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

Supplementary Information for

Hyperconjomer stereocontrol of cationic polyene cyclisations

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General experimental:

All reactions were performed under an inert atmosphere (nitrogen or argon) in oven dried glassware, unless otherwise stated. Dichloromethane and triethylamine were distilled from calcium hydride. Tetrahydrofuran, toluene, acetonitrile, methanol, diethyl ether, dichloromethane, tetrahydrofuran and dimethylformamide were purified using an Innovative Technology, Inc., PureSolv™ solvent purification system. All other solvents and reagents were used as received from commercial sources. Melting points were determined using a Stanford Research Systems Optimelt automated melting point system and are uncorrected. Infrared spectra were acquired on a Bruker ALPHA FT-IR as thin films, neat. Absorption maxima are expressed in wavenumbers (cm^{-1}). ^{1}H and ^{13}C NMR spectra were recorded in deuterochloroform on a Bruker AVANCE III 500, a Bruker AVANCE III 400, a Bruker AVANCE 300, or a Bruker AVANCE 200 spectrometer (^{1}H frequencies 500, 400, 300, 200 MHz; ^{13}C frequencies 125, 100, 75 and 50 MHz respectively). ^{1}H chemical shifts are expressed as parts per million (ppm) with residual chloroform (δ 7.26) as an internal reference and are reported as chemical shift (δ_H); relative integral; multiplicity (s = singlet, br = broad, d = doublet, t = triplet, dd = doublet of doublets, ddd = doublet of doublet of doublets, m = multiplet); and coupling constants (*J*) reported in Hz. ^{13}C NMR chemical shifts are expressed as parts per million (ppm) with residual chloroform (δ 77.1) as internal reference and are reported as chemical shift (δ_C); multiplicity (assigned from DEPT or HSQC experiments); and coupling constants (*J*) reported in Hz. High resolution mass spectra were recorded on a Bruker Apex II Fourier Transform Ion Cyclotron Resonance mass spectrometer with a 7.0 T magnet, fitted with an off-axis Analytica electrospray source. Column chromatography was performed using Grace Davison, Merck, or Scharlau 40-60 μm (230-400 mesh) silica gel using commercial solvents. Analytical thin layer chromatography was performed using preconditioned plates (Merck TLC silica gel 60 F_{254} on aluminium) and visualised using UV light (254 nm and 365 nm), ethanolic anisaldehyde, ethanolic vanillin, or potassium permanganate solution.

Computational details.

DFT calculations were carried out using Spartan 16 or Spartan 18 parallel suite.[1] Gas phase geometries were obtained using the ωB97X-D functional with the 6-31G* basis set.[2] The vibrational frequencies of stationary points were inspected to ensure that they corresponded to minima on the potential energy surface and the Intrinsic Reaction Coordinate (IRC) method was used to confirm that they corresponded to motion along the reaction coordinate.

Energies of calculated structures (ωB97X-D/6-31G*)

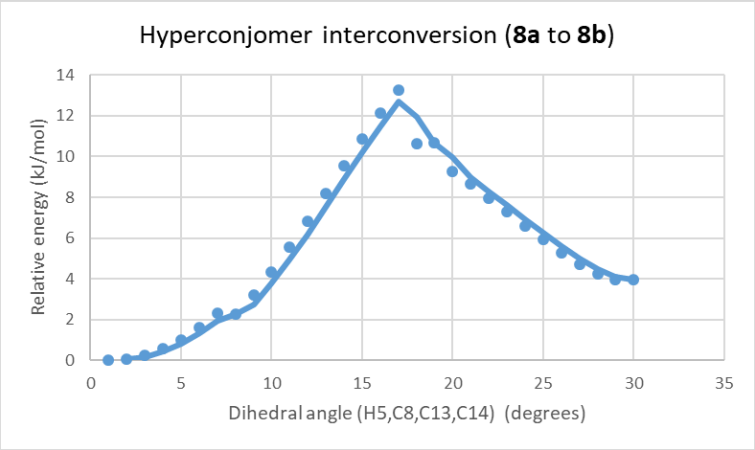
Molecule	Energy (au)	ZPE (kj/mol)	H (au)	G (au)	delta G (au)	delta G (kJmol)
16	-969.995158	1253.54	-969.494024	-969.576615	0	0
16a	-969.994183	1250.15	-969.494281	-969.57502	0.001595	4.186875
19	-969.986722	1249.63	-969.487067	-969.569954	0.006661	17.485125
19a	-969.98284	1249.65	-969.483033	-969.56794	0.008675	22.771875
TS8a	-969.971384	1247.67	-969.472443	-969.557611	0.019004	49.8855
TS8b (chair)	*not found*					
TS8b (boat)	-969.967075	1249.69	-969.467389	-969.54972	0.026895	70.599375
8a (H axial)	-970.009501	1262.74	-969.505687	-969.583548	-0.006933	-18.19913
8b boat (Bn axial)	-970.009764	1256.9	-969.507854	-969.590627	-0.014012	-36.78150
8b (Bn axial)	-970.010655	1255.97	-969.509075	-969.591218	-0.014603	-38.332875
TS17	-970.007752	1261.08	-969.504323	-969.582169	-0.005554	-14.57925
TS18	-969.987176	1262.91	-969.483183	-969.56105	0.01556	40.847625
TS20	-969.998979	1259.95	-969.49599	-969.575081	0.001534	4.02675
TS21	-970.009158	1261.98	-969.505469	-969.583407	-0.006792	-17.829
17	-970.016834	1259.860000	-969.514152	-969.593831	-0.017216	-45.192000
18	-970.011456	1262.040000	-969.508073	-969.587893	-0.011278	-29.604750
20	-970.025136	1262.670000	-969.521525	-969.600721	-0.024106	-63.278250
21	-970.019903	1264.530000	-969.515821	-969.593152	-0.016537	-43.409625
TS24	-969.990888	1257.68	-969.488482	-969.569212	0.007403	19.432875
24	-970.019575	1260.58	-969.516419	-969.594713	-0.018098	-47.50725

Molecule	Energy (au)	ZPE (kj/mol)	H (au)	G (au)	delta G (au)	delta G (kJ/mol)
28	-1126.02633	1585.210000	-1125.397680	-1125.484080	0.000000	0
29	-1126.01686	1584.85	-1125.3884	-1125.47378	0.010300	27.0375
TS30	-1126.00241	1587.770000	-1125.372830	-1125.456150	0.027930	73.31625
TS31	-1126.01738	1587.060000	-1125.388010	-1125.471390	0.012690	33.31125
syn anti TS	-1126.01335	1493.910000	-1125.418170	-1125.506650	0.012980	34.0725
syn syn TS	*not found*					
30	-1126.03852	1594.350000	-1125.406920	-1125.488650	-0.004570	-11.99625
31	-1126.04973	1596.900000	-1125.417280	-1125.497940	-0.013860	-36.3825
32	-1126.04961	1595.670000	-1125.417550	-1125.499770	-0.015690	-41.18625
33	-1126.04704	1595.550000	-1125.414990	-1125.496770	-0.012690	-33.31125
34	-1125.68606	1562.97000	-1125.066640	-1125.147950	0.000000	0
36	-1125.68821	1564.59	-1125.068390	-1125.149280	-0.001330	-3.49125

Molecule	Energy (au)	ZPE (kj/mol)	H (au)	G (au)	delta G (au)	delta G (kJ/mol)
37	-3500.60866	1031.72000	-3500.19408	-3500.27326	0.00000	0
39	-3500.61457	1030.64000	-3500.20039	-3500.27952	-0.00626	-16.4325
TS38	-3500.60805	1034.11000	-3500.19260	-3500.26749	0.00577	15.14625
TS40	-3500.60412	1036.51	-3500.18801	-3500.26293	0.01033	27.11625
38	-3500.62997	1040.74000	-3500.21265	-3500.28762	-0.01436	-37.695
40	-3500.65035	1042.50000	-3500.23225	-3500.30732	-0.03406	-89.4075

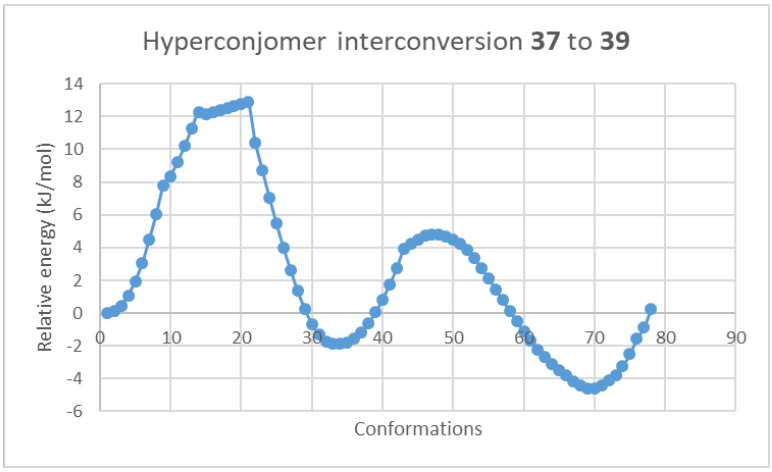
Molecule	Energy (au)	ZPE (kj/mol)	H (au)	G (au)	delta G (au)	delta G (kJ/mol)
42a	-930.722517	1188.34	-930.247807	-930.325353	0	0
42b	-930.72588	1185.67	-930.252181	-930.331283	-0.00593	-15.56625
TS43	-930.712984	1190.72	-930.237432	-930.311555	0.013798	36.21975
TS44	-930.710624	1190.83	-930.235028	-930.309619	0.015734	41.30175
43	-930.712984	1190.72	-930.237432	-930.311555	0.013798	36.21975
44	-930.71588	1189.66000	-930.24065	-930.31557	0.00978	25.6725
46a	-1084.49546	1340.09	-1083.95976	-1084.04741	0	0
46b	-1084.49097	1337.47	-1083.95618	-1084.04623	0.00118	3.0975
TS47	-1084.49067	1340.94	-1083.95464	-1084.03924	0.00817	21.44625
TS48	-1084.48577	1338.69	-1083.95052	-1084.03574	0.00969	25.43625
47	-1084.52116	1347.67	-1083.98302	-1084.06728	-0.01987	-52.15875
48	-1084.51465	1346.22	-1083.97713	-1084.06304	-0.01563	-41.02875
50a	-1045.20617	1269.44	-1044.69452	-1044.77887	0	0
50b	-1045.20166	1264.57	-1044.69559	-1044.78261	-0.00374	-9.8175
TS51	-1045.20191	1271.01	-1044.69369	-1044.77373	0.00514	13.4925
TS52	-1045.19944	1271.86	-1044.69105	-1044.7708	0.00807	21.18375
51	-1045.23042	1277.08	-1044.72046	-1044.80047	-0.0216	-56.7
52	-1045.22737	1275.92	-1044.7179	-1044.79855	-0.01968	-51.66

Estimated interconversion of hyperconjomers (PM3, gas phase)



Dihedral(H5,C8,C13,C14)	Energy (kJ/mol)	Relative Energy (kJ/mol)
104.68	379.9	0
101.73	379.96	0.07
98.77	380.15	0.25
95.82	380.47	0.57
92.87	380.91	1.01
89.91	381.49	1.6
86.96	382.21	2.31
84.01	382.15	2.25
81.05	383.11	3.21
78.1	384.21	4.31
75.15	385.43	5.53
72.19	386.73	6.83
69.24	388.09	8.19
66.29	389.45	9.55
63.33	390.77	10.87
60.38	392.02	12.13
57.43	393.16	13.26
54.47	390.55	10.65
51.52	390.58	10.68
48.57	389.19	9.29
45.61	388.54	8.64

Dihedral(H5,C8,C13,C14)	Energy (kJ/mol)	Relative Energy (kJ/mol)
48.57	389.19	9.29
45.61	388.54	8.64
42.66	387.86	7.96
39.71	387.17	7.28
36.75	386.49	6.59
33.8	385.82	5.92
30.85	385.19	5.29
27.89	384.61	4.72
24.94	384.14	4.24
21.99	383.86	3.96
19.03	383.87	3.97
16.08	384.19	4.29
13.26	383.42	3.52
10.39	384.12	4.22
7.48	385.09	5.19
4.56	386.27	6.37
1.59	385.79	5.89
-1.46	387.01	7.11
-4.37	388.42	8.52
-7.3	390.08	10.19
-10.22	391.99	12.09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Relative energy (kJ/mol)
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12
10
8
6
4
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-4
-6
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10
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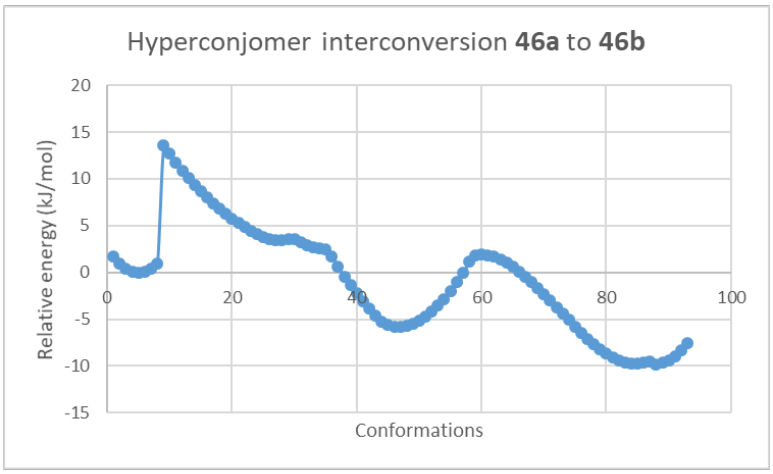
30
40
50
60
70
80
90
Conformations


Hyperconjomer interconversion 46a to 46b
Relative energy (kJ/mol)
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15
10
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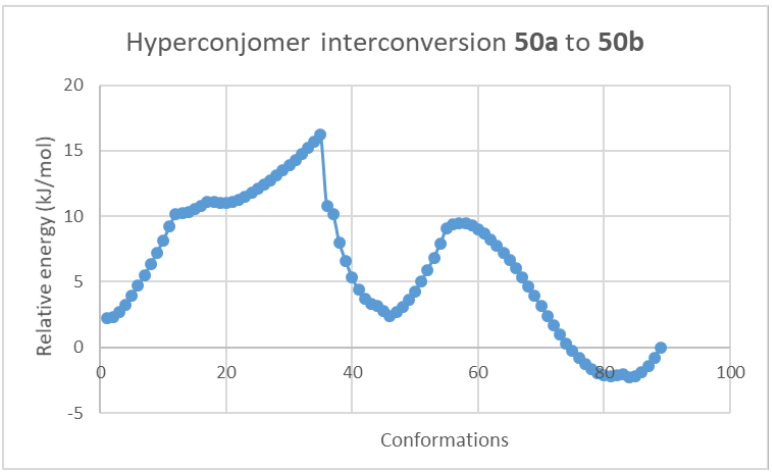
-15
0
20
40
60
80
100
Conformations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Relative energy (kJ/mol)
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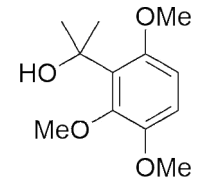
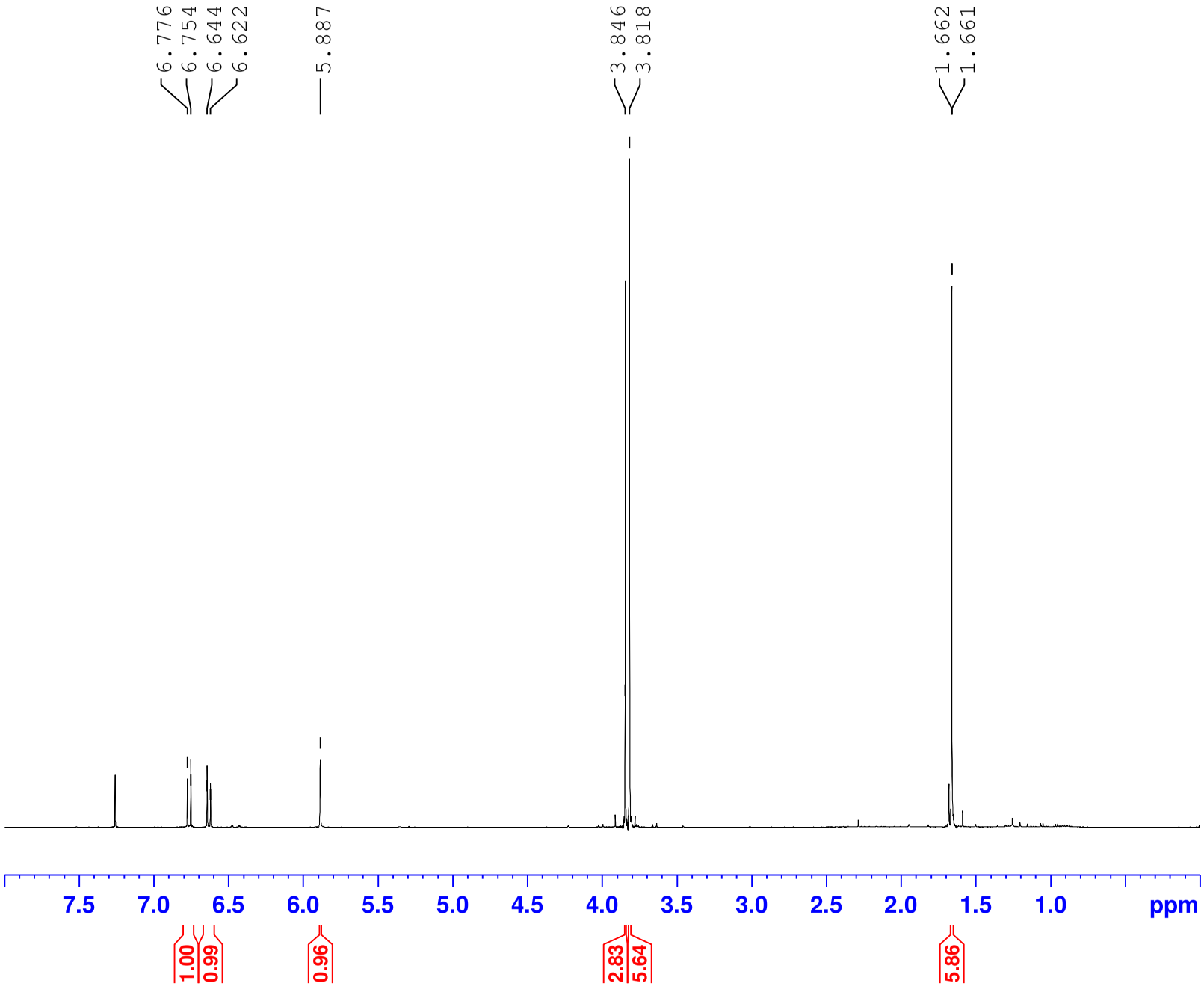
15
10
5
0
-5
0
20
40
60
80
100
Conformations

References

1. Except for molecular mechanics and semi-empirical models, the calculation methods used in Spartan have been documented in: Y.Shao, L.F. Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S.T. Brown, A.T.B. Gilbert, L.V. Slipchenko, S.V. Levchenko, D.P. O'Neill, R.A. DiStasio Jr., R.C. Lochan, T. Wang, G.J.O. Beran, N.A. Besley, J.M. Herbert, C.Y. Lin, T. Van Voorhis, S.H. Chien, A. Sodt, R.P. Steele, V.A. Rassolov, P.E. Maslen, P.P. Korambath, R.D. Adamson, B. Austin, J. Baker, E.F.C. Byrd, H. Dachsel, R.J. Doerksen, A. Dreuw, B.D. Dunietz, A.D. Dutoi, T.R. Furlani, S.R. Gwaltney, A. Heyden, S. Hirata, C-P. Hsu, G. Kedziora, R.Z. Khalliulin, P. Klunzinger, A.M. Lee, M.S. Lee, W.Z. Liang, I. Lotan, N. Nair, B. Peters, E.I. Proynov, P.A. Pieniazek, Y.M. Rhee, J. Ritchie, E. Rosta, C.D. Sherrill, A.C. Simmonett, J.E. Subotnik, H.L. Woodcock III, W. Zhang, A.T. Bell, A.K. Chakraborty, D.M. Chipman, F.J. Keil, A.Warshel, W.J. Hehre, H.F. Schaefer, J. Kong, A.I. Krylov, P.M.W. Gill and M. Head-Gordon, *Phys. Chem. Chem. Phys*., **2006**, *8*, 3172.
2. J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, **2008**, *10*, 6615-6620.

