Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

Unprecedented stereoselective synthesis of cyclopenta[*b*]benzofuran derivatives and their characterisation assisted by aligned media NMR and ^{13}C chemical shift *ab-initio* predictions

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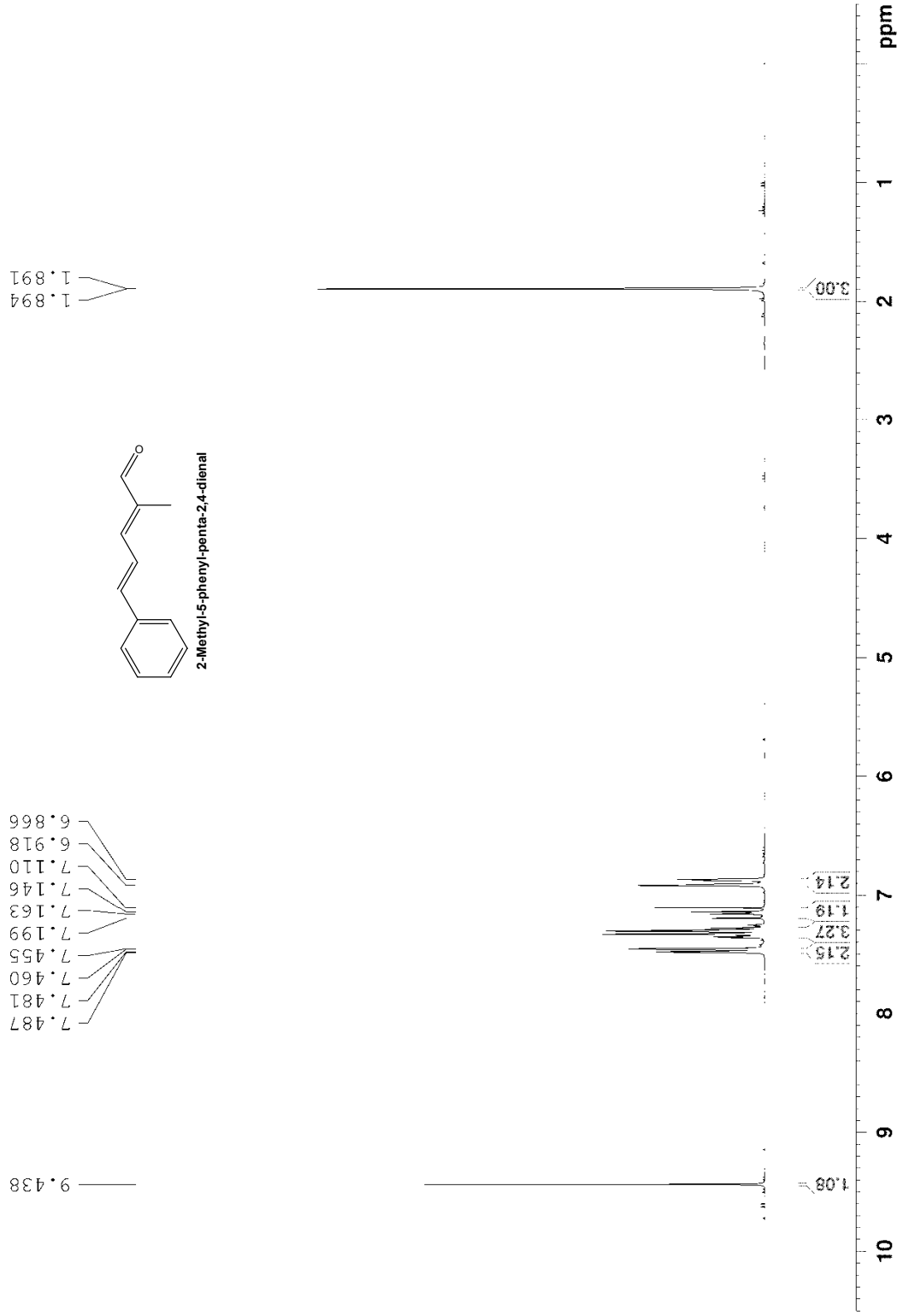
^{1}H NMR, ^{13}C NMR and other Spectra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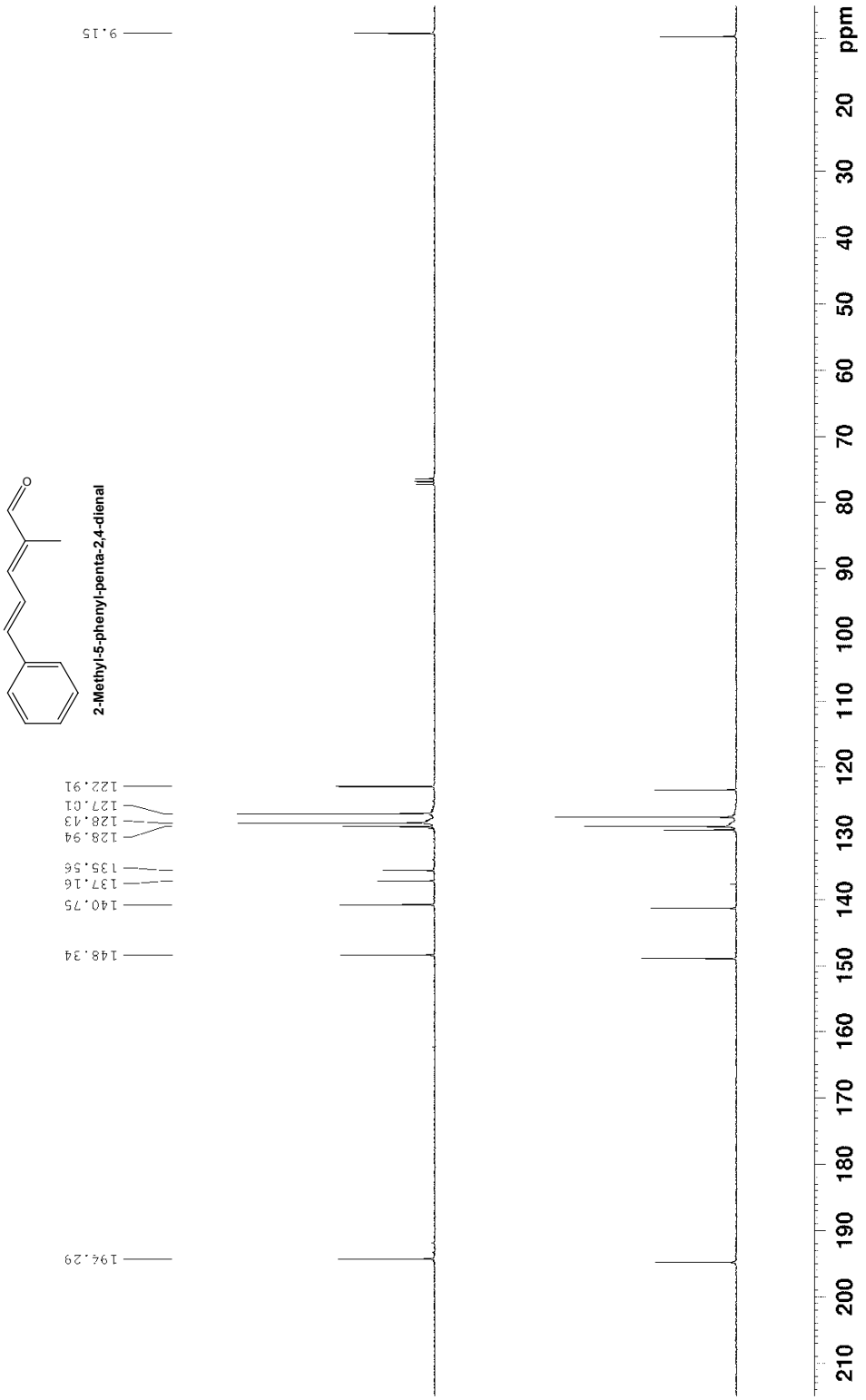
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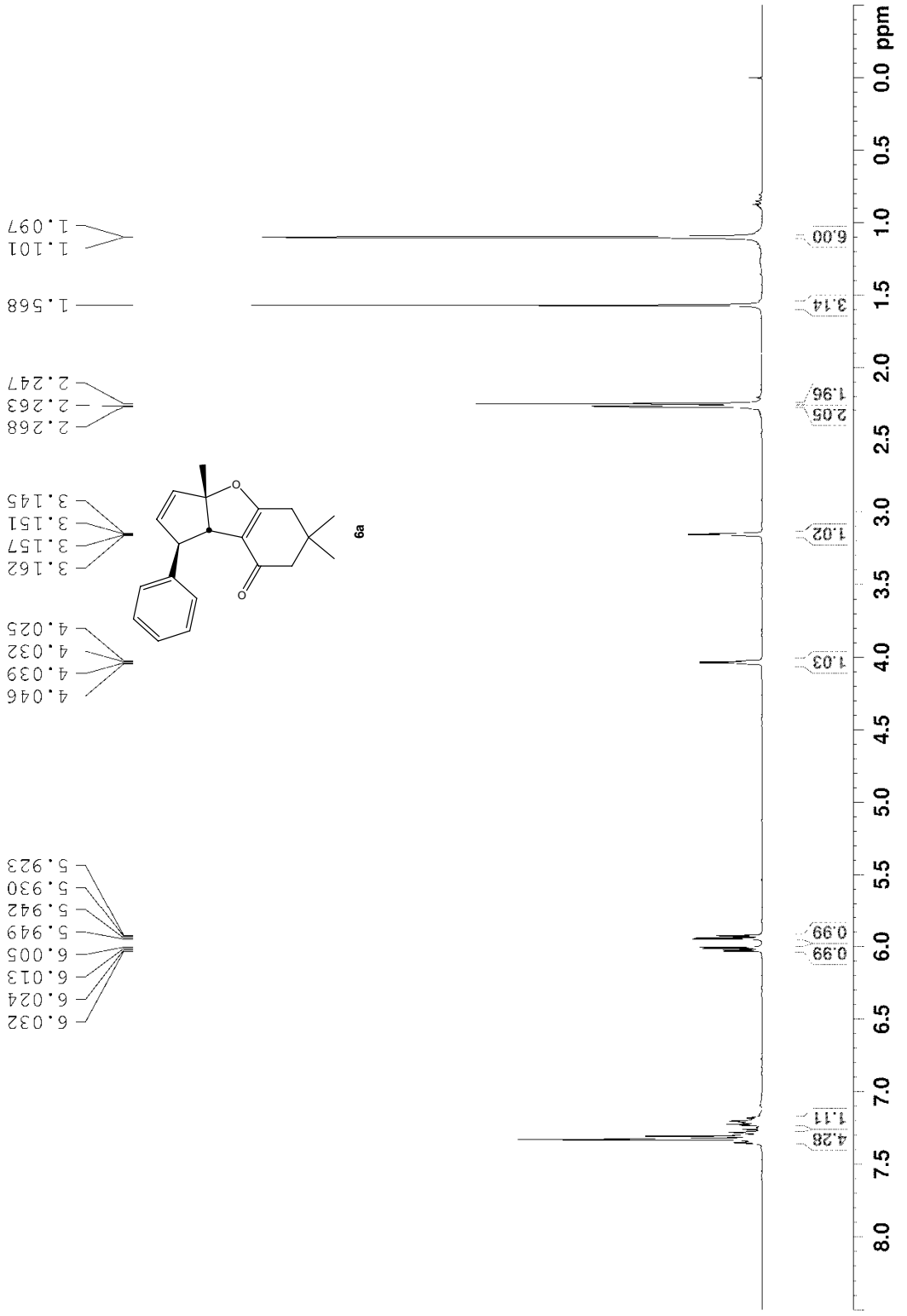
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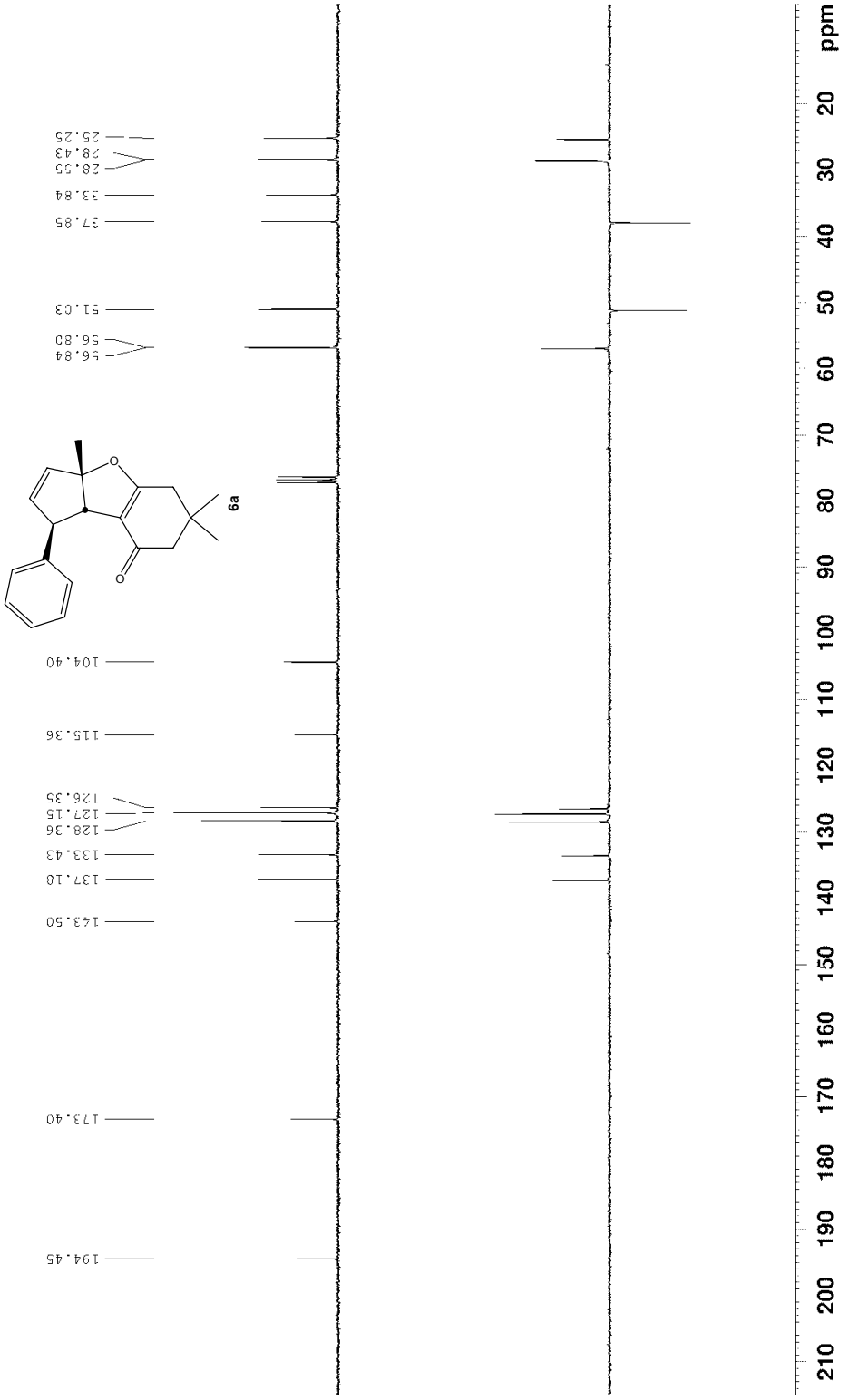
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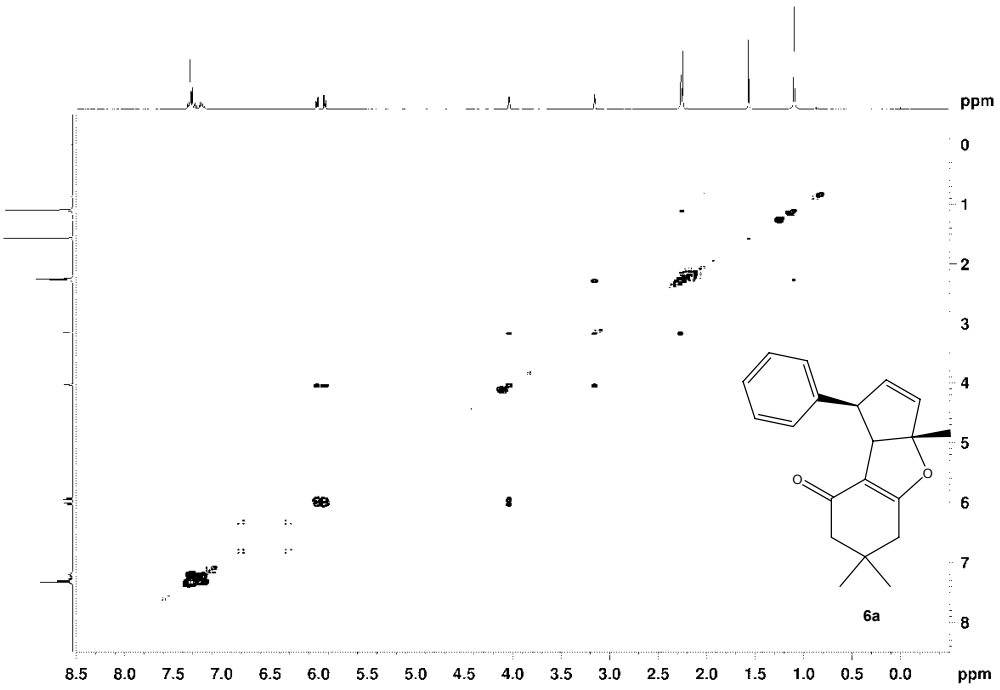

