000	5.491000	-9.871000
O	4.803000	5.920000	-9.156000
C	4.231000	4.529000	-11.043000
C	1.651000	3.928000	-8.158000
O	0.124000	5.517000	-9.175000
C	4.668000	5.345000	-12.276000
C	3.995000	-1.105000	-9.091000
H	4.020000	0.528000	-7.665000
H	0.653000	3.935000	-6.213000
H	1.154000	5.549000	-6.755000
H	2.370000	4.413000	-6.149000
H	2.216000	2.098000	-7.325000
H	2.111000	2.361000	-10.421000
H	1.799000	0.935000	-9.500000
H	4.022000	1.019000	-10.690000
H	4.789000	3.133000	-8.607000
H	5.476000	2.814000	-11.595000
H	6.258000	3.951000	-10.518000
H	1.284000	4.292000	-10.282000
H	2.471000	6.638000	-8.698000
H	2.135000	6.602000	-10.413000
H	3.306000	4.005000	-11.337000
H	-0.521000	4.818000	-9.044000
H	4.850000	4.693000	-13.151000
H	5.599000	5.913000	-12.092000
H	3.893000	6.073000	-12.582000
H	4.375000	-1.377000	-10.094000
H	2.897000	-1.227000	-9.111000
H	4.388000	-1.853000	-8.377000



Carbon	δC Theoretical	δC Experimental
1	67.1	68.0
2	46.9	43.2
3	203.4	211.5
4	42.3	46.8
5	39.0	37.0
6	75.0	81.8
7	51.6	49.3
8	26.9	30.2
9	118.7	121.2
10	138.1	138.2
11	40.8	41.9
12	166.2	177.3
13	14.6	13.7
14	18.2	18.2
15	20.8	18.8

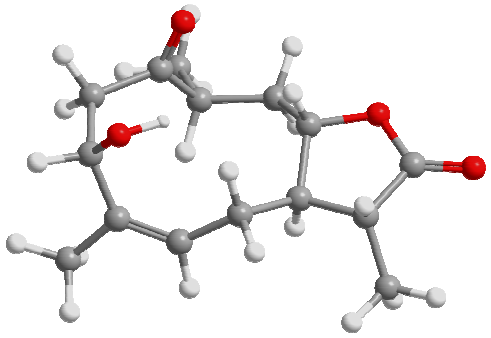
Free Energies = -885.458329 Hartrees



C3_b

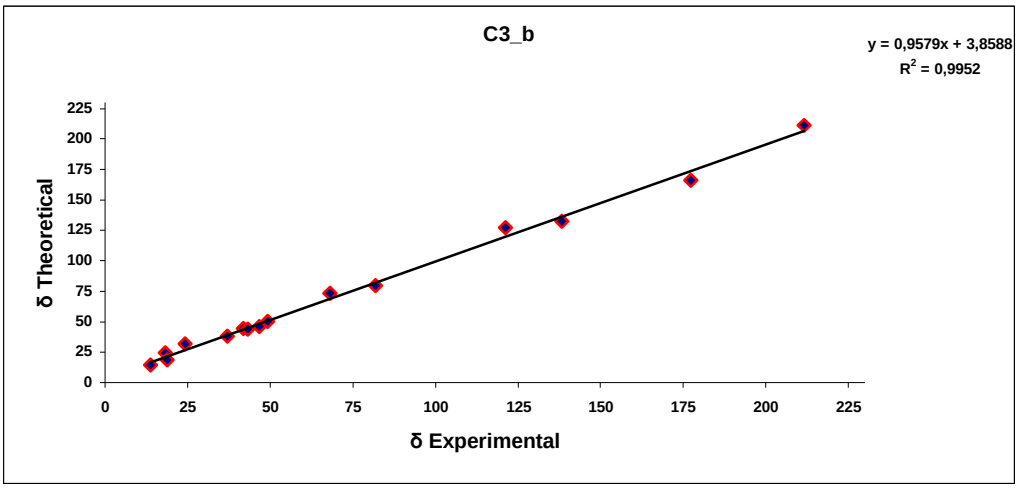
Cartesian coordinates (x, y, z)

C	5.025000	0.531000	-8.906000
C	6.440000	0.905000	-9.325000
O	7.390000	0.122000	-9.381000
C	-0.285000	3.673000	-9.828000
C	1.690000	2.432000	-9.098000
C	2.968000	1.992000	-8.405000
C	4.184000	1.748000	-9.354000
C	5.245000	2.881000	-9.391000
O	6.517000	2.245000	-9.611000
C	5.109000	3.980000	-10.480000
C	1.254000	4.767000	-8.054000
C	2.048000	5.892000	-8.764000
C	3.510000	5.586000	-9.147000
O	4.405000	5.919000	-8.367000
C	3.853000	4.895000	-10.492000
C	0.954000	3.553000	-8.950000
O	1.873000	4.452000	-6.810000
C	3.975000	5.954000	-11.607000
C	4.535000	-0.812000	-9.487000
H	5.036000	0.454000	-7.801000
H	-0.908000	2.759000	-9.798000
H	-0.010000	3.848000	-10.885000
H	-0.948000	4.508000	-9.532000
H	1.333000	1.695000	-9.822000
H	2.706000	1.052000	-7.883000
H	3.260000	2.665000	-7.581000
H	3.834000	1.564000	-10.391000
H	5.299000	3.372000	-8.399000
H	5.199000	3.494000	-11.470000
H	6.007000	4.625000	-10.406000
H	0.282000	5.217000	-7.777000
H	2.042000	6.788000	-8.115000
H	1.501000	6.213000	-9.671000
H	2.998000	4.255000	-10.771000
H	2.770000	4.183000	-7.020000
H	4.148000	5.488000	-12.595000
H	4.811000	6.656000	-11.426000
H	3.054000	6.559000	-11.703000
H	5.167000	-1.654000	-9.149000
H	4.546000	-0.817000	-10.593000
H	3.501000	-1.038000	-9.167000



Carbon	δC Theoretical	δC Experimental
1	73.3	68.0
2	43.9	43.2
3	211.4	211.5
4	46.1	46.8
5	38.2	37.0
6	79.6	81.8
7	50.1	49.3
8	31.9	24.2
9	127.2	121.2
10	132.8	138.2
11	44.7	41.9
12	166.0	177.3
13	14.6	13.7
14	24.6	18.2
15	18.8	18.8

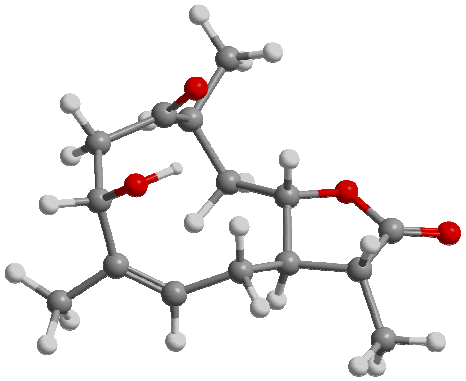
Free Energies = -885.457384 Hartrees



C3_c

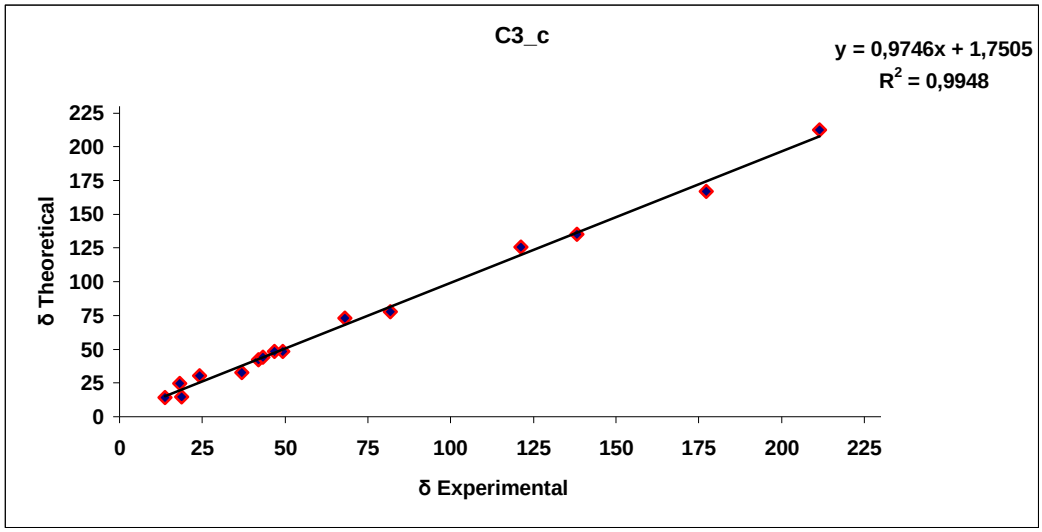
Cartesian coordinates (x, y, z)

C	4.910000	0.844000	-7.823000
C	6.119000	0.715000	-8.756000
O	7.069000	-0.048000	-8.579000
C	-0.340000	3.454000	-10.058000
C	1.532000	2.571000	-8.762000
C	2.813000	2.397000	-7.959000
C	3.892000	1.572000	-8.723000
C	4.843000	2.407000	-9.609000
O	5.997000	1.579000	-9.823000
C	4.249000	2.893000	-10.965000
C	1.343000	5.146000	-9.067000
C	2.234000	5.701000	-10.210000
C	3.724000	5.311000	-10.184000
O	4.410000	5.729000	-9.248000
C	4.365000	4.411000	-11.279000
C	0.925000	3.677000	-9.238000
O	1.916000	5.439000	-7.795000
C	5.813000	4.822000	-11.624000
C	4.404000	-0.503000	-7.266000
H	5.208000	1.492000	-6.977000
H	-1.183000	3.136000	-9.417000
H	-0.203000	2.673000	-10.831000
H	-0.672000	4.361000	-10.596000
H	1.052000	1.614000	-8.982000
H	2.536000	1.869000	-7.028000
H	3.232000	3.360000	-7.616000
H	3.399000	0.808000	-9.360000
H	5.187000	3.282000	-9.021000
H	3.180000	2.620000	-11.028000
H	4.699000	2.314000	-11.794000
H	0.414000	5.747000	-9.099000
H	2.189000	6.805000	-10.178000
H	1.795000	5.440000	-11.191000
H	3.784000	4.580000	-12.205000
H	2.835000	5.163000	-7.849000
H	6.216000	4.228000	-12.465000
H	6.500000	4.685000	-10.768000
H	5.874000	5.885000	-11.925000
H	4.119000	-1.208000	-8.070000
H	3.518000	-0.368000	-6.619000
H	5.177000	-1.002000	-6.652000



Carbon	δC Theoretical	δC Experimental
1	73.1	68.0
2	44.1	43.2
3	212.4	211.5
4	48.6	46.8
5	32.5	37.0
6	77.7	81.8
7	48.2	49.3
8	30.1	30.2
9	125.5	121.2
10	135.2	138.2
11	42.1	41.9
12	166.9	177.3
13	14.2	13.7
14	24.5	18.2
15	14.6	18.8

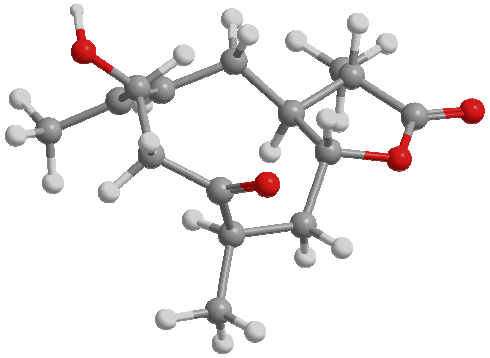
Free Energies = -885.457141 Hartrees



C4_a

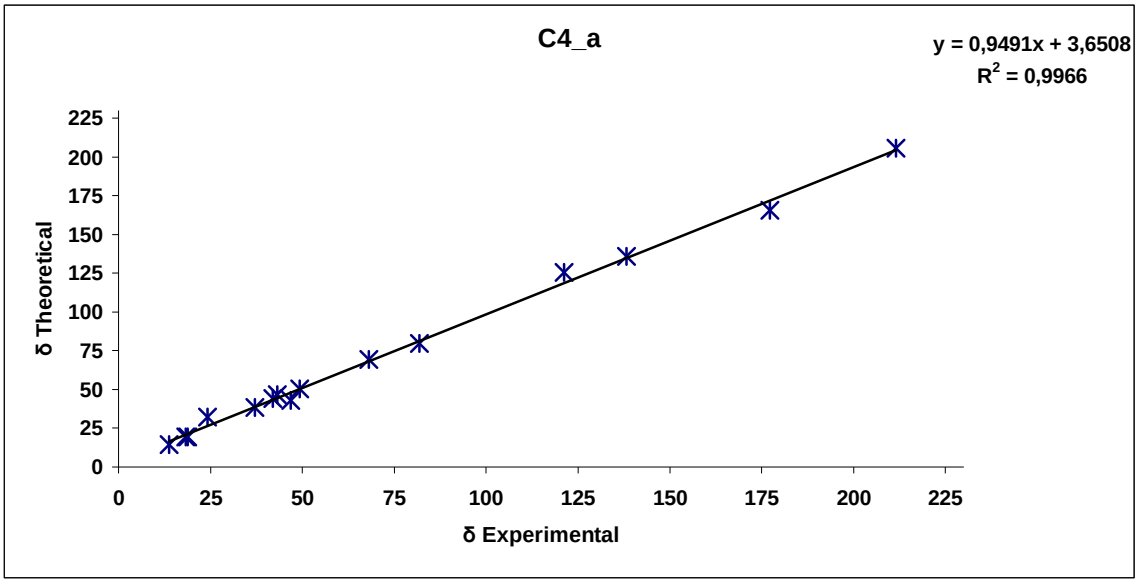
Cartesian coordinates (x, y, z)

C	4.614000	0.371000	-8.331000
C	5.786000	0.183000	-9.282000
O	6.522000	-0.805000	-9.309000
C	1.379000	5.682000	-7.490000
C	2.300000	3.431000	-7.758000
C	2.713000	2.085000	-8.326000
C	4.251000	1.867000	-8.482000
C	4.859000	2.223000	-9.869000
O	5.893000	1.256000	-10.130000
C	5.528000	3.616000	-10.038000
C	1.205000	4.490000	-9.818000
C	2.078000	5.416000	-10.702000
C	3.474000	4.868000	-11.059000
O	3.654000	4.416000	-12.193000
C	4.643000	4.892000	-10.041000
C	1.646000	4.450000	-8.347000
O	-0.145000	4.933000	-9.905000
C	5.504000	6.152000	-10.268000
C	4.920000	-0.053000	-6.879000
H	3.797000	-0.269000	-8.718000
H	0.788000	6.452000	-8.019000
H	2.322000	6.168000	-7.178000
H	0.817000	5.430000	-6.571000
H	2.593000	3.559000	-6.713000
H	2.191000	1.843000	-9.269000
H	2.310000	1.339000	-7.615000
H	4.795000	2.438000	-7.702000
H	4.092000	2.095000	-10.657000
H	6.094000	3.596000	-10.990000
H	6.308000	3.722000	-9.259000
H	1.221000	3.479000	-10.264000
H	2.185000	6.413000	-10.237000
H	1.540000	5.612000	-11.649000
H	4.224000	4.995000	-9.027000
H	-0.657000	4.334000	-9.356000
H	6.310000	6.235000	-9.515000
H	4.904000	7.078000	-10.192000
H	5.986000	6.154000	-11.264000
H	5.765000	0.515000	-6.447000
H	5.179000	-1.126000	-6.815000
H	4.047000	0.106000	-6.219000



Carbon	δC Theoretical	δC Experimental
1	69.4	68.0
2	46.8	43.2
3	205.7	211.5
4	43.0	46.8
5	38.4	37.0
6	79.9	81.8
7	50.3	49.3
8	32.0	30.2
9	125.4	121.2
10	135.8	138.2
11	44.4	41.9
12	165.6	177.3
13	14.7	13.7
14	19.4	18.2
15	19.5	18.8

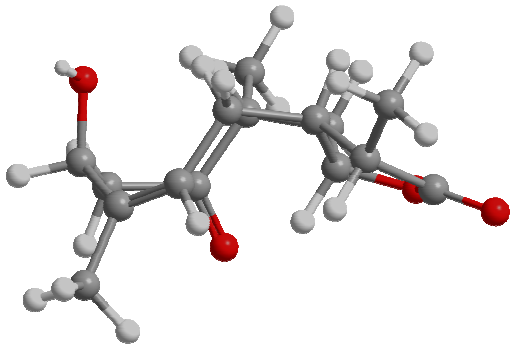
Free Energies = -885.457970 Hartrees



C4_b

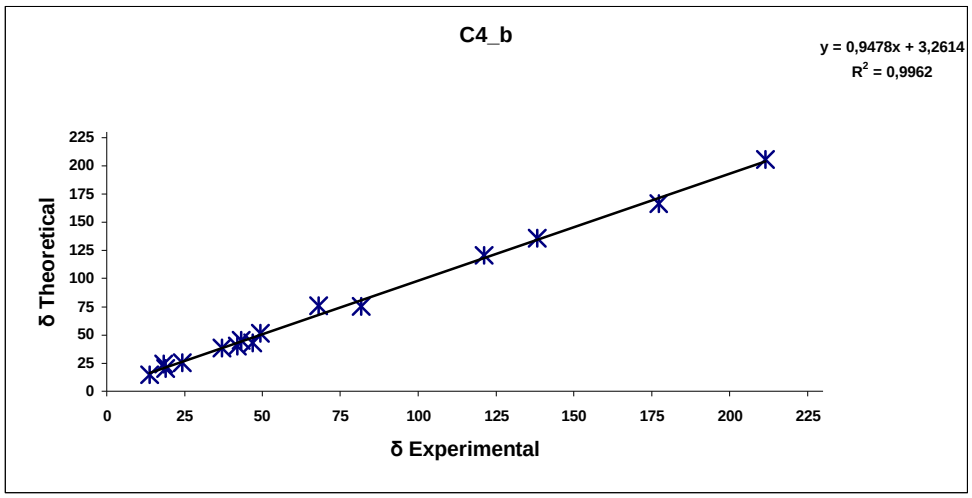
Cartesian coordinates (x, y, z)