2-(2,3,6-trimethoxyphenyl)-propan-2-ol



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DW               62.500 usec
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TE                298.0 K
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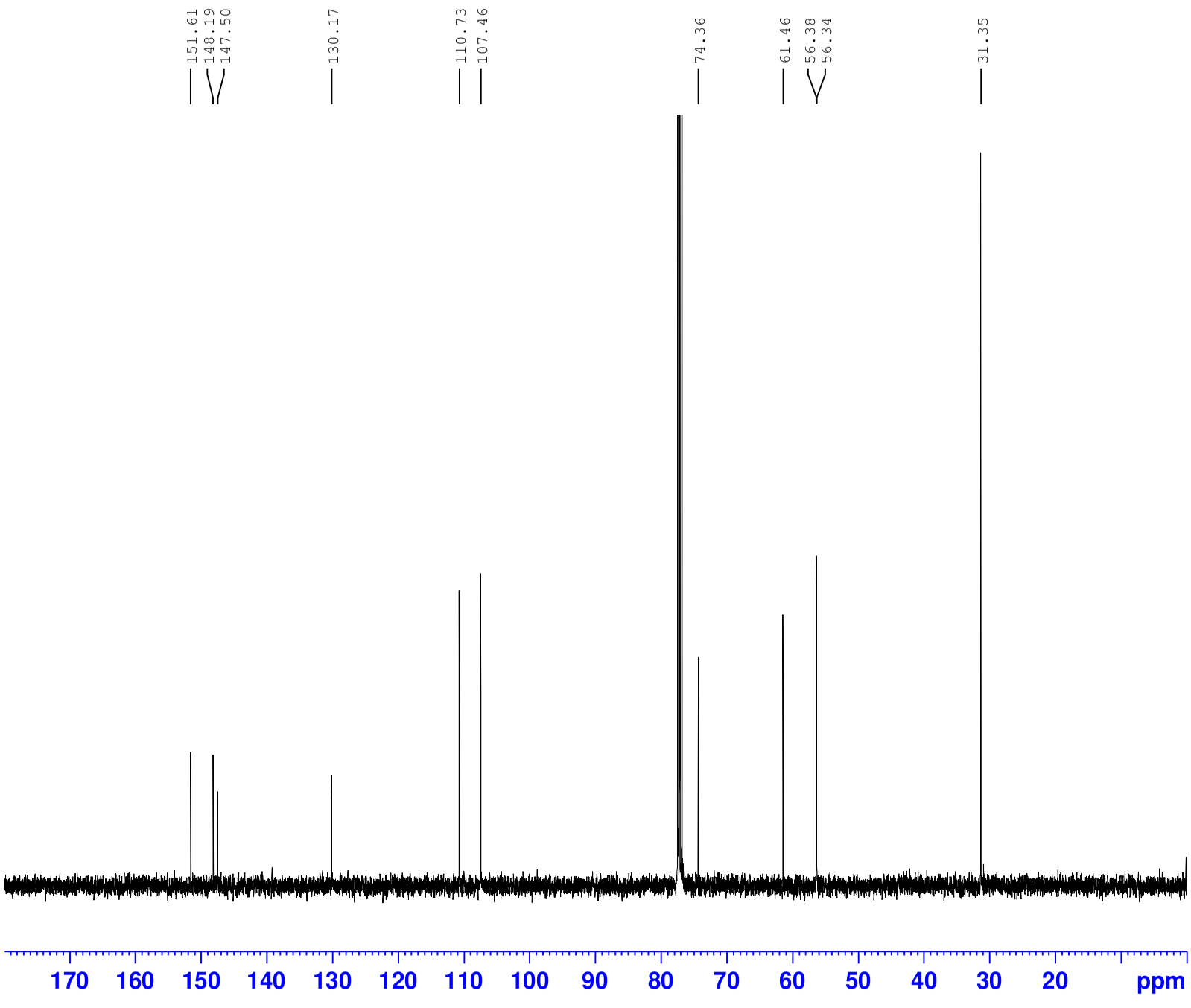
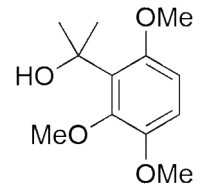
2-(2,3,6-trimethoxyphenyl)-propan-2-ol



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DE                 6.50 usec
TE                298.1 K
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D11          0.03000000 sec
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NUC2                1H
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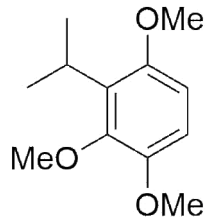
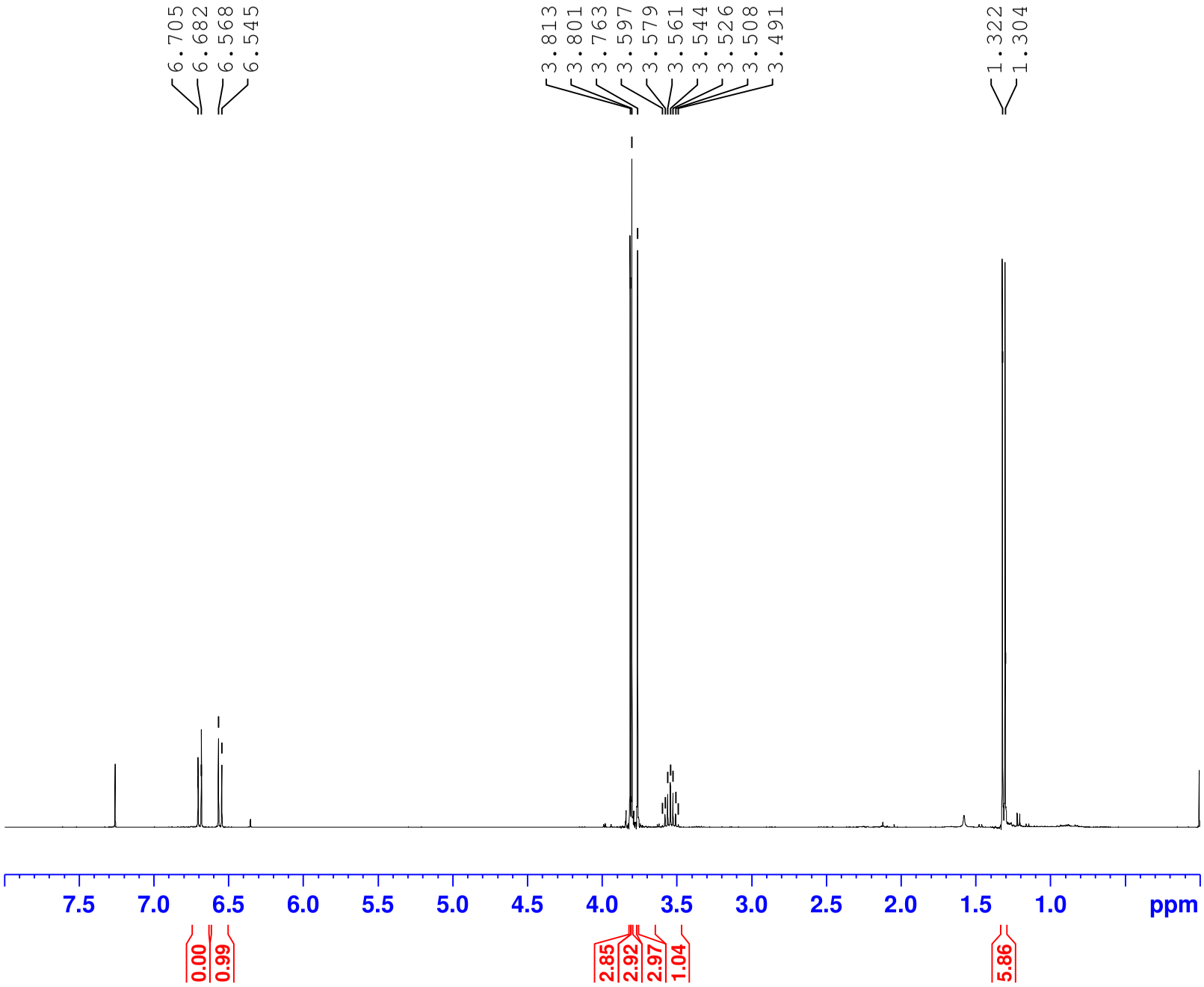
2-Isopropyl-1,3,4-trimethoxybenzene





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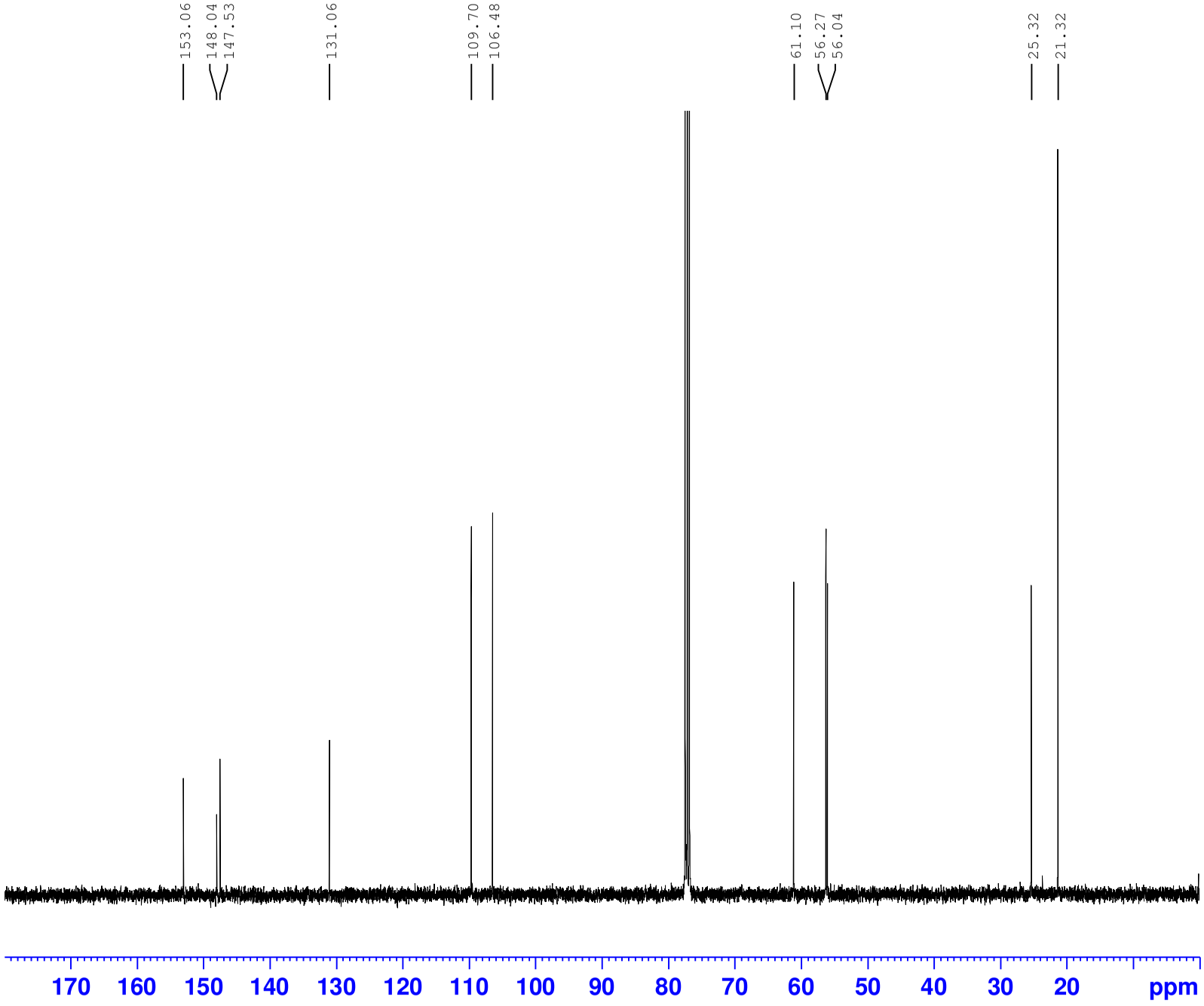
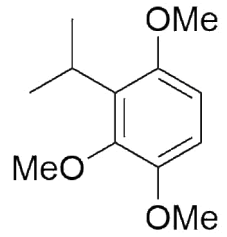
2-Isopropyl-1,3,4-trimethoxybenzene



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D11               0.03000000 sec
TD0                       25
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P1                    9.80 usec
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NUC2                     1H
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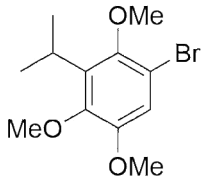
rr-10-9



6.932

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3.509
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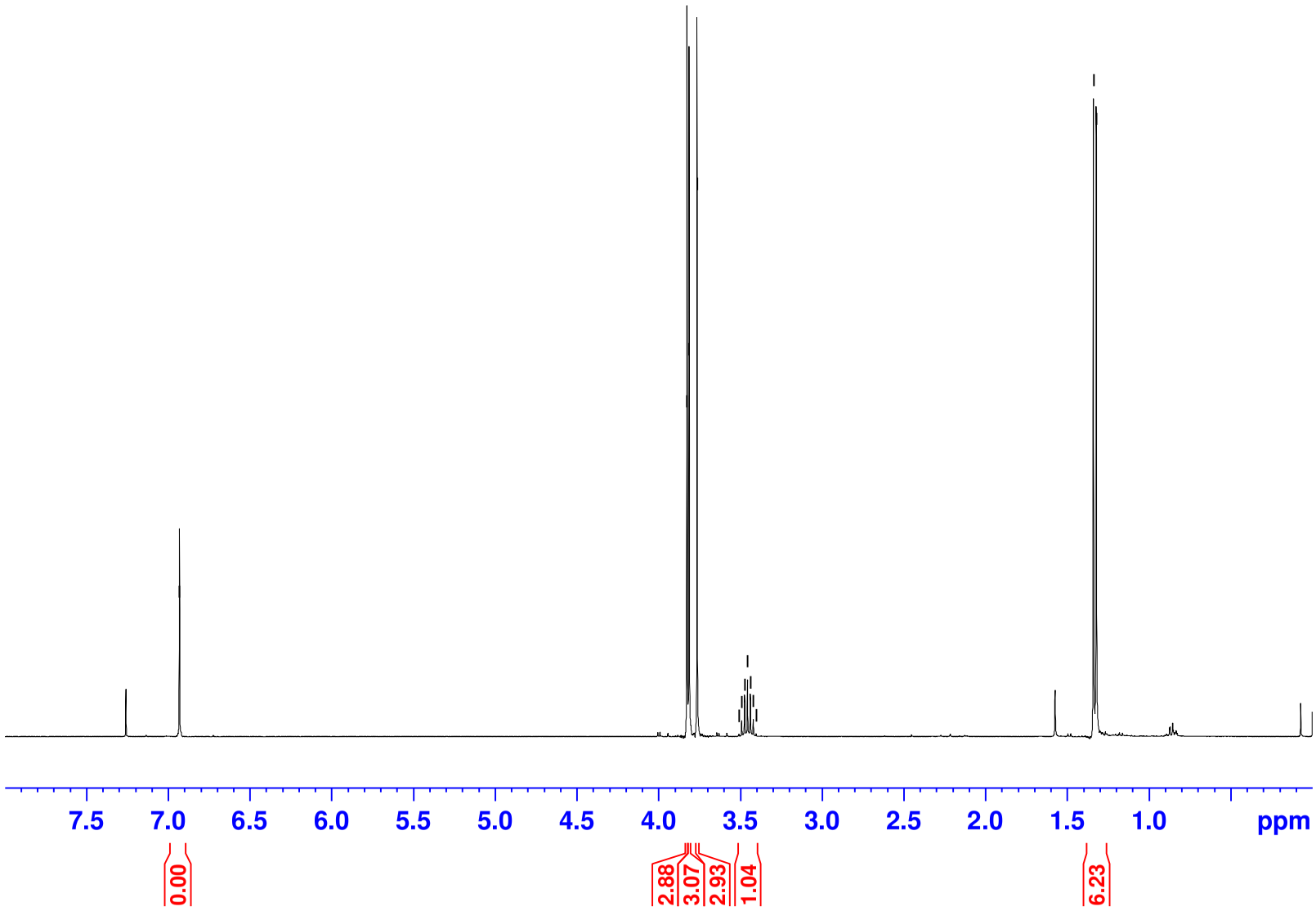
3.403

1.340
1.322

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TE                300.1 K
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NUC1                 1H
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PLW1         11.99499989 W

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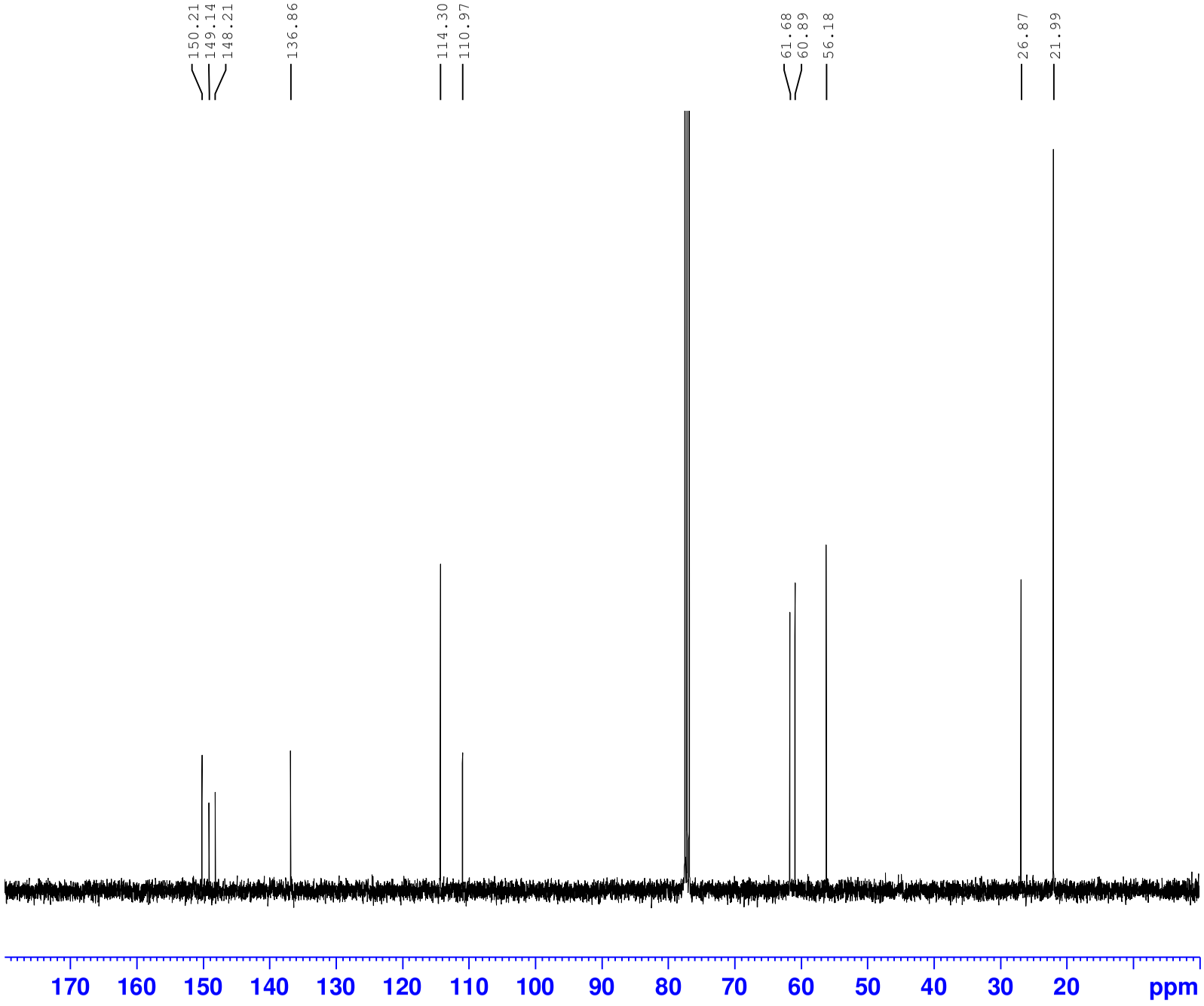
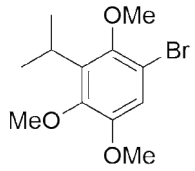
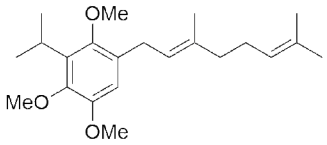
1-Bromo-3-isopropyl-2,4,5-trimethoxybenzene