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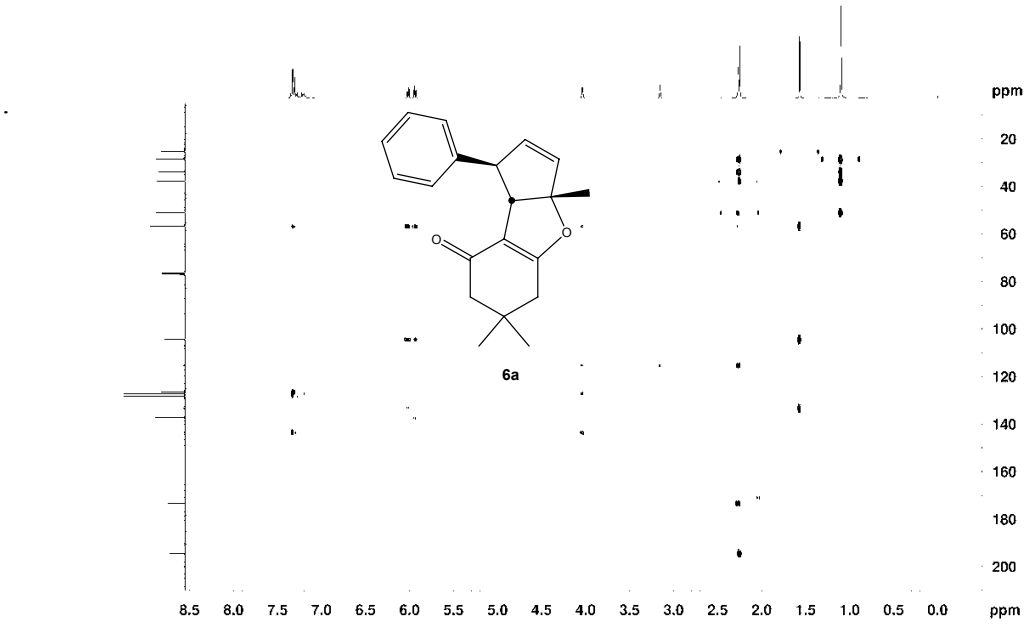

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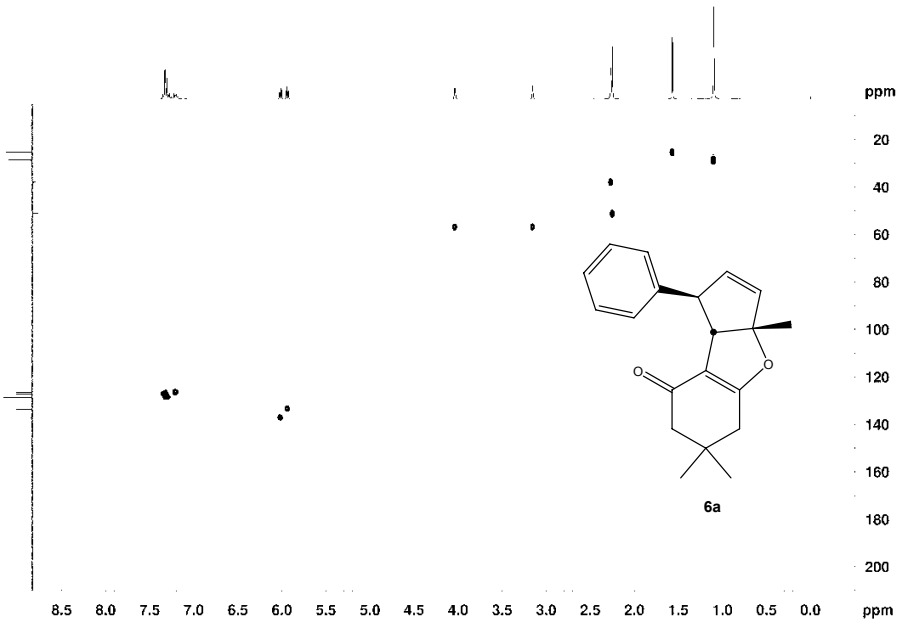