C	4.872000	2.110000	-7.049000
C	5.266000	0.761000	-7.650000
O	5.659000	-0.211000	-7.004000
C	0.080000	4.116000	-8.671000
C	2.462000	4.115000	-8.131000
C	3.975000	4.307000	-8.165000
C	4.847000	3.023000	-8.294000
C	4.505000	2.018000	-9.421000
O	5.112000	0.779000	-9.019000
C	4.987000	2.363000	-10.856000
C	1.691000	5.328000	-10.298000
C	1.713000	4.485000	-11.601000
C	2.717000	3.319000	-11.731000
O	2.262000	2.196000	-11.963000
C	4.253000	3.507000	-11.615000
C	1.511000	4.524000	-8.996000
O	2.789000	6.231000	-10.297000
C	4.861000	3.704000	-13.018000
C	5.816000	2.593000	-5.929000
H	3.854000	1.997000	-6.632000
H	-0.656000	4.487000	-9.409000
H	-0.241000	4.502000	-7.685000
H	-0.031000	3.016000	-8.646000
H	2.129000	3.548000	-7.259000
H	4.266000	4.842000	-7.242000
H	4.278000	5.005000	-8.958000
H	5.885000	3.368000	-8.474000
H	3.411000	1.843000	-9.447000
H	4.911000	1.441000	-11.465000
H	6.072000	2.581000	-10.820000
H	0.803000	5.982000	-10.391000
H	1.870000	5.163000	-12.460000
H	0.695000	4.082000	-11.763000
H	4.444000	4.444000	-11.067000
H	2.685000	6.774000	-9.511000
H	5.947000	3.908000	-12.966000
H	4.405000	4.562000	-13.546000
H	4.726000	2.813000	-13.660000
H	6.861000	2.695000	-6.278000
H	5.824000	1.890000	-5.075000
H	5.505000	3.576000	-5.531000



Carbon	δC Theoretical	δC Experimental
1	75.8	68.0
2	45.6	43.2
3	205.5	211.5
4	42.9	46.8
5	38.5	37.0
6	75.3	81.8
7	51.4	49.3
8	25.6	30.2
9	120.8	121.2
10	135.8	138.2
11	39.9	41.9
12	166.6	177.3
13	14.5	13.7
14	24.3	18.2
15	20.5	18.8

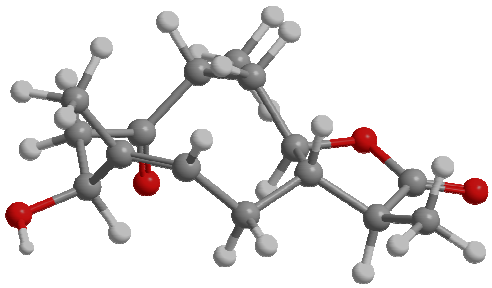
Free Energies = -885.456948 Hartrees



C4_c

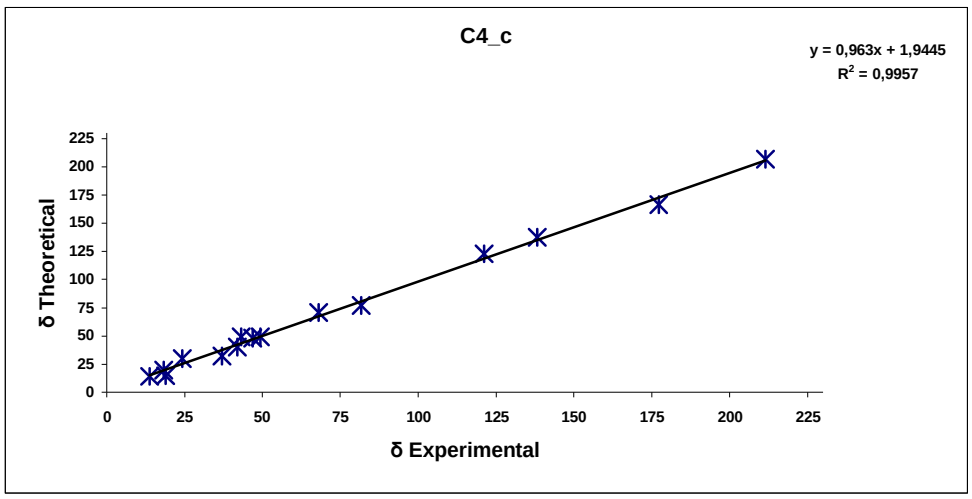
Cartesian coordinates (x, y, z)

C	4.028000	0.147000	-8.868000
C	5.400000	0.192000	-9.545000
O	6.112000	-0.789000	-9.762000
C	1.576000	5.671000	-7.174000
C	2.024000	3.330000	-7.711000
C	2.284000	2.020000	-8.439000
C	3.790000	1.625000	-8.498000
C	4.613000	2.343000	-9.592000
O	5.725000	1.485000	-9.890000
C	5.126000	3.766000	-9.218000
C	1.493000	4.907000	-9.675000
C	2.603000	5.803000	-10.294000
C	3.736000	5.035000	-10.998000
O	3.492000	4.552000	-12.107000
C	5.135000	4.832000	-10.347000
C	1.711000	4.548000	-8.196000
O	0.246000	5.585000	-9.802000
C	6.264000	4.573000	-11.370000
C	3.957000	-0.819000	-7.667000
H	3.298000	-0.181000	-9.633000
H	1.326000	6.644000	-7.637000
H	2.516000	5.825000	-6.611000
H	0.780000	5.459000	-6.436000
H	2.141000	3.239000	-6.628000
H	1.836000	2.010000	-9.449000
H	1.728000	1.237000	-7.890000
H	4.264000	1.818000	-7.513000
H	3.989000	2.397000	-10.506000
H	6.134000	3.687000	-8.768000
H	4.524000	4.177000	-8.389000
H	1.395000	3.990000	-10.285000
H	3.023000	6.502000	-9.546000
H	2.151000	6.466000	-11.056000
H	5.391000	5.794000	-9.865000
H	-0.414000	5.000000	-9.423000
H	7.255000	4.521000	-10.881000
H	6.322000	5.379000	-12.125000
H	6.119000	3.623000	-11.917000
H	2.956000	-0.809000	-7.198000
H	4.692000	-0.563000	-6.881000
H	4.156000	-1.863000	-7.975000



Carbon	δC Theoretical	δC Experimental
1	70.6	68.0
2	49.3	43.2
3	206.8	211.5
4	48.2	46.8
5	32.2	37.0
6	77.0	81.8
7	49.4	49.3
8	30.2	30.2
9	123.1	121.2
10	137.8	138.2
11	39.9	41.9
12	166.4	177.3
13	14.1	13.7
14	19.9	18.2
15	14.8	18.8

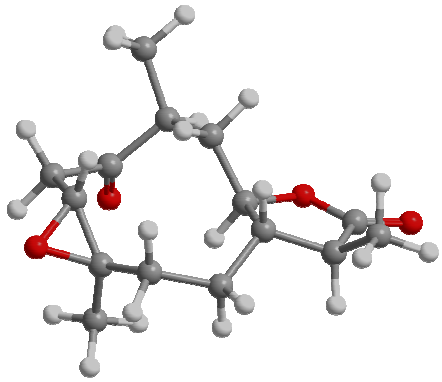
Free Energies = -885.456903 Hartrees



D1_a

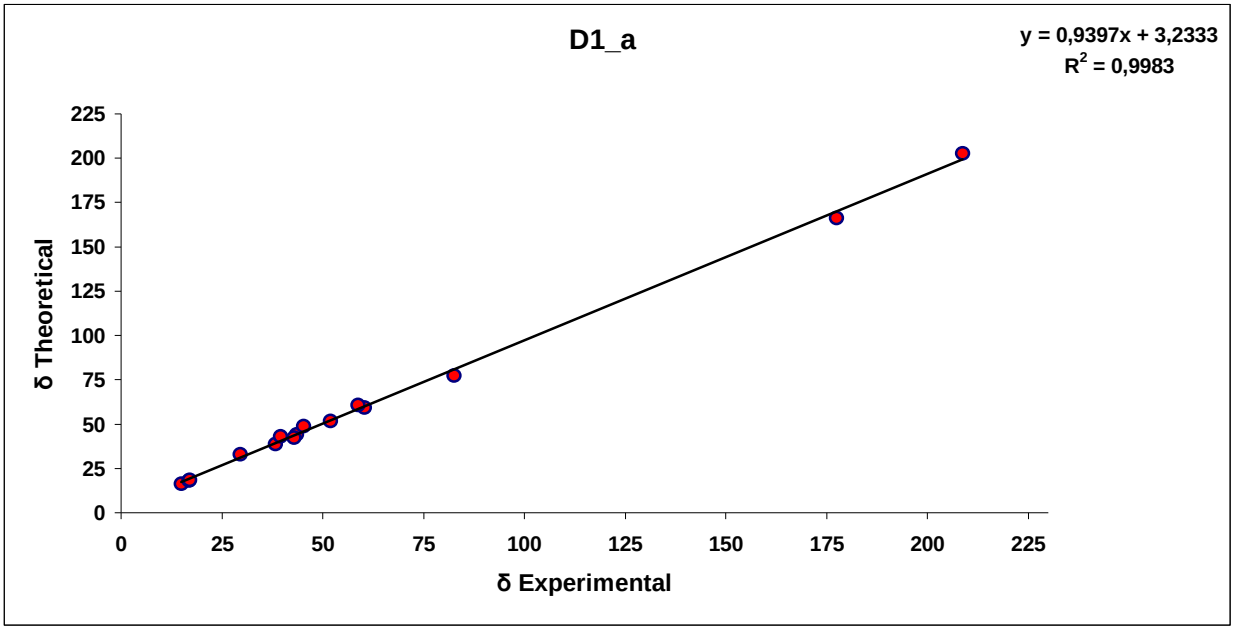
Cartesian coordinates (x, y, z)

C	0.865500	-2.543000	0.697500
C	2.212500	-2.287000	0.029500
O	3.110500	-3.122000	-0.075500
C	-2.307500	0.650000	-2.015500
C	-2.230500	0.005000	0.567500
C	-1.328500	-1.249000	0.425500
C	0.193500	-1.151000	0.765500
C	1.069500	-0.283000	-0.180500
O	2.275500	-1.010000	-0.470500
C	1.483500	1.098000	0.403500
C	-1.453500	2.375000	-0.131500
C	-0.681500	3.243000	-1.142500
C	0.654500	2.601000	-1.587500
O	0.798500	2.370000	-2.788500
C	1.821500	2.212000	-0.630500
C	-2.095500	1.073000	-0.545500
O	-2.883500	2.273000	-0.304500
C	2.388500	3.462000	0.071500
C	0.983500	-3.246000	2.065500
H	0.310500	-3.214000	0.013500
H	-1.474500	0.022000	-2.379500
H	-2.386500	1.510000	-2.705500
H	-3.235500	0.062000	-2.131500
H	-2.084500	0.444000	1.573500
H	-3.283500	-0.334000	0.571500
H	-1.458500	-1.677000	-0.586500
H	-1.764500	-2.017000	1.094500
H	0.287500	-0.759000	1.798500
H	0.532500	-0.145000	-1.137500
H	2.357500	0.941000	1.066500
H	0.711500	1.464000	1.100500
H	-1.201500	2.504000	0.936500
H	-0.475500	4.231000	-0.692500
H	-1.308500	3.460000	-2.027500
H	2.641500	1.817000	-1.260500
H	3.283500	3.219000	0.673500
H	1.652500	3.927000	0.755500
H	2.697500	4.236000	-0.655500
H	1.467500	-4.236000	1.974500
H	-0.011500	-3.415000	2.518500
H	1.577500	-2.655000	2.788500



Carbon	δC Theoretical	δC Experimental
1	60.8	58.8
2	42.3	42.8
3	202.7	208.7
4	48.7	45.3
5	43.1	39.6
6	77.4	82.6
7	51.6	51.9
8	32.8	29.5
9	38.5	38.3
10	59.1	60.3
11	44.1	43.5
12	166.3	177.5
13	16.1	14.9
14	18.2	16.9
15	18.4	17.0

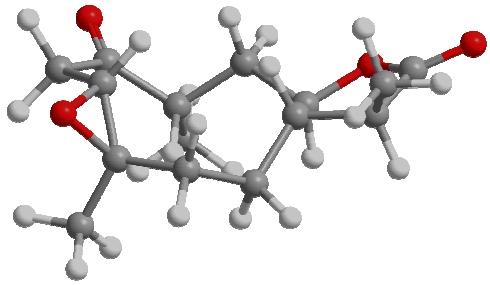
Free Energies = -885.442336 Hartrees



D1_b

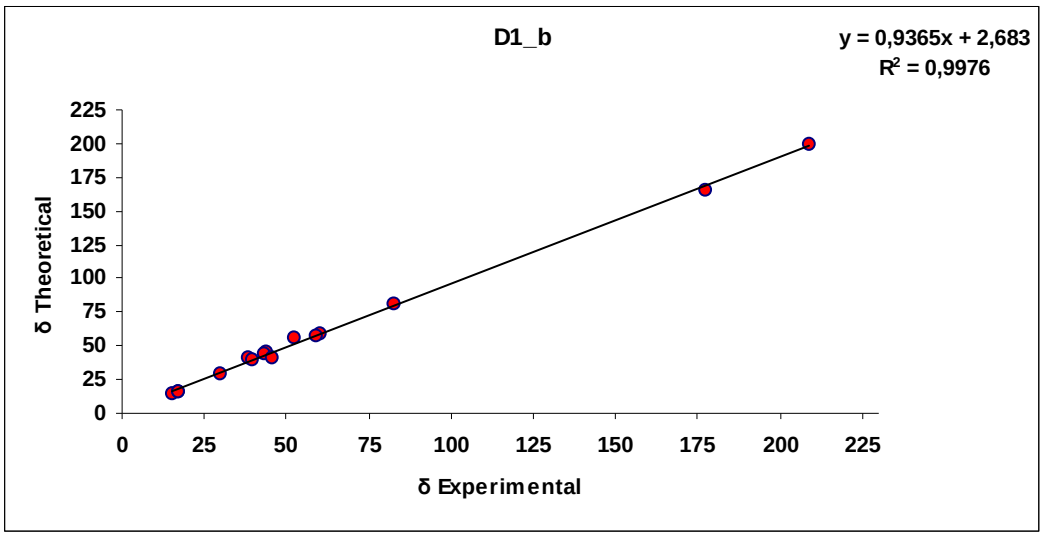
Cartesian coordinates (x, y, z)

C	0.654000	-2.559000	0.992000
C	2.036000	-2.309000	1.586000
O	2.637000	-3.088000	2.327000
C	-2.243000	1.345000	-2.340000
C	-2.142000	-0.550000	-0.499000
C	-0.758000	-1.216000	-0.718000
C	0.233000	-1.159000	0.491000
C	1.608000	-0.472000	0.250000
O	2.528000	-1.098000	1.164000
C	1.664000	1.058000	0.518000
C	-1.753000	1.898000	0.251000
C	-1.115000	3.267000	-0.069000
C	0.428000	3.217000	-0.115000
O	1.049000	4.192000	0.313000
C	1.209000	1.981000	-0.649000
C	-2.180000	0.955000	-0.847000
O	-3.150000	1.733000	-0.094000
C	2.372000	2.367000	-1.586000
C	-0.347000	-3.198000	1.976000
H	0.800000	-3.247000	0.137000
H	-2.998000	0.742000	-2.878000
H	-1.274000	1.177000	-2.843000
H	-2.518000	2.403000	-2.501000
H	-2.496000	-0.734000	0.534000
H	-2.888000	-1.066000	-1.132000
H	-0.284000	-0.819000	-1.636000
H	-0.958000	-2.272000	-0.984000
H	-0.254000	-0.635000	1.338000
H	1.969000	-0.684000	-0.776000
H	2.694000	1.341000	0.811000
H	1.082000	1.259000	1.439000
H	-1.532000	1.454000	1.240000
H	-1.431000	3.987000	0.708000
H	-1.490000	3.691000	-1.017000
H	0.509000	1.414000	-1.284000
H	3.150000	2.955000	-1.063000
H	2.021000	2.974000	-2.442000
H	2.867000	1.473000	-2.009000
H	-1.336000	-3.347000	1.506000
H	-0.501000	-2.576000	2.878000
H	-0.001000	-4.192000	2.318000



Carbon	δC Theoretical	δC Experimental
1	57.5	58.8
2	44.6	42.8
3	199.2	208.7
4	41.4	45.3
5	39.3	39.6
6	81.8	82.6
7	56.3	51.9
8	29.0	29.5
9	41.5	38.3
10	59.4	60.3
11	46.4	43.5
12	165.4	177.5
13	14.2	14.9
14	16.8	16.9
15	16.1	17.0

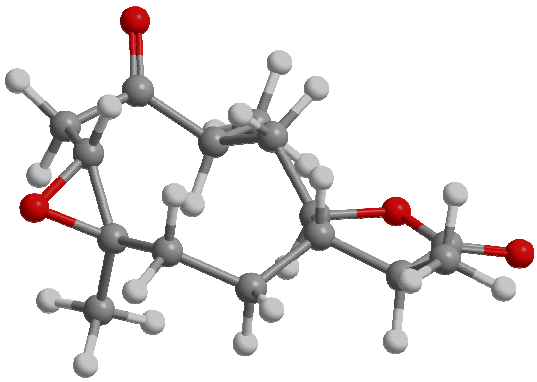
Free Energies = -885.441193 Hartrees



D1_c

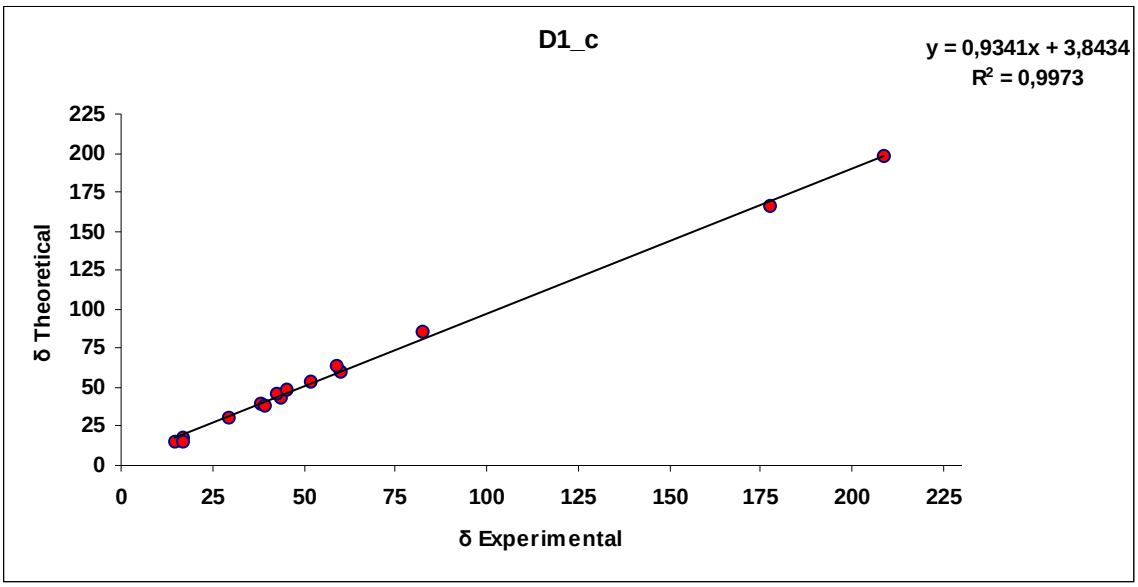
Cartesian coordinates (x, y, z)