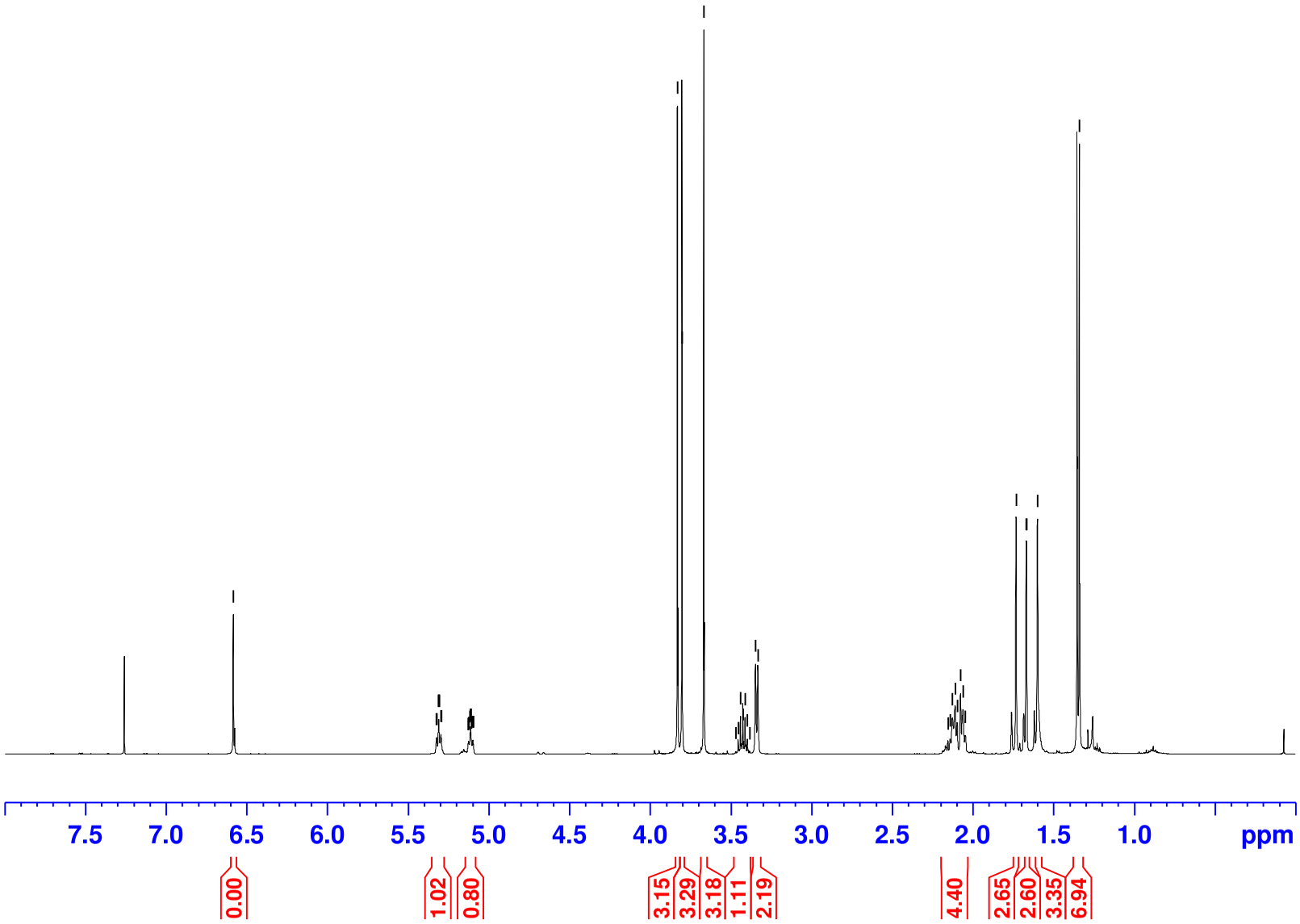



```
Current Data Parameters
NAME       rr-10-9-clean
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170704
Time               12.24 h
INSTRUM             spect
PROBHD   Z108618_0516 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  105
DS                    4
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ             1.2976128 sec
RG                  203
DW                19.800 usec
DE                 6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   25
SFO1         100.6228303 MHz
NUC1                13C
P1                 9.80 usec
PLW1         77.98300171 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.32877001 W
PLW13         0.16537000 W

F2 - Processing parameters
SI                 65536
SF           100.6127557 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

RR-14-55



6.584 5.326 5.323 5.314 5.312 5.309 5.307 5.297 5.295 5.129 5.126 5.124 5.118 5.116 5.113 5.110 5.108 5.102 5.099 5.097 3.832 3.803 3.668 3.469 3.455 3.441 3.426 3.412 3.398 3.384 3.347 3.333 2.155 2.141 2.127 2.110 2.098 2.077 2.061 2.048 1.732 1.670 1.668 1.599

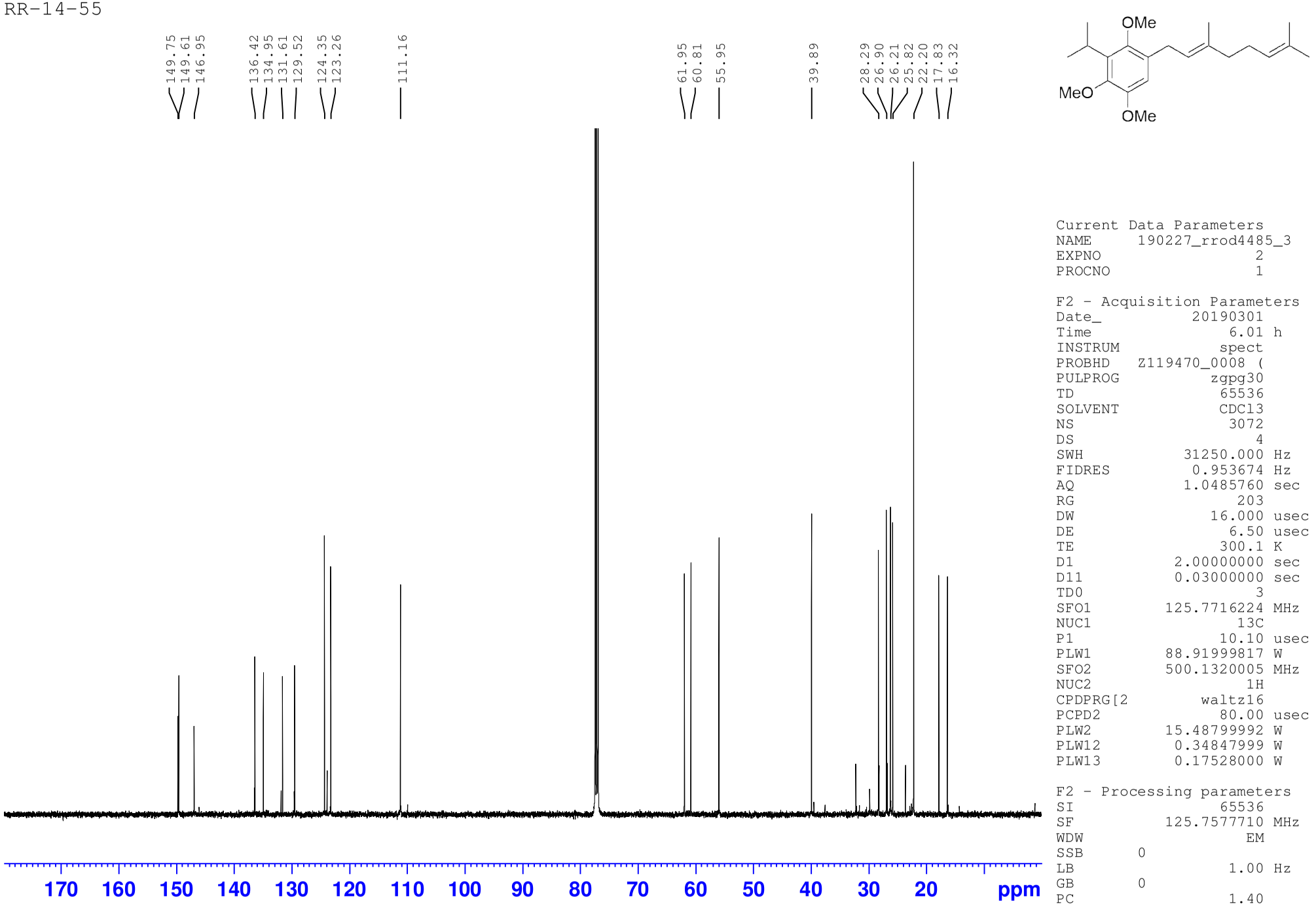


Current Data Parameters
NAME 190227_rrod4485_3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190301
Time 3.20 h
INSTRUM spect
PROBHD Z119470_0008 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 45.2
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
SFO1 500.1330008 MHz
NUC1 1H
P1 12.50 usec
PLW1 15.48799992 W

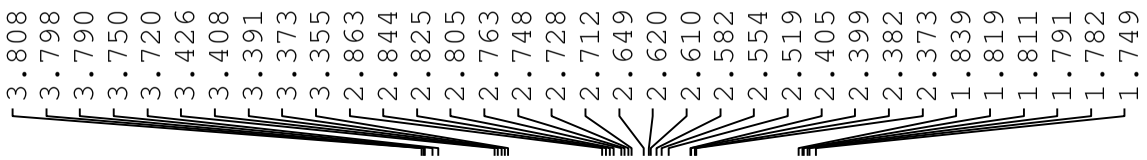
F2 - Processing parameters
SI 32768
SF 500.1300110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

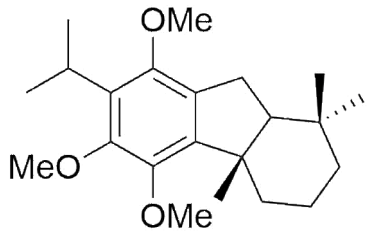
RR-14-55

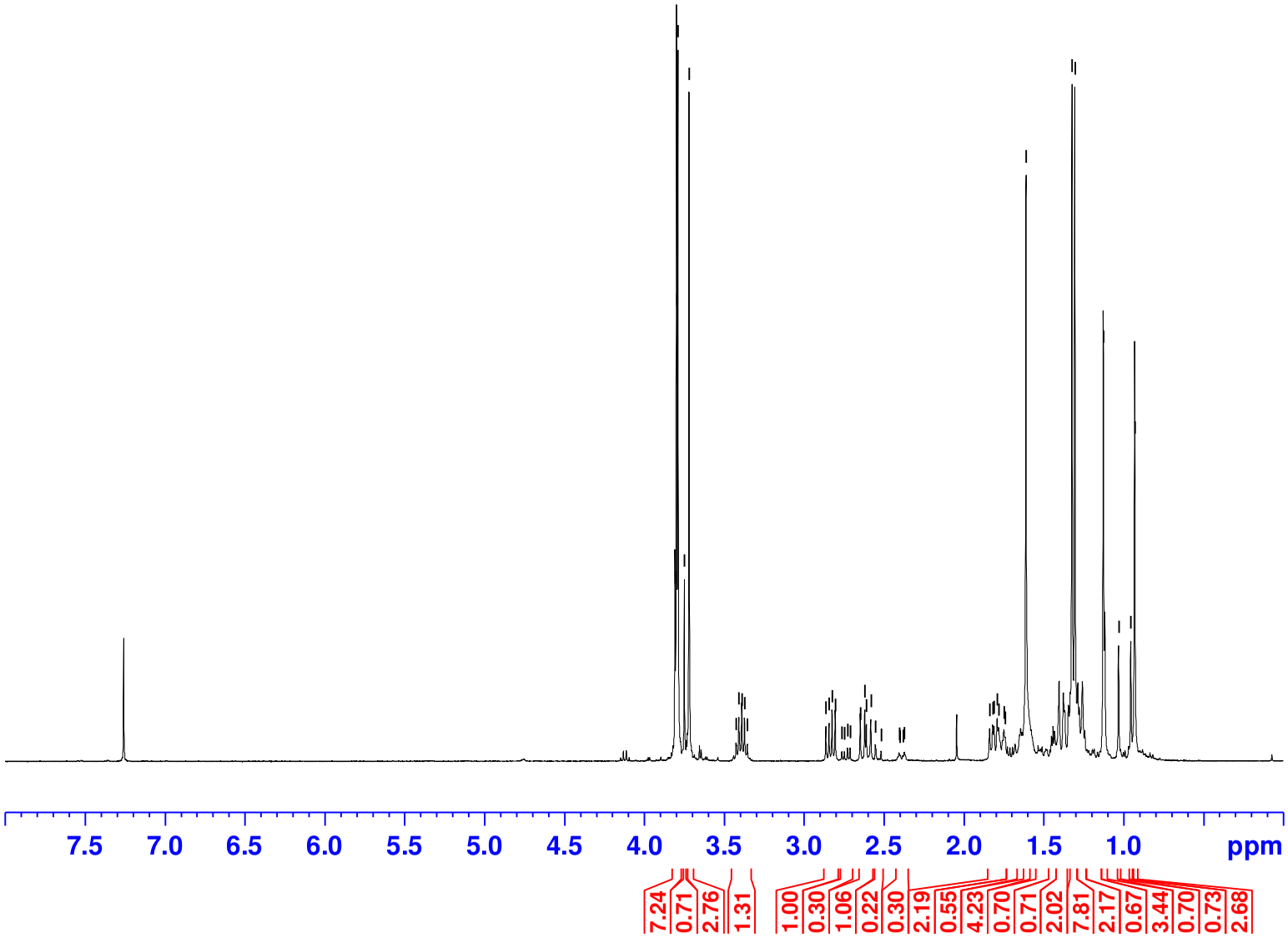



```
Current Data Parameters
NAME      190227_rrod4485_3
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20190301
Time                6.01 h
INSTRUM            spect
PROBHD   Z119470_0008 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           31250.000 Hz
FIDRES         0.953674 Hz
AQ            1.0485760 sec
RG                  203
DW               16.000 usec
DE                6.50 usec
TE                300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   3
SFO1        125.7716224 MHz
NUC1               13C
P1               10.10 usec
PLW1        88.91999817 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2            80.00 usec
PLW2        15.48799992 W
PLW12        0.34847999 W
PLW13        0.17528000 W

F2 - Processing parameters
SI                65536
SF          125.7577710 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC                1.40
```

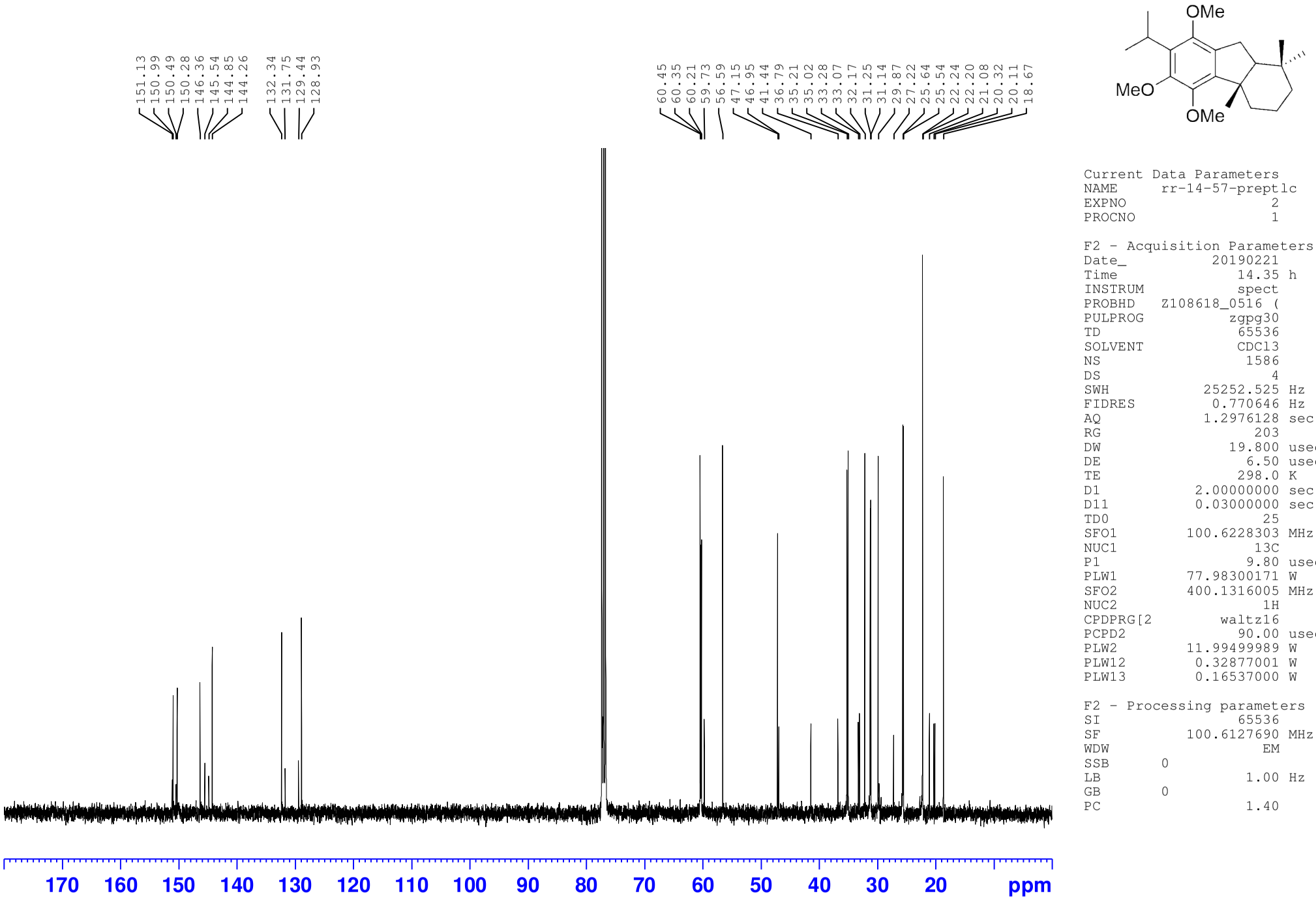
rr-14-57








```
Current Data Parameters
NAME      rr-14-57-preptlc
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190221
Time              13.03 h
INSTRUM            spect
PROBHD   Z108618_0516 (
PULPROG                zg
TD                  48076
SOLVENT             CDCl3
NS                      1
DS                      0
SWH            8000.000 Hz
FIDRES        0.332806 Hz
AQ            3.0047500 sec
RG                 80.6
DW               62.500 usec
DE               10.20 usec
TE               298.0 K
D1            5.00000000 sec
TD0                     1
SFO1         400.1324008 MHz
NUC1                   1H
P1               14.90 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                  32768
SF           400.1300099 MHz
WDW                    no
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```



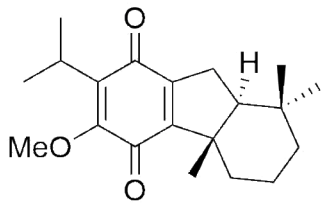
Current Data Parameters
NAME rr-14-57-preptlc
EXPNO 2
PROCNO 1

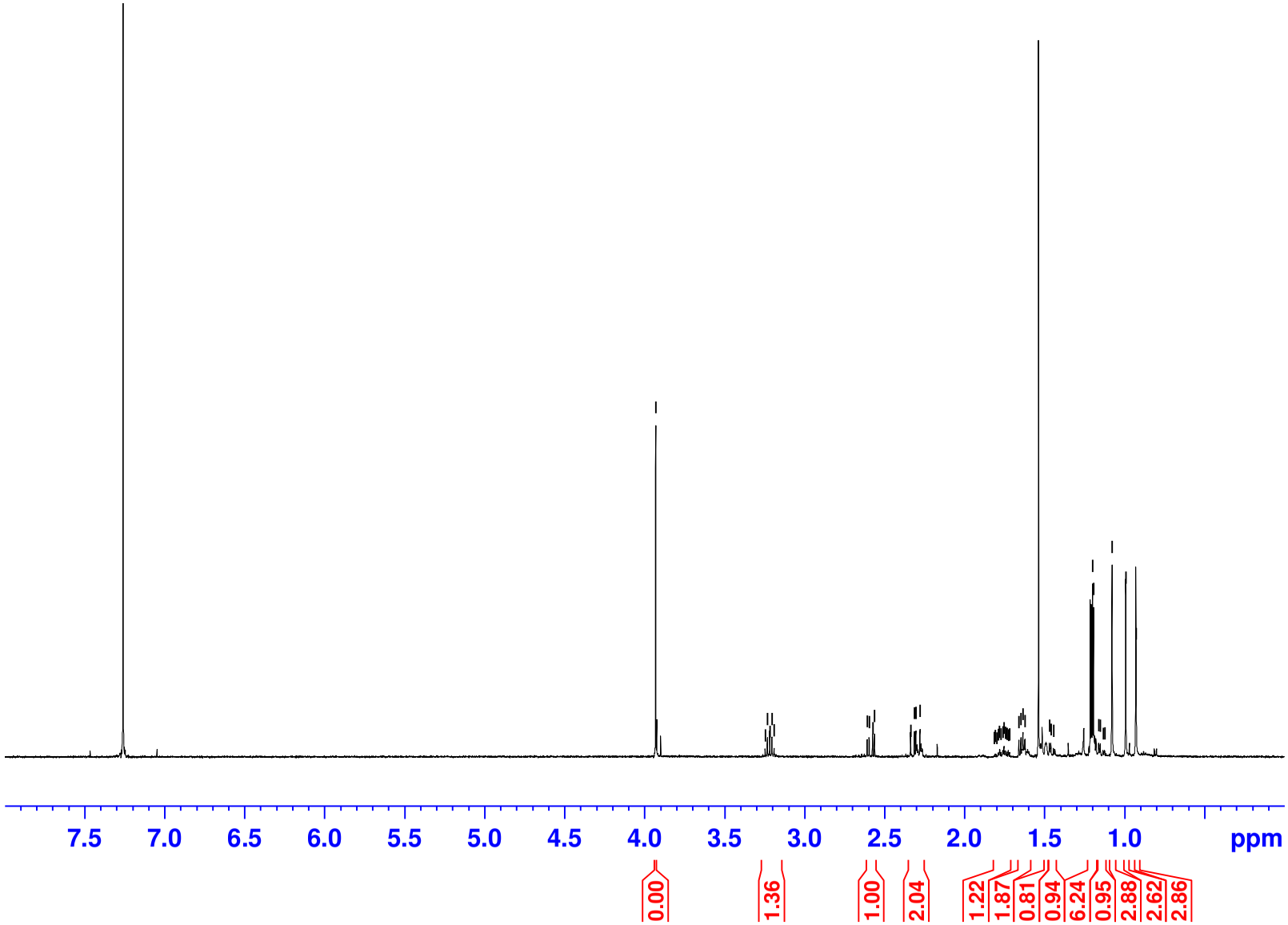
F2 - Acquisition Parameters
Date_ 20190221
Time 14.35 h
INSTRUM spect
PROBHD Z108618_0516 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1586
DS 4
SWH 25252.525 Hz
FIDRES 0.770646 Hz
AQ 1.2976128 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 25
SFO1 100.6228303 MHz
NUC1 13C
P1 9.80 usec
PLW1 77.98300171 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.99499989 W
PLW12 0.32877001 W
PLW13 0.16537000 W

F2 - Processing parameters
SI 65536
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

RR-taiG
nmrproton CDCl3 {C:\NMRDATA\MCERLEAN\mcerlean} {SHARED\nmrstaff} 5

3.931 3.247 3.233 3.218 3.204 3.190 2.609 2.596 2.575 2.562 2.338 2.313 2.304 2.279 1.816 1.808 1.800 1.789 1.782 1.773 1.760 1.753 1.744 1.735 1.726 1.718 1.660 1.648 1.635 1.623