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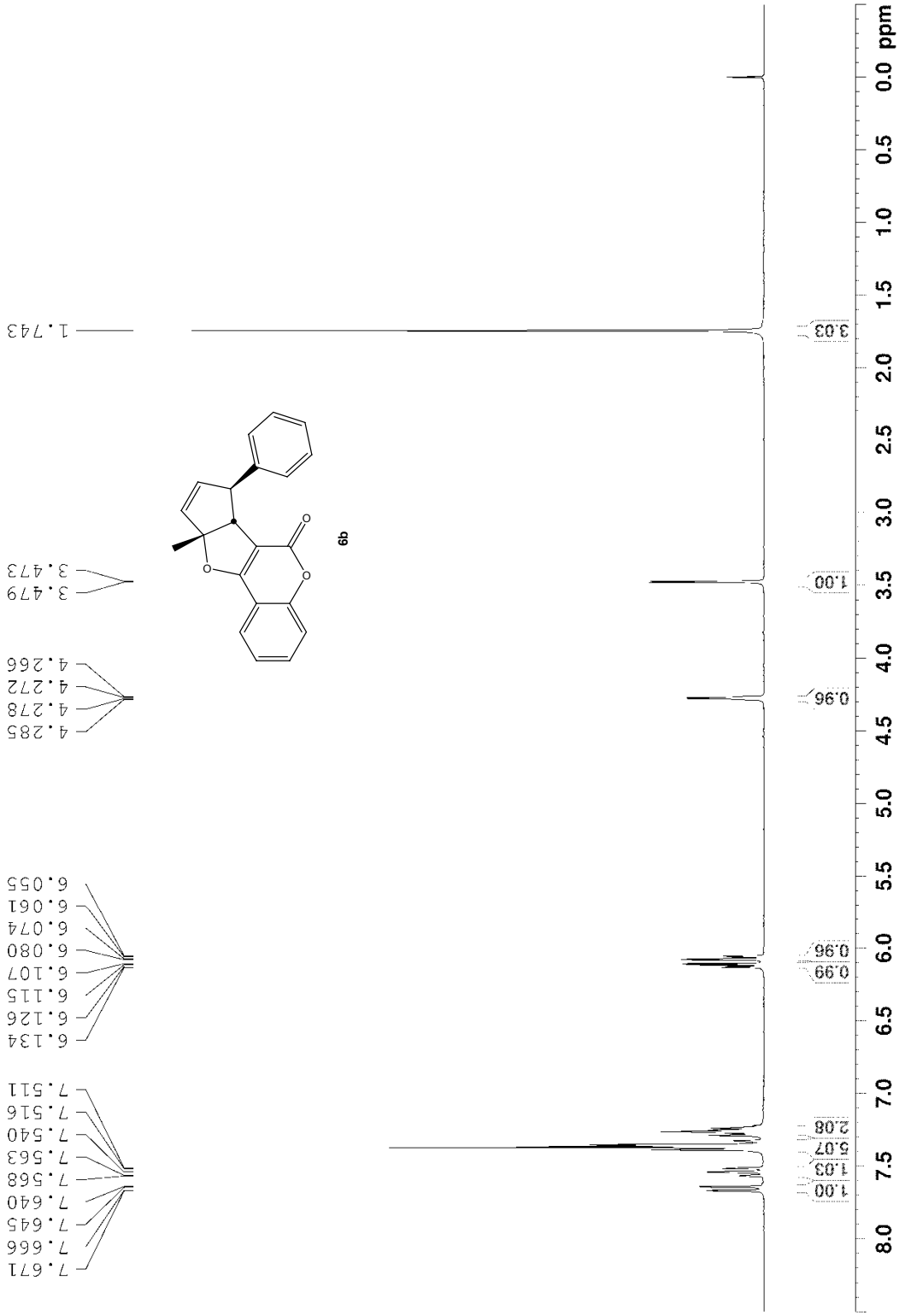
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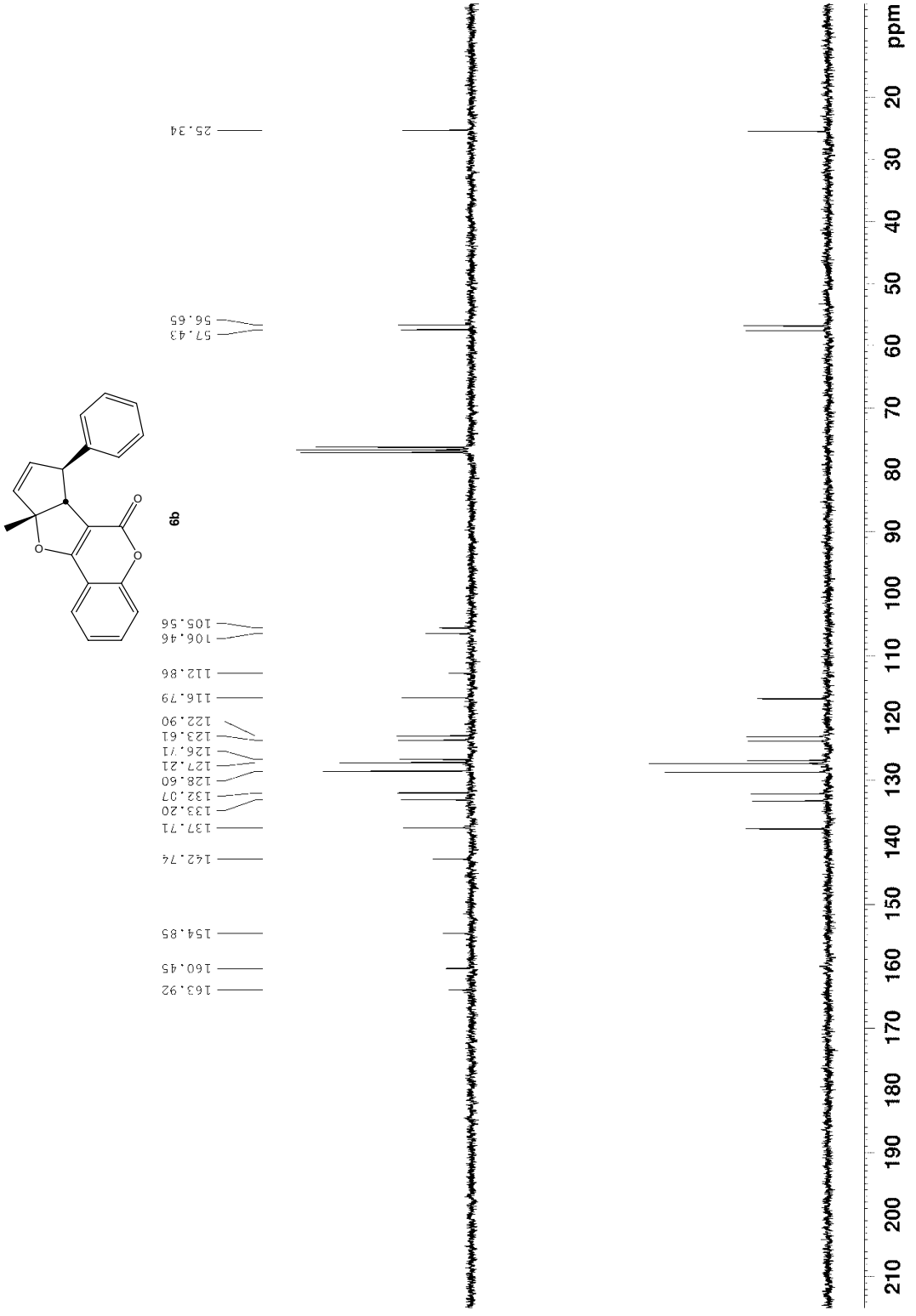
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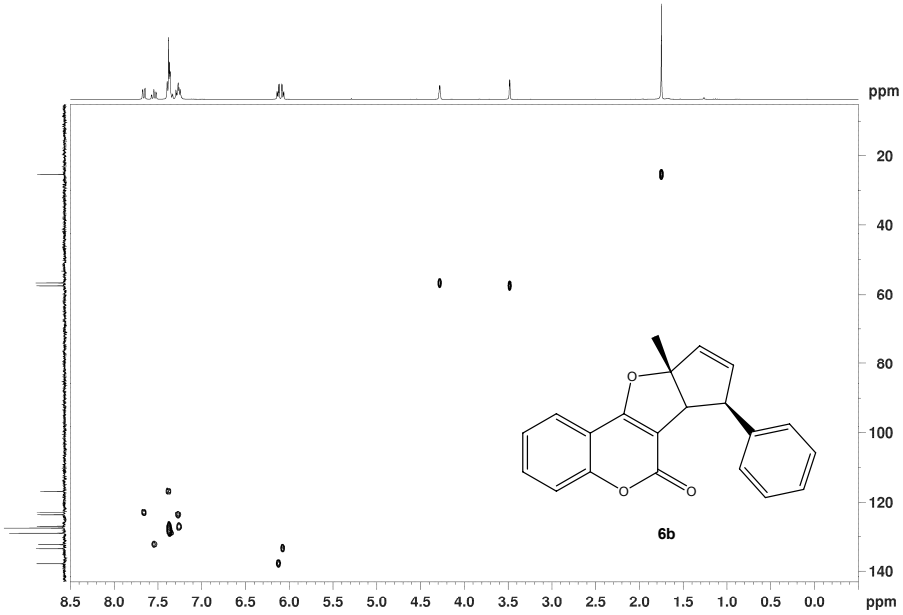

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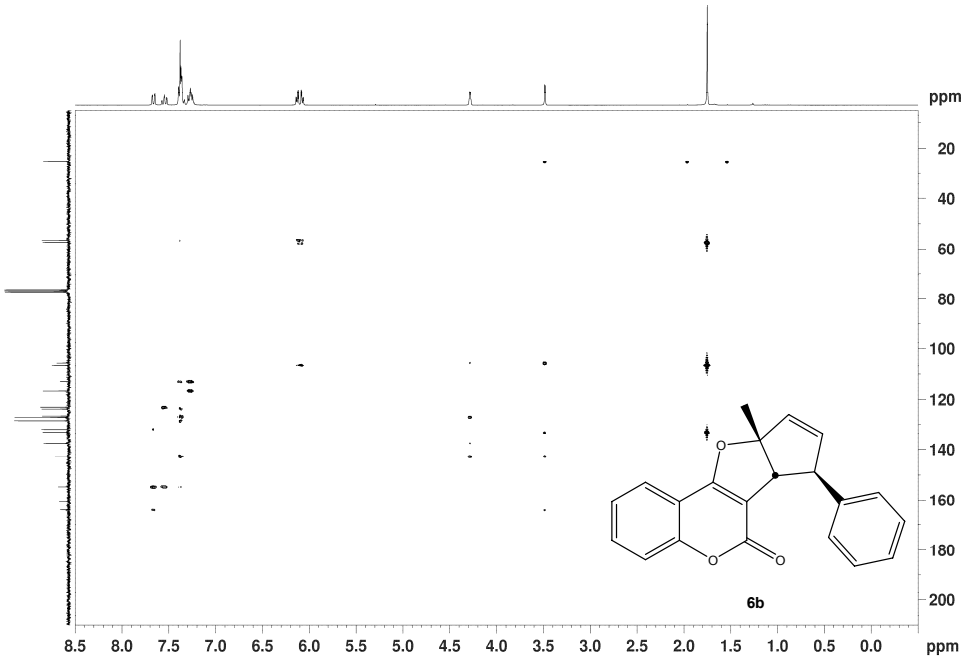
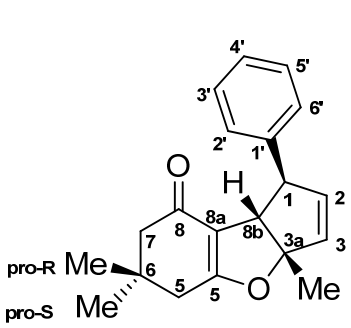
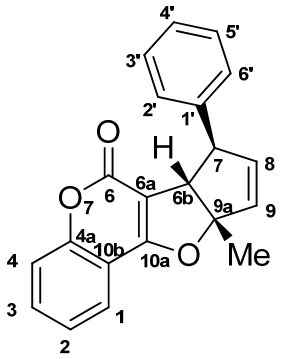


RDC measurements tables



6a



6b

Table 1. RDCs at several degrees of compression and linear fitting for compound **6a**