C	0.705500	-2.720000	0.899500
C	2.140500	-2.544000	0.409500
O	3.043500	-3.368000	0.565500
C	-2.326500	0.468000	-2.074500
C	-2.293500	-0.086000	0.523500
C	-1.428500	-1.371000	0.414500
C	0.094500	-1.307000	0.755500
C	1.023500	-0.659000	-0.308500
O	2.283500	-1.350000	-0.252500
C	1.296500	0.860000	-0.114500
C	-1.674500	2.331000	-0.223500
C	-0.965500	3.261000	-1.230500
C	0.566500	3.096000	-1.154500
O	1.253500	4.073000	-0.846500
C	1.229500	1.716000	-1.417500
C	-2.170500	0.956000	-0.617500
O	-3.077500	2.084000	-0.441500
C	2.599500	1.811000	-2.120500
C	0.606500	-3.303000	2.324500
H	0.219500	-3.424000	0.197500
H	-3.202500	-0.198000	-2.177500
H	-1.443500	-0.106000	-2.405500
H	-2.471500	1.290000	-2.798500
H	-2.119500	0.377000	1.513500
H	-3.353500	-0.402000	0.559500
H	-1.573500	-1.835000	-0.579500
H	-1.890500	-2.096000	1.111500
H	0.222500	-0.771000	1.716500
H	0.590500	-0.851000	-1.309500
H	2.264500	1.016000	0.399500
H	0.580500	1.243000	0.633500
H	-1.465500	2.504000	0.849500
H	-1.239500	4.308000	-1.005500
H	-1.301500	3.092000	-2.269500
H	0.561500	1.210000	-2.138500
H	2.530500	2.370000	-3.072500
H	3.000500	0.809000	-2.364500
H	3.353500	2.322000	-1.493500
H	1.116500	-2.665000	3.072500
H	1.064500	-4.308000	2.384500
H	-0.445500	-3.410000	2.646500



Carbon	δC Theoretical	δC Experimental
1	63.7	58.8
2	46.5	42.8
3	198.6	208.7
4	48.2	45.3
5	38.6	39.6
6	85.7	82.6
7	54.2	51.9
8	31.3	29.5
9	39.0	38.3
10	59.7	60.3
11	43.7	43.5
12	166.1	177.5
13	15.0	14.9
14	18.2	16.9
15	15.7	17.0

Free Energies = -885.441168 Hartrees

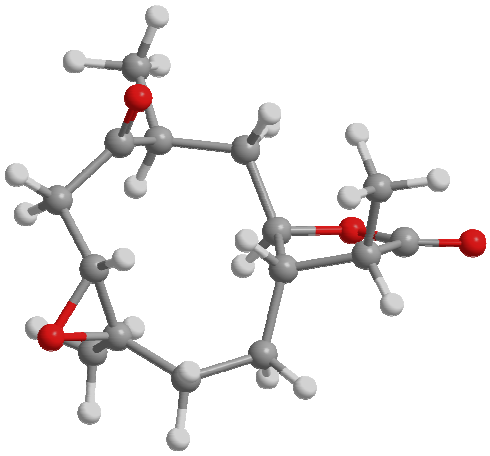


D1_d

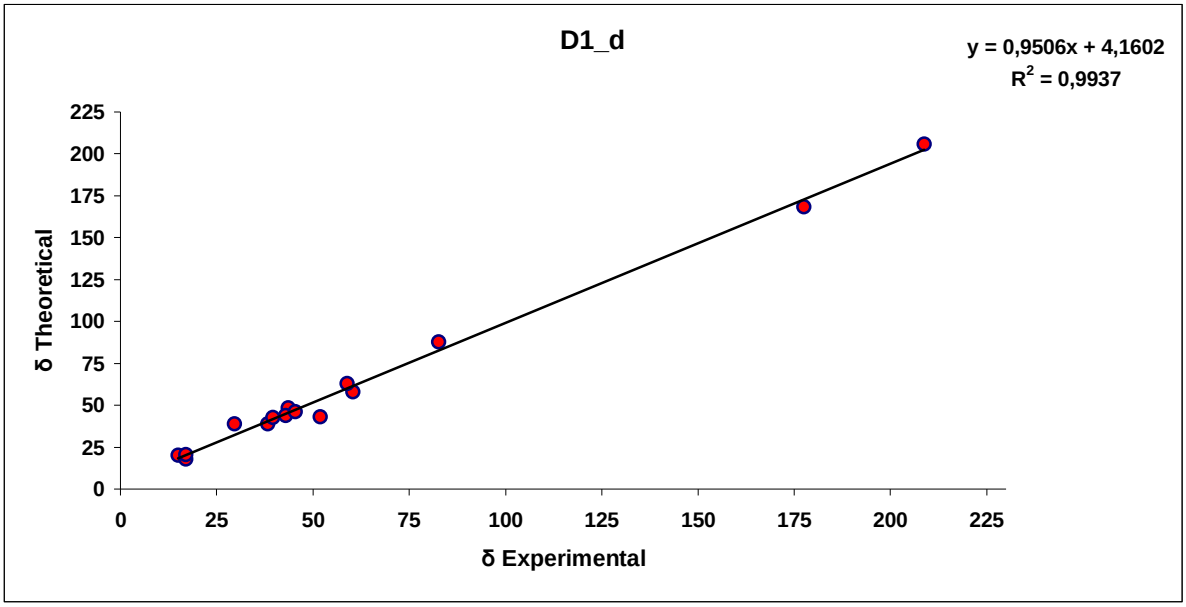
Cartesian coordinates (x, y, z)

C	0.029000	-2.196000	1.471000
C	1.306000	-2.772000	0.872000
O	1.845000	-3.813000	1.248000
C	-1.654000	0.728000	-2.866000
C	-2.698000	-0.711000	-0.891000
C	-1.540000	-1.679000	-0.538000
C	-0.411000	-1.146000	0.419000
C	0.917000	-0.825000	-0.333000
O	1.760000	-1.983000	-0.160000
C	1.730000	0.434000	0.101000
C	-2.152000	1.743000	-0.408000
C	-1.142000	2.889000	-0.551000
C	0.139000	2.500000	0.202000
O	0.211000	2.746000	1.409000
C	1.323000	1.807000	-0.516000
C	-2.271000	0.662000	-1.453000
O	-3.267000	1.715000	-1.329000
C	2.522000	2.779000	-0.563000
C	0.261000	-1.625000	2.886000
H	-0.711000	-3.011000	1.570000
H	-1.574000	1.760000	-3.255000
H	-2.268000	0.165000	-3.592000
H	-0.641000	0.291000	-2.891000
H	-3.334000	-0.584000	0.007000
H	-3.364000	-1.205000	-1.623000
H	-1.100000	-2.071000	-1.475000
H	-2.025000	-2.571000	-0.099000
H	-0.789000	-0.247000	0.940000
H	0.734000	-0.726000	-1.418000
H	2.777000	0.234000	-0.200000
H	1.786000	0.503000	1.203000
H	-2.487000	1.499000	0.619000
H	-1.565000	3.813000	-0.114000
H	-0.916000	3.135000	-1.604000
H	1.035000	1.632000	-1.569000
H	3.364000	2.359000	-1.144000
H	2.909000	3.014000	0.447000
H	2.257000	3.739000	-1.045000
H	-0.667000	-1.190000	3.299000
H	1.031000	-0.832000	2.906000
H	0.586000	-2.413000	3.592000

Free Energies = -885.439676 Hartrees



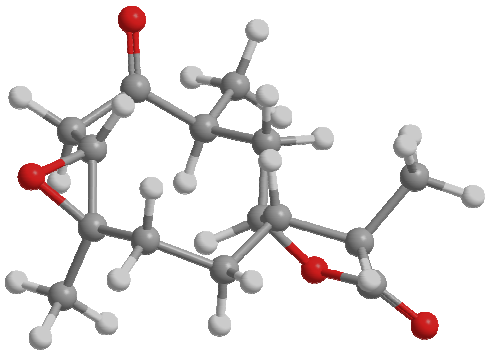
carbon	δC Theoretical	δC Experimental
1	62.9	58.8
2	44.0	42.8
3	206.1	208.7
4	46.1	45.3
5	42.7	39.6
6	87.8	82.6
7	43.1	51.9
8	39.1	29.5
9	39.0	38.3
10	58.1	60.3
11	48.4	43.5
12	168.5	177.5
13	20.1	14.9
14	17.8	16.9
15	20.5	17.0



D1_e

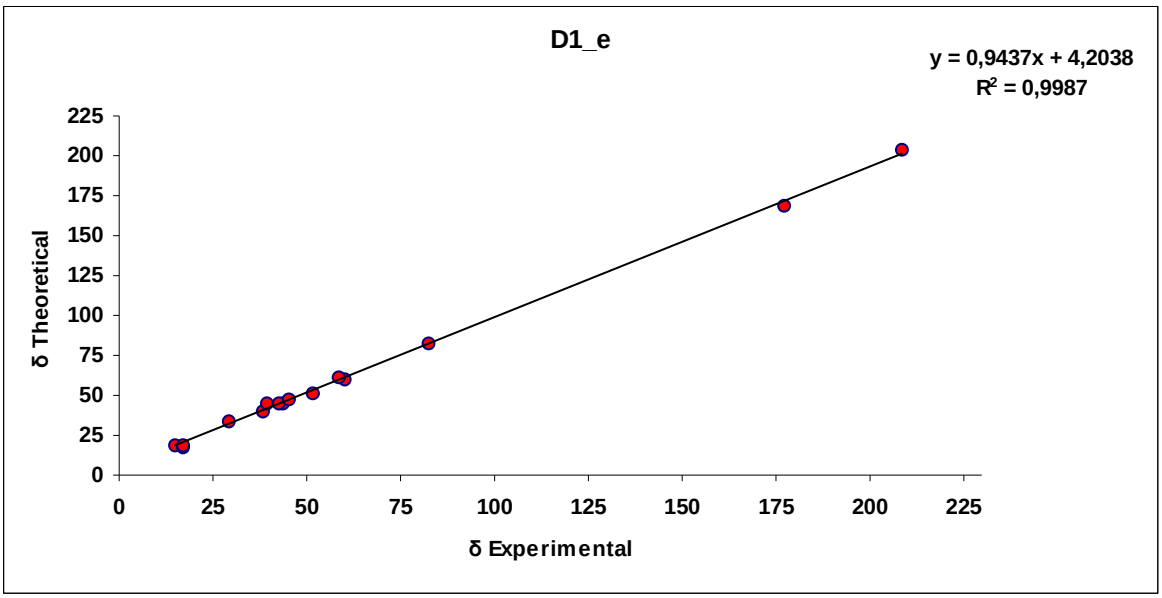
Cartesian coordinates (x, y, z)

C	0.345500	-2.585500	1.329000
C	1.532500	-2.726500	0.379000
O	2.276500	-3.706500	0.336000
C	-2.102500	-0.008500	-2.845000
C	-2.804500	-0.885500	-0.439000
C	-1.686500	-1.913500	-0.121000
C	-0.462500	-1.414500	0.718000
C	0.614500	-0.663500	-0.118000
O	1.645500	-1.618500	-0.431000
C	1.254500	0.589500	0.560000
C	-1.957500	1.539500	-0.639000
C	-0.996500	2.567500	-1.267000
C	0.221500	2.773500	-0.352000
O	0.179500	3.706500	0.454000
C	1.452500	1.820500	-0.380000
C	-2.397500	0.288500	-1.360000
O	-3.259500	1.449500	-1.269000
C	2.768500	2.566500	-0.063000
C	0.804500	-2.338500	2.781000
H	-0.232500	-3.528500	1.318000
H	-2.027500	0.906500	-3.461000
H	-2.903500	-0.624500	-3.293000
H	-1.156500	-0.566500	-2.969000
H	-3.225500	-0.509500	0.514000
H	-3.647500	-1.420500	-0.913000
H	-1.338500	-2.390500	-1.057000
H	-2.181500	-2.732500	0.434000
H	-0.867500	-0.768500	1.521000
H	0.178500	-0.347500	-1.080000
H	2.223500	0.277500	0.997000
H	0.672500	0.895500	1.450000
H	-2.088500	1.576500	0.460000
H	-1.522500	3.531500	-1.405000
H	-0.654500	2.268500	-2.274000
H	1.570500	1.458500	-1.419000
H	2.928500	3.420500	-0.747000
H	3.647500	1.903500	-0.171000
H	2.783500	2.963500	0.969000
H	-0.059500	-2.223500	3.461000
H	1.420500	-1.424500	2.880000
H	1.405500	-3.182500	3.167000



Carbon	δC Theoretical	δC Experimental
1	61.0	58.8
2	44.5	42.8
3	203.2	208.7
4	47.9	45.3
5	45.0	39.6
6	83.1	82.6
7	51.6	51.9
8	34.0	29.5
9	39.8	38.3
10	60.3	60.3
11	44.4	43.5
12	168.5	177.5
13	19.3	14.9
14	17.3	16.9
15	18.5	17.0

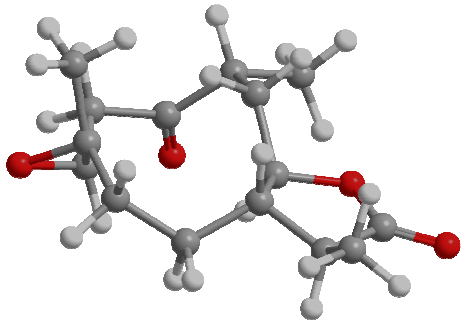
Free Energies = -885.439095 Hartrees



D2_a

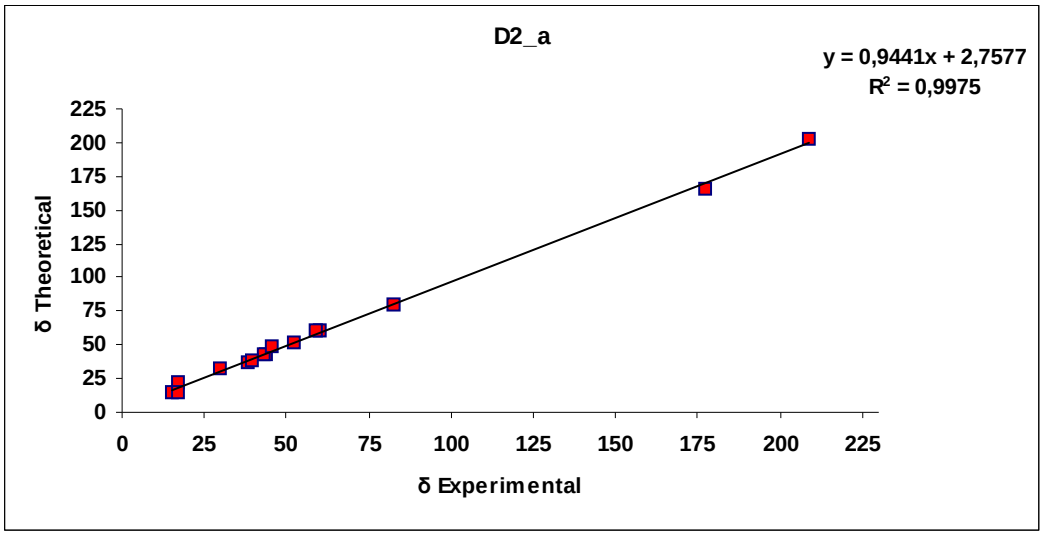
Cartesian coordinates (x, y, z)

C	4.510000	0.438000	-8.632000
C	5.892000	0.712000	-9.214000
O	6.811000	-0.107000	-9.260000
C	1.772000	5.388000	-7.544000
C	1.392000	2.873000	-8.224000
C	2.323000	1.774000	-8.804000
C	3.862000	1.838000	-8.524000
C	4.710000	2.671000	-9.528000
O	5.963000	1.990000	-9.709000
C	5.028000	4.132000	-9.094000
C	1.840000	4.596000	-10.143000
C	2.629000	5.822000	-10.643000
C	4.009000	5.376000	-11.160000
O	4.112000	5.134000	-12.365000
C	5.235000	5.199000	-10.209000
C	1.603000	4.344000	-8.669000
O	0.554000	4.849000	-9.546000
C	6.576000	4.990000	-10.948000
C	4.543000	-0.338000	-7.298000
H	3.977000	-0.179000	-9.381000
H	0.921000	5.346000	-6.838000
H	1.819000	6.429000	-7.910000
H	2.686000	5.206000	-6.951000
H	1.452000	2.812000	-7.121000
H	0.346000	2.586000	-8.445000
H	2.143000	1.666000	-9.890000
H	1.936000	0.825000	-8.386000
H	4.030000	2.228000	-7.500000
H	4.194000	2.675000	-10.508000
H	5.909000	4.126000	-8.422000
H	4.233000	4.498000	-8.430000
H	1.766000	3.736000	-10.834000
H	2.755000	6.600000	-9.870000
H	2.067000	6.310000	-11.461000
H	5.340000	6.168000	-9.686000
H	7.431000	4.956000	-10.247000
H	6.780000	5.812000	-11.660000
H	6.588000	4.047000	-11.526000
H	3.524000	-0.512000	-6.907000
H	5.108000	0.203000	-6.515000
H	5.016000	-1.330000	-7.417000