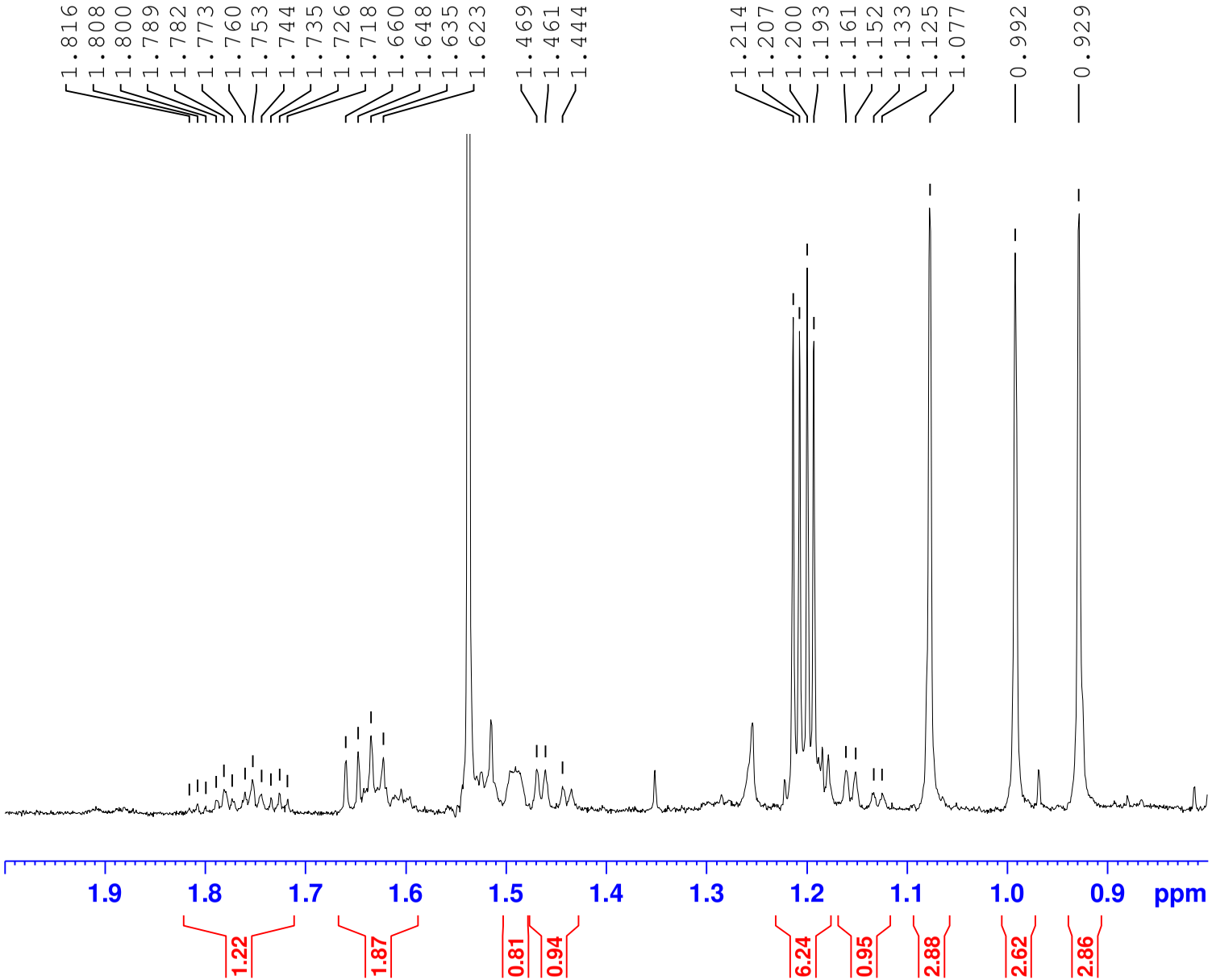


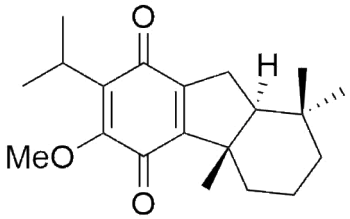
Current Data Parameters
NAME 190301_rrod4485_2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190301
Time 10.36 h
INSTRUM spect
PROBHD Z119470_0008 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
TD0 1
SFO1 500.1330008 MHz
NUC1 1H
P1 12.50 usec
PLW1 15.48799992 W

F2 - Processing parameters
SI 32768
SF 500.1300108 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

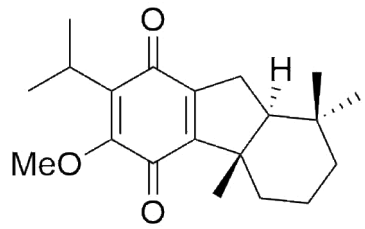
RR-taiG
nmrproton CDCl3 {C:\NMRDATA\MCERLEAN\mcerlean} {SHARED\nmrstaff} 5

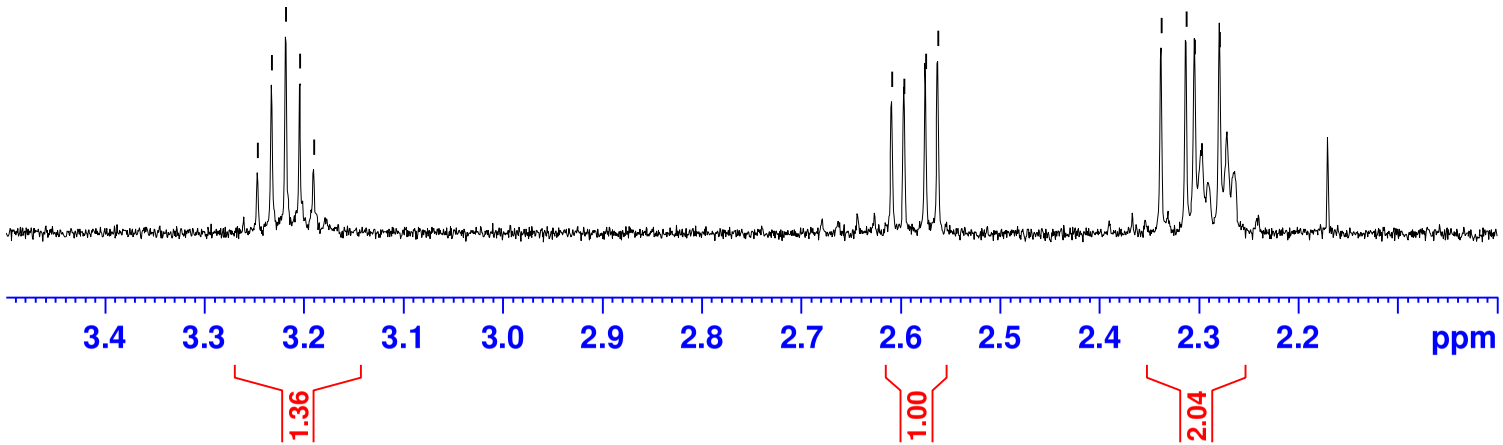





```
Current Data Parameters
NAME      190301_rrod4485_2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20190301
Time                10.36 h
INSTRUM             spect
PROBHD    Z119470_0008 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                      1
DS                      0
SWH             10000.000 Hz
FIDRES          0.305176 Hz
AQ              3.2767999 sec
RG                    101
DW                50.000 usec
DE                 6.50 usec
TE                300.1 K
D1             2.00000000 sec
TD0                     1
SFO1          500.1330008 MHz
NUC1                   1H
P1                12.50 usec
PLW1          15.48799992 W

F2 - Processing parameters
SI                  32768
SF            500.1300108 MHz
WDW                    no
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

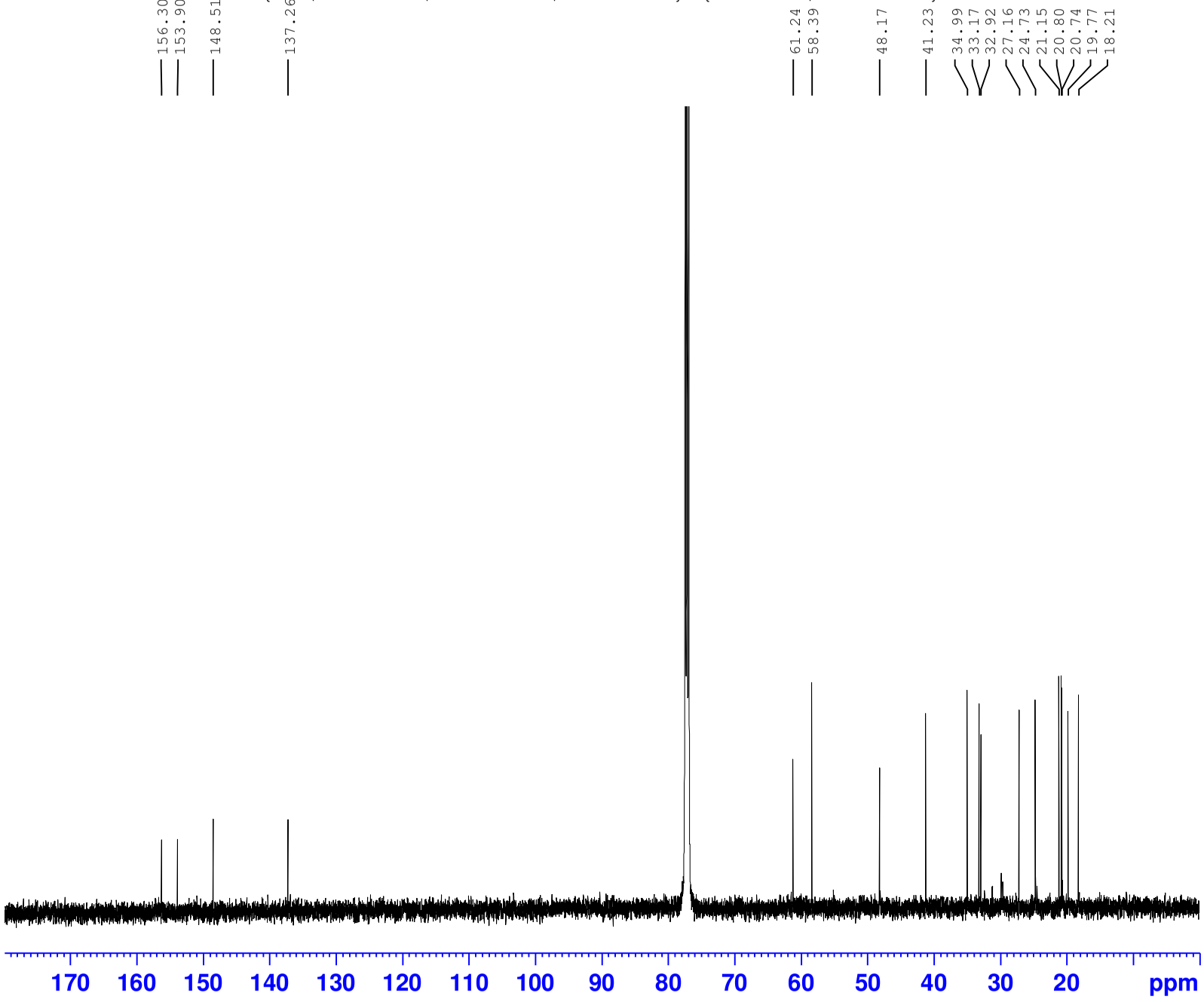
RR-taiG
nmrproton CDCl3 {C:\NMRDATA\MCERLEAN\mcerlean} {SHARED\nmrstaff} 5

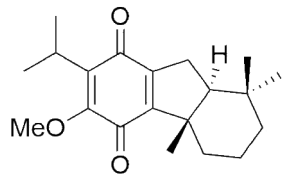





```
Current Data Parameters
NAME      190301_rrod4485_2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20190301
Time                10.36 h
INSTRUM             spect
PROBHD    Z119470_0008 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                      1
DS                      0
SWH             10000.000 Hz
FIDRES          0.305176 Hz
AQ              3.2767999 sec
RG                    101
DW                 50.000 usec
DE                  6.50 usec
TE                 300.1 K
D1             2.00000000 sec
TD0                     1
SFO1          500.1330008 MHz
NUC1                   1H
P1                 12.50 usec
PLW1          15.48799992 W

F2 - Processing parameters
SI                  32768
SF            500.1300108 MHz
WDW                    no
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

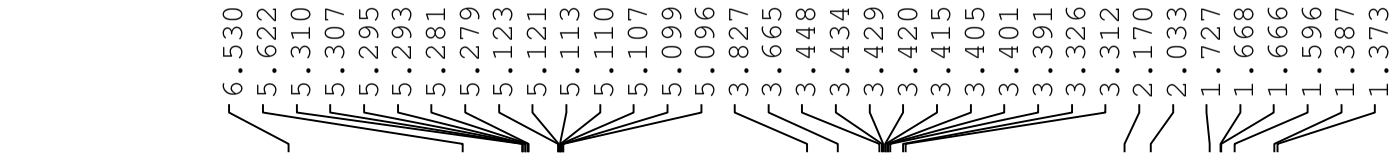
RR-taiG
nmr13c1hdec CDCl3 {C:\NMRDATA\MCERLEAN\mcerlean} {SHARED\nmrstaff} 5

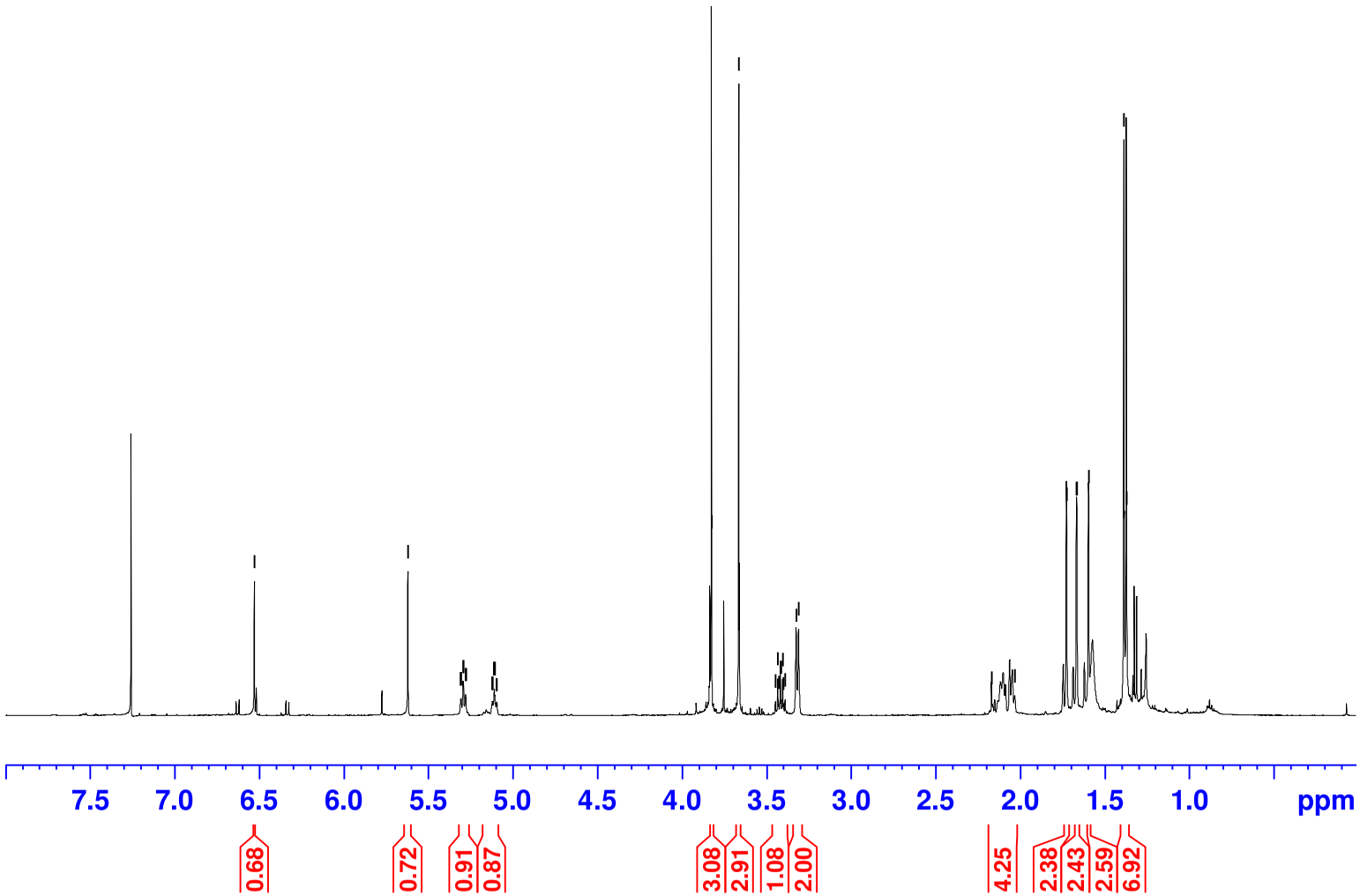


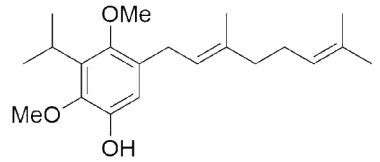



```
Current Data Parameters
NAME      190301_rrod4485_2
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_           20190302
Time                8.44 h
INSTRUM            spect
PROBHD   Z119470_0008 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                25600
DS                    4
SWH           31250.000 Hz
FIDRES         0.953674 Hz
AQ            1.0485760 sec
RG                  203
DW               16.000 usec
DE                6.50 usec
TE                299.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  25
SFO1         125.7716224 MHz
NUC1                13C
P1                10.10 usec
PLW1         88.91999817 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.48799992 W
PLW12         0.34847999 W
PLW13         0.17528000 W

F2 - Processing parameters
SI                65536
SF           125.7577691 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

RR-14-61
nmrproton CDCl3 {C:\NMRDATA\MCERLEAN\MCERLEAN} {SHARED\nmrstaff} 65

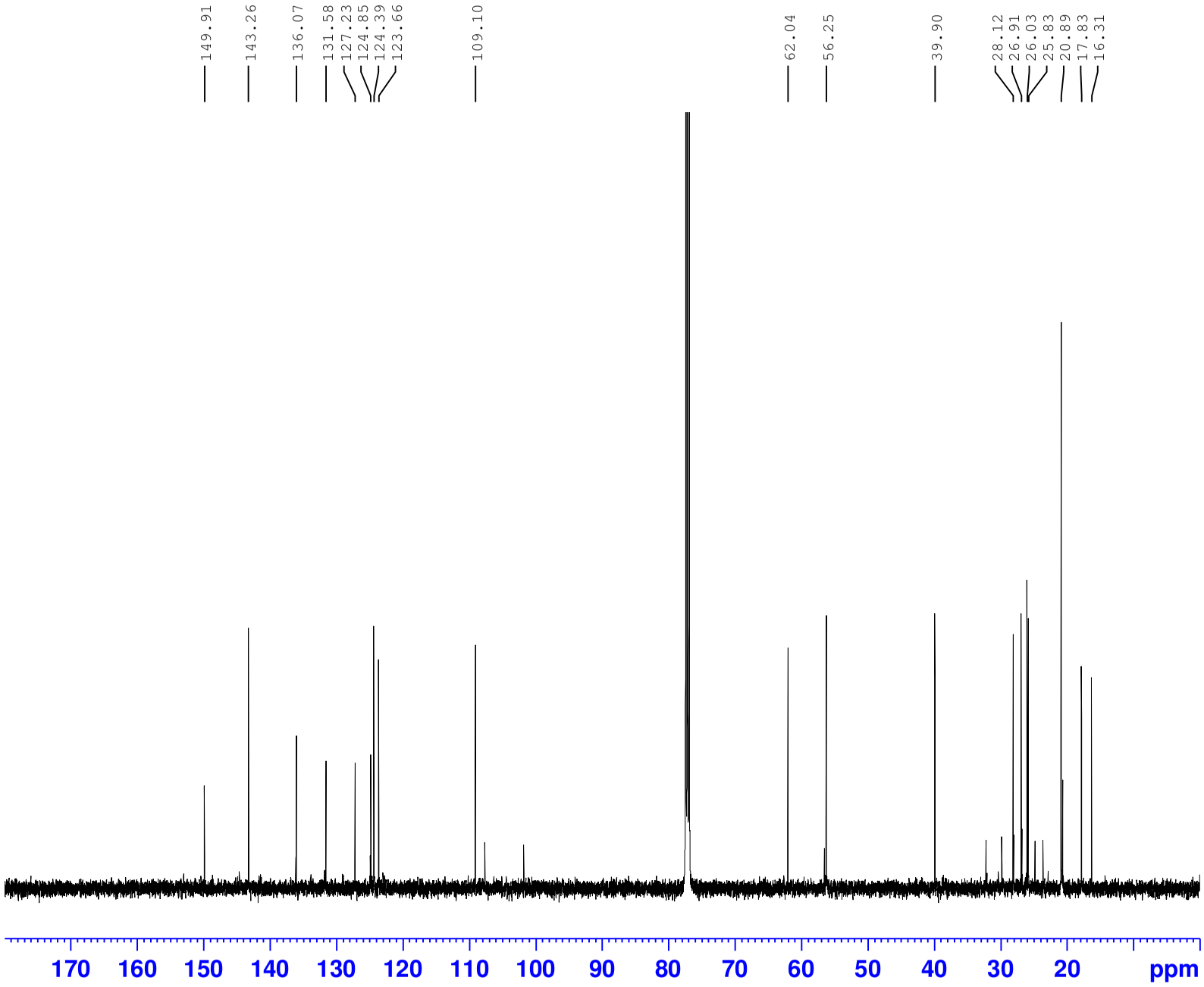


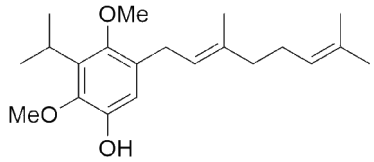





```
Current Data Parameters
NAME      190227_rrod4485_2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190228
Time              22.34 h
INSTRUM             spect
PROBHD   Z119470_0008 (
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                  45.2
DW                50.000 usec
DE                 6.50 usec
TE                300.1 K
D1           2.00000000 sec
TD0                    1
SFO1        500.1330008 MHz
NUC1                  1H
P1                12.50 usec
PLW1        15.48799992 W

F2 - Processing parameters
SI                 32768
SF          500.1300110 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