	$^1T_{CH}$ (Hz)										
ΔQ_ν (Hz)	C3	C2	C1	C8b	C5	C7	C2'	C3'	C4'	C6-Me2	C3a(Me)
41.6	165.1	149.5	136.7	134.6	112.3	116.2	167.4	168.2	172.8	126.1	128.7
38.6	165.2	152.4	136.6	135	113	117.4	167.2	167.6	171.6	125.8	128.3
36.7	165.5	154.1	136.2	135.6	113.8	117.6	166.2	167.1	170.2	126	130
29	165.7	156.7	135.9	136.8	115.4	118.5	164.9	166.2	168.3	126	129
21	167.3	160.2	135.6	137.6	117.9	121.6	163.3	165.1	165.2	126.1	127.6
14.5	167.3	162.2	134.7	139.4	119.6	123	162.8	163.7	164	126	127.5
10.5	167.7	163.3	134	140.1	122.7	124	162	161	162	125.8	127.1
2.7	167.5	164.2	133.8	140.5	128.1	126.4	160.1	159.8	160.2	126.1	127.6
D/*Q*	-0.0745	-0.372	0.0776	-0.161	-0.369	-0.2549	0.1815	0.2107	0.3209	-0.0006	0.0507
$^1J_{CH}$(fit)	168.2	166.87	133.55	141.4	126.83	126.79	159.82	159.71	158.98	126	126.99
$^1J_{CH}$(iso)	167.7	165.5	134.4	140.7	129.2	126	159.5	158.4	159.3	127	128
δ*J*	-0.5	-1.37	0.85	-0.67	2.37	-0.79	-0.32	-1.31	0.32	1	1.01
$\frac{\delta J}{^1J_{CH}(iso)}$ %	0.29815	0.8278	0.63244	0.476	1.8344	0.627	0.20063	0.827	0.2009	0.787	0.7891

Table 2. . RDCs at several degrees of compression and linear fitting for compound **6b**

	$^1T_{CH}$ (Hz)											
ΔQ_v (Hz)	C9	C8	C7	C6b	C1	C2	C3	C4	C2'	C3'	C4'	C9a(Me)
9.5	166.1	160.2	134.5	140.7	165.6	166.3	167.3	167.3	157.5	159	164.2	128.6
18.6	166.7	158.5	134	137.8	166	170	172.6	170	160.1	159	165.6	128.8
28.6	165.3	150.2	134.2	132.3	169.8	175.5	179.5	170.6	162.7	163.1	173.7	131
40	166.8	147.8	133.3	125.2	171.2	173.7	182.2	173.4	165.2	165.5	176	133.6
D/Q	0.07	-4.55	0.34	-5.2	-0.34[a]	2.77[a]	5.16	1.89	2.57	2.36	4.35	1.72
$^1J_{CH}$(fit)	166.1	165.6	134.9	147	134.9	164.5	162.5	165.6	154.95	155.75	159	126.2
$^1J_{CH}$(iso)	168	165.2	134.5	142.6	164.1	163	162.4	165.2	158.1	159.3	159.5	127.6
δ*J*	-1.95	0.35	0.35	4.4	-29.25	1.45	0.1	0.4	-3.15	-3.55	-0.5	-1.4
$\frac{\delta J}{^1J_{CH}(iso)}$ %	-1.16	0.212	0.26	3.086	-17.82	0.89	0.0616	0.242	-1.992	-2.228	-0.3135	-1.0972

a) Not used for the RDC analysis due to strong coupling artifacts

^{13}C Chemical shift prediction

Isotropic OPBE/pcsS-1//OPBE/6-31G* shieldings are transformed into chemical shifts by choosing an appropriate reference

$$\delta_{calc} \simeq \sigma_{ref} - \sigma_{calc}$$

σ_{ref} is determined by minimizing the quadratic deviation between the experimentally observed and computed shits

$$\frac{\delta}{\delta\sigma_{ref}} \sum (\delta_{\exp} - \delta_{calc})^2 = 0$$

Solving the corresponding linear equation results in

$$\sigma_{ref} = \frac{\sum_{i=1}^{N} (\delta_{\exp} + \sigma_{calc})}{N}$$

Being *N* the number of determined shifts.

Experimental shifts are reported downfield from TMS.

Table 3. Experimental and computed OPBE/pcS-1 ^{13}C chemical shifts for compound **6a**

	expt	SRR	SRS	SSR	SSS
C5	37.85	40.04	40.77	39.61	39.22
C6	33.84	35.01	34.15	34.01	35.01
C4a	173.4	180.79	181.85	173.11	171.74
C7	51.04	51.10	51.43	50.69	51.54
C8a	115.36	114.91	114.90	112.74	114.71
C8	194.45	184.90	185.53	185.89	186.86
C3a	104.4	103.20	104.23	106.92	106.27
C8b	56.8	63.65	58.62	55.38	58.72
C3	133.43	139.41	141.80	135.29	137.01
Me(C3a)	25.25	18.96	20.77	25.69	25.28
C1	56.84	48.27	48.28	60.77	59.11
C2	137.19	146.04	144.54	142.82	139.90
C1'	143.5	139.85	138.16	139.11	141.64
C2'	127.15	127.81	128.18	130.11	126.75
C3'	128.36	126.59	126.83	126.62	126.90
C4'	126.35	125.46	125.01	125.81	125.37
MeC6-proR	28.55	29.48	25.63	30.64	28.43
Me(C6)-proS	28.44	26.74	31.60	26.92	27.70

Table 4. Experimental and computed OPBE/pcS-1 ^{13}C chemical shifts for compound **6b**

	expt	SRR	SRS	SSR	SSS
C3	132.07	131.45	131.63	131.53	131.47
C2	123.61	122.85	123.13	122.88	122.76
C1	122.9	121.85	122.03	122.39	122.47
C10b	112.86	111.47	111.32	110.77	110.3
C4a	154.85	154.61	154.37	154.74	154.19
C4	116.79	116.66	116.67	116.6	116.28
C10a	163.92	168.88	169.37	161.72	160.09
C6a	105.56	104.59	104.86	102.35	104.96
C6	160.45	153.65	155.36	154.64	155.12
C9a	106.46	105.43	105.94	108.6	107.79
C6b	57.43	64.02	59.92	57.04	60.35
C9	133.2	139.95	142.39	135.56	137.56
C9a(Me)	25.34	19.57	20.83	26.14	26.26
C7	56.65	49.01	49.22	62.27	60.27
C8	137.71	147.49	146.05	144.82	141.26
C1'	142.74	140.18	138.48	138.04	141.64
C2'	127.21	128.84	129.13	130.31	127.71
C3'	128.6	127.8	128.06	127.5	128.01
C4'	126.71	126.77	126.37	127.15	126.65

DP4 probability computations

DP4 probabilities were computed from chemical shift tensors exactly according to the procedure described in the original paper (Ref. 13) making use of the t distribution option in the authors Java applet implementation (http://www-jmg.ch.cam.ac.uk/tools/nmr/DP4/).

RDC Analysis

OPBE/6-31G* geometries and RDC fitting results for diastereisomers of compound 6a