Carbon	δC Theoretical	δC Experimental
1	61.1	58.8
2	42.5	42.8
3	203.1	208.7
4	49.0	45.3
5	38.1	39.6
6	79.7	82.6
7	51.9	51.9
8	32.8	29.5
9	36.4	38.3
10	60.9	60.3
11	43.3	43.5
12	165.8	177.5
13	14.9	14.9
14	22.4	16.9
15	15.4	17.0

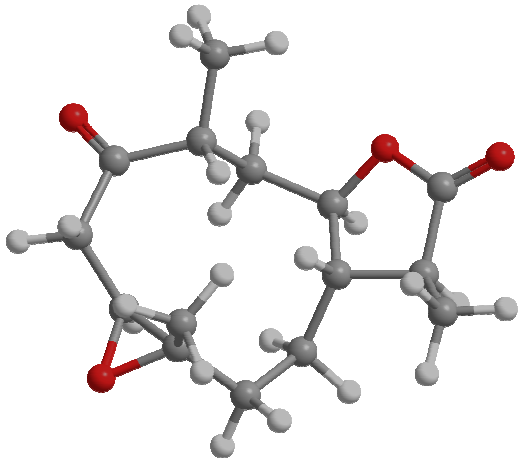
Free Energies = -885.440434 Hartrees



D2_b

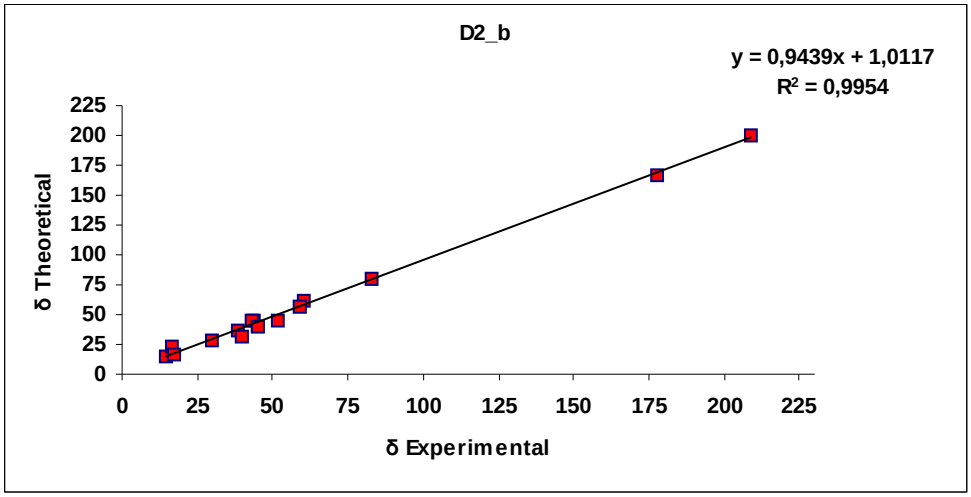
Cartesian coordinates (x, y, z)

C	4.587000	0.908000	-8.078000
C	6.069000	1.176000	-8.383000
O	7.011000	0.791000	-7.689000
C	2.073000	4.940000	-7.613000
C	1.358000	2.638000	-8.722000
C	2.417000	1.701000	-9.364000
C	3.903000	1.962000	-8.967000
C	4.902000	2.035000	-10.145000
O	6.200000	1.910000	-9.545000
C	4.809000	3.263000	-11.092000
C	1.742000	4.704000	-10.273000
C	2.542000	5.986000	-10.597000
C	3.939000	5.679000	-11.180000
O	4.258000	6.213000	-12.245000
C	4.922000	4.696000	-10.481000
C	1.610000	4.166000	-8.866000
O	0.528000	4.896000	-9.509000
C	6.376000	5.211000	-10.460000
C	4.219000	1.014000	-6.584000
H	4.348000	-0.112000	-8.435000
H	1.930000	6.032000	-7.703000
H	3.143000	4.769000	-7.398000
H	1.507000	4.627000	-6.717000
H	1.263000	2.378000	-7.651000
H	0.368000	2.386000	-9.148000
H	2.303000	1.772000	-10.462000
H	2.143000	0.652000	-9.145000
H	3.967000	2.919000	-8.422000
H	4.749000	1.142000	-10.787000
H	3.846000	3.156000	-11.628000
H	5.554000	3.144000	-11.902000
H	1.561000	4.001000	-11.107000
H	2.658000	6.642000	-9.718000
H	1.965000	6.585000	-11.326000
H	4.609000	4.669000	-9.425000
H	6.448000	6.207000	-9.985000
H	6.800000	5.301000	-11.477000
H	7.037000	4.535000	-9.887000
H	3.138000	0.844000	-6.422000
H	4.461000	2.009000	-6.163000
H	4.758000	0.261000	-5.980000



Carbon	δC Theoretical	δC Experimental
1	56.3	58.8
2	45.5	42.8
3	199.9	208.7
4	39.7	45.3
5	31.2	39.6
6	80.5	82.6
7	44.4	51.9
8	28.4	29.5
9	36.5	38.3
10	61.0	60.3
11	45.6	43.5
12	166.7	177.5
13	14.9	14.9
14	22.7	16.9
15	17.5	17.0

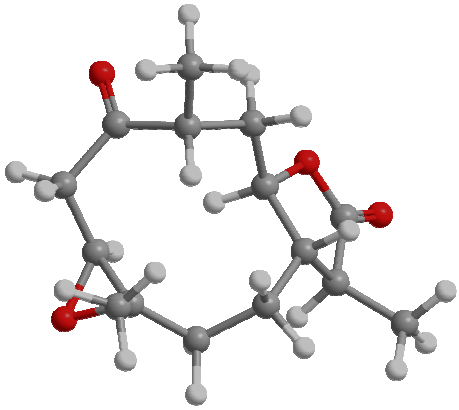
Free Energies = -885.439273 Hartress



D2_c

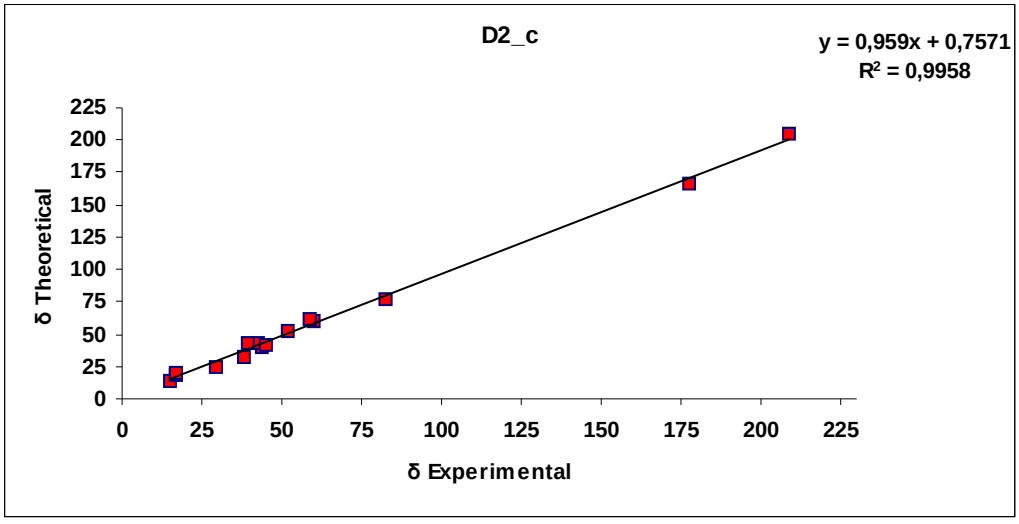
Cartesian coordinates (x, y, z)

C	4.904000	0.688000	-8.599000
C	5.867000	0.645000	-9.786000
O	6.467000	-0.359000	-10.174000
C	1.250000	4.988000	-7.799000
C	2.085000	2.488000	-8.132000
C	3.513000	2.629000	-7.530000
C	4.770000	2.206000	-8.350000
C	5.014000	2.782000	-9.769000
O	5.970000	1.889000	-10.367000
C	5.562000	4.234000	-9.885000
C	1.705000	3.904000	-10.240000
C	2.025000	5.271000	-10.872000
C	3.549000	5.420000	-11.051000
O	3.993000	5.541000	-12.196000
C	4.535000	5.404000	-9.845000
C	1.538000	3.799000	-8.745000
O	0.406000	3.677000	-9.651000
C	5.254000	6.764000	-9.728000
C	5.396000	-0.120000	-7.379000
H	3.941000	0.265000	-8.942000
H	0.651000	5.785000	-8.277000
H	2.180000	5.457000	-7.432000
H	0.680000	4.658000	-6.911000
H	1.391000	2.183000	-7.326000
H	2.046000	1.648000	-8.851000
H	3.527000	2.044000	-6.592000
H	3.669000	3.662000	-7.169000
H	5.642000	2.514000	-7.738000
H	4.098000	2.692000	-10.375000
H	6.131000	4.318000	-10.832000
H	6.327000	4.378000	-9.099000
H	2.012000	3.004000	-10.803000
H	1.637000	6.119000	-10.282000
H	1.521000	5.342000	-11.854000
H	3.950000	5.295000	-8.917000
H	5.893000	6.974000	-10.607000
H	5.904000	6.806000	-8.834000
H	4.536000	7.600000	-9.637000
H	5.515000	-1.192000	-7.625000
H	4.680000	-0.064000	-6.539000
H	6.372000	0.241000	-7.005000



Carbon	δC Theoretical	δC Experimental
1	61.6	58.8
2	43.9	42.8
3	205.2	208.7
4	42.0	45.3
5	42.6	39.6
6	76.9	82.6
7	53.1	51.9
8	23.9	29.5
9	32.3	38.3
10	59.7	60.3
11	40.7	43.5
12	166.0	177.5
13	14.1	14.9
14	18.4	16.9
15	20.4	17.0

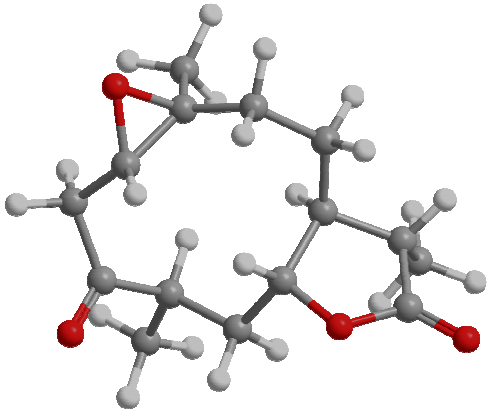
Free Energies = -885.438912 Hartrees



D2_d

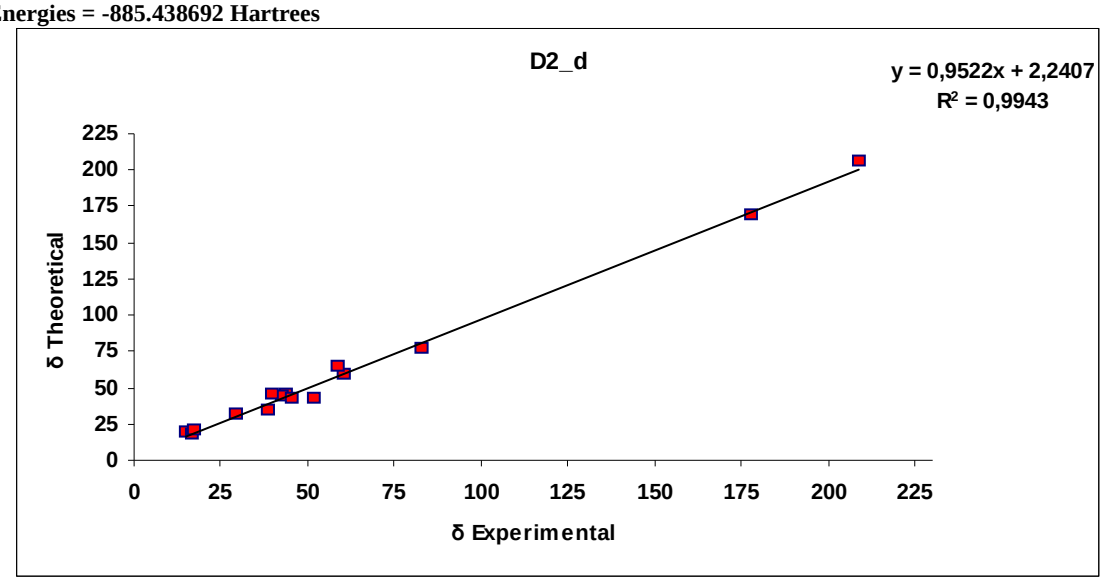
Cartesian coordinates (x, y, z)

C	5.120000	1.181000	-7.887000
C	5.709000	0.579000	-9.161000
O	6.390000	-0.446000	-9.195000
C	1.529000	4.665000	-7.616000
C	1.431000	2.366000	-8.962000
C	2.634000	1.639000	-8.302000
C	4.090000	2.201000	-8.433000
C	4.600000	2.486000	-9.876000
O	5.349000	1.320000	-10.267000
C	5.522000	3.734000	-10.057000
C	1.737000	4.526000	-10.311000
C	2.441000	5.884000	-10.447000
C	3.912000	5.634000	-10.817000
O	4.263000	5.808000	-11.986000
C	4.941000	5.150000	-9.763000
C	1.451000	3.913000	-8.961000
O	0.401000	4.527000	-9.761000
C	6.071000	6.190000	-9.613000
C	6.199000	1.782000	-6.962000
H	4.625000	0.370000	-7.318000
H	0.838000	4.225000	-6.874000
H	1.258000	5.733000	-7.704000
H	2.543000	4.624000	-7.182000
H	0.503000	2.025000	-8.467000
H	1.330000	1.980000	-9.995000
H	2.611000	0.591000	-8.659000
H	2.413000	1.560000	-7.221000
H	4.124000	3.125000	-7.830000
H	3.752000	2.590000	-10.575000
H	5.922000	3.723000	-11.090000
H	6.418000	3.579000	-9.429000
H	1.784000	3.853000	-11.188000
H	2.380000	6.495000	-9.529000
H	1.948000	6.479000	-11.237000
H	4.434000	5.117000	-8.782000
H	6.663000	6.301000	-10.541000
H	6.776000	5.911000	-8.808000
H	5.676000	7.191000	-9.353000
H	6.913000	1.010000	-6.619000
H	5.746000	2.224000	-6.056000
H	6.791000	2.577000	-7.451000



carbon	δC Theoretical	δC Experimental
1	64.1	58.8
2	44.6	42.8
3	205.4	208.7
4	42.5	45.3
5	45.2	39.6
6	76.4	82.6
7	42.8	51.9
8	31.3	29.5
9	34.9	38.3
10	58.6	60.3
11	44.9	43.5
12	168.3	177.5
13	19.7	14.9
14	17.8	16.9
15	20.4	17.0

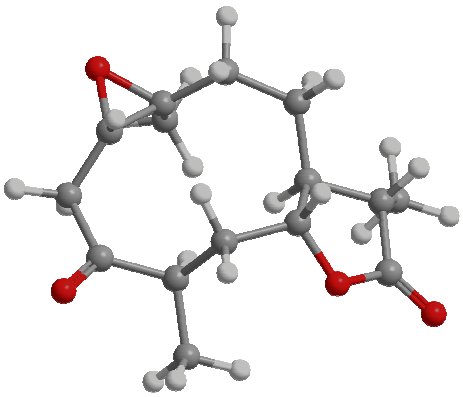
Free Energies = -885.438692 Hartrees



D2_e

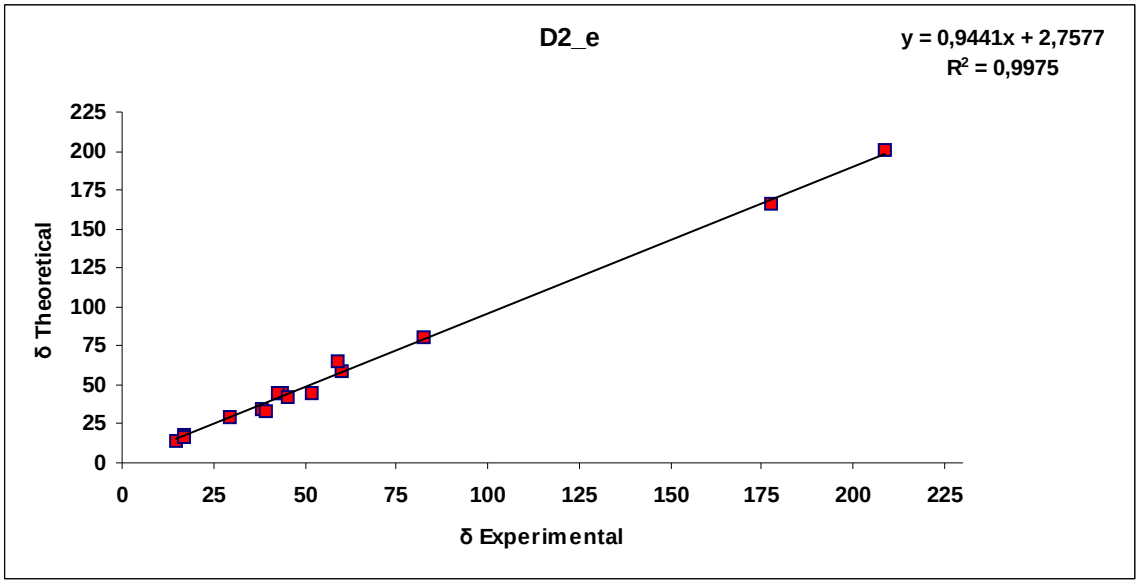
Cartesian coordinates (x, y, z)