RR-14-61
nmr13c1hdec CDCl3 {C:\NMRDATA\MCERLEAN\MCERLEAN} {SHARED\nmrstaff} 65



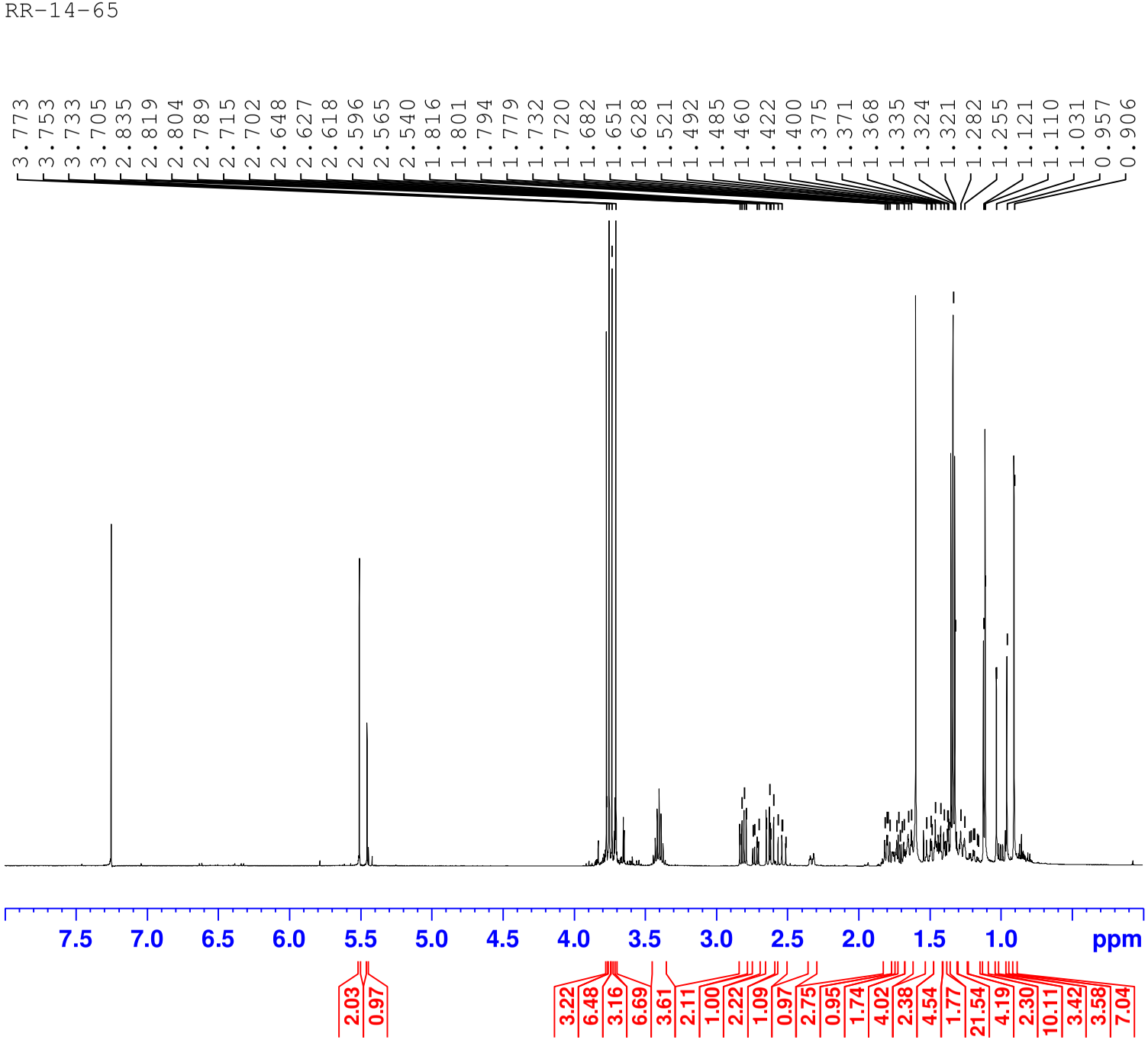


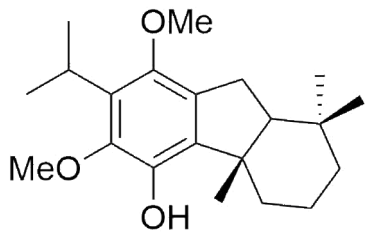
Current Data Parameters
NAME 190227_rrod4485_2
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190301
Time 3.15 h
INSTRUM spect
PROBHD Z119470_0008 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3072
DS 4
SWH 31250.000 Hz
FIDRES 0.953674 Hz
AQ 1.0485760 sec
RG 203
DW 16.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 3
SFO1 125.7716224 MHz
NUC1 13C
P1 10.10 usec
PLW1 88.91999817 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.48799992 W
PLW12 0.34847999 W
PLW13 0.17528000 W

F2 - Processing parameters
SI 65536
SF 125.7577704 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

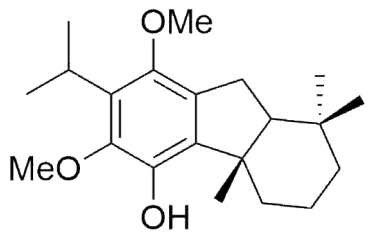
RR-14-65

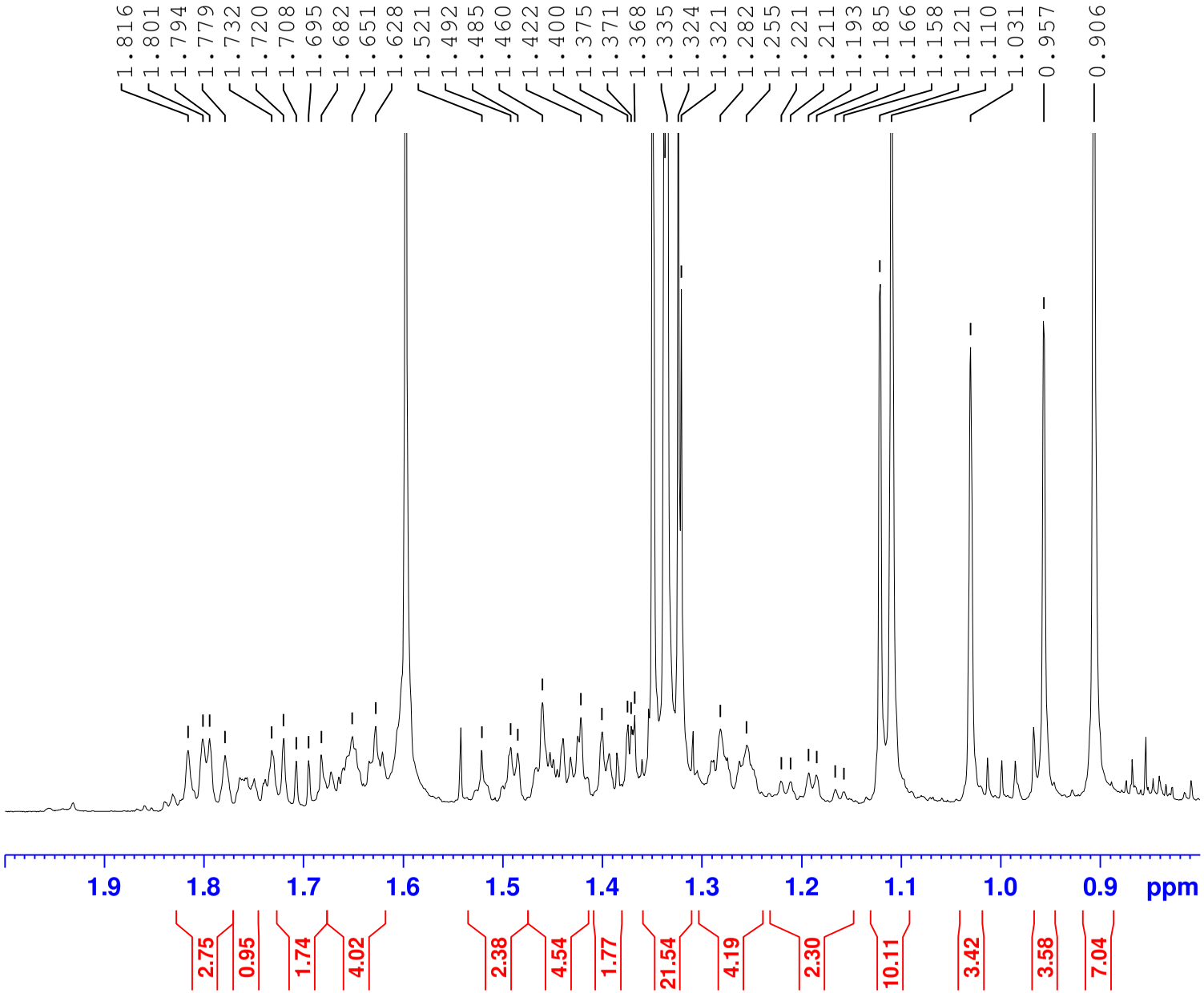





```
Current Data Parameters
NAME      190301_rrod4485_1
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20190301
Time                 7.48 h
INSTRUM              spect
PROBHD    Z119470_0008 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                      1
DS                      0
SWH             10000.000 Hz
FIDRES          0.305176 Hz
AQ              3.2767999 sec
RG                   22.6
DW                 50.000 usec
DE                  6.50 usec
TE                 300.1 K
D1            2.00000000 sec
TD0                     1
SFO1          500.1330008 MHz
NUC1                   1H
P1                 12.50 usec
PLW1          15.48799992 W

F2 - Processing parameters
SI                  32768
SF            500.1300137 MHz
WDW                    no
SSB       0
LB        0 Hz
GB        0
PC                   1.00
```