6a1

```
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C       3.703390   -2.502527   -0.043281
C       1.907082   -0.791895   -0.418036
C       2.532477   -3.509774   -0.023974
C       0.930885   -1.578197    0.143707
C       1.168665   -2.979996    0.440099
O       0.344713   -3.724999    0.971346
O       1.551833    0.502466   -0.655076
C       0.342127    0.670211    0.171148
C      -0.296624   -0.709476    0.046620
C      -0.825087    1.537674   -0.208053
C       0.863141    1.097704    1.552549
C      -1.671242   -0.525319    0.715398
H      -0.572404   -0.769203   -1.024754
C      -1.938974    0.894533    0.204291
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H       1.353082    2.076415    1.458786
H       0.046626    1.198612    2.276312
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H      -1.568169   -0.499651    1.813772
H      -0.766073    2.572065   -0.546392
H      -2.941216    1.326507    0.215791
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C      -3.394798   -1.498563   -0.881914
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H      3.597477   -0.726649   -1.704420
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C15,H22 -37.20[0.50]   -12.11[0.38]
C11,H21 -7.45[0.50]    1.51[0.40]
C10,H14 -16.10[0.50]   -15.87[0.29]
C1,H35  -36.91[0.50]   12.33[0.33]
C1,H36  -36.91[0.50]   -1.49[0.31]
C4,H37  -25.49[0.50]   -9.39[0.38]
C4,H38  -25.49[0.50]   -17.41[0.29]
C23,H28 18.15[0.50]    -3.00[0.29]
C24,H29 18.15[0.50]    -3.00[0.29]
C27,H32 21.07[0.50]    -2.96[0.29]
C25,H30 21.07[0.50]    -2.96[0.29]
C26,H31 32.09[0.50]    20.53[0.39]
C33,H39 -0.06[0.50]    2.61[0.08]
C33,H40 -0.06[0.50]    2.61[0.08]
C33,H41 -0.06[0.50]    2.61[0.08]
C34,H42 -0.06[0.50]    3.44[0.09]
C34,H43 -0.06[0.50]    3.44[0.09]
C34,H44 -0.06[0.50]    3.44[0.09]
C12,H16 5.07[0.50]     5.04[0.11]
C12,H17 5.07[0.50]     5.04[0.11]
C12,H18 5.07[0.50]     5.04[0.11]

6a2
44
DG298.15K(OPBE/6-31G*)=-925.05502
C      3.454445   -0.641870    0.722129
C      3.844209   -2.136287    0.817420
C      2.002753   -0.477841    0.445556
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C      3.202997   -2.893814   -0.364306
C      1.171088   -1.419048   -0.116329
C      1.705479   -2.672177   -0.611230
O      1.057497   -3.494242   -1.265822
O      1.432698    0.726445    0.708089
C     -0.016257    0.437698    0.657265
C     -0.063216   -0.616063   -0.445641
C     -1.027481    1.412536    0.115339
C     -0.375482    0.034092    2.091654
C     -1.568897   -0.771725   -0.764260
H      0.261895   -0.041649   -1.335464
C     -1.930686    0.707998   -0.600021
H      0.237710   -0.811353    2.426191
H     -0.183579    0.887841    2.756345
H     -1.428518   -0.245444    2.180322
C     -2.424362   -1.750750    0.035890
H     -1.680866   -1.060683   -1.822808
H     -1.106014    2.463736    0.392551
H     -2.847020    1.127988   -1.019253
C     -3.548697   -1.342520    0.771522
C     -2.131672   -3.125075   -0.022303
C     -2.928209   -4.053680    0.650866
C     -4.040667   -3.634345    1.387776
C     -4.348551   -2.273681    1.443006
H     -3.807258   -0.284472    0.828297
H     -1.267477   -3.464793   -0.593566
H     -2.676874   -5.114540    0.595006
H     -4.663221   -4.362268    1.910821
H     -5.215971   -1.929323    2.009373
C      3.368118   -2.731989    2.153659
C      5.373614   -2.259569    0.739495
H      4.019924   -0.159139   -0.094666
H      3.725177   -0.100455    1.641229
H      3.703892   -2.594367   -1.301973
H      3.366879   -3.976373   -0.269492
H      2.277677   -2.682032    2.262981
H      3.820163   -2.201462    3.004225
H      3.660457   -3.788839    2.227480
H      5.764993   -1.852644   -0.204239
H      5.684320   -3.311958    0.804237
H      5.857734   -1.718324    1.565857
44
DG298.15K(OPBE/6-31G*)=-925.05604
C      3.445517   -0.648098    0.762291
C      4.080881   -1.784489   -0.073361
C      2.001933   -0.478394    0.447006
C      3.119620   -2.994658   -0.078290
C      1.166655   -1.421642   -0.106437
C      1.697343   -2.692236   -0.561095
O      1.078671   -3.492848   -1.268024
O      1.433753    0.729405    0.700053
C     -0.014862    0.436476    0.655556
C     -0.059935   -0.614296   -0.451394
C     -1.029607    1.410749    0.121594
C     -0.365850    0.022057    2.089365
C     -1.565936   -0.769741   -0.770742
H      0.267383   -0.038568   -1.339330
C     -1.932001    0.707443   -0.595636
H      0.259697   -0.816919    2.419342
H     -0.185347    0.875466    2.757632
H     -1.414386   -0.273761    2.178311
C     -2.419976   -1.757084    0.020320
H     -1.676856   -1.050729   -1.831491
H     -1.111317    2.459967    0.405326
H     -2.850759    1.126842   -1.010182
C     -3.537356   -1.356937    0.770961
C     -2.133336   -3.131334   -0.062839
C     -2.928514   -4.068304    0.600015
C     -4.034245   -3.657078    1.351516
C     -4.336258   -2.296379    1.432092
H     -3.791029   -0.298950    0.847754
```

```
H     -1.274495   -3.464542   -0.645669
H     -2.681934   -5.129007    0.524185
H     -4.656274   -4.391329    1.866264
H     -5.198401   -1.958458    2.010253
C      5.420729   -2.190073    0.557011
C      4.328101   -1.302626   -1.513236
H      3.973072    0.305156    0.606144
H      3.539925   -0.873699    1.839431
H      3.515560   -3.802879   -0.707806
H      3.040642   -3.399478    0.945920
H      5.288664   -2.561353    1.583684
H      6.115530   -1.337986    0.593559
H      5.902091   -2.986825   -0.027361
H      3.402395   -0.968195   -1.999753
H      4.750254   -2.112182   -2.124702
H      5.040006   -0.464851   -1.529128
Conformationall averaged solution 25% 75 %
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=0.5 Hz
Alignment tensor
<Axx>=-0.000108957 stdved=6.3842e-06
 <Ayy>=-0.000841287 stdved=9.62774e-06
 <Azz>=0.000950244 stdved=1.01194e-05
Conformationally averaged quality factors statistic
<Q>=0.782591StdDev(Q)=0.00064706
Highest Q=0.784771
Lowest Q=0.780624
        Exp [Std.Dev]  Hz     Comp [Std.Dev] Hz
C13,H20 7.76[0.50]     -2.96[0.34]
C15,H22 -37.20[0.50]   -18.47[0.38]
C11,H21 -7.45[0.50]    -17.21[0.47]
C10,H14 -16.10[0.50]   -15.79[0.35]
C1,H35  -36.91[0.50]   4.65[0.28]
C1,H36  -36.91[0.50]   -21.33[0.28]
C4,H37  -25.49[0.50]   10.49[0.30]
C4,H38  -25.49[0.50]   -32.33[0.35]
C23,H28 18.15[0.50]    5.91[0.27]
C24,H29 18.15[0.50]    5.91[0.27]
C27,H32 21.07[0.50]    5.74[0.27]
C25,H30 21.07[0.50]    5.74[0.27]
C26,H31 32.09[0.50]    12.30[0.31]
C33,H39 -0.06[0.50]    2.83[0.07]
C33,H40 -0.06[0.50]    2.83[0.07]
C33,H41 -0.06[0.50]    2.83[0.07]
C34,H42 -0.06[0.50]    0.81[0.09]
C34,H43 -0.06[0.50]    0.81[0.09]
C34,H44 -0.06[0.50]    0.81[0.09]
C12,H16 5.07[0.50]     3.36[0.12]
C12,H17 5.07[0.50]     3.36[0.12]
C12,H18 5.07[0.50]     3.36[0.12]

6a3
44
DG298.15K(OPBE/6-31G*)=-925.10000
C      2.598419   -1.909710   -1.104014
C      3.149783   -2.985760   -0.135769
C      1.594396   -1.041909   -0.427444
C      1.971781   -3.629427    0.629161
C      0.819344   -1.400506    0.635416
C      1.029713   -2.652338    1.339934
O      0.495907   -2.932266    2.414592
O      1.421408    0.212001   -0.870648
C      0.458311    0.868915    0.056174
C     -0.080192   -0.255865    0.991282
C     -0.740858    1.335160   -0.711447
C      1.237182    1.980659    0.747100
C     -1.621024   -0.394415    0.679114
H      0.035198    0.015715    2.049845
C     -1.851386    0.676619   -0.352447
H      2.075618    1.566000    1.322392
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H      1.638895    2.690202    0.011443
H      0.579696    2.529292    1.434390
C     -2.132367   -1.755948    0.236637
H     -2.174925   -0.131327    1.595644
H     -0.684883    2.141149   -1.443795
H     -2.846250    0.864190   -0.760553
C     -2.794445   -2.594404    1.147369
C     -1.979700   -2.203289   -1.086587
C     -2.472372   -3.449028   -1.485147
C     -3.129264   -4.272972   -0.566727
C     -3.286623   -3.840701    0.753286
H     -2.911706   -2.273056    2.183705
H     -1.477387   -1.565112   -1.814409
H     -2.346887   -3.773803   -2.519915
H     -3.517455   -5.244374   -0.877622
H     -3.793842   -4.475933    1.481383
C      4.133111   -2.341874    0.856666
C      3.888202   -4.059433   -0.947935
H      2.108510   -2.398036   -1.964229
H      3.412072   -1.295899   -1.517650
H      1.348926   -4.203397   -0.079215
H      2.337795   -4.345555    1.377399
H      3.654526   -1.551293    1.449061
H      4.991087   -1.899853    0.329800
H      4.522264   -3.093343    1.557724
H      3.217699   -4.554436   -1.665396
H      4.301323   -4.834330   -0.286664
H      4.725658   -3.624354   -1.513559
44
DG298.15K(OPBE/6-31G*)=-925.09868
C      2.686774   -1.844288   -1.057522
C      2.565588   -3.344945   -0.700838
C      1.610114   -1.031968   -0.427352
C      2.241899   -3.480830    0.802442
C      0.814260   -1.413261    0.612764
C      1.077293   -2.640327    1.343109
O      0.499520   -2.958375    2.384093
O      1.436309    0.225477   -0.857702
C      0.453605    0.864238    0.056870
C     -0.084149   -0.269097    0.985498
C     -0.740056    1.315875   -0.727491
C      1.205457    1.987021    0.760232
C     -1.635590   -0.363226    0.713402
H      0.061214   -0.014572    2.044942
C     -1.854493    0.671963   -0.355988
H      2.042299    1.583917    1.346270
H      1.606430    2.704091    0.031372
H      0.530481    2.524333    1.439441
C     -2.236975   -1.718066    0.377915
H     -2.144815   -0.021057    1.630875
H     -0.677511    2.107125   -1.475135
H     -2.848197    0.860306   -0.766543
C     -2.773851   -2.521067    1.397300
C     -2.318386   -2.184193   -0.944594
C     -2.919869   -3.411882   -1.238713
C     -3.449200   -4.199483   -0.213193
C     -3.370049   -3.749794    1.108298
H     -2.708979   -2.186166    2.433506
H     -1.912668   -1.576859   -1.754863
H     -2.976975   -3.750894   -2.274854
H     -3.921217   -5.156516   -0.441760
H     -3.775410   -4.357205    1.919229
C      3.903121   -4.037470   -1.004114
C      1.462628   -4.005626   -1.544498
H      2.678603   -1.693534   -2.148268
H      3.655972   -1.447392   -0.707398
H      2.042677   -4.529190    1.064495
H      3.126348   -3.183933    1.393543
H      4.725265   -3.607589   -0.413414
H      4.167084   -3.941679   -2.067982
H      3.849384   -5.110298   -0.771158
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H      0.482305   -3.547697   -1.371578
H      1.378895   -5.073302   -1.297277
H      1.691994   -3.929994   -2.617551
Conformationall averaged solution 80% 20%
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=0.5 Hz
Alignment tensor
<Axx>=0.00024924 stdved=6.09964e-06
 <Ayy>=0.000910372 stdved=6.25803e-06
 <Azz>=-0.00115961 stdved=8.65864e-06
Conformationally averaged quality factors statistic
<Q>=0.541743StdDev(Q)=0.00170271
Highest Q=0.547351
Lowest Q=0.535567
        Exp [Std.Dev]  Hz     Comp [Std.Dev] Hz
C13,H20 7.76[0.50]     19.98[0.33]
C15,H22 -37.20[0.50]   -45.53[0.39]
C11,H21 -7.45[0.50]    -1.14[0.40]
C10,H14 -16.10[0.50]   -18.11[0.34]
C1,H35  -36.91[0.50]   -28.77[0.31]
C1,H36  -36.91[0.50]   -28.75[0.45]
C4,H37  -25.49[0.50]   -17.94[0.27]
C4,H38  -25.49[0.50]   -19.30[0.32]
C23,H28 18.15[0.50]    -6.98[0.24]
C24,H29 18.15[0.50]    -6.98[0.24]
C27,H32 21.07[0.50]    -6.60[0.24]
C25,H30 21.07[0.50]    -6.60[0.24]
C26,H31 32.09[0.50]    24.90[0.37]
C33,H39 -0.06[0.50]    9.68[0.09]
C33,H40 -0.06[0.50]    9.68[0.09]
C33,H41 -0.06[0.50]    9.68[0.09]
C34,H42 -0.06[0.50]    -13.67[0.11]
C34,H43 -0.06[0.50]    -13.67[0.11]
C34,H44 -0.06[0.50]    -13.67[0.11]
C12,H16 5.07[0.50]     1.45[0.11]
C12,H17 5.07[0.50]     1.45[0.11]
C12,H18 5.07[0.50]     1.45[0.11]

6a4
44
DG298.15K(OPBE/6-31G*)=-925.10506
C      3.340525   -0.356599    0.073435
C      3.869460   -1.764318    0.439375
C      1.873720   -0.253691    0.305562
C      2.919322   -2.824095   -0.159321
C      0.989887   -1.291463    0.339689
C      1.430145   -2.661018    0.168811
O      0.682549   -3.642373    0.225051
O      1.343007    0.958517    0.501203
C     -0.127176    0.780032    0.636815
C     -0.390420   -0.759330    0.611947
C     -0.779932    1.272710   -0.624044
C     -0.527415    1.522622    1.902453
C     -1.436477   -1.013610   -0.527192
H     -0.779810   -1.132964    1.569164
C     -1.472612    0.306837   -1.243977
H     -0.008912    1.104097    2.775287
H     -0.274996    2.588905    1.827927
H     -1.608870    1.431272    2.062868
C     -2.789977   -1.501225   -0.022373
H     -1.048784   -1.793336   -1.199950
H     -0.676335    2.305007   -0.960160
H     -2.038665    0.444229   -2.167219
C     -3.869752   -0.632225    0.200417
C     -2.966623   -2.868545    0.255876
C     -4.184805   -3.348623    0.741232
C     -5.255006   -2.473467    0.954165
C     -5.091681   -1.113084    0.682302
H     -3.758734    0.432814   -0.008166
H     -2.131781   -3.554220    0.105165
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H     -4.298577   -4.413696    0.951563
H     -6.208691   -2.849661    1.328300
H     -5.919090   -0.419203    0.843061
C      3.941470   -1.920496    1.968312
C      5.277787   -1.941437   -0.146363
H      3.536540   -0.145675   -0.992439
H      3.865593    0.425716    0.641760
H      3.000393   -2.802921   -1.260604
H      3.216676   -3.835319    0.150620
H      2.960032   -1.788739    2.441835
H      4.630572   -1.183968    2.406366
H      4.309066   -2.921000    2.235970
H      5.274987   -1.846184   -1.241956
H      5.681762   -2.932838    0.102501
H      5.972226   -1.188825    0.255488
44
DG298.15K(OPBE/6-31G*)=-925.10527
C      3.343187   -0.368795    0.090466
C      3.717217   -1.703079   -0.598527
C      1.873379   -0.260585    0.302489
C      2.944985   -2.852137    0.085975
C      0.988646   -1.296961    0.351754
C      1.426901   -2.669718    0.199749
O      0.668966   -3.644569    0.204113
O      1.344759    0.954133    0.489774
C     -0.124672    0.778161    0.639872
C     -0.392380   -0.760068    0.609015
C     -0.783501    1.279350   -0.614369
C     -0.511810    1.514679    1.913303
C     -1.433903   -1.009951   -0.536109
H     -0.789241   -1.133358    1.563348
C     -1.472327    0.315921   -1.242428
H      0.014261    1.090235    2.778773
H     -0.257639    2.580803    1.842288
H     -1.591873    1.425246    2.084656
C     -2.788120   -1.502007   -0.038207
H     -1.041589   -1.784773   -1.211260
H     -0.683179    2.314545   -0.942380
H     -2.039792    0.459576   -2.163839
C     -3.854973   -0.628583    0.225972
C     -2.977659   -2.875617    0.196277
C     -4.196124   -3.357627    0.679376
C     -5.253209   -2.477900    0.934056
C     -5.076849   -1.110978    0.706112
H     -3.732873    0.441272    0.050976
H     -2.152341   -3.565354    0.015287
H     -4.320215   -4.427738    0.855560
H     -6.206898   -2.855458    1.306788
H     -5.894015   -0.413450    0.900030
C      5.227731   -1.937527   -0.453224
C      3.362380   -1.641915   -2.094515
H      3.700787    0.493564   -0.492122
H      3.840088   -0.300082    1.074018
H      3.126887   -3.805826   -0.428165
H      3.322244   -2.978724    1.116231
H      5.525723   -2.002519    0.603261
H      5.802279   -1.121477   -0.915946
H      5.527809   -2.874604   -0.943126
H      2.294514   -1.446770   -2.256700
H      3.606421   -2.593037   -2.588147
H      3.930989   -0.847930   -2.599974
Conformationall averaged solution 44% 56 %
Distribution size=512
Distribution type=Gaussian
RDC general Std.Dev=0.5 Hz
Alignment tensor
<Axx>=0.000177447 stdved=8.04704e-06
 <Ayy>=0.000782238 stdved=5.14812e-06
 <Azz>=-0.000959686 stdved=8.52479e-06
Conformationally averaged quality factors statistic
<Q>=0.185575StdDev(Q)=0.000669634
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Highest Q=0.188162
Lowest Q=0.184245

        Exp [Std.Dev]  Hz     Comp [Std.Dev] Hz
C13,H20 7.76[0.50]     6.82[0.37]
C15,H22 -37.20[0.50]   -36.41[0.35]
C11,H21 -7.45[0.50]    -12.24[0.44]
C10,H14 -16.10[0.50]   -23.88[0.38]
C1,H35  -36.91[0.50]   -26.01[0.30]
C1,H36  -36.91[0.50]   -37.84[0.39]
C4,H37  -25.49[0.50]   -21.37[0.27]
C4,H38  -25.49[0.50]   -24.86[0.26]
C23,H28 18.15[0.50]    23.04[0.25]
C24,H29 18.15[0.50]    23.04[0.25]
C27,H32 21.07[0.50]    22.65[0.25]
C25,H30 21.07[0.50]    22.65[0.25]
C26,H31 32.09[0.50]    34.13[0.36]
C33,H39 -0.06[0.50]    -2.60[0.09]
C33,H40 -0.06[0.50]    -2.60[0.09]
C33,H41 -0.06[0.50]    -2.60[0.09]
C34,H42 -0.06[0.50]    1.24[0.08]
C34,H43 -0.06[0.50]    1.24[0.08]
C34,H44 -0.06[0.50]    1.24[0.08]
C12,H16 5.07[0.50]     5.15[0.13]
C12,H17 5.07[0.50]     5.15[0.13]
C12,H18 5.07[0.50]     5.15[0.13]
```