C	4.881000	0.901000	-8.066000
C	6.256000	1.150000	-8.690000
O	7.322000	0.727000	-8.240000
C	1.726000	4.455000	-7.584000
C	1.422000	2.505000	-9.401000
C	2.484000	1.554000	-8.786000
C	3.995000	1.950000	-8.773000
C	4.746000	2.116000	-10.122000
O	6.137000	1.905000	-9.833000
C	4.578000	3.440000	-10.917000
C	1.665000	4.916000	-10.257000
C	2.517000	6.196000	-10.158000
C	3.920000	5.932000	-10.753000
O	4.289000	6.614000	-11.712000
C	4.834000	4.803000	-10.192000
C	1.506000	4.017000	-9.050000
O	0.410000	4.835000	-9.557000
C	6.328000	5.192000	-10.178000
C	4.878000	0.998000	-6.525000
H	4.573000	-0.122000	-8.358000
H	1.133000	3.834000	-6.889000
H	1.429000	5.505000	-7.401000
H	2.783000	4.370000	-7.279000
H	0.422000	2.139000	-9.100000
H	1.436000	2.355000	-10.497000
H	2.374000	0.565000	-9.271000
H	2.177000	1.375000	-7.739000
H	4.096000	2.885000	-8.200000
H	4.426000	1.296000	-10.796000
H	3.559000	3.408000	-11.337000
H	5.209000	3.387000	-11.825000
H	1.558000	4.468000	-11.263000
H	2.616000	6.563000	-9.121000
H	2.018000	7.009000	-10.716000
H	4.547000	4.709000	-9.132000
H	6.732000	5.321000	-11.200000
H	6.946000	4.425000	-9.676000
H	6.497000	6.140000	-9.636000
H	3.870000	0.819000	-6.109000
H	5.209000	1.993000	-6.170000
H	5.550000	0.247000	-6.071000



Carbon	δC Theoretical	δC Experimental
1	64.9	58.8
2	45.3	42.8
3	200.1	208.7
4	41.7	45.3
5	33.6	39.6
6	80.4	82.6
7	44.5	51.9
8	29.0	29.5
9	34.9	38.3
10	59.0	60.3
11	44.8	43.5
12	166.1	177.5
13	14.6	14.9
14	17.9	16.9
15	17.0	17.0

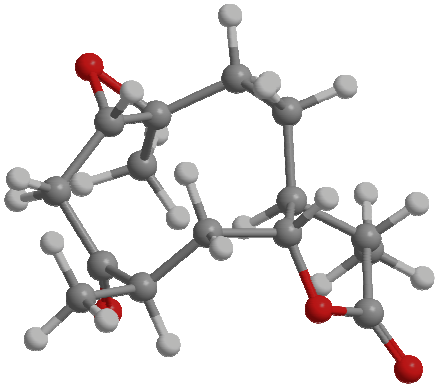
Free Energies = -885.438069 Hartrees



D2_f

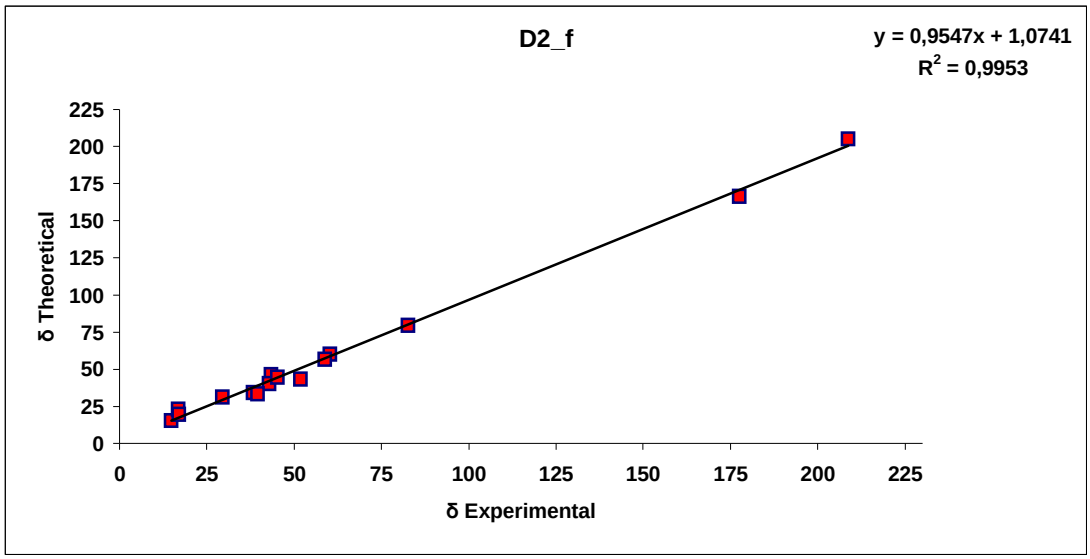
Cartesian coordinates (x, y, z)

C	4.943000	1.126000	-8.306000
C	6.319000	1.430000	-8.909000
O	7.396000	1.191000	-8.362000
C	2.062000	4.619000	-7.288000
C	1.483000	2.312000	-8.464000
C	2.533000	1.517000	-9.292000
C	4.020000	1.990000	-9.185000
C	4.796000	2.012000	-10.519000
O	6.186000	2.005000	-10.156000
C	4.489000	3.146000	-11.542000
C	1.679000	4.420000	-9.947000
C	2.537000	5.665000	-10.242000
C	4.051000	5.355000	-10.142000
O	4.635000	5.722000	-9.121000
C	4.891000	4.621000	-11.226000
C	1.587000	3.861000	-8.544000
O	0.475000	4.573000	-9.158000
C	4.929000	5.467000	-12.516000
C	4.835000	1.429000	-6.798000
H	4.738000	0.051000	-8.472000
H	3.112000	4.375000	-7.044000
H	1.451000	4.352000	-6.407000
H	2.000000	5.717000	-7.398000
H	1.556000	1.994000	-7.407000
H	0.470000	1.994000	-8.774000
H	2.212000	1.560000	-10.349000
H	2.450000	0.442000	-9.045000
H	4.060000	3.017000	-8.784000
H	4.591000	1.057000	-11.046000
H	3.424000	3.100000	-11.834000
H	5.018000	2.847000	-12.467000
H	1.506000	3.722000	-10.786000
H	2.276000	6.495000	-9.559000
H	2.299000	6.042000	-11.252000
H	5.936000	4.589000	-10.862000
H	3.938000	5.537000	-13.001000
H	5.625000	5.040000	-13.262000
H	5.275000	6.500000	-12.322000
H	3.819000	1.217000	-6.415000
H	5.057000	2.488000	-6.567000
H	5.537000	0.810000	-6.209000



Carbon	δC Theoretical	δC Experimental
1	56.9	58.8
2	40.6	42.8
3	205.1	208.7
4	44.9	45.3
5	33.7	39.6
6	79.7	82.6
7	43.3	51.9
8	31.5	29.5
9	34.6	38.3
10	60.3	60.3
11	46.4	43.5
12	166.7	177.5
13	15.3	14.9
14	23.1	16.9
15	20.0	17.0

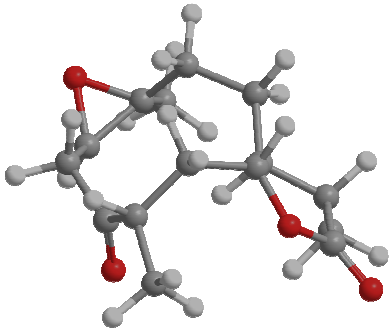
Free Energies = -885.436865 Hartrees



D3_a

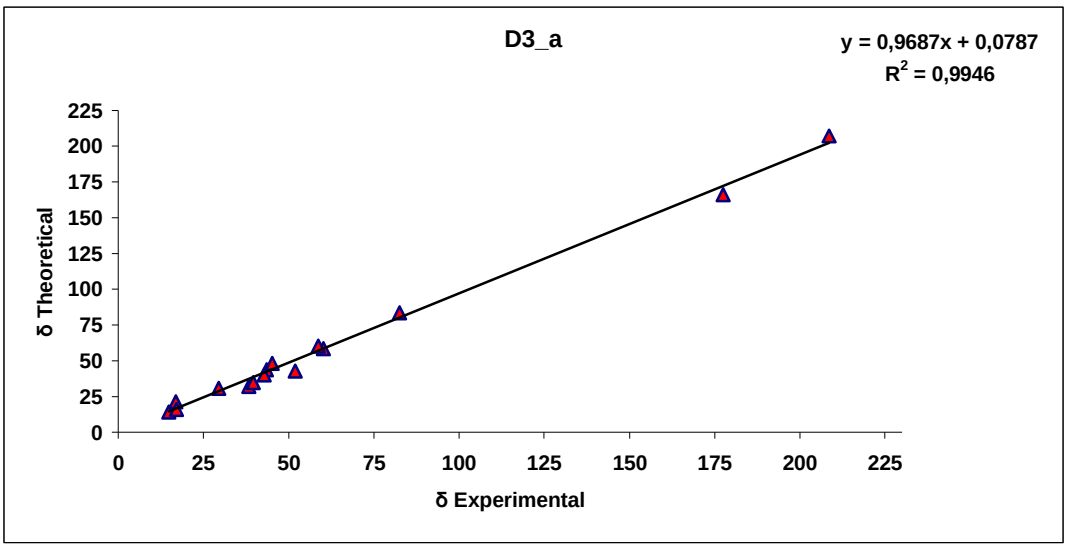
Cartesian coordinates (x, y, z)

C	4.775000	1.648000	-7.893000
C	6.273000	1.947000	-7.982000
O	7.081000	1.783000	-7.067000
C	0.364000	3.666000	-8.766000
C	2.016000	2.664000	-10.580000
C	2.895000	1.774000	-9.668000
C	4.210000	2.400000	-9.117000
C	5.430000	2.379000	-10.071000
O	6.597000	2.415000	-9.235000
C	5.540000	3.442000	-11.202000
C	1.900000	5.309000	-10.085000
C	3.106000	5.708000	-10.962000
C	4.454000	5.621000	-10.225000
O	4.539000	6.097000	-9.089000
C	5.689000	4.964000	-10.899000
C	1.379000	3.903000	-9.900000
O	0.812000	4.796000	-10.891000
C	7.033000	5.314000	-10.219000
C	4.138000	2.065000	-6.551000
H	4.653000	0.556000	-8.022000
H	0.858000	3.250000	-7.869000
H	-0.419000	2.949000	-9.073000
H	-0.153000	4.592000	-8.451000
H	1.194000	2.036000	-10.972000
H	2.578000	2.948000	-11.485000
H	3.133000	0.837000	-10.207000
H	2.265000	1.441000	-8.822000
H	4.009000	3.438000	-8.798000
H	5.439000	1.395000	-10.583000
H	4.691000	3.302000	-11.893000
H	6.407000	3.150000	-11.826000
H	1.542000	6.067000	-9.364000
H	2.965000	6.748000	-11.307000
H	3.139000	5.108000	-11.890000
H	5.751000	5.447000	-11.893000
H	7.894000	4.880000	-10.762000
H	7.082000	4.949000	-9.177000
H	7.196000	6.407000	-10.184000
H	3.054000	1.850000	-6.532000
H	4.261000	3.146000	-6.348000
H	4.589000	1.519000	-5.701000



Carbon	δC Theoretical	δC Experimental
1	60.1	58.8
2	40.1	42.8
3	207.1	208.7
4	48.0	45.3
5	35,.0	39.6
6	83.4	82.6
7	42.6	51.9
8	30.8	29.5
9	32.2	38.3
10	58.3	60.3
11	43.8	43.5
12	166.1	177.5
13	14.4	14.9
14	21.6	16.9
15	16.3	17.0

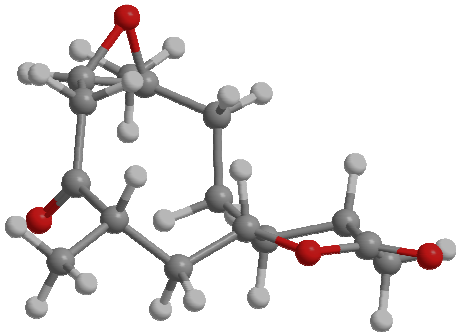
Free Energies = -885.447336 Hartrees



D3_b

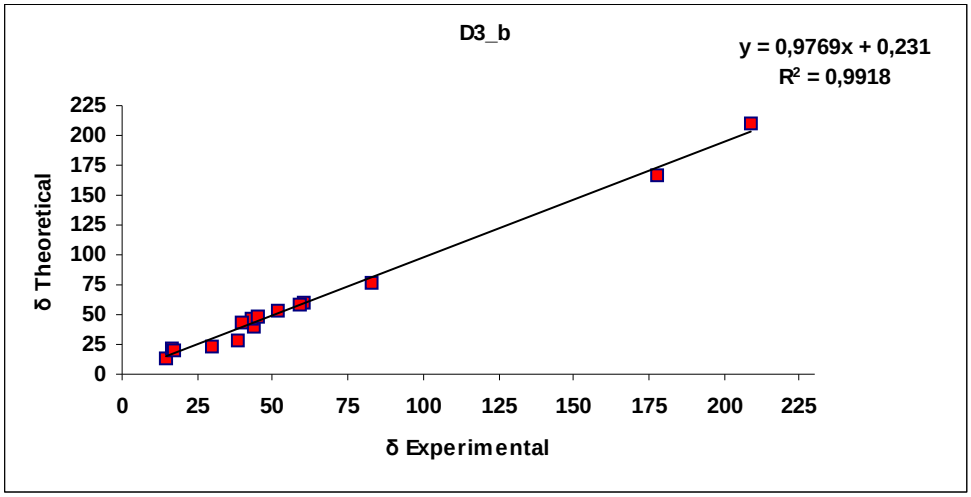
Cartesian coordinates (x, y, z)

C	4.083000	0.833000	-8.779000
C	5.549000	0.464000	-9.024000
O	5.987000	-0.687000	-9.068000
C	0.194000	4.848000	-9.738000
C	2.316000	3.288000	-10.041000
C	2.918000	3.186000	-8.615000
C	4.199000	2.329000	-8.427000
C	5.454000	2.753000	-9.230000
O	6.313000	1.599000	-9.193000
C	6.216000	4.009000	-8.711000
C	2.399000	5.866000	-10.702000
C	3.923000	5.879000	-10.963000
C	4.797000	5.959000	-9.695000
O	4.394000	6.592000	-8.715000
C	6.181000	5.260000	-9.639000
C	1.611000	4.641000	-10.298000
O	1.696000	5.058000	-11.683000
C	7.282000	6.269000	-9.249000
C	3.392000	-0.019000	-7.695000
H	3.544000	0.701000	-9.736000
H	-0.256000	5.808000	-10.055000
H	0.197000	4.839000	-8.633000
H	-0.489000	4.046000	-10.072000
H	1.607000	2.455000	-10.202000
H	3.092000	3.127000	-10.809000
H	2.132000	2.820000	-7.929000
H	3.147000	4.197000	-8.230000
H	4.466000	2.401000	-7.353000
H	5.190000	2.908000	-10.294000
H	7.275000	3.720000	-8.565000
H	5.878000	4.282000	-7.693000
H	1.905000	6.844000	-10.554000
H	4.165000	6.745000	-11.606000
H	4.221000	4.996000	-11.558000
H	6.435000	4.922000	-10.662000
H	7.302000	7.139000	-9.934000
H	8.288000	5.812000	-9.291000
H	7.145000	6.662000	-8.224000
H	3.907000	0.049000	-6.718000
H	3.364000	-1.087000	-7.978000
H	2.345000	0.300000	-7.538000



Carbon	δC Theoretical	δC Experimental
1	57.9	58.8
2	47.1	42.8
3	210.8	208.7
4	48.7	45.3
5	43.0	39.6
6	76.7	82.6
7	52.6	51.9
8	22.7	29.5
9	27.7	38.3
10	60.6	60.3
11	40.1	43.5
12	166.7	177.5
13	14.0	14.9
14	22.0	16.9
15	19.2	17.0

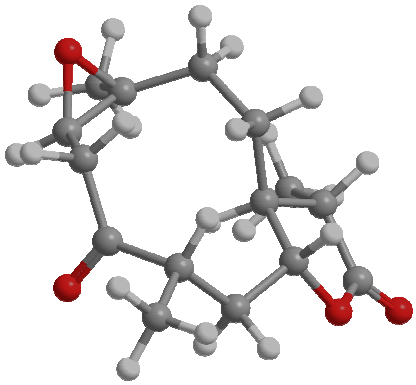
Free Energies = -885.446744 Hartrees



D3_c

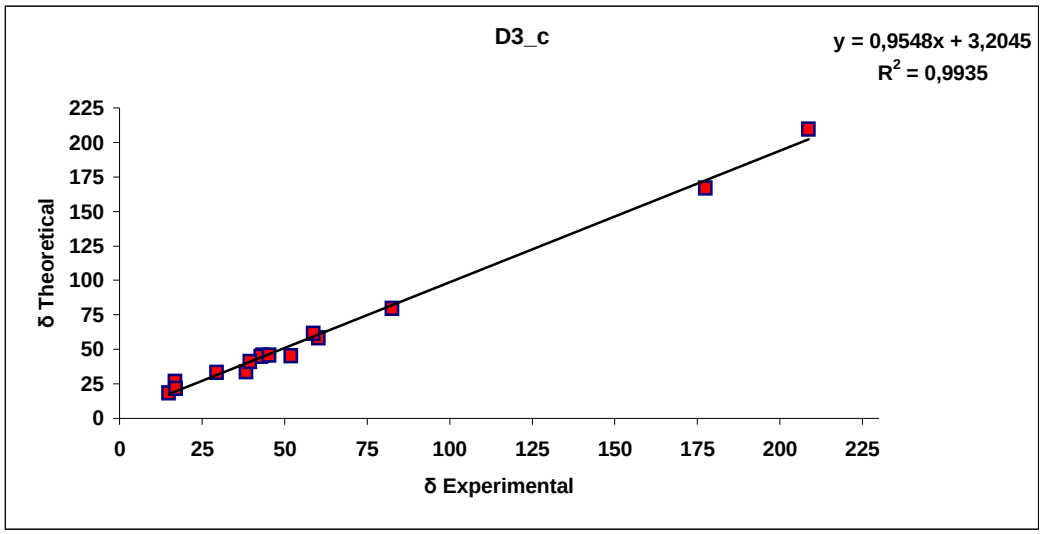
Cartesian coordinates (x, y, z)