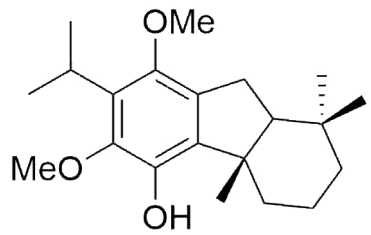
RR-14-65

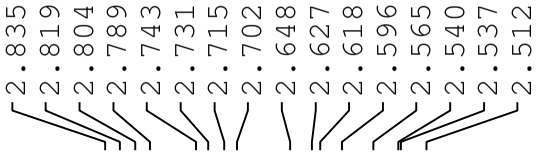


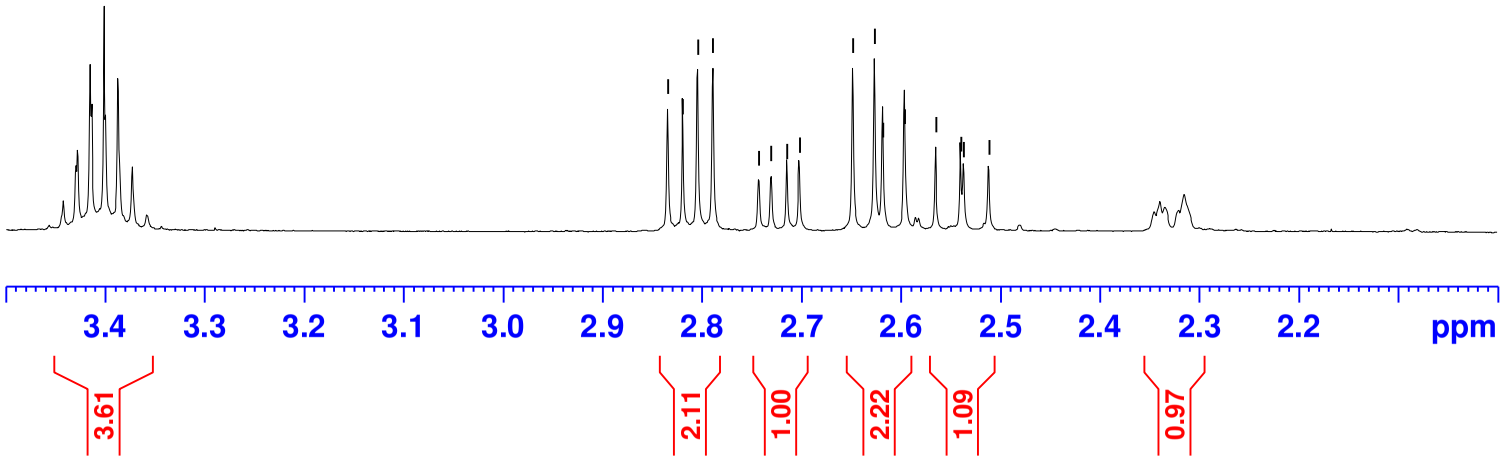



```
Current Data Parameters
NAME      190301_rrod4485_1
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20190301
Time                  7.48 h
INSTRUM              spect
PROBHD    Z119470_0008 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                       1
DS                       0
SWH             10000.000 Hz
FIDRES          0.305176 Hz
AQ              3.2767999 sec
RG                    22.6
DW                 50.000 usec
DE                  6.50 usec
TE                 300.1 K
D1              2.00000000 sec
TD0                      1
SFO1          500.1330008 MHz
NUC1                   1H
P1                 12.50 usec
PLW1          15.48799992 W

F2 - Processing parameters
SI                   32768
SF            500.1300137 MHz
WDW                    no
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```

RR-14-65





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EXPNO                    1
PROCNO                   1

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PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                    1
DS                    0
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                 22.6
DW                50.000 usec
DE                 6.50 usec
TE                300.1 K
D1            2.00000000 sec
TD0                   1
SFO1         500.1330008 MHz
NUC1                 1H
P1                12.50 usec
PLW1         15.48799992 W

F2 - Processing parameters
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RR-14-65
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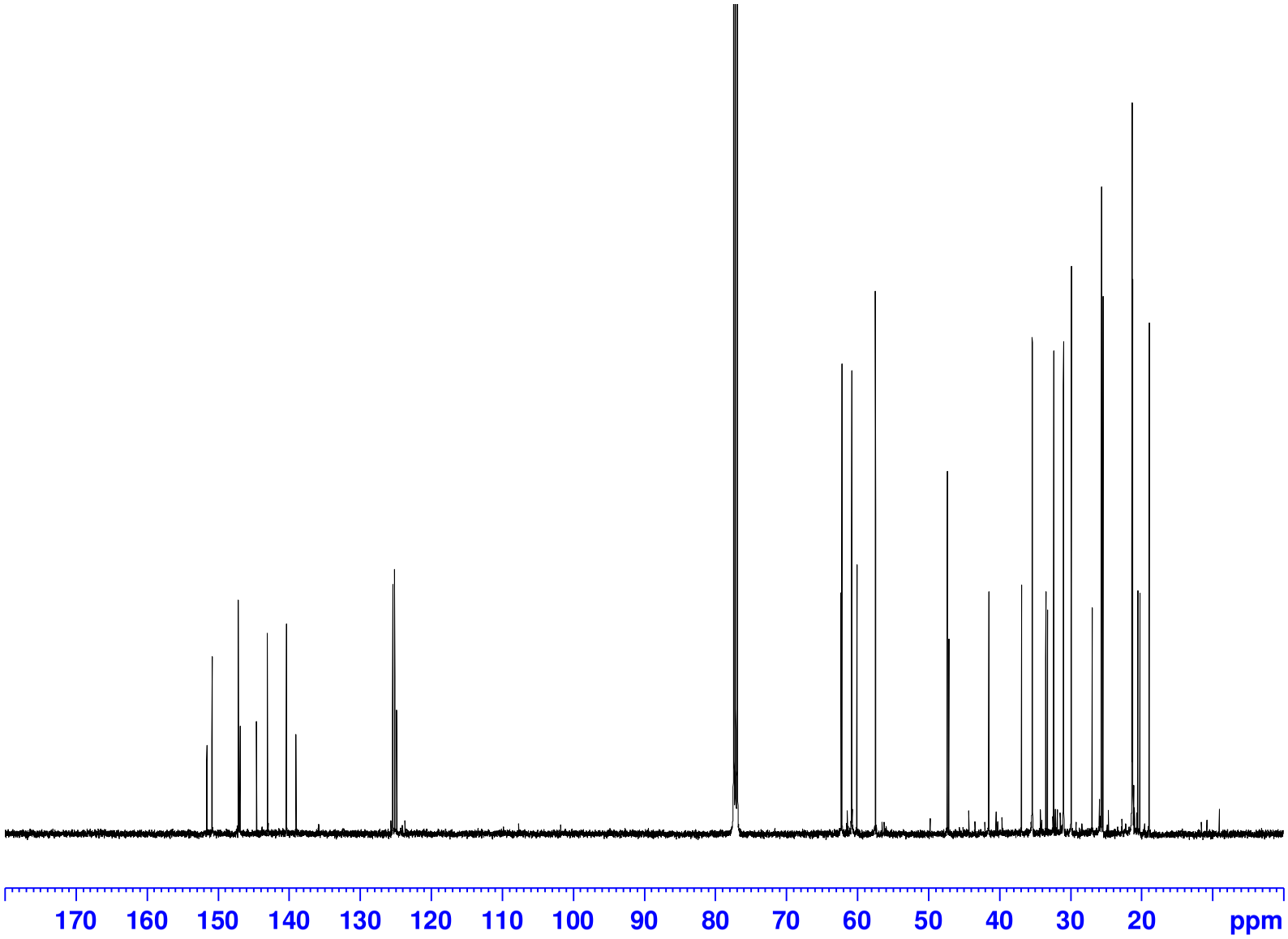

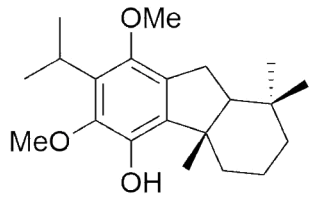

Current Data Parameters
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EXPNO 2
PROCNO 1

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TD	65536
SOLVENT	CDCl3
NS	3072
DS	4
SWH	31250.000 Hz
FIDRES	0.953674 Hz
AQ	1.0485760 sec
RG	203
DW	16.000 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	3
SFO1	125.7716224 MHz
NUC1	13C
P1	10.10 usec
PLW1	88.91999817 W
SFO2	500.1320005 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	80.00 usec
PLW2	15.48799992 W
PLW12	0.34847999 W
PLW13	0.17528000 W

F2 - Processing parameters

SI	65536
SF	125.7577720 MHz
WDW	EM
SSB	0
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GB	0
PC	1.40

Cartesian co-ordinates for calculated structures

Compound 16:

C	-0.575083	-0.721666	1.054015
C	-3.030288	0.468738	0.611682
C	-1.552653	-1.464580	0.387497
C	-0.767993	0.605063	1.464227
C	-2.013079	1.176881	1.242988
C	-2.802789	-0.838609	0.179024
C	1.129325	2.234401	1.038065
C	2.456219	2.149912	0.766851
C	3.330309	1.055259	1.316877
C	0.373132	1.405524	2.048976
C	3.146202	3.220778	-0.033476
C	3.385490	2.767128	-1.481151
C	2.040848	2.429663	-2.118111
C	1.279094	1.293221	-1.536550
C	-0.197119	1.330015	-1.680165
C	1.913686	-0.033477	-1.387230
O	0.676524	-1.275390	1.260692
C	0.780324	-2.052752	2.451615
C	-1.250797	-2.866081	-0.119653
C	-1.325156	-2.945261	-1.652420
C	-2.119915	-3.941418	0.547746
O	-3.736492	-1.579682	-0.458616
C	-5.027898	-1.036047	-0.657577
H	-3.992866	0.942721	0.464425
H	-2.201325	2.197848	1.565835
H	0.583607	3.090846	0.640394
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H	3.708487	1.348347	2.304128
H	4.205544	0.888842	0.681073
H	1.061027	0.756786	2.591842
H	-0.031869	2.116067	2.780953
H	2.551248	4.140189	-0.039796
H	4.108176	3.459585	0.433438
H	4.063471	1.908086	-1.514255
H	3.863302	3.565583	-2.055023
H	1.406241	3.319592	-2.178690
H	2.210908	2.093807	-3.157458
H	-0.632867	2.277917	-1.361150
H	-0.372793	1.252646	-2.766554
H	-0.700407	0.491633	-1.200339
H	3.002795	-0.003900	-1.372659
H	1.588014	-0.626357	-2.257448
H	1.537942	-0.570395	-0.508854
H	0.113371	-2.920487	2.413754
H	1.815747	-2.390345	2.513822
H	0.532115	-1.448474	3.332111
H	-0.210631	-3.071054	0.149005
H	-2.342429	-2.780853	-2.013961

H	-0.995624	-3.932790	-1.991261
H	-0.669792	-2.196729	-2.115012
H	-3.170990	-3.827708	0.274415
H	-2.045458	-3.889064	1.639249
H	-1.788547	-4.936344	0.233069
H	-4.992839	-0.143330	-1.293575
H	-5.600957	-1.814326	-1.160560
H	-5.507333	-0.790623	0.296832

Compound TS8a:

C	-0.917343	-1.227154	-0.142987
C	0.252424	-3.009846	-1.896733
C	-1.150605	-2.588756	0.057625
C	-0.064660	-0.732544	-1.140505
C	0.501374	-1.646069	-2.018614
C	-0.541103	-3.481922	-0.852129
C	0.958957	1.306784	-0.034800
C	2.254672	1.692039	-0.000721
C	3.185020	1.517426	-1.178330
C	0.230811	0.753195	-1.236683
C	2.824925	2.338341	1.232999
C	2.681645	3.875583	1.181136
C	1.214622	4.294601	1.383937
C	0.290262	4.106981	0.253284
C	-1.109002	3.718712	0.522999
C	0.636608	4.653068	-1.081004
O	-1.522628	-0.287172	0.678560
C	-2.838534	0.036602	0.254012
C	-1.958720	-3.067802	1.254072
C	-1.073753	-3.852166	2.236557
C	-3.218431	-3.859866	0.875464
O	-0.773639	-4.799742	-0.642366
C	-0.088031	-5.747303	-1.437786
H	0.689903	-3.694282	-2.613430
H	1.138267	-1.298967	-2.828500
H	0.397977	1.283833	0.897069
H	3.082802	2.303091	-1.941003
H	3.002126	0.557961	-1.674941
H	4.229053	1.520139	-0.850985
H	-0.709699	1.311535	-1.343887
H	0.806139	0.937914	-2.149374
H	2.332445	1.967940	2.139025
H	3.890846	2.108554	1.329060
H	3.065936	4.268715	0.232635
H	3.274441	4.334937	1.976592
H	0.806450	3.858960	2.300188
H	1.204348	5.393601	1.521437
H	-1.181649	2.864480	1.198814
H	-1.561402	4.573154	1.058675
H	-1.691824	3.552152	-0.384452
H	1.136148	3.853849	-1.651303

H	1.348432	5.484541	-1.014332
H	-0.253719	4.948973	-1.646786
H	-3.501751	-0.834570	0.300667
H	-3.211159	0.805736	0.934566
H	-2.840190	0.419258	-0.776126
H	-2.282818	-2.166175	1.781940
H	-0.726523	-4.790045	1.796777
H	-1.640443	-4.088469	3.143518
H	-0.198327	-3.261749	2.526961
H	-2.964554	-4.813859	0.408242
H	-3.851135	-3.298889	0.178584
H	-3.808341	-4.066665	1.775158
H	0.998066	-5.611701	-1.368670
H	-0.355969	-6.724577	-1.035986
H	-0.398751	-5.692368	-2.488120

Compound 8a:

C	-0.557461	1.179561	-0.834195
C	0.873957	-0.215796	-2.747112
C	0.045450	1.906469	-1.862880
C	-0.435007	-0.214690	-0.708521
C	0.282794	-0.891469	-1.686863
C	0.760692	1.172819	-2.834915
C	-1.057604	-0.964529	0.448578
C	-0.050221	-1.681496	1.379041
C	-0.625303	-2.949488	2.111025
C	0.472595	-3.581113	2.987224
C	1.057581	-2.621960	4.011945
C	1.580854	-1.353387	3.334524
C	0.760806	-0.793667	2.244056
C	0.896884	0.630573	1.959933
C	-1.050660	-4.004645	1.079120
C	-1.838104	-2.535991	2.959302
O	-1.248705	1.848252	0.158308
C	-2.619137	2.089197	-0.151767
C	-0.051633	3.423823	-1.899871
C	-0.808268	3.938602	-3.133133
C	1.326351	4.089109	-1.759523
O	1.318990	1.895958	-3.829307
C	2.028324	1.227264	-4.854701
H	1.413901	-0.778596	-3.498250
H	0.373294	-1.975428	-1.639119
H	-1.727253	-1.728001	0.047581
H	0.050994	-4.451254	3.500798
H	1.274247	-3.963726	2.339916
H	0.306201	-2.341540	4.756469
H	1.878320	-3.091421	4.559819
H	1.852700	-0.566941	4.044799
H	2.526448	-1.585050	2.800638
H	1.296361	0.737815	0.937581

H	-0.090960	1.110543	1.857604
H	1.527154	1.161782	2.671759
H	-0.226162	-4.261906	0.404055
H	-1.348869	-4.919685	1.600296
H	-1.905125	-3.692833	0.473513
H	-1.598932	-1.737839	3.672507
H	-2.661790	-2.181182	2.332903
H	-2.207257	-3.393932	3.530130
H	-3.155280	1.145428	-0.310581
H	-2.713778	2.708524	-1.049594
H	-3.043524	2.617452	0.702648
H	-0.626088	3.714535	-1.015924
H	-0.955547	5.020485	-3.052745
H	-1.794133	3.468807	-3.221454
H	-0.253548	3.736401	-4.052005
H	1.964219	3.873243	-2.619271
H	1.837119	3.744658	-0.853592
H	1.206731	5.174839	-1.685449
H	2.365948	2.007260	-5.536364
H	2.898738	0.693657	-4.455038
H	1.380977	0.527481	-5.395620
H	0.774408	-2.071853	0.737283
H	-1.682690	-0.295120	1.044436

Compound TS17:

C	1.463947	1.282069	-2.990651
C	-0.160856	-0.463511	-4.005803
C	-0.180890	-1.304432	-2.684499
C	1.406709	0.377121	-1.720973
C	1.127720	0.350321	-4.179461
H	-1.039390	0.189814	-4.032803
H	0.624316	-2.042886	-2.730736
H	2.127283	-0.420293	-1.939413
H	1.965923	-0.343440	-4.328746
H	-0.275010	-1.168841	-4.834057
H	-1.138954	-1.818581	-2.575034
H	1.052335	0.945498	-5.096211
C	0.508830	2.482106	-2.936841
H	0.697959	3.135009	-3.794427
H	0.664665	3.080985	-2.033485
H	-0.546662	2.198973	-2.974864
C	2.900749	1.803212	-3.130902
H	3.015280	2.342368	-4.076783
H	3.628997	0.984397	-3.121340
H	3.152522	2.496996	-2.321823
C	1.742019	0.923880	-0.330592
H	1.339450	1.926187	-0.160462
H	2.822327	0.975686	-0.164625
C	1.037628	-0.049107	0.594622
C	0.269756	0.405129	1.675309
C	-0.667465	-0.406109	2.319985

C	-0.800526	-1.760386	1.881457
O	0.346667	1.729330	2.000707
O	-1.698593	-2.499293	2.550379
C	1.421360	2.061964	2.877672
H	1.308512	1.548448	3.839330
H	1.371207	3.140079	3.028271
H	2.388520	1.795080	2.434754
C	-1.875023	-3.861035	2.194181
H	-2.645620	-4.241890	2.862556
H	-0.949819	-4.428907	2.341466
H	-2.211962	-3.955724	1.155393
C	-1.534937	0.171573	3.419485
H	-1.236328	1.217752	3.515847
C	-3.023984	0.167786	3.037026
H	-3.595341	0.695802	3.806468
H	-3.418406	-0.847242	2.955810
H	-3.186733	0.686662	2.086238
C	-1.284300	-0.506687	4.776513
H	-1.831271	0.034377	5.554729
H	-0.221345	-0.489372	5.039552
H	-1.623366	-1.544355	4.778567
C	-0.023969	-2.246415	0.843307
H	-0.079605	-3.283691	0.537799
C	-1.158004	0.398487	-1.095057
H	-0.946808	1.358230	-0.622884
H	-1.669488	-0.245333	-0.366063
H	-1.867463	0.545429	-1.917523
C	0.868952	-1.388024	0.178534
H	1.581947	-1.840136	-0.501695
C	0.056537	-0.295065	-1.618200

Compound 17:

C	1.487141	1.244670	-2.983556
C	0.388016	-0.887281	-3.990860
C	0.088761	-0.456049	-1.533835
C	0.235946	-1.539062	-2.604025
C	1.291258	0.517259	-1.640706
C	1.539317	0.126627	-4.055623
H	-0.553300	-0.407255	-4.281480
H	1.128952	-2.144019	-2.392852
H	2.173094	-0.140829	-1.569985
H	2.488443	-0.415105	-3.938452
H	0.560793	-1.673412	-4.732676
H	-0.625243	-2.218133	-2.600358
H	1.567534	0.583900	-5.051289
C	0.408360	2.286022	-3.317334
H	0.727804	2.874951	-4.183246
H	0.250465	2.989711	-2.491856
H	-0.557162	1.845426	-3.570779
C	2.843759	1.966653	-2.950637
H	3.090738	2.359232	-3.942415

H	3.653566	1.291604	-2.649278
H	2.829138	2.815583	-2.257022
C	1.268089	1.302399	-0.319895
H	0.639686	2.202675	-0.364091
H	2.262654	1.633985	-0.006886
C	0.342917	-0.936022	-0.049211
H	1.307529	-1.483472	-0.104094
C	0.636360	0.330972	0.638669
C	0.154442	0.570571	1.908313
C	-0.743024	-0.352916	2.511760
C	-1.113964	-1.565462	1.822410
O	0.375611	1.716561	2.584704
O	-1.975613	-2.350466	2.486343
C	1.689674	2.272519	2.611142
H	2.448199	1.484222	2.567229
H	1.771151	2.803390	3.559565
H	1.833086	2.980566	1.790939
C	-2.406245	-3.557306	1.873788
H	-3.108147	-4.006843	2.573933
H	-1.562859	-4.237860	1.712230
H	-2.913910	-3.353823	0.923917
C	-1.322590	-0.017502	3.859061
H	-0.874305	0.931521	4.153256
C	-2.847040	0.202756	3.782369
H	-3.190989	0.565057	4.755411
H	-3.380922	-0.719273	3.548435
H	-3.100044	0.961166	3.035372
C	-0.933225	-1.058333	4.928875
H	-1.256412	-0.680535	5.903176
H	0.150999	-1.201642	4.969858
H	-1.411277	-2.022910	4.755885
C	-0.591274	-1.852971	0.594978
H	-0.817803	-2.780534	0.081438
C	-1.309518	0.184170	-1.578928
H	-1.368412	1.114793	-1.005645
H	-2.050099	-0.509614	-1.167938
H	-1.620106	0.409667	-2.598104

Compound TS18:

C	-2.661414	-1.847452	-0.600547
C	-1.688689	-1.803205	1.813612
C	-1.741351	0.254107	0.473243
C	-1.219735	-0.298430	1.752854
C	-1.565863	-0.747547	-0.663708
C	-2.898408	-2.137023	0.916245
H	-1.928663	-2.036549	2.853797
H	-0.122033	-0.274010	1.750271
H	-0.645399	-1.289181	-0.423409
H	-3.143352	-3.196135	1.045332
H	-0.845743	-2.444050	1.537808
H	-1.571293	0.275409	2.614204

H	-3.779931	-1.589830	1.270903
C	-3.965570	-1.465322	-1.306991
H	-4.693236	-2.277818	-1.210543
H	-3.797499	-1.300360	-2.376903
H	-4.430300	-0.565417	-0.894701
C	-2.079758	-3.097691	-1.281447
H	-2.825018	-3.898936	-1.303075
H	-1.197175	-3.471226	-0.750191
H	-1.786532	-2.886775	-2.315459
C	-1.189984	0.073556	-1.902435
H	-2.004805	0.702434	-2.273256
H	-0.816493	-0.546772	-2.716487
C	-0.516626	1.897689	-0.326069
H	-1.395757	2.481025	-0.569365
C	-0.106556	0.885060	-1.218290
C	1.186097	0.362339	-1.071680
C	2.071361	0.825317	-0.093845
C	1.643118	1.892566	0.759100
O	1.522431	-0.718869	-1.836489
O	2.551400	2.318851	1.651162
C	2.106818	-0.389919	-3.096740
H	1.422487	0.220865	-3.698137
H	2.298207	-1.336560	-3.601622
H	3.049303	0.152300	-2.958918
C	2.207244	3.379097	2.528304
H	1.987089	4.295902	1.970038
H	3.082558	3.537489	3.156190
H	1.350100	3.107605	3.155795
C	3.426077	0.167933	0.064833
H	3.456693	-0.636466	-0.673601
C	4.580249	1.133466	-0.253192
H	4.652283	1.933529	0.486194
H	4.459291	1.587225	-1.242579
H	5.522973	0.577973	-0.251355
C	3.587482	-0.492638	1.444077
H	4.523123	-1.059539	1.463416
H	2.769824	-1.194547	1.641278
H	3.618833	0.246148	2.247043
C	0.379428	2.432501	0.626709
H	0.060775	3.274335	1.228788
C	-2.974916	1.103838	0.572354
H	-2.821081	1.948580	1.247984
H	-3.752947	0.478931	1.029293
H	-3.349118	1.456197	-0.389794

Compound 18:

C	-2.804434	-1.473384	-0.899304
C	-3.462360	-1.061791	1.591130
C	-1.745971	0.467184	0.564242
C	-2.190303	-0.234601	1.853534
C	-1.575142	-0.628058	-0.529581

C	-3.306091	-2.069243	0.441601
H	-4.306782	-0.392379	1.393258
H	-1.390570	-0.903501	2.200494
H	-0.894218	-1.356381	-0.056946
H	-2.594428	-2.845726	0.755643
H	-3.724586	-1.605125	2.504556
H	-2.376628	0.491631	2.654589
H	-4.261502	-2.579255	0.272211
C	-3.919199	-0.712233	-1.632729
H	-4.631904	-1.428343	-2.054527
H	-3.524603	-0.119587	-2.466240
H	-4.487508	-0.044301	-0.983863
C	-2.347458	-2.626441	-1.808582
H	-3.156837	-3.353079	-1.934282
H	-1.485826	-3.157151	-1.386684
H	-2.073154	-2.266625	-2.806811
C	-0.704675	0.045779	-1.612441
H	-1.254304	0.813392	-2.171866
H	-0.260404	-0.649591	-2.328049
C	-0.293117	1.075057	0.559151
H	-0.405715	2.172579	0.389841
C	0.328176	0.627542	-0.698579
C	1.696720	0.536476	-0.822362
C	2.519887	0.680148	0.321563
C	1.918917	0.883562	1.621525
O	2.267138	0.119353	-1.979162
O	2.792558	0.885384	2.640964
C	2.097963	0.974449	-3.111590
H	1.039800	1.113217	-3.356031
H	2.597742	0.474005	-3.940081
H	2.566685	1.947130	-2.929690
C	2.293664	1.062151	3.959027
H	1.578234	0.271787	4.213787
H	1.824184	2.046006	4.071420
H	3.161258	0.996067	4.613034
C	4.010611	0.512670	0.249223
H	4.407942	0.879851	1.196743
C	4.331184	-0.999134	0.177113
H	5.417344	-1.125336	0.197504
H	3.947897	-1.435886	-0.748710
H	3.910712	-1.537401	1.031297
C	4.695680	1.293032	-0.883190
H	5.768815	1.326035	-0.674761
H	4.339679	2.327089	-0.937121
H	4.555583	0.816023	-1.853604
C	0.571984	1.061881	1.748401
H	0.115527	1.300240	2.702176
C	-2.710283	1.619017	0.226140
H	-2.582129	2.425350	0.957846
H	-3.755872	1.320456	0.267839
H	-2.529881	2.040003	-0.769064

Compound 19:

C	-0.144511	-0.624069	-1.106869
C	2.560587	-1.022167	-0.729790
C	0.746873	0.195503	-1.814455
C	0.265920	-1.642299	-0.232223
C	1.634882	-1.813033	-0.056037
C	2.123427	-0.042050	-1.623007
C	-0.603068	-2.554690	1.979221
C	-1.342474	-1.865234	2.855420
C	-1.182113	-2.083110	4.340079
C	-0.728502	-2.544600	0.473249
C	-2.408470	-0.873664	2.441302
C	-2.259213	0.498673	3.119437
C	-0.860868	1.105162	2.949727
C	-0.417969	1.546034	1.617257
C	-1.368941	2.029163	0.632533
C	1.018366	1.511702	1.335341
O	-1.503888	-0.376970	-1.208398
C	-2.175473	-1.062229	-2.266061
C	0.236634	1.250377	-2.786694
C	0.507996	0.837300	-4.243073
C	0.773123	2.666565	-2.526563
O	2.969786	0.734963	-2.338005
C	4.361442	0.485576	-2.262355
H	3.617871	-1.199469	-0.574193
H	1.995699	-2.590306	0.611956
H	-0.842428	-1.183337	4.869764
H	-0.464530	-2.879393	4.551828
H	-2.141086	-2.365465	4.791858
H	-0.574780	-3.570292	0.116732
H	-2.414631	-0.740394	1.354640
H	-3.397334	-1.265244	2.713197
H	-2.433874	0.408819	4.195479
H	-3.030108	1.180920	2.747665
H	-0.817649	2.067966	3.502289
H	-0.087936	0.478439	3.407034
H	-0.937260	2.757716	-0.056401
H	-1.623047	1.140998	-0.000280
H	-2.310034	2.372057	1.066763
H	1.321483	2.101900	0.471742
H	1.256901	0.449621	1.128614
H	1.599150	1.763514	2.230314
H	-2.024794	-2.143560	-2.178967
H	-3.235514	-0.827614	-2.163332
H	-1.814385	-0.722491	-3.241631
H	-0.848270	1.295371	-2.650132
H	1.581908	0.813572	-4.445005
H	0.045638	1.552697	-4.930952
H	0.101579	-0.155908	-4.459349
H	1.841193	2.737497	-2.736095

H	0.615529	2.983076	-1.488444
H	0.248017	3.380923	-3.168525
H	4.746820	0.667767	-1.251996
H	4.598731	-0.539546	-2.568292
H	4.824730	1.187014	-2.955396
H	-1.742204	-2.272232	0.178245
H	0.141068	-3.241522	2.380832

Compound TS8b:

C	-0.380955	-1.176113	0.312849
C	1.108942	-2.646403	2.107523
C	-0.441837	-2.566611	0.221024
C	0.432089	-0.496348	1.231174
C	1.174490	-1.257381	2.121027
C	0.319528	-3.297282	1.160473
C	1.488005	1.344557	-0.040339
C	2.201192	2.458814	-0.242388
C	3.124531	2.586472	-1.426621
C	0.596138	1.001195	1.136936
C	2.139507	3.661147	0.673871
C	0.756015	4.323306	0.754114
C	0.081974	4.455566	-0.661970
C	-0.881055	3.389025	-0.952906
C	-2.113786	3.335385	-0.144946
C	-0.753313	2.447646	-2.061835
O	-1.141428	-0.393653	-0.556878
C	-2.501827	-0.304449	-0.159127
C	-1.249042	-3.250814	-0.872818
C	-2.393661	-4.115354	-0.323101
C	-0.349815	-4.051277	-1.828245
O	0.230814	-4.644932	1.072383
C	0.987992	-5.441145	1.962393
H	1.692247	-3.208953	2.825727
H	1.823647	-0.763795	2.839014
H	2.882539	3.464031	-2.041765
H	3.100481	1.699441	-2.065227
H	4.158237	2.727791	-1.088199
H	1.024787	1.391018	2.068485
H	2.431320	3.384020	1.694951
H	2.866399	4.408047	0.338795
H	0.847306	5.326363	1.177025
H	0.101838	3.759141	1.424015
H	-0.519714	5.378545	-0.636652