OPBE/6-31G* geometries and RDC fitting results for diastereisomers of compound 6b

6b1

```
40
DG298.15K(OPBE/6-31G*)= -1034.79905
C       5.360572   -1.234022   -0.493976
C       5.253135    0.116644   -0.867507
C       4.028524    0.765358   -0.771441
C       2.894575    0.071275   -0.305458
C       3.013364   -1.289935    0.070233
C       4.253952   -1.937306   -0.026656
H       6.322620   -1.743072   -0.568421
H       6.128966    0.654963   -1.230351
H       3.925111    1.812566   -1.053443
C       1.579812    0.618859   -0.156025
O       1.972705   -2.017234    0.538900
H       4.323748   -2.983715    0.267922
C       0.511332   -0.130867    0.298037
C       0.645184   -1.513420    0.653417
O      -0.200040   -2.288570    1.048090
O       1.292078    1.911918   -0.459789
C       0.004937    2.125489    0.235044
C      -0.664237    0.766490    0.039533
C      -1.082705    3.027212   -0.275407
C       0.389905    2.537523    1.664049
C      -2.098225    0.995848    0.545624
H      -0.808591    0.703194   -1.057035
C      -2.256933    2.422126    0.007088
H       0.912828    3.502589    1.624205
H       1.057640    1.801589    2.129002
H      -0.494536    2.660902    2.299094
C      -3.146119    0.010369    0.068619
H      -2.120361    1.022249    1.648427
H      -0.951247    4.057648   -0.604589
H      -3.239092    2.886277   -0.096459
C      -3.637134   -0.980522    0.932183
C      -3.641499    0.057131   -1.244776
C      -4.603520   -0.857131   -1.681328
C      -5.086781   -1.837121   -0.809708
C      -4.597654   -1.896887    0.498217
H      -3.250137   -1.047226    1.950108
H      -3.272030    0.818059   -1.935083
H      -4.976378   -0.802389   -2.705636
H      -5.837865   -2.552363   -1.148780
```

```
H     -4.961530   -2.662867    1.184868

        Exp [Std.Dev]  Hz     Comp [Std.Dev] Hz
C19,H29 0.07[0.50]     1.61[0.32]
C23,H30 -4.55[0.50]    -1.45[0.41]
C21,H28 0.34[0.50]     -2.40[0.30]
C18,H22 -5.20[0.50]    -4.01[0.40]
C20,H24 1.72[0.50]     1.64[0.21]
C20,H25 1.72[0.50]     1.64[0.21]
C20,H26 1.72[0.50]     1.64[0.21]
C1,H7          5.16[0.50]     -0.48[0.29]
C6,H12  1.89[0.50]     -0.73[0.42]
C31,H36 2.57[0.50]     -0.07[0.29]
C32,H37 2.57[0.50]     -0.07[0.29]
C35,H40 2.36[0.50]     -0.07[0.29]
C33,H38 2.36[0.50]     -0.07[0.29]
C34,H39 4.35[0.50]     1.60[0.44]

Gaussian distribution size=512
RDC Error=1.5 Hz
Alignment tensor
<Axx>=4.75316e-05 stdved=1.12541e-05
 <Ayy>=8.93551e-05 stdved=1.26361e-05
 <Azz>=-0.000136887 stdved=1.83975e-05
Quality factors statistic
<Q>=0.851192
StdDev(Q)=0.00850618
Highest Q=0.880825
Lowest Q=0.833705
```

6b2

```
40
DG(298.15K)= -1034.79352
C       5.430087   -0.648299    0.693575
C       5.147237    0.716753    0.872857
C       3.872055    1.200100    0.608795
C       2.863407    0.325205    0.159180
C       3.160354   -1.047381   -0.022004
C       4.448549   -1.530022    0.249784
H       6.431305   -1.027538    0.903057
H       5.926451    1.394912    1.221292
H       3.631638    2.253581    0.746869
C       1.508827    0.688749   -0.130097
O       2.242969   -1.943239   -0.457237
H       4.654115   -2.589850    0.104792
C       0.561451   -0.232407   -0.540887
C       0.918961   -1.591195   -0.826001
O       0.248111   -2.469684   -1.332971
O       1.076005    1.970451   -0.047419
C      -0.395645    1.822948   -0.021631
C      -0.585243    0.640292   -0.971743
C      -1.317258    2.815452   -0.676594
C      -0.740537    1.651443    1.461245
C      -2.107407    0.602837   -1.243236
H      -0.222054    1.048688   -1.935775
C      -2.306668    2.121472   -1.279017
H      -0.451788    2.566385    1.996657
H      -0.194071    0.806734    1.899172
H      -1.810654    1.485444    1.609012
C      -3.036930   -0.156641   -0.299253
H      -2.280068    0.186414   -2.249756
H      -1.277998    3.896478   -0.544493
H      -3.185328    2.575880   -1.740278
C      -4.075222    0.476542    0.403088
C      -2.908203   -1.551621   -0.178747
C      -3.777843   -2.281777    0.633877
C      -4.803150   -1.638832    1.334854
C      -4.949274   -0.255698    1.213694
H      -4.205853    1.556484    0.325012
H      -2.115085   -2.068384   -0.718320
H      -3.652440   -3.362895    0.716071
```

```
H     -5.483340   -2.211827    1.967150
H     -5.746794    0.261756    1.750125

        Exp [Std.Dev]  Hz     Comp [Std.Dev] Hz
C19,H29 0.07[0.50]     -0.34[0.38]
C23,H30 -4.55[0.50]    -4.75[0.41]
C21,H28 0.34[0.50]     -1.97[0.41]
C18,H22 -5.20[0.50]    -5.54[0.44]
C20,H24 1.72[0.50]     1.56[0.16]
C20,H25 1.72[0.50]     1.56[0.16]
C20,H26 1.72[0.50]     1.56[0.16]
C1,H7          5.16[0.50]     2.72[0.32]
C6,H12  1.89[0.50]     -0.14[0.32]
C31,H36 2.57[0.50]     3.48[0.28]
C32,H37 2.57[0.50]     3.48[0.28]
C35,H40 2.36[0.50]     3.42[0.28]
C33,H38 2.36[0.50]     3.42[0.28]
C34,H39 4.35[0.50]     1.85[0.36]

Gaussian distribution size=512
RDC Error=1.5 Hz
Alignment tensor
<Axx>=-4.63266e-05 stdved=7.09406e-06
 <Ayy>=-0.000182544 stdved=1.08972e-05
 <Azz>=0.00022887 stdved=1.27834e-05
Quality factors statistic
<Q>=0.473464
StdDev(Q)=0.00869274
Highest Q=0.508268
Lowest Q=0.459023
```