C	4.305000	1.211000	-8.370000
C	5.710000	1.159000	-7.776000
O	6.049000	0.438000	-6.837000
C	0.562000	3.822000	-8.669000
C	2.007000	2.617000	-10.515000
C	3.523000	2.329000	-10.586000
C	4.354000	2.462000	-9.275000
C	5.870000	2.647000	-9.539000
O	6.554000	2.011000	-8.446000
C	6.416000	4.098000	-9.642000
C	2.066000	5.332000	-10.151000
C	3.242000	5.673000	-11.088000
C	4.575000	5.794000	-10.327000
O	4.628000	6.551000	-9.353000
C	5.855000	5.031000	-10.760000
C	1.524000	3.947000	-9.864000
O	0.936000	4.807000	-10.879000
C	6.919000	6.044000	-11.234000
C	3.193000	1.238000	-7.302000
H	4.186000	0.295000	-8.979000
H	0.127000	4.791000	-8.359000
H	1.077000	3.404000	-7.785000
H	-0.286000	3.152000	-8.902000
H	1.532000	1.766000	-9.993000
H	1.600000	2.543000	-11.541000
H	3.950000	2.977000	-11.366000
H	3.666000	1.318000	-11.012000
H	4.009000	3.344000	-8.699000
H	6.154000	2.104000	-10.463000
H	7.510000	3.992000	-9.783000
H	6.330000	4.595000	-8.656000
H	1.749000	6.136000	-9.461000
H	3.034000	6.644000	-11.574000
H	3.320000	4.958000	-11.925000
H	5.623000	4.411000	-11.645000
H	7.250000	6.716000	-10.419000
H	6.541000	6.684000	-12.054000
H	7.820000	5.535000	-11.623000
H	2.189000	1.239000	-7.762000
H	3.259000	2.131000	-6.652000
H	3.238000	0.350000	-6.645000



Carbon	δC Theoretical	δC Experimental
1	61.6	58.8
2	45.0	42.8
3	209.9	208.7
4	45.8	45.3
5	41.3	39.6
6	79.7	82.6
7	45.3	51.9
8	33.4	29.5
9	33.7	38.3
10	58.2	60.3
11	45.9	43.5
12	166.9	177.5
13	18.4	14.9
14	27.0	16.9
15	21.6	17.0

Free Energies = -885.441423 Hartrees

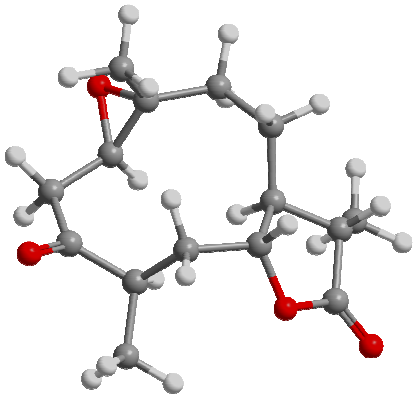


D4_a

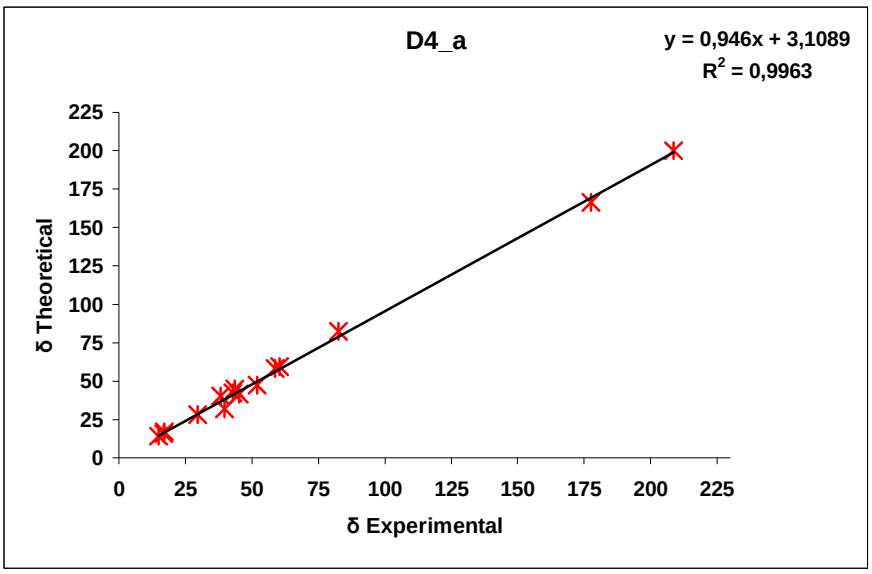
Cartesian coordinates (x, y, z)

C	3.996000	0.571000	-8.536000
C	5.480000	0.659000	-8.909000
O	6.384000	0.028000	-8.360000
C	0.720000	4.630000	-10.931000
C	1.033000	2.927000	-8.924000
C	1.896000	1.791000	-9.532000
C	3.422000	1.840000	-9.197000
C	4.376000	1.986000	-10.409000
O	5.663000	1.541000	-9.952000
C	4.471000	3.383000	-11.077000
C	2.314000	5.189000	-8.835000
C	3.067000	6.333000	-9.546000
C	4.210000	5.867000	-10.476000
O	4.451000	6.552000	-11.473000
C	5.027000	4.567000	-10.225000
C	1.277000	4.334000	-9.523000
O	0.899000	5.411000	-8.623000
C	6.544000	4.771000	-10.419000
C	3.732000	0.483000	-7.018000
H	3.586000	-0.335000	-9.023000
H	0.875000	5.676000	-11.249000
H	-0.368000	4.442000	-10.973000
H	1.188000	3.985000	-11.696000
H	1.171000	2.937000	-7.826000
H	-0.034000	2.670000	-9.060000
H	1.736000	1.756000	-10.626000
H	1.471000	0.834000	-9.176000
H	3.614000	2.679000	-8.503000
H	4.046000	1.281000	-11.199000
H	3.458000	3.616000	-11.451000
H	5.061000	3.288000	-12.009000
H	2.789000	4.767000	-7.930000
H	3.493000	7.008000	-8.782000
H	2.363000	6.966000	-10.118000
H	4.907000	4.325000	-9.154000
H	7.114000	3.860000	-10.162000
H	6.932000	5.583000	-9.775000
H	6.798000	5.032000	-11.464000
H	4.179000	-0.430000	-6.582000
H	2.649000	0.449000	-6.798000
H	4.152000	1.348000	-6.471000

Free Energies = -885.443905 Hartrees



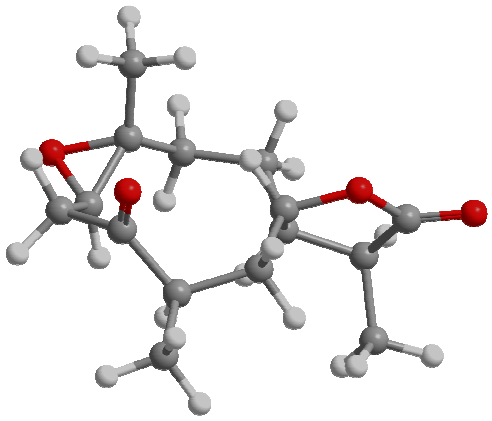
Carbon	δC Theoretical	δC Experimental
1	58.1	58.8
2	42.4	42.8
3	199.9	208.7
4	41.5	45.3
5	32.0	39,.6
6	82.2	82.6
7	47.2	51.9
8	28.1	29.5
9	40.5	38.3
10	59.5	60.3
11	45.0	43.5
12	166.4	177.5
13	14.2	14.9
14	15.6	16.9
15	17.0	17.0



D4_b

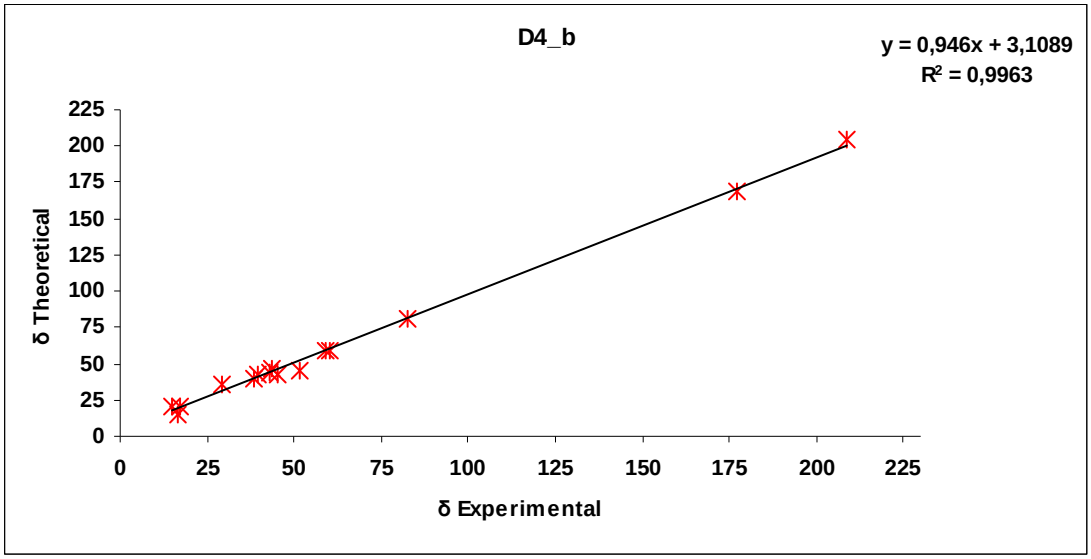
Cartesian coordinates (x, y, z)

C	4.243000	0.737000	-8.403000
C	4.723000	0.207000	-9.752000
O	5.110000	-0.944000	-9.950000
C	0.793000	4.190000	-11.006000
C	1.084000	3.115000	-8.595000
C	1.982000	1.885000	-8.877000
C	3.538000	2.067000	-8.778000
C	4.205000	2.431000	-10.140000
O	4.632000	1.183000	-10.720000
C	5.435000	3.391000	-10.130000
C	2.190000	5.398000	-9.040000
C	2.959000	6.329000	-9.992000
C	4.201000	5.640000	-10.586000
O	4.376000	5.702000	-11.805000
C	5.222000	4.870000	-9.702000
C	1.263000	4.321000	-9.543000
O	0.755000	5.569000	-8.993000
C	6.564000	5.629000	-9.660000
C	5.392000	0.883000	-7.383000
H	3.533000	0.004000	-7.978000
H	0.859000	5.139000	-11.569000
H	-0.263000	3.866000	-11.054000
H	1.386000	3.442000	-11.560000
H	1.227000	3.421000	-7.541000
H	0.026000	2.794000	-8.639000
H	1.710000	1.440000	-9.853000
H	1.657000	1.124000	-8.142000
H	3.744000	2.840000	-8.012000
H	3.461000	2.875000	-10.823000
H	5.872000	3.386000	-11.148000
H	6.224000	2.945000	-9.498000
H	2.611000	5.259000	-8.026000
H	3.280000	7.231000	-9.440000
H	2.306000	6.704000	-10.802000
H	4.850000	4.858000	-8.662000
H	7.287000	5.140000	-8.981000
H	6.438000	6.665000	-9.293000
H	7.041000	5.689000	-10.657000
H	5.865000	-0.092000	-7.166000
H	5.022000	1.281000	-6.420000
H	6.192000	1.562000	-7.730000



Carbon	δC Theoretical	δC Experimental
1	59.5	58.8
2	44.2	42.8
3	203.9	208.7
4	42.0	45.3
5	42.6	39.6
6	80.8	82.6
7	45.1	51.9
8	36.1	29.5
9	40.4	38.3
10	58.5	60.3
11	47.0	43.5
12	168.4	177.5
13	19.9	14.9
14	15.6	16.9
15	20.2	17.0

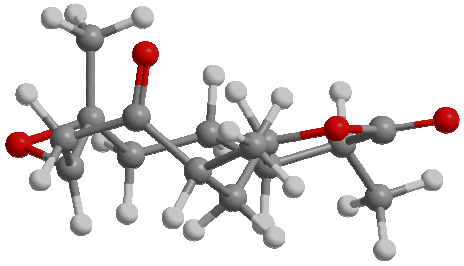
Free Energies = -885.443340 Hartrees



D4_c

Cartesian coordinates (x, y, z)

C	4.285000	0.313000	-9.409000
C	5.512000	0.735000	-10.209000
O	6.364000	-0.039000	-10.646000
C	0.702000	3.951000	-10.643000
C	1.300000	2.770000	-8.331000
C	2.122000	1.599000	-8.933000
C	3.684000	1.642000	-8.895000
C	4.387000	2.712000	-9.778000
O	5.521000	2.093000	-10.408000
C	4.903000	3.958000	-8.998000
C	1.935000	5.264000	-8.638000
C	2.512000	6.340000	-9.578000
C	3.692000	5.799000	-10.414000
O	3.536000	5.727000	-11.635000
C	5.025000	5.310000	-9.765000
C	1.213000	4.057000	-9.189000
O	0.499000	5.150000	-8.544000
C	6.221000	5.305000	-10.743000
C	4.600000	-0.703000	-8.291000
H	3.601000	-0.171000	-10.133000
H	0.489000	4.936000	-11.098000
H	-0.234000	3.366000	-10.695000
H	1.440000	3.449000	-11.294000
H	1.669000	2.984000	-7.310000
H	0.266000	2.411000	-8.175000
H	1.780000	1.409000	-9.968000
H	1.808000	0.693000	-8.381000
H	3.998000	1.789000	-7.842000
H	3.692000	3.025000	-10.579000
H	5.879000	3.713000	-8.536000
H	4.266000	4.122000	-8.114000
H	2.400000	5.167000	-7.639000
H	2.853000	7.205000	-8.982000
H	1.725000	6.739000	-10.245000
H	5.278000	6.070000	-9.002000
H	7.167000	5.044000	-10.233000
H	6.371000	6.298000	-11.207000
H	6.081000	4.579000	-11.566000
H	3.688000	-0.985000	-7.734000
H	5.324000	-0.304000	-7.557000
H	5.028000	-1.638000	-8.700000



Carbon	δC Theoretical	δC Experimental
1	61.0	58.8
2	46.6	42.8
3	202.2	208.7
4	47.0	45.3
5	40.4	39.6
6	76.9	82.6
7	52.3	51.9
8	32.9	29.5
9	38.6	38.3
10	59.2	60.3
11	43.7	43.5
12	166.2	177.5
13	16.1	14.9
14	18.1	16.9
15	16.4	17.0

Free Energies = -885.442195 Hartrees

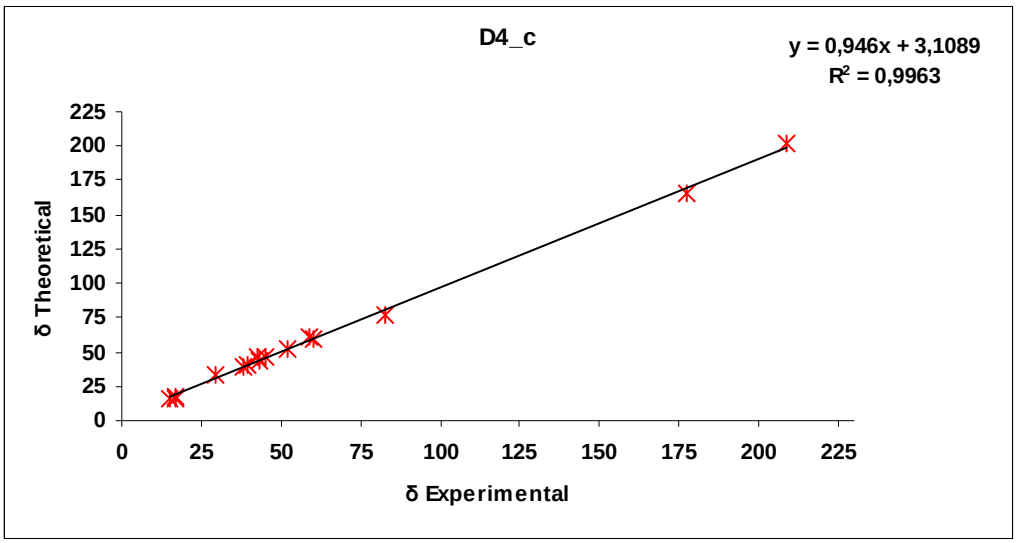
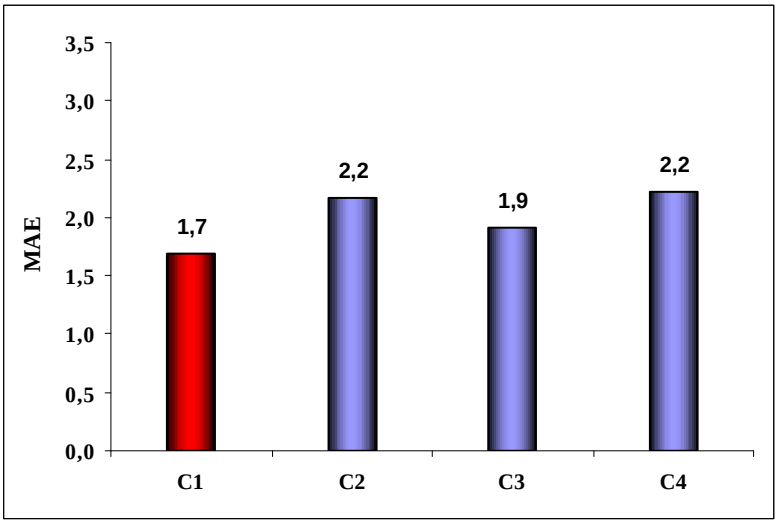


Table S1. Boltzmann averages of GIAO values for ^{13}C NMR chemical of C1-C4 compared to experimental