H	0.835783	4.549197	-1.444897
H	-2.858676	3.911099	-0.722469
H	-2.511872	2.322951	-0.054912
H	-2.021679	3.816644	0.830139
H	-1.689618	2.428737	-2.638982
H	-0.691654	1.429996	-1.620007
H	0.108989	2.629041	-2.702337
H	-3.023469	0.267469	-0.932241

H	-2.967940	-1.291299	-0.085072
H	-2.594283	0.194549	0.816080
H	-1.693851	-2.452630	-1.474850
H	-2.005774	-4.975833	0.226170
H	-3.012205	-4.484212	-1.148344
H	-3.039165	-3.547479	0.357052
H	0.121414	-4.894759	-1.319819
H	0.437395	-3.415900	-2.247087
H	-0.948584	-4.441663	-2.658143
H	2.062714	-5.258117	1.844768
H	0.695974	-5.263754	3.004106
H	0.765783	-6.474560	1.697086
H	-0.392083	1.473066	1.035523
H	1.579212	0.550456	-0.780527

Compound 8b:

C	0.706736	-0.324743	1.176928
C	-1.699902	-1.269949	2.196606
C	0.751880	-1.329560	2.142875
C	-0.502919	0.274095	0.761564
C	-1.694509	-0.214708	1.295643
C	-0.487756	-1.821908	2.618746
C	-0.485269	1.464477	-0.136250
C	-0.180766	1.210533	-1.708885
C	0.020858	2.530809	-2.513299
C	-1.319767	3.272797	-2.649517
C	-2.418341	2.412604	-3.269496
C	-2.564868	1.057416	-2.553197
C	-1.297051	0.405338	-2.167711
C	-1.230816	-1.047587	-2.044894
C	0.563101	2.118544	-3.894461
C	1.057401	3.435013	-1.838202
O	1.850911	0.200723	0.625119
C	2.563832	-0.648979	-0.263846
C	2.076919	-1.812509	2.714367
C	2.387406	-3.271671	2.350246
C	2.173229	-1.574620	4.230234
O	-0.415257	-2.835390	3.500579
C	-1.603854	-3.333704	4.089210
H	-2.642909	-1.631012	2.586764
H	-2.639088	0.249463	1.020185
H	0.349349	2.109675	0.141136
H	-1.641975	3.635191	-1.665160
H	-1.167971	4.165382	-3.265618
H	-3.379821	2.930644	-3.233855
H	-2.207050	2.223421	-4.326560
H	-3.065028	1.217091	-1.576602
H	-3.210765	0.363098	-3.097242
H	-0.267730	-1.444872	-2.379961
H	-1.240855	-1.228143	-0.944690

H	-2.065704	-1.579402	-2.501825
H	-0.086458	1.396397	-4.405117
H	0.662386	2.993663	-4.544189
H	1.553110	1.658676	-3.801408
H	0.666644	3.924556	-0.941096
H	1.957179	2.873475	-1.561050
H	1.360410	4.226221	-2.531074
H	3.097502	-1.446016	0.261020
H	3.286381	-0.015061	-0.780482
H	1.887770	-1.110924	-0.996488
H	2.849198	-1.178868	2.270388
H	3.392916	-3.536074	2.692910
H	2.344727	-3.436390	1.267505
H	1.676259	-3.953006	2.823004
H	1.487791	-2.216362	4.786402
H	1.952816	-0.531416	4.476946
H	3.192298	-1.792051	4.565657
H	-1.284845	-4.114633	4.778222
H	-2.128786	-2.548798	4.644916
H	-2.270924	-3.765976	3.334710
H	0.744141	0.628806	-1.713197
H	-1.412169	2.036226	-0.046514

Compound TS20:

C	-3.277318	-1.019305	-0.991287
C	-3.041325	-2.257501	1.314023
C	-1.102882	-1.163303	0.407342
C	-2.002730	-1.131316	1.587995
C	-1.729628	-1.131964	-0.975647
C	-3.846218	-2.066490	0.005099
H	-3.705634	-2.287627	2.181755
H	-1.452752	-1.318676	2.513306
H	-1.507704	-2.137232	-1.370345
H	-3.904419	-3.035624	-0.501918
H	-2.516752	-3.219042	1.300668
H	-2.536274	-0.188253	1.690495
H	-4.878274	-1.787385	0.240023
C	-3.829419	0.382273	-0.667520
H	-4.908307	0.389091	-0.851616
H	-3.395683	1.158134	-1.306613
H	-3.694604	0.685917	0.374109
C	-3.751526	-1.378850	-2.409113
H	-4.844558	-1.428021	-2.440836
H	-3.364696	-2.353051	-2.728038
H	-3.435687	-0.630303	-3.143741
C	-0.928546	-0.090551	-1.799211
H	-1.592987	0.618175	-2.300798
H	-0.336508	-0.580816	-2.571235
C	-0.558174	1.195823	0.334572
H	-1.620416	1.408957	0.368285
C	-0.012363	0.609518	-0.813631

C	1.387339	0.508966	-0.904060
C	2.230991	0.919557	0.126926
C	1.633147	1.502930	1.284569
O	1.911333	-0.132715	-1.992869
O	2.486581	1.895920	2.242812
C	2.202716	0.724878	-3.095235
H	2.610670	0.088060	-3.879979
H	2.941633	1.483297	-2.812808
H	1.293960	1.222334	-3.455806
C	1.975948	2.503831	3.417989
H	1.441845	3.430772	3.182044
H	2.845566	2.732187	4.032295
H	1.314429	1.818548	3.960499
C	3.729131	0.708767	0.015705
H	3.892103	0.222052	-0.948743
C	4.506980	2.034225	0.002324
H	5.562374	1.834053	-0.206796
H	4.440132	2.549116	0.962906
H	4.131723	2.707516	-0.775791
C	4.253921	-0.258011	1.089320
H	5.311704	-0.468011	0.903637
H	3.714779	-1.211273	1.055780
H	4.160832	0.162484	2.093015
C	0.255814	1.650573	1.377776
H	-0.200727	2.130887	2.234012
C	0.194577	-1.856180	0.595836
H	0.833726	-1.288454	1.285603
H	0.732824	-2.046904	-0.333185
H	-0.020668	-2.811983	1.096103

Compound 20:

C	-2.945744	-0.817359	-1.372813
C	-3.654424	-0.299871	1.032575
C	-1.317267	-1.322438	0.688042
C	-2.520039	-1.133586	1.619131
C	-1.695500	-1.574844	-0.808549
C	-4.074297	-0.860931	-0.324807
H	-3.364203	0.755883	0.946665
H	-2.911478	-2.133976	1.844267
H	-1.922999	-2.641245	-0.910197
H	-4.395210	-1.903115	-0.188196
H	-4.504193	-0.316465	1.722139
H	-2.183218	-0.725910	2.581182
H	-4.943484	-0.317379	-0.712267
C	-2.701805	0.649390	-1.786242
H	-3.599331	1.031155	-2.283004
H	-1.879223	0.759199	-2.500599
H	-2.512120	1.326499	-0.947484
C	-3.403595	-1.571979	-2.632186
H	-4.301405	-1.108456	-3.054191
H	-3.643433	-2.616194	-2.404068

H	-2.633935	-1.566508	-3.413091
C	-0.386713	-1.252651	-1.567314
H	-0.522722	-0.885188	-2.588339
H	0.255379	-2.137915	-1.666247
C	-0.411629	-0.049483	0.545658
H	-1.116623	0.759855	0.253478
C	0.337537	-0.292787	-0.683375
C	1.619015	0.185669	-0.843939
C	2.292122	0.794563	0.238505
C	1.616665	0.949159	1.508705
O	2.286204	-0.079800	-1.998321
O	2.353479	1.526389	2.470117
C	2.065993	0.871235	-3.041959
H	2.603222	0.497495	-3.912482
H	2.457369	1.855393	-2.759265
H	0.998126	0.958276	-3.275196
C	1.781914	1.687643	3.760218
H	2.558446	2.145775	4.370134
H	1.502926	0.717686	4.187330
H	0.908364	2.348260	3.722447
C	3.723336	1.220290	0.053509
H	3.981712	0.970665	-0.977307
C	3.896751	2.742386	0.223941
H	4.919565	3.005906	-0.060227
H	3.733113	3.057365	1.255291
H	3.214749	3.299583	-0.426575
C	4.677743	0.416499	0.958869
H	5.706136	0.672293	0.688250
H	4.550805	-0.659888	0.809584
H	4.529407	0.649666	2.014015
C	0.329267	0.522234	1.670348
H	-0.201020	0.667346	2.604706
C	-0.449504	-2.470244	1.230921
H	-0.176206	-2.283837	2.275023
H	0.478380	-2.610242	0.665740
H	-1.006401	-3.411469	1.197449

Compound TS21:

C	1.593158	1.366919	-2.861935
C	-0.754005	0.349970	-3.102651
C	0.806433	-0.628815	-1.509677
C	-0.641755	-0.340103	-1.709493
C	1.742684	0.562294	-1.519386
C	0.099412	1.617101	-3.151156
H	-1.809512	0.591308	-3.256034
H	-1.238634	-1.254804	-1.674965
H	2.773511	0.193855	-1.474220
H	0.005432	2.084828	-4.137417
H	-0.474797	-0.348849	-3.898189
H	-1.034854	0.360863	-0.970841
H	-0.302127	2.341790	-2.431040

C	2.333030	2.703841	-2.712049
H	2.289246	3.258508	-3.654699
H	3.389463	2.545460	-2.468574
H	1.891993	3.337722	-1.937174
C	2.248978	0.593645	-4.017887
H	2.220079	1.196115	-4.931122
H	1.755185	-0.355019	-4.246793
H	3.300195	0.378320	-3.797969
C	1.430865	1.357304	-0.235630
H	0.676973	2.127561	-0.416095
H	2.320692	1.865755	0.147914
C	1.314649	-0.969277	0.710708
H	2.308051	-1.187724	0.331890
C	0.856016	0.355047	0.737563
C	-0.308030	0.639569	1.470877
C	-1.028315	-0.349443	2.139058
C	-0.530168	-1.688427	2.089584
O	-0.806810	1.911456	1.408840
O	-1.255782	-2.599312	2.756648
C	-0.229065	2.816726	2.347153
H	-0.415672	2.480893	3.373533
H	-0.711245	3.780098	2.182110
H	0.852166	2.912690	2.188609
C	-0.820945	-3.948577	2.775760
H	-1.563717	-4.488747	3.360672
H	0.159812	-4.039812	3.255664
H	-0.781192	-4.364037	1.761983
C	-2.315868	0.004353	2.855866
H	-2.456767	1.076844	2.703063
C	-3.533798	-0.695984	2.231723
H	-4.447928	-0.311841	2.694535
H	-3.501729	-1.776637	2.385044
H	-3.593944	-0.495297	1.156726
C	-2.223314	-0.236880	4.371435
H	-3.124116	0.154790	4.853855
H	-1.359199	0.278124	4.804419
H	-2.144438	-1.300106	4.607023
C	0.632536	-1.987526	1.401404
H	1.043891	-2.989338	1.402241
C	1.270729	-1.965957	-1.982273
H	0.726384	-2.771832	-1.483999
H	2.346700	-2.111160	-1.874518
H	1.019463	-2.038240	-3.050116

Compound 21:

C	-1.543852	2.948419	-1.297362
C	0.453270	3.417708	0.252443
C	-0.953411	1.341321	0.721657
C	0.452609	1.973294	0.757862
C	-1.614664	1.523196	-0.685475

C	-0.112005	3.506971	-1.166591
H	1.478817	3.800005	0.265744
H	0.847852	1.923033	1.779276
H	-2.676716	1.257448	-0.581642
H	-0.105828	4.547551	-1.510218
H	-0.117163	4.059213	0.933662
H	1.140573	1.387176	0.131040
H	0.558519	2.962017	-1.846724
C	-1.938143	2.888768	-2.782738
H	-1.947080	3.897118	-3.208566
H	-2.942934	2.467852	-2.909118
H	-1.240165	2.293632	-3.380709
C	-2.549012	3.887382	-0.607101
H	-2.576011	4.849123	-1.129433
H	-2.304160	4.097228	0.435665
H	-3.560848	3.467755	-0.634814
C	-0.949892	0.431569	-1.562141
H	-0.082958	0.808501	-2.121023
H	-1.620920	0.005956	-2.315859
C	-0.815967	-0.229302	0.762342
H	-1.869212	-0.580689	0.850018
C	-0.439585	-0.581332	-0.601443
C	0.442211	-1.606260	-0.863600
C	1.110163	-2.256116	0.197821
C	0.822770	-1.877710	1.565573
O	0.788960	-1.870037	-2.151033
O	1.516482	-2.557349	2.491405
C	-0.069153	-2.796697	-2.820425
H	-0.019144	-3.783843	-2.346429
H	0.294843	-2.861802	-3.844811
H	-1.106636	-2.443058	-2.818278
C	1.329247	-2.227275	3.860181
H	2.005894	-2.875686	4.413898
H	0.297268	-2.422505	4.172529
H	1.588580	-1.179071	4.047810
C	2.146070	-3.297002	-0.127683
H	2.179695	-3.358827	-1.216942
C	3.552690	-2.872450	0.338578
H	4.275671	-3.596376	-0.048150
H	3.631541	-2.851564	1.426175
H	3.820367	-1.888585	-0.058134
C	1.746556	-4.686623	0.407875
H	2.458916	-5.421281	0.021580
H	0.747680	-4.977266	0.066572
H	1.769132	-4.723087	1.497712
C	-0.087866	-0.899293	1.841934
H	-0.335639	-0.633971	2.862986
C	-1.807402	1.810684	1.899501
H	-1.417601	1.417313	2.845164
H	-2.848888	1.487604	1.796572
H	-1.803526	2.897218	1.992864

Compound TS24:

C	-1.177561	-0.775110	0.331294
C	1.063417	-2.409799	0.203787
C	-0.784235	-1.454640	1.491975
C	-0.533912	-0.962268	-0.913316
C	0.568061	-1.809396	-0.946629
C	0.392221	-2.234439	1.413194
C	-1.062428	-0.296067	-2.169884
C	-0.023936	1.657284	-1.298521
C	1.230763	1.905397	-0.727849
C	2.462456	1.553405	-1.541222
C	2.193266	1.554116	-3.045876
C	1.020186	0.628787	-3.365337
C	-0.285177	0.996103	-2.622817
C	-1.208364	1.841236	-3.510908
C	1.397272	1.911982	0.773509
C	0.585701	3.440318	-1.230888
O	-2.277413	0.050205	0.302517
C	-2.415626	1.089769	1.259003
C	-1.651491	-1.479375	2.746648
C	-0.987929	-0.832927	3.971089
C	-2.141024	-2.903872	3.060868
O	0.792173	-2.818497	2.563888
C	1.859906	-3.747011	2.532035
H	1.933001	-3.051350	0.135623
H	1.048021	-2.035799	-1.894091
H	-2.111918	-0.033437	-2.021445
H	-1.016428	-0.991736	-3.014492
H	3.282247	2.227287	-1.270154
H	2.759334	0.547305	-1.217782
H	1.998561	2.572933	-3.406808
H	3.088224	1.214544	-3.573670
H	0.820188	0.615989	-4.441120
H	1.319670	-0.386482	-3.094307
H	-2.064408	2.237232	-2.953264
H	-0.669111	2.675852	-3.974610
H	-1.600316	1.218904	-4.320326
H	1.626414	0.886590	1.083038
H	2.223548	2.560741	1.075362
H	0.485891	2.222470	1.290263
H	-0.127995	3.580676	-2.050229
H	0.212463	3.929270	-0.335043
H	1.525508	3.865501	-1.586161
H	-3.350904	0.963437	1.809950
H	-2.464948	2.051131	0.729268
H	-1.580592	1.108135	1.964995
H	-2.555802	-0.912556	2.518319
H	-1.697728	-0.793644	4.803645
H	-0.656983	0.191922	3.764024
H	-0.116485	-1.407313	4.291938

H	-1.320631	-3.554173	3.369622
H	-2.629597	-3.348434	2.188372
H	-2.871859	-2.866380	3.875293
H	1.952673	-4.124925	3.549776
H	1.642301	-4.579060	1.852677
H	2.800104	-3.265469	2.238254
H	-0.898766	1.775636	-0.663475

Compound 24:

C	-0.142027	-0.038739	-1.068527
C	-1.820118	-1.929401	0.055093
C	-1.520629	0.215356	-1.083311
C	0.427699	-1.178672	-0.465272
C	-0.451477	-2.133491	0.044422
C	-2.356694	-0.754349	-0.492428
C	1.913073	-1.383362	-0.358995
C	2.551121	-0.989555	1.004286
C	0.957264	0.905394	1.510653
C	0.103969	0.066815	2.360219
C	0.650330	-1.280185	2.848930
O	0.711823	0.880179	-1.640712
C	0.948670	0.676491	-3.034332
C	-2.080480	1.459783	-1.757593
C	-2.914278	2.348141	-0.821551
C	-2.877666	1.105839	-3.024115
O	-3.678289	-0.500062	-0.519719
C	-4.583642	-1.454919	0.007938
H	-2.468538	-2.695631	0.462000
H	-0.052993	-3.057973	0.452564
H	2.434128	-0.835362	-1.148258
H	-0.187219	0.718479	3.202589
H	-0.848004	-0.045562	1.811602
H	0.790110	-1.222496	3.931782
H	-0.133062	-2.023366	2.691742
H	1.668897	1.436764	-3.338164
H	0.025118	0.794569	-3.609452
H	1.362455	-0.321818	-3.215126
H	-1.215775	2.054232	-2.066939
H	-3.176797	3.276306	-1.338871
H	-2.357232	2.620612	0.081024
H	-3.837816	1.854496	-0.515407
H	-3.791994	0.562447	-2.773512
H	-2.291276	0.483432	-3.708101
H	-3.159638	2.020599	-3.555047
H	-5.575497	-1.027514	-0.133316
H	-4.516700	-2.405612	-0.532195
H	-4.408161	-1.620146	1.077266
C	1.978023	-1.764916	2.213108
H	2.140684	-2.444054	-0.516685
H	1.883942	-2.818694	1.931655
H	2.750484	-1.740421	2.989423

C	4.048214	-1.327222	0.920244
H	4.176597	-2.414395	0.931469
H	4.603833	-0.919168	1.771449
H	4.504914	-0.955093	-0.000841
C	0.434322	2.216960	1.094678
H	-0.610505	2.359671	1.369865
H	0.573492	2.343663	0.012659
H	1.045785	2.998989	1.567660
C	2.365070	0.544797	1.271459
H	2.750623	0.664958	2.309646
C	3.157811	1.487947	0.366577
H	2.795489	1.439010	-0.661743
H	4.215073	1.221304	0.383019
H	3.087492	2.524945	0.705186

Compound 28:

C	-1.369701	2.236835	-0.801612
C	-0.838140	1.115337	-2.863168
C	-0.487993	1.462295	-1.563330
C	-2.582241	2.673381	-1.320529
C	0.798997	0.973881	-0.933187
C	0.512233	-0.233032	-0.019964
C	0.439309	-1.538100	-0.669873
H	1.217158	1.781326	-0.329632
H	1.536925	0.736283	-1.701829
C	-0.253393	-2.601408	0.056751
C	1.574122	-0.484677	1.210117
H	-0.430365	-0.049985	0.507054
H	-0.393737	-3.505050	-0.538776
H	-1.208559	-2.261450	0.466098
C	1.158650	-1.850153	-1.897212
H	0.583850	-1.339273	-2.704389
H	1.224276	-2.918543	-2.104692
H	2.138649	-1.365657	-1.945237
C	-2.925404	2.315130	-2.628838
C	0.948571	-1.617535	2.078112
C	0.712401	-2.890106	1.268528
H	1.645607	-3.326539	0.898441
H	0.213700	-3.659415	1.861047
H	-1.089326	2.518425	0.212121
H	-3.873950	2.653064	-3.032380
O	-2.317818	1.135806	-4.667893
C	-3.535847	1.534076	-5.271839
H	-3.524494	1.104274	-6.272902
H	-3.606081	2.625632	-5.343850
H	-4.398104	1.144677	-4.718342
C	2.966394	-0.769050	0.631214
H	3.176501	-0.094489	-0.205765
H	3.744151	-0.585283	1.371950
H	3.094179	-1.797162	0.279972
C	1.608105	0.814209	2.039765

H	0.579090	1.150841	2.225350
H	2.114732	1.610231	1.485697
C	1.626914	-1.866043	3.464142
C	2.316229	0.614137	3.384834
H	2.259920	1.552681	3.945439
H	3.384166	0.423883	3.229517
C	1.686134	-0.510760	4.199056
H	0.661800	-0.218830	4.471039
H	2.230775	-0.640537	5.141208
H	-0.050747	-1.239396	2.345413
C	3.021106	-2.507758	3.381887
H	3.783638	-1.843918	2.971432
H	3.014493	-3.424586	2.782375
H	3.348492	-2.786561	4.388791
C	0.732423	-2.803192	4.297162
H	-0.315961	-2.482352	4.283245
H	1.064476	-2.797811	5.340325
H	0.780890	-3.841828	3.953922
C	-2.069667	1.538392	-3.403506
O	-0.002939	0.317696	-3.610916
C	0.667443	0.981249	-4.683740
H	-0.052775	1.342758	-5.420844
H	1.321982	0.238840	-5.142647
H	1.264665	1.816606	-4.300904
C	-3.544860	3.478458	-0.480441
H	-4.032913	4.234908	-1.104735
H	-2.990672	4.021671	0.292807
C	-4.611577	2.595229	0.178798
H	-5.300051	3.198897	0.777339
H	-4.149177	1.851626	0.836854
H	-5.196654	2.057741	-0.574831

Compound 29:

C	0.223470	-0.954637	-2.165742
C	1.334925	1.173676	-2.337689
C	1.149610	-0.034669	-1.664648
C	-0.544421	-0.669769	-3.292246
C	1.898877	-0.264814	-0.368735
C	1.151512	0.249109	0.942259
C	0.318351	1.395843	0.539808
H	2.854619	0.257423	-0.413278
H	2.105825	-1.325471	-0.213654
C	-1.111392	1.182122	0.343505
C	0.385247	-0.813003	1.818377
H	1.951575	0.662885	1.568726
H	-1.203923	0.413975	-0.440418
H	-1.627874	2.081833	0.005222
C	0.875163	2.747917	0.492404
H	0.460765	3.334366	-0.332403
H	1.963021	2.779511	0.488742
H	0.500779	3.212970	1.424571

C	-0.390830	0.567831	-3.924967
C	-0.662415	0.018228	2.623005
C	-1.716384	0.622009	1.680431
H	-2.478447	-0.112838	1.415358
H	-2.222999	1.453186	2.175781
H	0.110134	-1.919475	-1.683899
H	-1.003518	0.793505	-4.791295
O	0.762673	2.705799	-4.002037
C	0.033873	3.068480	-5.163345
H	0.383477	4.064291	-5.433259
H	-1.042691	3.102993	-4.960170
H	0.231997	2.374573	-5.987989
C	-0.257702	-1.944039	1.005134
H	0.497018	-2.501406	0.443989
H	-0.740242	-2.663682	1.664389
H	-1.015169	-1.600213	0.297059
C	1.426139	-1.415956	2.786129
H	2.034181	-0.603964	3.209612
H	2.113593	-2.066395	2.230514
C	-1.280719	-0.638246	3.899284
C	0.790118	-2.167235	3.954997
H	1.582820	-2.539317	4.611805
H	0.248905	-3.053122	3.604480
C	-0.133627	-1.238353	4.740170
H	0.468895	-0.416269	5.153175
H	-0.564337	-1.766114	5.598737
H	-0.078842	0.865154	3.028285
C	-2.347262	-1.716647	3.635219
H	-1.946606	-2.630289	3.192333
H	-3.157346	-1.357242	2.993048
H	-2.803461	-2.002084	4.588730
C	-1.952149	0.467854	4.734958
H	-1.274598	1.313120	4.905033
H	-2.238203	0.073745	5.715557
H	-2.865036	0.847177	4.263306
C	0.543306	1.489980	-3.463231
O	2.255381	2.077062	-1.875404
C	3.413492	2.225274	-2.700662
H	4.068108	2.925826	-2.181215
H	3.144302	2.629278	-3.679074
H	3.922507	1.262148	-2.820676
C	-1.493628	-1.697629	-3.859962
H	-2.381778	-1.197122	-4.261896
H	-1.840105	-2.360346	-3.058978
C	-0.833271	-2.533522	-4.964316
H	-1.535335	-3.272455	-5.361173
H	0.042852	-3.065126	-4.579655
H	-0.503198	-1.897697	-5.792115

Compound TS30:

C	-1.081700	-2.680917	0.267860

C	1.697839	-3.224088	0.238344
C	-0.752764	-0.960779	-1.537668
C	-0.159233	0.139992	-0.644576
H	-0.362946	-0.954237	-2.559951
C	1.876197	0.482259	0.733175
C	-0.502070	1.669426	-0.814095
H	-0.552138	-0.088699	0.351340
H	2.955340	0.339297	0.825208
H	1.366543	0.021552	1.584456
C	0.904313	-3.692154	1.265946
C	0.047426	2.314517	0.502051
C	1.539978	2.023596	0.716962
H	2.160464	2.513976	-0.040735
H	1.872101	2.404121	1.685565
H	1.323209	-4.278862	2.077456
O	-1.093515	-3.982877	2.355282
C	-2.449869	-3.724580	2.720524