6b3

```
40
DG298.15K(OPBE/6-31G*)= -1034.83697
C      4.500538   -1.582670   -0.551635
C      4.401961   -0.410531   -1.319854
C      3.303785    0.427295   -1.165629
C      2.288949    0.102663   -0.245052
C      2.400750   -1.078211    0.528807
C      3.511770   -1.919208    0.368427
H      5.362516   -2.240449   -0.672493
H      5.184847   -0.157908   -2.035311
H      3.209373    1.339980   -1.753141
C      1.101789    0.871939    0.003074
O      1.480468   -1.445042    1.451158
H      3.577151   -2.822332    0.973938
C      0.138018    0.462076    0.886465
C      0.304151   -0.695174    1.718670
O     -0.409200   -1.092446    2.616219
O      0.865135    2.042631   -0.599839
C     -0.373582    2.599435    0.016585
C     -0.979553    1.455277    0.887747
C     -1.394873    2.844437   -1.051146
C      0.063129    3.841365    0.781339
C     -2.346984    1.052260    0.210414
H     -1.188483    1.806506    1.907826
C     -2.454652    2.033559   -0.925660
H      0.542640    4.563415    0.107238
H      0.777918    3.577275    1.571870
H     -0.807711    4.324664    1.243648
C     -2.519216   -0.389818   -0.238545
H     -3.151870    1.256693    0.935625
H     -1.268756    3.618825   -1.808119
H     -3.328883    2.045587   -1.578907
C     -3.311100   -1.273303    0.511862
C     -1.916793   -0.870815   -1.413256
C     -2.097200   -2.195166   -1.820749
C     -2.887155   -3.063834   -1.062566
C     -3.493408   -2.597499    0.107174
H     -3.780703   -0.924107    1.433254
H     -1.303821   -0.201489   -2.017565
```

```
H     -1.618989   -2.547722   -2.736347
H     -3.029152   -4.097868   -1.380876
H     -4.109243   -3.266683    0.710226

        Exp [Std.Dev]  Hz     Comp [Std.Dev] Hz
C19,H29 0.07[0.50]     0.22[0.34]
C23,H30 -4.55[0.50]    -5.13[0.38]
C21,H28 0.34[0.50]     1.40[0.33]
C18,H22 -5.20[0.50]    -5.34[0.50]
C20,H24 1.72[0.50]     -0.09[0.13]
C20,H25 1.72[0.50]     -0.09[0.13]
C20,H26 1.72[0.50]     -0.09[0.13]
C1,H7          5.16[0.50]     4.50[0.46]
C6,H12  1.89[0.50]     1.95[0.37]
C31,H36 2.57[0.50]     0.30[0.25]
C32,H37 2.57[0.50]     0.30[0.25]
C35,H40 2.36[0.50]     0.38[0.25]
C33,H38 2.36[0.50]     0.38[0.25]
C34,H39 4.35[0.50]     4.00[0.42]


Gaussian distribution size=512
RDC Error=1.5 Hz
Alignment tensor
<Axx>=-4.86824e-05 stdved=8.38947e-06
 <Ayy>=-8.87854e-05 stdved=6.11116e-06
 <Azz>=0.000137468 stdved=8.22237e-06
Quality factors statistic
<Q>=0.373457
StdDev(Q)=0.016479
Highest Q=0.428026
Lowest Q=0.343741
```

6b4

```
40
DG298.15K(OPBE/6-31G*)= -1034.84214
C     -5.640411   -0.642209    0.151213
C     -5.380058    0.737618    0.099530
C     -4.070812    1.191103   -0.005202
C     -3.005870    0.271613   -0.058339
C     -3.279049   -1.116349   -0.006067
C     -4.602432   -1.568278    0.099159
H     -6.668364   -0.998287    0.233041
H     -6.203249    1.451127    0.141206
H     -3.849255    2.256955   -0.047174
C     -1.614563    0.607054   -0.171224
O     -2.306797   -2.058598   -0.052531
H     -4.789778   -2.640615    0.138234
C     -0.631475   -0.345980   -0.213698
C     -0.927309   -1.747904   -0.160253
O     -0.157551   -2.689129   -0.190935
O     -1.188988    1.869711   -0.260829
C      0.296456    1.829643   -0.317651
C      0.705695    0.319886   -0.352102
C      0.830111    2.310484    1.002022
C      0.695252    2.668175   -1.522213
C      1.692158    0.095309    0.846130
H      1.191690    0.040758   -1.297290
C      1.567786    1.377521    1.619793
H      0.345501    3.703116   -1.410894
H      0.262458    2.252951   -2.441946
H      1.787468    2.679479   -1.624625
C      3.112367   -0.254203    0.416119
H      1.328060   -0.744438    1.457278
H      0.615493    3.311349    1.377571
H      2.064070    1.515604    2.581961
C      4.115635    0.717718    0.274925
C      3.433512   -1.591678    0.124329
C      4.717457   -1.943680   -0.297286
C      5.709315   -0.966773   -0.431118
C      5.402886    0.365299   -0.143197
```

```
H       3.893092    1.761900    0.499287
H       2.662899   -2.358314    0.214720
H       4.943961   -2.988006   -0.519473
H       6.714014   -1.242720   -0.755568
H       6.168718    1.137055   -0.241195

        Exp [Std.Dev]  Hz     Comp [Std.Dev] Hz
C19,H29 0.07[0.50]     -0.00[0.37]
C23,H30 -4.55[0.50]    -4.73[0.40]
C21,H28 0.34[0.50]     0.14[0.43]
C18,H22 -5.20[0.50]    -5.26[0.49]
C20,H24 1.72[0.50]     0.94[0.16]
C20,H25 1.72[0.50]     0.94[0.16]
C20,H26 1.72[0.50]     0.94[0.16]
C1,H7          5.16[0.50]     5.26[0.45]
C6,H12  1.89[0.50]     1.91[0.28]
C31,H36 2.57[0.50]     2.36[0.24]
C32,H37 2.57[0.50]     2.36[0.24]
C35,H40 2.36[0.50]     2.35[0.24]
C33,H38 2.36[0.50]     2.35[0.24]
C34,H39 4.35[0.50]     4.16[0.38]


Gaussian distribution size=512
RDC Error=1.5 Hz
Alignment tensor
<Axx>=-2.72611e-05 stdved=4.57323e-06
 <Ayy>=-8.77263e-05 stdved=6.18103e-06
 <Azz>=0.000114987 stdved=6.39032e-06
Quality factors statistic
<Q>=0.133002
StdDev(Q)=0.0261081
Highest Q=0.235545
Lowest Q=0.0839539
```

M06/6-31+G geometries and free energies for cyclization of compound 6a.**

Trienone 5a s-trans conformation

E(RM06) = -925.19906
Sum of electronic and thermal Free Energies= -924.88478

XYZ coordinates:
44
trienone s-trans

C	4.499698	0.433986	-0.724501
C	4.767013	-0.740217	0.215302
C	3.055600	0.856427	-0.861998
C	3.774032	-1.849849	-0.137514
C	2.008831	-0.005611	-0.280334
C	2.325811	-1.440665	-0.059105
O	1.457332	-2.274502	0.179180
O	2.780006	1.856950	-1.518213
C	0.156092	1.689415	0.233041
C	0.734646	0.390894	0.031759
C	-1.209439	1.807367	0.314350
C	0.998724	2.906927	0.475728
C	-3.525965	1.090309	0.237542
H	0.083068	-0.453651	0.264844
C	-2.207563	0.801386	0.115955
H	1.866274	2.669160	1.104763
H	1.393731	3.326115	-0.454571
H	0.409955	3.676001	0.986035
C	-4.646334	0.177737	0.082296
H	-3.795927	2.123189	0.472211
H	-1.600384	2.803518	0.537319
H	-1.899416	-0.209920	-0.146818
C	-5.948845	0.685771	0.214605
C	-4.489270	-1.192209	-0.192122
C	-5.596835	-2.016237	-0.331389
C	-6.885572	-1.495080	-0.199080
C	-7.057972	-0.140391	0.074981
H	-6.083505	1.744995	0.428776
H	-3.493773	-1.618189	-0.295912
H	-5.457506	-3.073496	-0.543400
H	-7.750101	-2.145077	-0.308766
H	-8.057877	0.273257	0.180259
C	4.609985	-0.313905	1.676544
C	6.188517	-1.249110	0.000226
H	4.842617	0.184525	-1.741906
H	5.073557	1.324130	-0.428010
H	3.955715	-2.182693	-1.173877
H	3.907286	-2.733329	0.500637
H	3.619298	0.108742	1.890664
H	5.356754	0.448780	1.932446
H	4.759291	-1.170431	2.346624
H	6.338031	-1.590605	-1.032398
H	6.407369	-2.090120	0.671096
H	6.919916	-0.456150	0.204530

trienone 5a s-cis s-trans ts

SCF Done: E(RM06) = -925.184231566
Sum of electronic and thermal Free Energies= -924.87039

XYZ Coordinates:
44
trienone 5a s-trans s-cis ts

C	-4.163402	0.174893	0.956290
C	-4.417669	-0.984858	-0.005871
C	-2.768061	0.751630	0.941563
C	-3.266164	-1.981485	0.151540
C	-1.725119	0.057996	0.152825
C	-1.899747	-1.401267	-0.103259
O	-0.982573	-2.106771	-0.503772

```
O   -2.505164  1.727956  1.634209
C   -0.215946  2.021811 -0.532966
C   -0.596911  0.634378 -0.346431
C    1.087079  2.282123 -0.802049
C   -1.221903  3.134811 -0.538875
C    3.042701  1.075380  0.125545
H    0.111534 -0.090071 -0.757114
C    2.179241  1.295993 -0.875365
H   -2.126248  2.841712 -1.088134
H   -1.542101  3.403349  0.471806
H   -0.800073  4.019506 -1.025850
C    4.178332  0.149047  0.125472
H    2.903912  1.636579  1.053132
H    1.362910  3.325721 -0.977844
H    2.285211  0.760097 -1.823393
C    4.974978  0.066655  1.275350
C    4.508778 -0.662215 -0.970723
C    5.597424 -1.522829 -0.913741
C    6.382119 -1.593827  0.238437
C    6.066394 -0.794998  1.333923
H    4.729406  0.689773  2.134342
H    3.909622 -0.623892 -1.878409
H    5.836680 -2.144411 -1.773516
H    7.233272 -2.269192  0.279134
H    6.670034 -0.842061  2.237261
C   -4.509905 -0.484364 -1.448963
C   -5.729158 -1.670077  0.363381
H   -4.346893 -0.149739  1.993271
H   -4.862395  1.005095  0.777561
H   -3.259249 -2.366990  1.185611
H   -3.389348 -2.852993 -0.504592
H   -3.614955  0.067900 -1.765316
H   -5.369698  0.188080 -1.563562
H   -4.644678 -1.325469 -2.141180
H   -5.696329 -2.070460  1.385052
H   -5.940351 -2.501924 -0.321022
H   -6.566736 -0.962891  0.302763
```

trienone 5a s-cis conformation

```
E(RM06) =  -925.19644
Sum of electronic and thermal Free Energies=         -924.88145

XYZ coordinates:
44
trienone s-cis
C   -3.788106 -0.204505  1.092076
C   -4.121206 -1.099522 -0.099938
C   -2.480404  0.547281  1.010116
C   -2.893499 -1.966475 -0.386471
C   -1.500606  0.145927 -0.015881
C   -1.627322 -1.191687 -0.646200
O   -0.741673 -1.668177 -1.350225
O   -2.233945  1.422325  1.836256
C   -0.152199  2.309976 -0.236615
C   -0.424027  0.905242 -0.391913
C    1.138022  2.760029 -0.335220
C   -1.269539  3.307508 -0.128327
C    2.493183  0.763564  0.243777
H    0.298215  0.365133 -1.012055
C    2.336390  1.971072 -0.354392
H   -2.146251  2.988714 -0.705425
H   -1.600335  3.430491  0.907671
H   -0.941387  4.280646 -0.508018
C    3.678372 -0.080363  0.187455
H    1.691686  0.397511  0.888919
H    1.279005  3.839909 -0.407972
```

```
H    3.191850  2.425353 -0.856781
C    3.770867 -1.175788  1.060457
C    4.735491  0.150042 -0.709154
C    5.850795 -0.675591 -0.714748
C    5.932899 -1.754915  0.166991
C    4.887263 -2.004272  1.052921
H    2.953064 -1.370900  1.752647
H    4.679411  0.974505 -1.416698
H    6.659499 -0.483904 -1.415848
H    6.806641 -2.401853  0.156782
H    4.940894 -2.846265  1.738639
C   -4.488441 -0.258496 -1.324253
C   -5.301619 -1.997555  0.254926
H   -3.731226 -0.814312  2.008986
H   -4.581103  0.534758  1.274533
H   -2.696747 -2.614652  0.484792
H   -3.059191 -2.635534 -1.241186
H   -3.690845  0.438968 -1.613064
H   -5.389743  0.334750 -1.122990
H   -4.694882 -0.903986 -2.187755
H   -5.073114 -2.632870  1.120686
H   -5.561128 -2.651994 -0.587453
H   -6.187260 -1.396486  0.499698
```