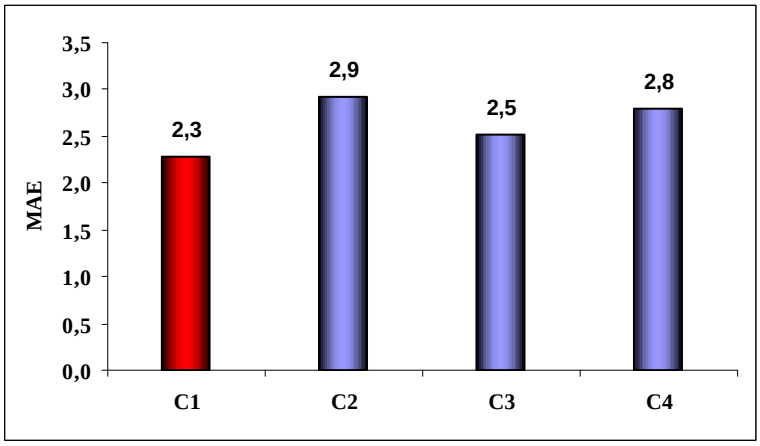
Carbon	C1	C2	C3	C4	Experimental
1	69.1	73.8	69.5	69.6	68.0
2	46.0	43.5	45.7	47.1	43.2
3	209.2	208.6	206.7	204.5	211.5
4	47.1	47.6	44.2	43.6	46.8
5	37.6	36.,5	37.7	37.5	37.0
6	80.4	79.6	76.5	75.5	81.8
7	50.2	49.2	50.7	51.1	49.3
8	30.1	30.4	28.6	27.3	30.2
9	122.3	124.7	121.8	120.0	121.2
10	135.5	135.0	136.4	137.6	138.2
12	166.6	166.8	166.3	166.3	177.3
11	44.2	44.0	41.9	40.5	41.9
13	15.0	15.0	14.5	14.5	13.7
14	21.6	23.6	20.7	19.8	18.2
15	20.3	19.2	19.3	19.6	18.8

Table S2. Boltzmann averages of GIAO values for ^{13}C NMR chemical of D1-D4 compared to experimental

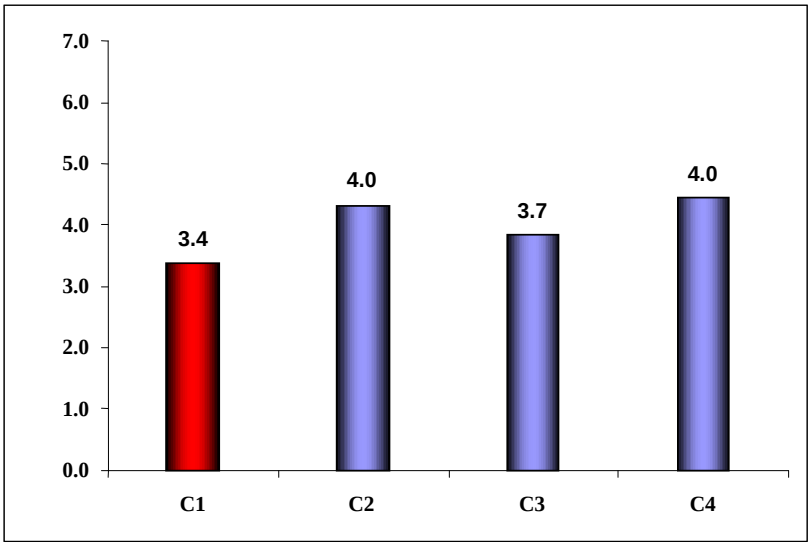
Carbon	D1	D2	D3	D4	Experimental
1	60.8	60.7	59.3	58.8	58.8
2	43.6	43.4	42.5	43.4	42.8
3	201.5	202.9	208.4	201.4	208,7
4	47.2	45.7	48.2	42.2	45.3
5	41.6	37.8	37.8	36.2	39.6
6	80.1	79.2	81.0	81.2	82.6
7	52.6	49.4	46.1	47.0	51.9
8	32.1	30.8	28.0	31.1	29.5
9	39.1	35.7	30.6	40,3	38.3
10	59.2	60.4	59.1	59.1	60.3
11	44.6	43.7	42.5	45.5	43.5
12	166.2	166.2	166.3	167.0	177.5
13	15.8	15.2	14.2	16.2	14.9
14	17.9	21.3	21.8	15.9	16.9
15	17.6	16.9	17.3	18.0	17.0



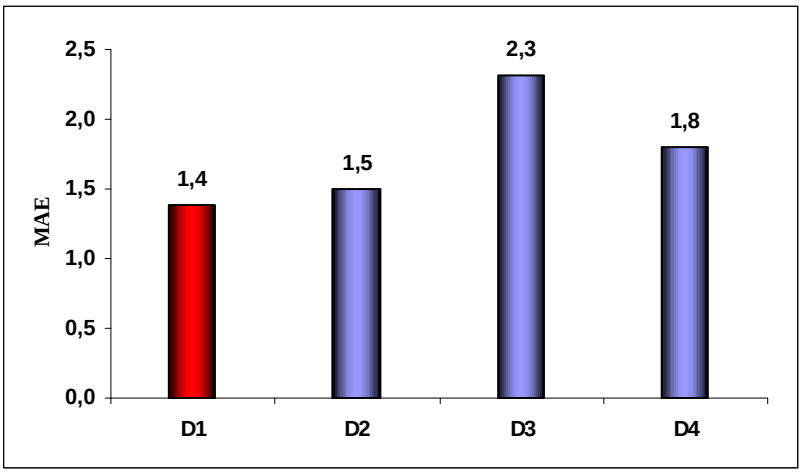
Mean absolute error relative to stereoisomers C1-C4, in Δδ (ppm) units obtained **by excluding** C-12 values



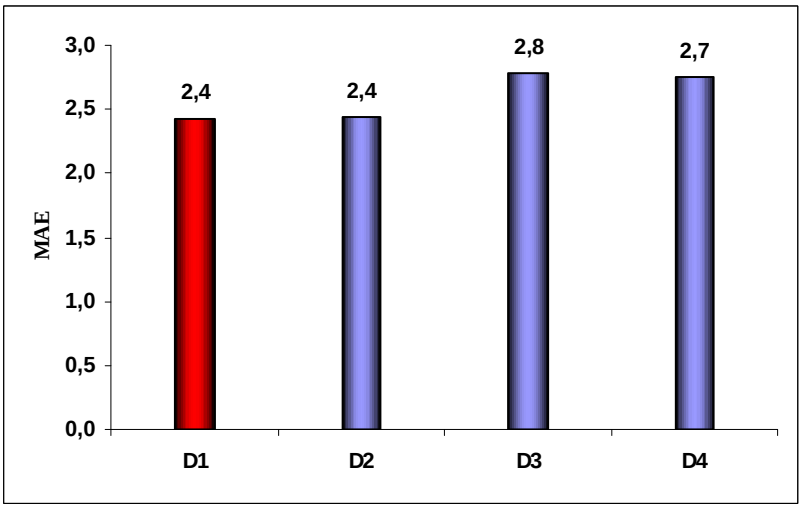
Mean absolute error relative to stereoisomers C1-C4, in Δδ (ppm) units obtained **without** excluding C-12 values



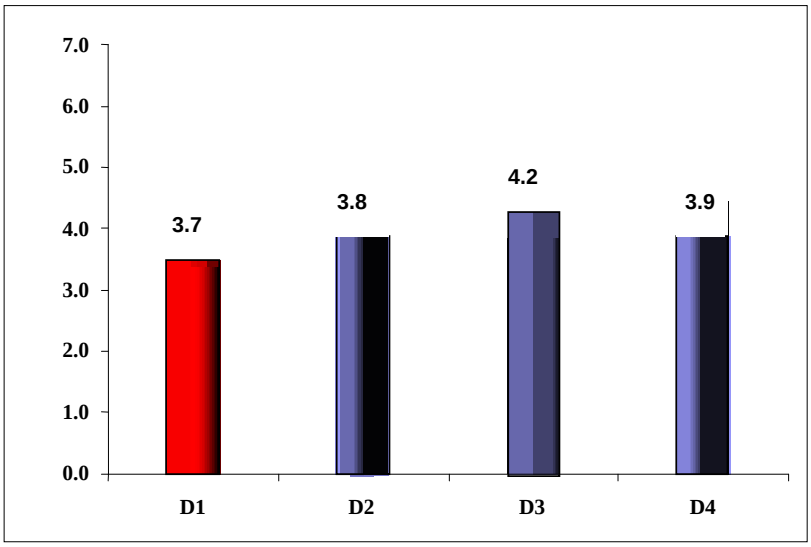
RMSD values relative to stereoisomers C1-C4, in Δδ (ppm) units obtained **without** excluding C-12 values



Mean absolute error relative to stereoisomers D1-D4, in Δδ (ppm) units obtained **by excluding** C-3 and C-12 values



Mean absolute error relative to stereoisomers D1-D4, in Δδ (ppm) units obtained **without** excluding C-3 and C-12 values



RMSD values relative to stereoisomers D1-D4, in Δδ (ppm) units obtained **without** excluding C-12 values

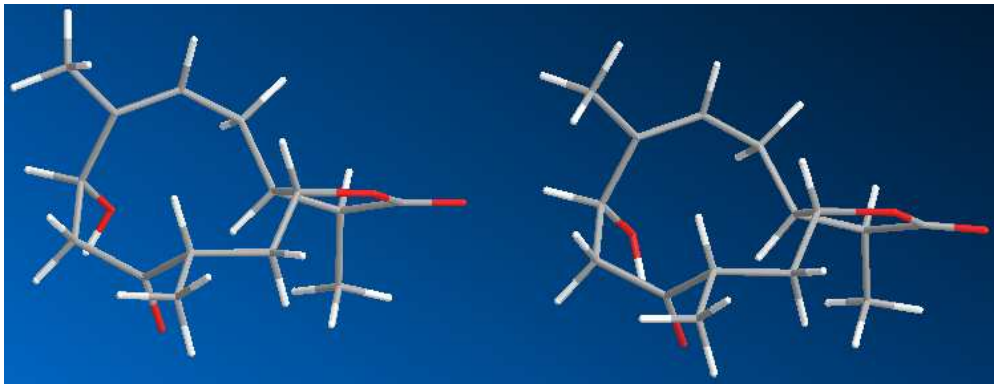
Table S3. Measured interatomic distances for the major conformational families of C1-C4 (geometries optimized at DFT level)

Structures	**H1-H4 distance (in Å)**	**H4-H6 distance (in Å)**
C1_a	4.4	2.3
C1_b	2.1	2.3
C1_c	2.2	2.4
C1_d	4.0	2.7
C1_e	3.8	2.6
C2_a	3.5	2.4
C2_b	3.8	2.4
C2_c	4.4	4.4
C2_d	4.8	2.4
C2_e	4.2	2.4
C2_f	5.5	2.8
C2_g	3.8	2.2
C3_a	3.3	3.0
C3_b	3.9	4.5
C3_c	3.5	4.2
C3_d	3.6	4.7
C3_e	3.7	4.9
C4_a	3.5	3.4
C4_b	4.0	3.2
C4_c	5.7	3.7
C4_d	4.4	3.7
C4_e	5.6	3.9
C4_f	5.4	3.9
C4_g	5.5	3.9

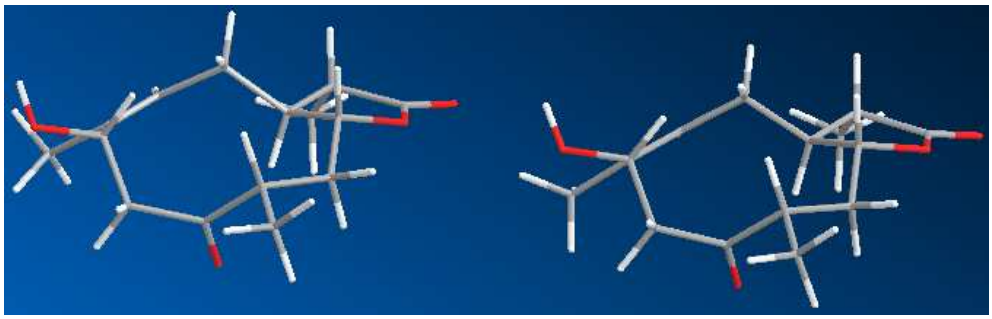
Table S4. Measured interatomic distances for the major conformational families of D1-D4 (geometries optimized at DFT level).

Structures	**H4-H6 distance (in Å)**	**$H_3$14-H4 distance (in Å)**	**$H_3$14-H6 distance (in Å)**
D1_a	2.9	4.5	2.3
D1_b	2.5	2.3	3.8
D1_c	2.2	2.4	2.3
D1_d	2.3	2.6	2.2
D1_e	2.3	3.9	2.2
D2_a	3.7	4.0	4.5
D2_b	3.7	2.6	5.1
D2_c	3.0	2.3	4.4
D2_d	3.1	2.6	4.0
D2_e	3.7	2.6	4.8
D2_f	3.7	4.6	5.4
D2_g	3.8	4.7	4.9
D3_a	4.2	6.4	5.4
D3_b	2.4	6.4	5.3
D3_c	2.6	5.9	5.7
D3_d	2.4	6.2	5.3
D4_a	3.8	4.6	3.6
D4_b	3.2	4.7	2.2
D4_c	3.7	5.2	2.3
D4_d	3.7	5.2	3.4
D4_e	3.7	5.6	2.2

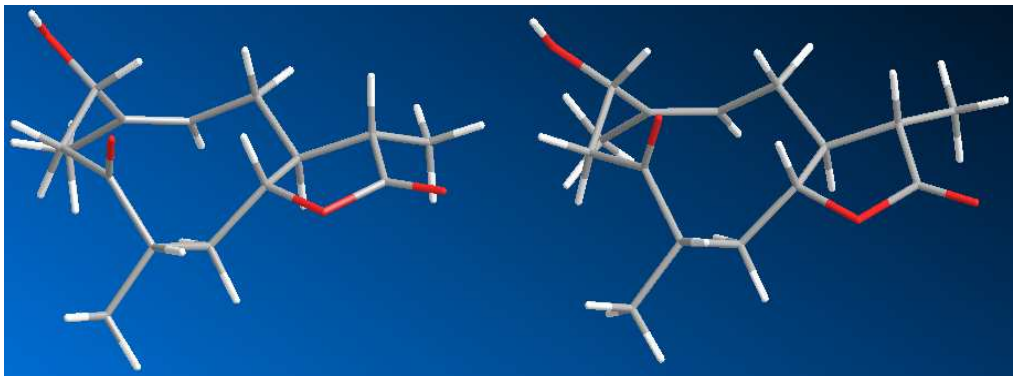
Comparison between AM1 (left) and DFT (right) output for the five conformers of structure C1 (H1-H4 and H4-H6 distances are reported)



Conformer C1_a.
AM1: H1-H4 4.4 Å; H4-H6 2.3 Å
DFT: H1-H4 4.4 Å; H4-H6 2.3 Å

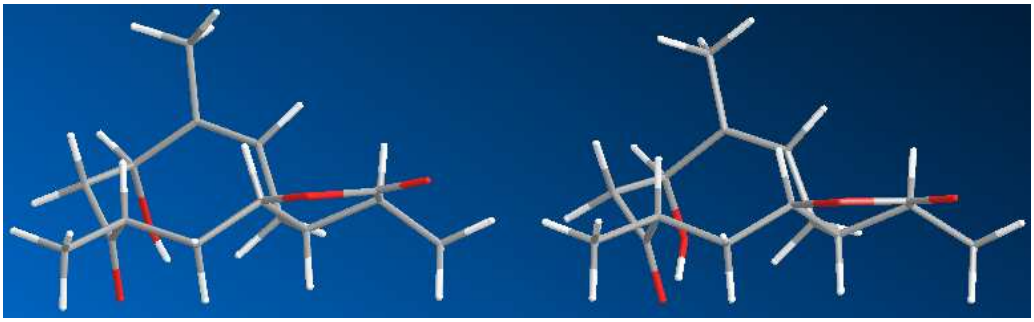


Conformer C1_b.
AM1: H1-H4 2.1 Å; H4-H6 2.3 Å
DFT: H1-H4 2.1 Å; H4-H6 2.3 Å



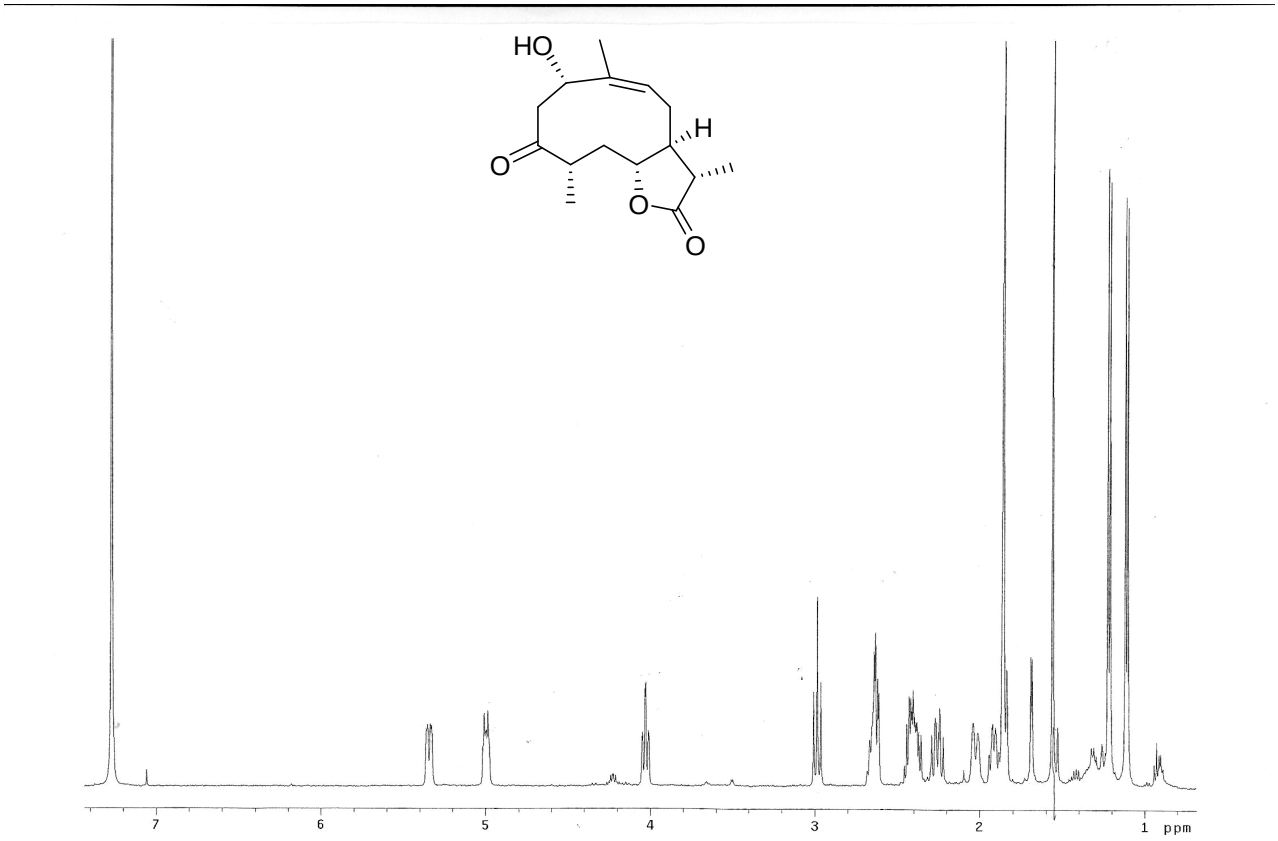
Conformer C1_c.
AM1: H1-H4 2.3 Å; H4-H6 2.3 Å
DFT: H1-H4 2.2 Å; H4-H6 2.4 Å

Conformer C1_d.
AM1: H1-H4 3.9 Å; H4-H6 2.9 Å
DFT: H1-H4 4.0 Å; H4-H6 2.7 Å

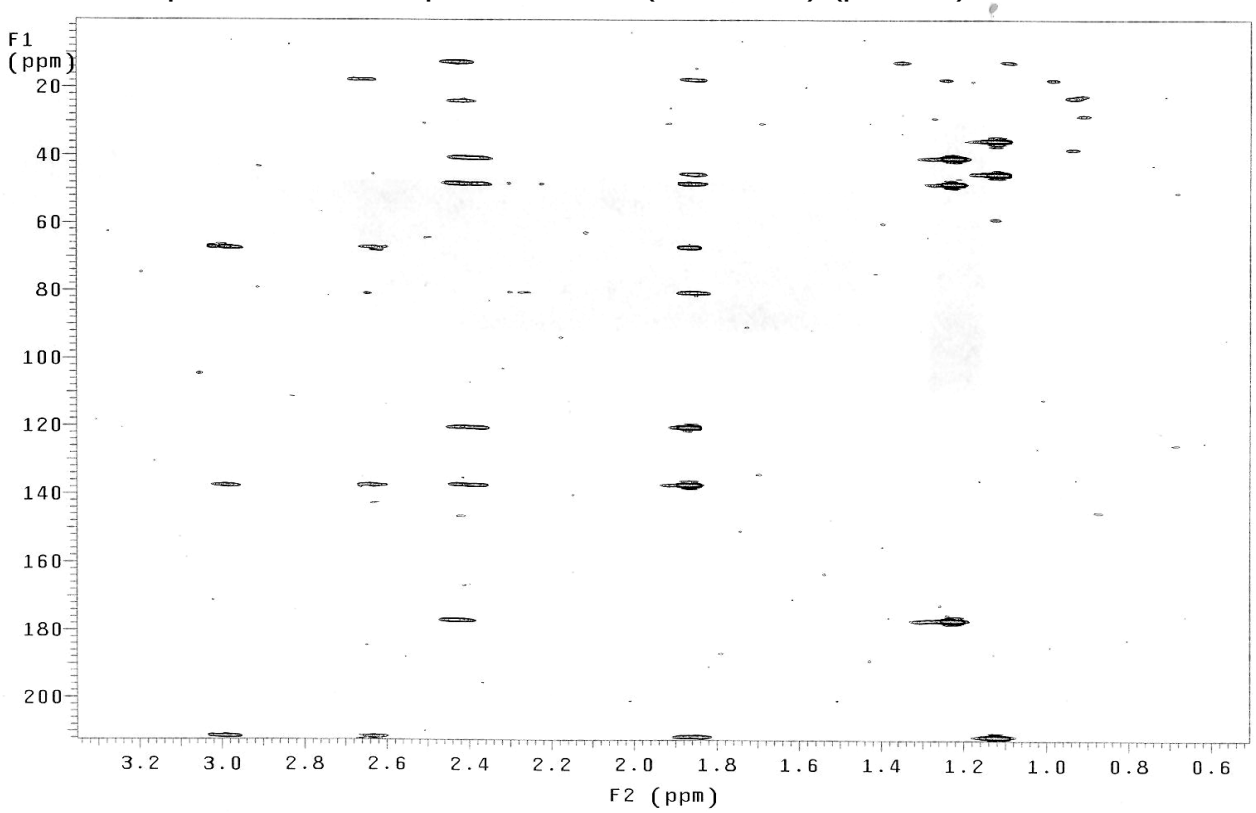


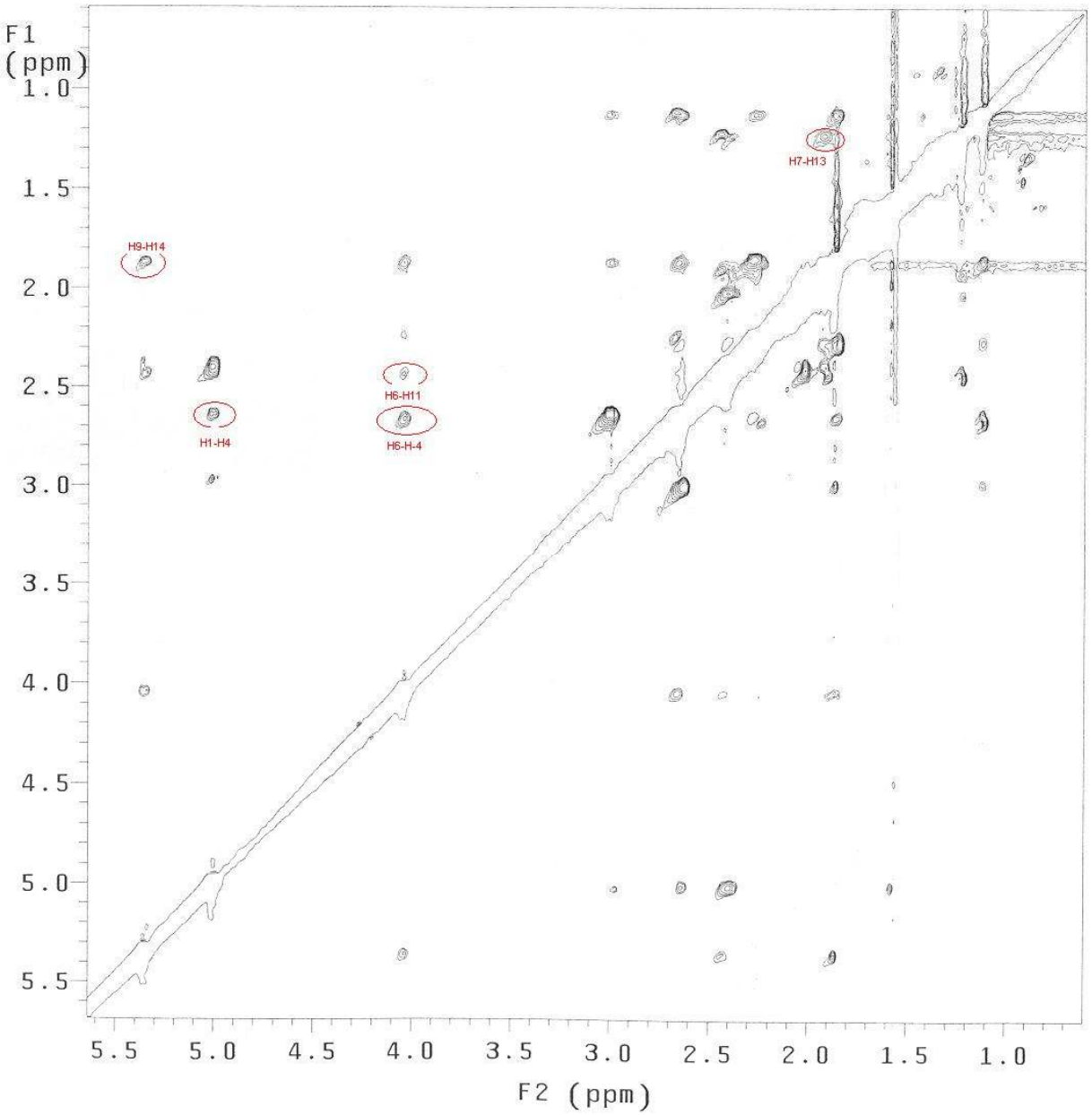
Conformer C1_e.
AM1: H1-H4 3.9 Å; H4-H6 2.6 Å
DFT: H1-H4 3.8 Å; H4-H6 2.6 Å

^{1}H NMR spectrum of ketopelenolide C (in $CDCl_3$)



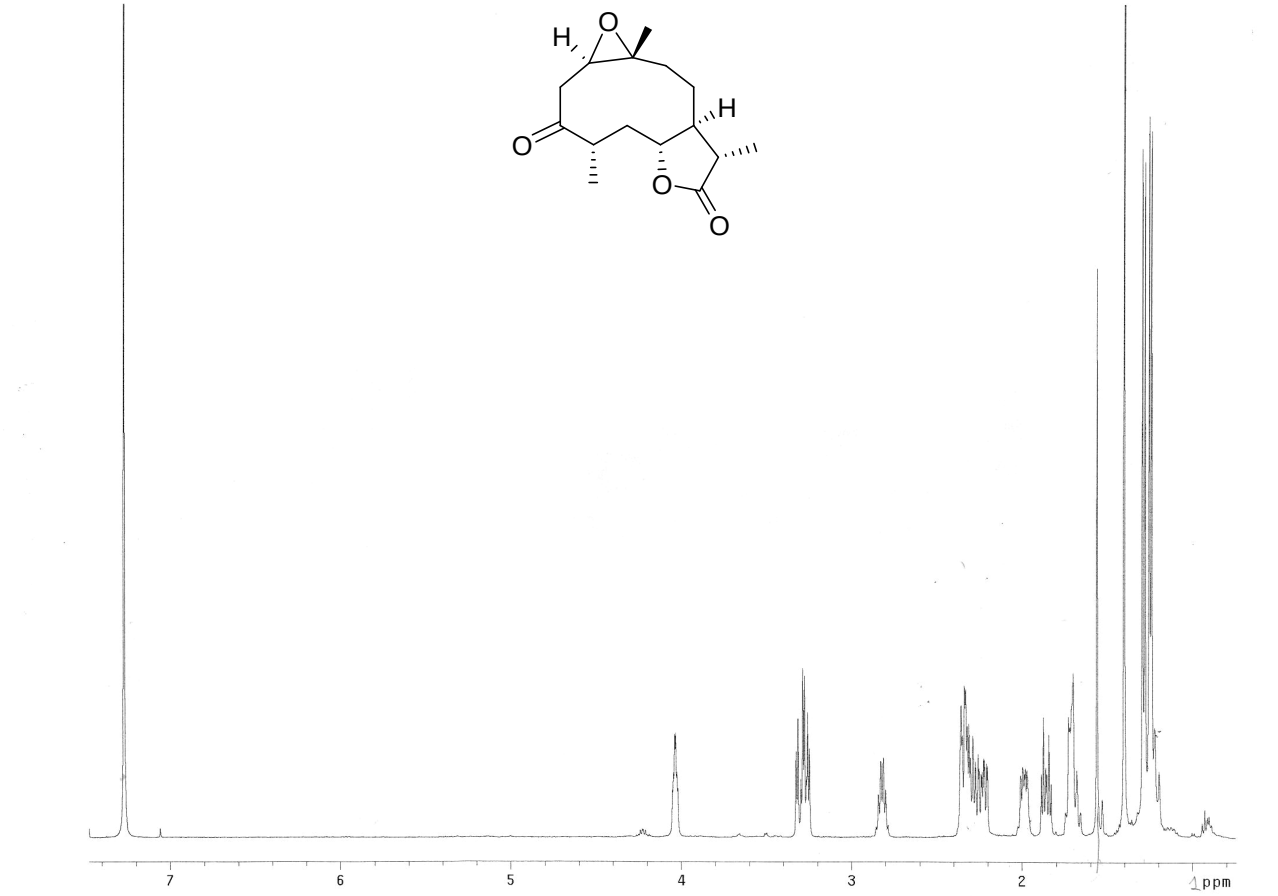
2D HMBC spectrum of ketopelenolide C (in $CDCl_3$) (portion)



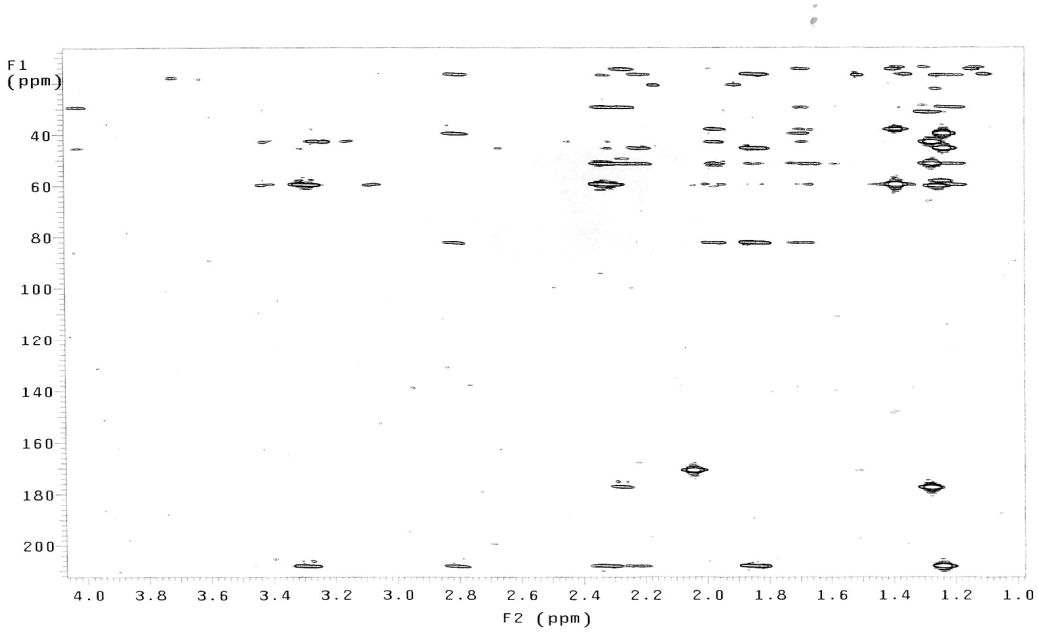


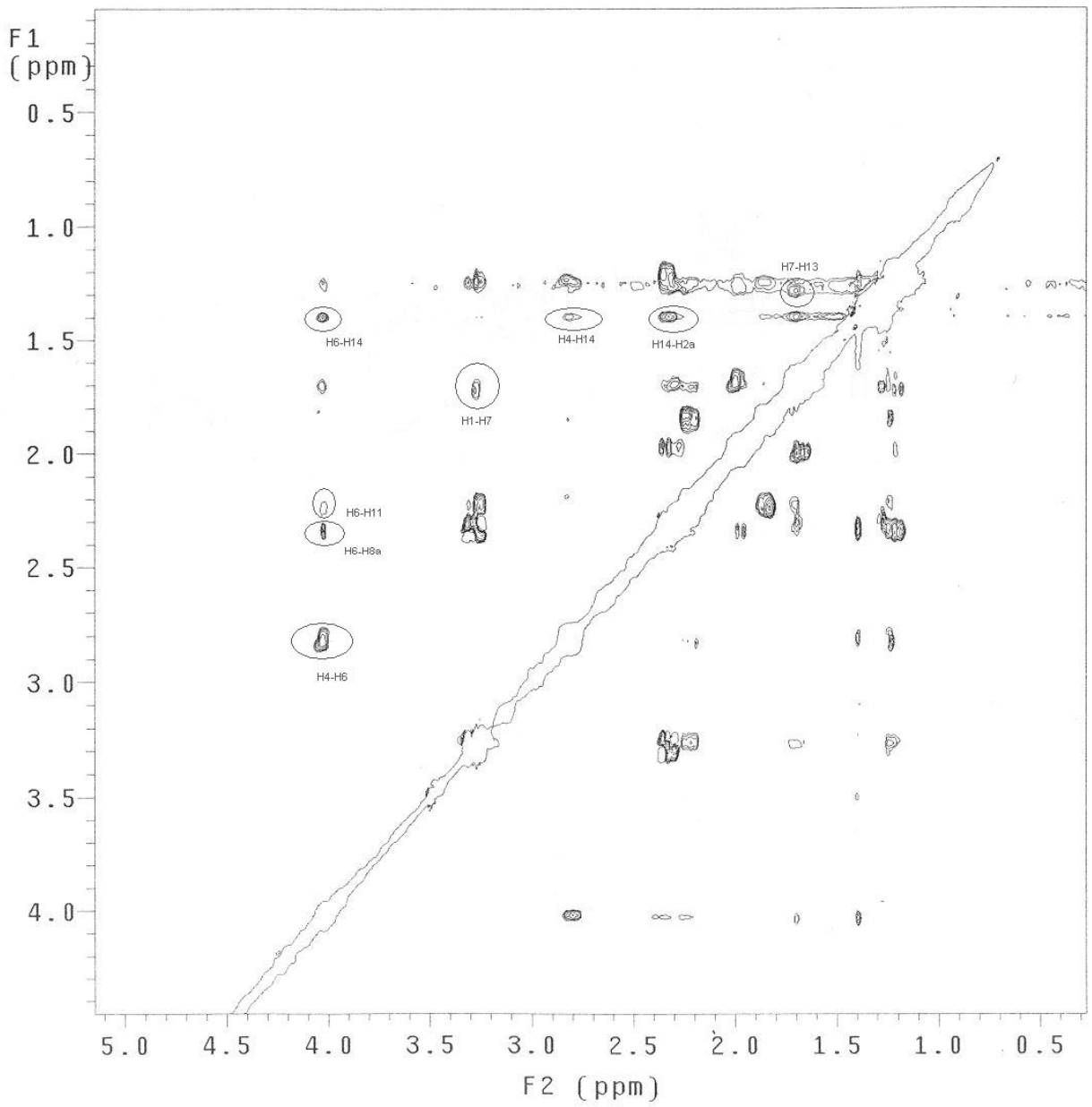
2D ROESY spectrum of ketopelenolide C (in $CDCl_3$)

^{1}H NMR spectrum of ketopelenolide D (in $CDCl_3$)



2D HMBC spectrum of ketopelenolide D (in $CDCl_3$)





2D ROESY spectrum of ketopelenolide D (in $CDCl_3$)