TS 5a->6a

```
E(RM06) =  -925.17835
Sum of electronic and thermal Free Energies=         -924.86176
44
cyclization ts
C    2.557917 -0.447703 -1.242410
C    3.158001 -1.162907 -0.031734
C    1.508515  0.588704 -0.918752
C    2.005998 -1.681137  0.831660
C    0.812658  0.498970  0.336939
C    0.979010 -0.641964  1.216855
O    0.298360 -0.802595  2.239192
O    1.209698  1.445109 -1.771723
C   -0.290214  2.813240  0.306189
C   -0.251443  1.389573  0.604699
C   -1.558004  3.296248  0.029557
C    0.936467  3.646967  0.333490
C   -1.895656  1.047506 -0.576730
H   -0.845450  1.102642  1.478687
C   -2.480445  2.275623 -0.222993
H    1.614952  3.338594  1.137470
H    1.478290  3.512908 -0.612952
H    0.688977  4.707211  0.442062
C   -2.500847 -0.271246 -0.416077
H   -1.135287  1.109725 -1.363147
H   -1.802766  4.355055  0.036750
H   -3.552832  2.394632 -0.070297
C   -1.981068 -1.346891 -1.149403
C   -3.531744 -0.510665  0.503422
C   -4.050905 -1.789303  0.659398
C   -3.531747 -2.851197 -0.082733
C   -2.492688 -2.629308 -0.984220
H   -1.168686 -1.166102 -1.853915
H   -3.915091  0.307286  1.111973
H   -4.852389 -1.964787  1.372617
H   -3.932524 -3.853172  0.049492
H   -2.081702 -3.456018 -1.558308
C    4.045514 -0.207796  0.769767
C    4.005600 -2.339157 -0.505566
H    2.071401 -1.187915 -1.901359
H    3.337307  0.034627 -1.849225
H    1.461818 -2.465132  0.276057
```

```
H    2.376736 -2.153920  1.751452
H    3.496658  0.673500  1.126252
H    4.881553  0.146313  0.152407
H    4.466284 -0.717918  1.646189
H    3.405753 -3.055998 -1.081906
H    4.444643 -2.873164  0.347679
H    4.828367 -1.993819 -1.145896
```

cyclization product 6a

```
E(RM06) =  -925.22781
Sum of electronic and thermal Free Energies=         -924.90603
XYZ coordinates
44
cyclization product
C    3.336355  0.789342 -0.284661
C    3.843255 -0.613735  0.096479
C    1.877267  0.907858 -0.062797
C    2.892474 -1.674740 -0.480921
C    0.995426 -0.120864 -0.002897
C    1.425353 -1.484375 -0.148484
O    0.656437 -2.446791 -0.057973
O    1.336912  2.114355  0.102205
C   -0.132885  1.939897  0.231564
C   -0.384830  0.406295  0.240949
C   -0.780517  2.406447 -1.035799
C   -0.545703  2.691066  1.472495
C   -1.399017  0.118704 -0.906699
H   -0.790445  0.060157  1.203386
C   -1.451656  1.427658 -1.644019
H   -0.029103  2.289693  2.352046
H   -0.311344  3.757429  1.380152
H   -1.625989  2.584185  1.625625
C   -2.742939 -0.359143 -0.401549
H   -0.995504 -0.672000 -1.556530
H   -0.696705  3.436941 -1.373517
H   -2.021599  1.543781 -2.563746
C   -3.749279  0.532926 -0.022027
C   -2.973789 -1.730707 -0.256436
C   -4.180912 -2.200522  0.253180
C   -5.179587 -1.302381  0.626820
C   -4.959366  0.065788  0.488398
H   -3.588594  1.605252 -0.131386
H   -2.187471 -2.430630 -0.538891
H   -4.343322 -3.271075  0.357499
H   -6.124716 -1.667615  1.021925
H   -5.733304  0.774472  0.775218
C    3.921154 -0.750880  1.618262
C    5.237721 -0.814003 -0.487138
H    3.539480  0.987241 -1.349953
H    3.867665  1.567188  0.281696
H    2.967094 -1.667463 -1.581541
H    3.191925 -2.679143 -0.153164
H    2.948885 -0.597858  2.102489
H    4.624023 -0.018146  2.035308
H    4.277066 -1.752188  1.892226
H    5.227584 -0.740077 -1.582339
H    5.633131 -1.801624 -0.217168
H    5.933287 -0.056812 -0.101515
```

trienone 6b s-trans conformation

E(RM06) = -1034.87284
Sum of electronic and thermal Free Energies= -1034.61257
XYZ Coordinates:
40
trienone s-trans

C	-6.583644	-0.925641	0.089366
C	-6.444108	0.394678	0.530740
C	-5.179469	0.946318	0.652592
C	-4.042012	0.198825	0.324140
C	-4.206709	-1.115680	-0.109125
C	-5.467996	-1.688973	-0.227596
H	-7.573497	-1.364735	-0.004844
H	-7.323739	0.982189	0.778226
H	-5.036877	1.967405	0.997759
C	-2.690212	0.766807	0.443730
O	-3.140209	-1.923197	-0.406299
H	-5.553675	-2.719220	-0.561562
C	-1.609322	-0.049895	-0.124142
C	-1.848408	-1.476294	-0.405762
O	-0.994213	-2.297831	-0.664347
O	-2.490392	1.831841	1.026013
C	0.259579	1.674184	-0.465601
C	-0.316040	0.371296	-0.342065
C	1.631453	1.793400	-0.438363
C	-0.557966	2.899323	-0.752366
C	3.936352	1.094829	-0.194251
H	0.365208	-0.455938	-0.544382
C	2.614044	0.790508	-0.181060
H	-0.999829	3.321767	0.154375
H	-1.389879	2.671371	-1.428614
H	0.068295	3.661153	-1.228013
C	5.050208	0.192092	0.030982
H	4.210923	2.134813	-0.388228
H	2.033926	2.794651	-0.612140
H	2.296916	-0.227664	0.040391
C	4.887085	-1.183730	0.271878
C	6.353084	0.716411	0.005409
C	7.457303	-0.100674	0.215571
C	7.278872	-1.461252	0.454813
C	5.990026	-1.998366	0.481580
H	3.891418	-1.620957	0.294052
H	6.491227	1.780233	-0.181299
H	8.457779	0.323862	0.192653
H	8.139881	-2.104242	0.619451
H	5.847708	-3.060178	0.666421

trienone 5b s-trans s-cis ts

E(RM06) = -1034.85709
Sum of electronic and thermal Free Energies= -1034.59723
XYZ Coordinates:
40
ts for s-trans s-cis isomerization

C	-6.147372	-1.378859	0.286147
C	-6.121864	-0.090011	0.829569
C	-4.923128	0.600076	0.899650
C	-3.741855	0.023677	0.416794
C	-3.792593	-1.262733	-0.118271
C	-4.984688	-1.974234	-0.184950
H	-7.084698	-1.926514	0.232899

```
H   -7.037513  0.365001  1.196288
H   -4.868625  1.600866  1.320910
C   -2.458866  0.737545  0.479729
O   -2.671338 -1.912092 -0.569083
H   -4.981692 -2.978364 -0.599395
C   -1.352143  0.113922 -0.270470
C   -1.446312 -1.315754 -0.641927
O   -0.528817 -2.001324 -1.032790
O   -2.315860  1.757392  1.147265
C    0.224674  2.111163 -0.675486
C   -0.181304  0.722408 -0.625142
C    1.555449  2.355930 -0.788975
C   -0.751929  3.248870 -0.718705
C    3.392027  1.051532  0.243076
H    0.566315  0.026271 -1.011520
C    2.634402  1.354310 -0.820099
H   -1.154464  3.482432  0.270111
H   -1.608694  3.006464 -1.358441
H   -0.264526  4.140225 -1.125896
C    4.509991  0.105414  0.290293
H    3.169495  1.552018  1.188777
H    1.863889  3.402757 -0.861142
H    2.825247  0.881977 -1.788379
C    4.939437 -0.632817 -0.822957
C    5.185300 -0.072174  1.505183
C    6.254573 -0.956772  1.610408
C    6.669341 -1.682730  0.497405
C    6.005948 -1.516296 -0.719397
H    4.436199 -0.519063 -1.781131
H    4.862277  0.494239  2.377702
H    6.763437 -1.078677  2.563685
H    7.503679 -2.375640  0.574391
H    6.323262 -2.080614 -1.593232
```

trienone 5b s-cis

```
E(RM06) =  -1034.87052
Sum of electronic and thermal Free Energies=        -1034.60950
XYZ coordinates:
40
trienone s-cis conformation
C    5.710655 -1.648661 -0.249692
C    5.677023 -0.544523 -1.108510
C    4.524421  0.217910 -1.198617
C    3.398205 -0.099447 -0.429496
C    3.455186 -1.206165  0.416970
C    4.601389 -1.987760  0.513200
H    6.611455 -2.252667 -0.177035
H    6.550357 -0.289115 -1.701984
H    4.464436  1.079222 -1.859414
C    2.166402  0.700272 -0.509531
O    2.384390 -1.601462  1.175238
H    4.604061 -2.845822  1.179582
C    1.127467  0.359523  0.469154
C    1.214291 -0.895013  1.231712
O    0.337313 -1.358149  1.929856
O    2.015983  1.567492 -1.369784
C   -0.331226  2.458331  0.367075
C   -0.020725  1.090942  0.670076
C   -1.648949  2.837775  0.289971
C    0.738315  3.510257  0.303608
C   -2.786806  0.728495 -0.321222
```

H	-0.786601	0.568809	1.249893
C	-2.788580	1.975488	0.218738
H	1.161956	3.593681	-0.701747
H	1.568487	3.277546	0.979922
H	0.320742	4.481334	0.589362
C	-3.902508	-0.203091	-0.352846
H	-1.892027	0.399414	-0.854006
H	-1.855369	3.909276	0.277500
H	-3.728100	2.393912	0.582321
C	-5.064597	-0.028308	0.417825
C	-3.813158	-1.330891	-1.184065
C	-4.855800	-2.246666	-1.259718
C	-6.006811	-2.053285	-0.499102
C	-6.105774	-0.942268	0.340778
H	-5.147674	0.821488	1.092019
H	-2.912322	-1.480864	-1.777084
H	-4.769913	-3.112852	-1.910907
H	-6.823517	-2.768845	-0.553145
H	-6.997965	-0.795057	0.944400