H	-3.145897	-4.174065	2.008780
H	-2.640004	-2.653935	2.804208
H	-2.564856	-4.204991	3.691632
C	0.057636	2.236525	-2.131698
H	0.036771	1.475991	-2.919467
H	-0.548522	3.068167	-2.492461
H	1.080535	2.611820	-2.047718
C	-2.039571	1.800883	-0.816268
H	-2.454742	1.179373	-0.010418
H	-2.443344	1.412569	-1.758988
C	-0.360888	3.797522	0.748092
C	-2.490426	3.250953	-0.614436
H	-3.583754	3.275919	-0.560039
H	-2.222970	3.859000	-1.486414
C	-1.902325	3.862672	0.656261
H	-2.321317	3.336846	1.526158
H	-2.219745	4.908163	0.745964
H	-0.475113	1.771712	1.306385
C	0.286581	4.803509	-0.216676
H	-0.070081	4.708756	-1.243690
H	1.378502	4.710466	-0.228762
H	0.055471	5.821950	0.112647
C	0.032145	4.203747	2.179888
H	-0.283104	3.453061	2.914552
H	-0.455362	5.148033	2.443589
H	1.110542	4.360628	2.287323
C	-0.483582	-3.457583	1.295963
O	-2.404522	-2.325649	0.333976
C	-3.253942	-3.086384	-0.522241
H	-2.964920	-2.967042	-1.573124
H	-4.264504	-2.704794	-0.372529
H	-3.218497	-4.151919	-0.266177
C	3.160981	-3.572042	0.152753
H	3.556980	-3.743811	1.159184

H	3.715093	-2.721910	-0.266090
C	3.406633	-4.813879	-0.716207
H	4.475821	-5.036012	-0.771038
H	3.036489	-4.663827	-1.735881
H	2.896047	-5.686302	-0.297561
C	-0.286327	-2.172404	-0.749068
C	1.096182	-2.441567	-0.770756
H	1.652855	-2.263898	-1.682571
C	1.329494	-0.004302	-0.543891
H	-1.837930	-0.877063	-1.579829
C	2.250084	0.047870	-1.716494
H	1.793733	-0.248974	-2.660127
H	3.150142	-0.543447	-1.529836
H	2.588355	1.088124	-1.814044

Compound 30:

C	2.259871	-1.371653	-2.156717
C	-0.450227	-0.823033	-3.052732
C	1.394330	-1.235041	0.214610
C	0.298020	-0.174905	0.424223
H	1.192892	-2.161606	0.765448
C	-1.925453	0.418007	-0.516521
C	0.051061	0.433977	1.820840
H	0.630617	0.679856	-0.187566
H	-2.862226	0.068926	-0.966815
H	-1.501192	1.181122	-1.183071
C	0.602283	-0.753209	-3.908884
C	-0.971416	1.589132	1.555299
C	-2.233733	1.081625	0.838969
H	-2.794634	0.390115	1.477452
H	-2.909357	1.918791	0.645167
H	0.460755	-0.492054	-4.952450
O	2.796469	-0.945948	-4.495540
C	4.202684	-1.272843	-4.432845
H	4.331638	-2.311961	-4.127815
H	4.716134	-0.600255	-3.749700
H	4.548436	-1.134806	-5.455036
C	-0.404115	-0.625135	2.847757
H	0.010047	-1.611081	2.612590
H	-0.054829	-0.377321	3.851505
H	-1.488792	-0.728619	2.911124
C	1.371714	1.065357	2.315835
H	1.818788	1.648193	1.496704
H	2.089717	0.275200	2.571561
C	-1.234039	2.548155	2.753107
C	1.171015	1.990118	3.518483
H	2.128424	2.455180	3.776819
H	0.875523	1.410210	4.400864
C	0.135971	3.077010	3.233090
H	0.535540	3.746343	2.457191
H	-0.010817	3.694881	4.127079

H	-0.459446	2.234182	0.820525
C	-2.008921	1.912358	3.918583
H	-1.433132	1.161693	4.463054
H	-2.937099	1.442000	3.575533
H	-2.287723	2.690117	4.637807
C	-2.046832	3.762501	2.268319
H	-1.630948	4.184655	1.345123
H	-2.029294	4.549715	3.029641
H	-3.097797	3.514047	2.088289
C	1.944141	-1.051009	-3.521738
O	3.563903	-1.423664	-1.773427
C	4.005780	-2.678961	-1.253748
H	3.442928	-2.957126	-0.357167
H	5.055958	-2.545314	-0.996786
H	3.904032	-3.469037	-2.006702
C	-1.842077	-0.614271	-3.579139
H	-1.775737	-0.350933	-4.638600
H	-2.296363	0.240731	-3.069777
C	-2.751098	-1.840317	-3.415323
H	-3.710479	-1.652602	-3.902928
H	-2.953178	-2.057563	-2.363253
H	-2.306501	-2.728485	-3.875173
C	1.234686	-1.395857	-1.264538
C	-0.207233	-1.300816	-1.653661
H	-0.532331	-2.357525	-1.748558
C	-0.928885	-0.735870	-0.353402
H	2.398842	-0.892690	0.471671
C	-1.629862	-1.936075	0.311048
H	-0.932421	-2.736305	0.579188
H	-2.365319	-2.362949	-0.378758
H	-2.168692	-1.657358	1.213871

Compound TS31:

C	-1.549807	-2.492816	-1.630377
C	1.178071	-3.225274	-1.425555
C	-1.357630	-1.092455	0.460064
C	-0.201665	-0.117275	0.712875
H	-1.695646	-1.529146	1.404792
H	-2.221984	-0.601961	0.005367
C	2.003851	0.505971	-0.277633
C	-0.498982	1.340627	1.260347
H	0.441299	-0.556297	1.481957
H	2.601232	0.557107	-1.190737
H	2.517884	-0.104626	0.469617
C	0.449097	-3.522221	-2.560769
C	0.910217	1.942518	1.563318
C	1.806416	1.948349	0.320007
H	1.416645	2.610511	-0.459937
H	2.810736	2.304168	0.560248
O	-1.446056	-3.543244	-3.854568
C	-2.809922	-3.333446	-4.216125

H	-2.888167	-3.734030	-5.226361
H	-3.066478	-2.273828	-4.209235
H	-3.482354	-3.887163	-3.555528
C	-1.346952	2.139442	0.255799
H	-2.122617	1.509095	-0.189784
H	-1.868176	2.961379	0.745618
H	-0.761733	2.575339	-0.558580
C	-1.271767	1.184028	2.584989
H	-0.770908	0.425145	3.202720
H	-2.284577	0.815235	2.383506
C	0.918284	3.279354	2.365519
C	-1.331468	2.495715	3.373446
H	-1.835889	2.311453	4.327564
H	-1.949331	3.231978	2.846855
C	0.064112	3.061166	3.634205
H	0.603625	2.370143	4.297771
H	-0.014630	4.010421	4.176848
H	1.371041	1.223230	2.259965
C	0.422260	4.501065	1.574656
H	-0.649260	4.482087	1.368777
H	0.946920	4.608797	0.618858
H	0.620939	5.409478	2.152807
C	2.357155	3.581619	2.824331
H	2.831529	2.703577	3.279011
H	2.345954	4.376859	3.576734
H	2.991309	3.930225	2.002329
C	-0.912811	-3.183647	-2.686265
O	-2.836209	-2.038512	-1.767832
C	-3.806118	-2.753788	-1.007427
H	-4.770140	-2.296242	-1.231103
H	-3.604800	-2.678886	0.067620
H	-3.823306	-3.812404	-1.291538
C	2.629615	-3.622617	-1.310702
H	2.768455	-4.620845	-1.739056
H	2.907797	-3.693842	-0.253299
C	3.559372	-2.631224	-2.021911
H	4.602438	-2.947066	-1.932931
H	3.473691	-1.629417	-1.586166
H	3.315834	-2.559073	-3.086962
C	-0.810492	-2.129742	-0.506103
C	0.544756	-2.498621	-0.403224
H	1.083166	-2.342601	0.526401
C	0.629607	0.035858	-0.515219
C	0.071474	0.233726	-1.873293
H	-1.015723	0.193043	-1.918866
H	0.480959	-0.538121	-2.542398
H	0.431300	1.193085	-2.266142
H	0.898556	-4.061364	-3.389291

Compound 31:

C	1.756128	-2.584134	1.630661

C	-1.144287	-2.609091	1.672962
C	1.646221	-0.751575	-0.133206
C	0.395922	-0.002640	-0.621896
H	2.244645	-1.143151	-0.962169
H	2.324885	-0.142638	0.476683
C	-2.040767	0.147875	-0.082888
C	0.516436	1.441293	-1.153440
H	0.037679	-0.580284	-1.488276
H	-2.818946	0.077483	0.685420
H	-2.324409	-0.535196	-0.895963
C	-0.432169	-3.318896	2.584291
C	-0.909395	1.765623	-1.713384
C	-1.997449	1.581953	-0.642372
H	-1.866903	2.300186	0.175087
H	-2.979406	1.796671	-1.072146
O	1.489898	-4.037653	3.571593
C	2.889946	-4.275270	3.837053
H	2.882447	-4.913934	4.717845
H	3.402669	-3.337353	4.037888
H	3.347717	-4.798441	2.997078
C	1.027030	2.417782	-0.073072
H	1.700426	1.918281	0.631101
H	1.599458	3.234925	-0.514782
H	0.224311	2.875155	0.508201
C	1.512925	1.434492	-2.333363
H	1.275283	0.587266	-2.994005
H	2.531248	1.267895	-1.957250
C	-1.024626	3.072216	-2.551915
C	1.464060	2.721064	-3.159465
H	2.143356	2.626930	-4.013404
H	1.839190	3.567966	-2.573167
C	0.049964	3.011808	-3.660494
H	-0.237096	2.224437	-4.372543
H	0.039638	3.953852	-4.221979
H	-1.093146	0.969564	-2.455572
C	-0.890343	4.366340	-1.732991
H	0.116051	4.530118	-1.343383
H	-1.584894	4.380310	-0.885562
H	-1.136053	5.226104	-2.365927
C	-2.396424	3.110465	-3.250335
H	-2.623948	2.158571	-3.745254
H	-2.401889	3.892089	-4.017454
H	-3.210719	3.338609	-2.555093
C	0.996921	-3.330047	2.600271
O	3.108376	-2.498681	1.757652
C	3.871628	-3.157517	0.745544
H	4.917049	-3.008656	1.013668
H	3.684156	-2.723822	-0.241049
H	3.643474	-4.229475	0.718408
C	-2.647056	-2.692654	1.637766
H	-2.932653	-3.750291	1.668111

H	-3.019109	-2.289950	0.692391
C	-3.319527	-1.965964	2.813903
H	-4.401728	-2.108185	2.761071
H	-3.120296	-0.891044	2.792833
H	-2.972143	-2.357894	3.774321
C	1.066319	-1.838494	0.727991
C	-0.420453	-1.816384	0.651027
H	-0.707106	-2.262640	-0.319608
C	-0.674637	-0.261904	0.474691
C	-0.416406	0.409476	1.834760
H	0.624438	0.323687	2.162193
H	-1.041795	-0.050696	2.605951
H	-0.663003	1.470087	1.813130
H	-0.921113	-3.936021	3.331864

Compound 32:

C	1.639122	-1.365218	2.109054
C	-1.207586	-1.300120	2.684578
C	1.037663	-1.856479	-0.313283
C	-0.064177	-1.006723	-0.997691
H	0.926136	-2.917080	-0.572749
H	2.053940	-1.562503	-0.580809
C	-1.352531	0.668110	0.440827
C	0.478483	0.302232	-1.664825
H	-0.488735	-1.595070	-1.816509
H	-0.455189	0.978915	0.987163
H	-2.190477	0.811353	1.132173
C	-0.299969	-0.962259	3.633588
C	-0.778598	1.132380	-2.043191
C	-1.568024	1.566454	-0.786983
H	-1.307411	2.589181	-0.498409
H	-2.634478	1.592343	-1.032086
O	1.805717	-0.558379	4.402249
C	3.246446	-0.458869	4.471017
H	3.431230	-0.057947	5.465327
H	3.617094	0.214278	3.701267
H	3.694367	-1.447668	4.372588
C	1.466031	1.095501	-0.769642
H	1.959305	0.470071	-0.019445
H	2.267003	1.532212	-1.370856
H	0.989868	1.924153	-0.241285
C	1.212777	-0.140263	-2.954148
H	0.598997	-0.890841	-3.471269
H	2.157129	-0.636452	-2.693195
C	-0.568038	2.286201	-3.070354
C	1.472653	0.999074	-3.938254
H	1.934564	0.590471	-4.843203
H	2.195828	1.714208	-3.528114
C	0.168324	1.708057	-4.296054
H	-0.495789	0.990834	-4.799938

H	0.358145	2.512868	-5.016362
H	-1.416306	0.418191	-2.588651
C	0.210269	3.500263	-2.533314
H	1.240807	3.266874	-2.259523
H	-0.272712	3.952774	-1.661051
H	0.248369	4.272626	-3.309142
C	-1.947833	2.786079	-3.531310
H	-2.573353	1.959118	-3.888544
H	-1.836883	3.498322	-4.355986
H	-2.487258	3.299457	-2.727841
C	1.109836	-0.961268	3.384220
O	2.976658	-1.286493	1.869553
C	3.644899	-2.539944	1.713265
H	4.680330	-2.301640	1.471937
H	3.203264	-3.124464	0.899449
H	3.603080	-3.122539	2.641431
C	-2.678822	-1.391855	2.978839
H	-3.032565	-2.360750	2.602604
H	-3.193500	-0.644798	2.361322
C	-3.092145	-1.215535	4.436679
H	-4.173917	-1.338039	4.526817
H	-2.843762	-0.217437	4.810695
H	-2.617915	-1.959664	5.083883
C	0.745827	-1.672376	1.134921
C	-0.723336	-1.659686	1.321406
H	-1.066059	-2.692253	1.135486
C	-1.217221	-0.812566	0.067718
H	-0.593780	-0.694714	4.641792
C	-2.542823	-1.365637	-0.466854
H	-2.453804	-2.425236	-0.731922
H	-2.844802	-0.826101	-1.368873
H	-3.354344	-1.263735	0.259814

Compound 33:

C	1.999617	-2.109281	-1.982477
C	-0.887907	-2.249940	-1.993734
C	1.842153	-0.449612	-0.066206
C	0.729423	0.622777	0.033113
H	2.021339	-0.944908	0.897758
C	-1.816996	0.253682	0.096644
C	0.468717	1.183283	1.456463
H	1.070371	1.483670	-0.552166
H	-1.838559	-0.489268	0.898882
H	-2.700621	0.058212	-0.520810
C	-0.166061	-2.905638	-2.945739
C	-0.638333	2.258628	1.266415
C	-1.951618	1.658650	0.705774
H	-2.714694	1.595232	1.487798
H	-2.360343	2.343461	-0.044389
H	-0.680891	-3.492894	-3.697501

O	1.989125	-3.446613	-3.860436
C	1.404053	-4.171320	-4.955598
H	0.770336	-3.509104	-5.549641
H	0.838396	-5.028149	-4.582071
H	2.249756	-4.510746	-5.549112
C	0.088556	0.076882	2.475269
H	0.306383	-0.930412	2.099576
H	0.648817	0.183672	3.408154
H	-0.969012	0.093879	2.744273
C	1.773316	1.880563	1.905969
H	2.155242	2.485311	1.070946
H	2.541374	1.126422	2.122286
C	-0.859671	3.233488	2.462095
C	1.586615	2.801717	3.110420
H	2.536208	3.299642	3.333314
H	1.335341	2.219199	4.005140
C	0.506232	3.846377	2.835689
H	0.840232	4.489819	2.008842
H	0.382601	4.500556	3.706891
H	-0.234485	2.910740	0.475352
C	-1.488897	2.592547	3.711031
H	-0.830799	1.871398	4.200434
H	-2.434526	2.085879	3.490077
H	-1.712063	3.375667	4.443652
C	-1.786582	4.369223	1.997268
H	-1.409791	4.841415	1.082037
H	-1.853913	5.144487	2.768197
H	-2.804079	4.013218	1.802226
C	1.258579	-2.853149	-2.963596
O	3.339551	-1.989719	-2.125526
C	4.110393	-3.024237	-1.509833
H	3.937953	-3.041506	-0.427697
H	5.152852	-2.782989	-1.712457
H	3.871377	-4.002391	-1.939891
C	-2.381135	-2.393931	-1.956152
H	-2.708481	-2.944827	-2.842919
H	-2.840148	-1.400952	-2.013231
C	-2.884671	-3.111674	-0.693361
H	-3.966909	-3.246894	-0.757967
H	-2.676518	-2.534733	0.211606
H	-2.424937	-4.099313	-0.590841
C	1.300427	-1.440980	-1.034680
C	-0.179596	-1.464615	-0.945770
H	-0.418671	-1.960974	0.012927
C	-0.536508	0.062960	-0.726968
C	-0.653675	0.761490	-2.088059
H	0.255255	0.629694	-2.686718
H	-0.798611	1.836431	-1.942776
H	-1.504127	0.391523	-2.670917
H	2.803239	-0.051029	-0.397278

Compound 34:

C	0.750641	0.242926	1.708577
C	-0.967856	0.089030	3.431196
C	-0.540876	-0.113232	2.130100
C	1.633571	0.858773	2.600178
C	-1.370542	-0.654699	0.991470
C	-0.565437	-0.128183	-0.204011
H	-2.399510	-0.284138	1.014445
H	-1.426834	-1.750667	1.025080
C	1.767913	0.604207	-0.712748
C	-0.897770	-0.568224	-1.644477
H	-0.760359	0.956160	-0.195561
H	2.837940	0.467686	-0.514780
C	1.188783	1.054221	3.914945
C	-0.006153	0.348315	-2.546761
C	1.482130	0.230284	-2.179144
H	1.848420	-0.783293	-2.382355
H	2.075554	0.893680	-2.816042
H	1.839003	1.530444	4.644384
O	-0.438693	0.925455	5.641799
C	-0.648596	-0.240460	6.426000
H	-0.895576	0.106323	7.431223
H	0.264083	-0.848831	6.464820
H	-1.470853	-0.845526	6.030098
C	-0.693443	-2.084244	-1.853939
H	-0.894229	-2.633223	-0.929128
H	0.317299	-2.341439	-2.176093
H	-1.376974	-2.482599	-2.607555
C	-2.377361	-0.229246	-1.926497
H	-2.580042	0.791681	-1.570620
H	-3.025686	-0.897872	-1.345669
C	-0.313774	0.307376	-4.072247
C	-2.735255	-0.308274	-3.411551
H	-3.778238	-0.001705	-3.553057
H	-2.678841	-1.345398	-3.763724
C	-1.823548	0.580427	-4.256724
H	-2.014752	1.629828	-3.987717
H	-2.080796	0.481356	-5.319620
H	-0.297742	1.371795	-2.254497
C	0.085142	-1.006147	-4.764440
H	-0.531673	-1.854514	-4.461681
H	1.130672	-1.263002	-4.560396
H	-0.019184	-0.896676	-5.850547
C	0.440660	1.446936	-4.781607
H	0.310003	2.400900	-4.256453
H	0.057731	1.571808	-5.801457
H	1.513989	1.246546	-4.861209
C	-0.074360	0.670260	4.342938
O	-2.236971	-0.290178	3.793245
C	-3.101190	0.798870	4.086562

H	-2.742361	1.369149	4.949754
H	-4.078373	0.365430	4.308463
H	-3.187584	1.466972	3.220146
C	3.033255	1.324371	2.253903
H	3.280966	2.169903	2.906359
H	3.067879	1.712297	1.233217
C	4.107484	0.244923	2.429313
H	5.106910	0.663860	2.270513
H	3.972536	-0.574563	1.717309
H	4.070235	-0.179061	3.438201
H	1.544637	1.670263	-0.569190
C	0.918942	-0.227781	0.256841
C	1.480055	-1.666093	0.340494
H	2.403180	-1.660239	0.926729
H	1.715860	-2.086151	-0.638882
H	0.785959	-2.346799	0.842077

Compound 35:

C	0.998055	0.011322	1.371596
C	-0.604777	-0.972249	2.919390
C	-0.241504	0.016131	2.020287
C	1.934964	-0.991333	1.653020
C	-1.092514	1.177730	1.579512
C	-0.428559	1.585483	0.249099
H	-1.041029	1.995368	2.309781
H	-2.149203	0.914114	1.491605
C	1.894457	1.259387	-0.800286
C	-1.079472	0.871329	-0.990438
H	-0.536971	2.663911	0.073252
H	2.905771	0.886655	-0.625204
C	1.547488	-1.997003	2.546458
C	-0.154291	1.127990	-2.217001
C	1.232439	0.526326	-1.960542
H	1.165090	-0.547574	-1.750944
H	1.870024	0.627915	-2.844730
H	2.215300	-2.815566	2.791105
O	0.010619	-3.022375	4.043746
C	-0.998729	-3.907297	3.579739
H	-1.113769	-4.674052	4.348574
H	-0.694042	-4.379862	2.637262
H	-1.949988	-3.384962	3.432485
C	-1.326814	-0.629228	-0.732497
H	-1.971756	-0.775298	0.138562
H	-0.408845	-1.189191	-0.545509
H	-1.831668	-1.098506	-1.576533
C	-2.440708	1.553499	-1.251990
H	-2.293915	2.643521	-1.257856
H	-3.133493	1.336884	-0.429802
C	-0.740116	0.834261	-3.634510
C	-3.072044	1.154220	-2.585723

H	-4.019498	1.690202	-2.716629
H	-3.326686	0.087519	-2.588167
C	-2.135124	1.484348	-3.745394
H	-2.004857	2.576222	-3.780540
H	-2.590496	1.195534	-4.701831
H	-0.009674	2.222431	-2.221736
C	-0.815063	-0.658401	-4.002756
H	-1.626920	-1.187143	-3.499044
H	0.119632	-1.177901	-3.766691
H	-0.986317	-0.761771	-5.080950
C	0.158429	1.509745	-4.689137
H	0.356110	2.557908	-4.434599
H	-0.334831	1.490907	-5.668218
H	1.121324	1.000809	-4.802689
C	0.304774	-2.005830	3.168206
O	-1.853661	-0.943525	3.489238
C	-1.846267	-0.694656	4.887668
H	-1.316858	-1.486416	5.427914
H	-2.891659	-0.667445	5.201301
H	-1.375602	0.272521	5.105944
C	3.315601	-1.017985	1.020919
H	3.773724	-0.028207	1.137945
H	3.211655	-1.173499	-0.060464
C	4.285546	-2.062852	1.569532
H	5.261975	-1.953470	1.087574
H	3.936317	-3.082878	1.378255
H	4.428790	-1.950121	2.649402
H	2.018329	2.307508	-1.108252
C	1.084375	1.278556	0.506557
C	1.697618	2.384930	1.396719
H	2.753250	2.166676	1.595896
H	1.192349	2.464563	2.363754
H	1.643718	3.360171	0.898363

Compound 37:

C	0.274248	-1.278578	0.928532
C	-0.482498	-2.805463	2.799691
C	-0.767822	-0.280199	2.954391
C	-1.315368	-1.681809	3.405026
C	-0.703618	-0.355783	1.490904
C	-0.375322	-2.747583	1.253817
C	2.046261	1.018012	-0.191736
C	1.006232	0.366044	-0.864156
C	0.673333	-1.072791	-0.544762
C	0.272232	1.076093	-1.817566
C	0.579220	2.414027	-2.099519
C	1.620023	3.038244	-1.423342
C	2.361587	2.339241	-0.453763
C	0.630547	-3.781726	0.738941
C	-1.724003	-2.943224	0.552358

Br	-1.227051	-4.499690	3.437855
H	1.170601	-1.253326	1.559423
C	-1.676636	0.367083	0.681282
O	-0.762554	0.407538	-2.409671
O	3.369992	2.942591	0.211497
O	2.023488	4.318914	-1.600551
C	1.408469	5.091686	-2.616060
C	-1.425564	1.018680	-3.501335
H	2.655999	0.488030	0.535877
H	0.527691	-2.781982	3.218057
H	0.232100	-0.151343	3.380822
H	-1.431197	0.509705	3.312496
H	-1.271062	-1.707909	4.495807
H	-2.366586	-1.778370	3.120888
H	1.554112	-1.697564	-0.724294
H	-0.107321	-1.425757	-1.220803
H	0.014337	2.960861	-2.842487
H	1.631514	-3.619523	1.153264
H	0.694235	-3.765619	-0.351001
H	0.297337	-4.781008	1.034545
H	-2.043002	-3.982422	0.660236
H	-2.524051	-2.314107	0.954503
H	-1.642215	-2.739250	-0.518354
H	-1.183575	1.345069	0.506255
H	-2.606193	0.568505	1.220003
H	-1.838051	-0.053087	-0.313777
H	3.465992	3.839687	-0.142562
H	1.913436	6.056482	-2.607087
H	0.342158	5.236692	-2.406472
H	1.535113	4.620906	-3.597687
H	-1.968603	1.918912	-3.188692
H	-0.719921	1.274489	-4.300189
H	-2.138042	0.280622	-3.870605

Compound TS38:

C	0.704805	0.988298	-2.615115
C	-0.411537	-1.305962	-3.083262
C	-0.274402	-1.737551	-1.581547
C	0.865503	0.432753	-1.142863
C	0.667598	-0.298702	-3.480602
H	-1.411151	-0.900466	-3.262854
H	0.683066	-2.249909	-1.460040
H	1.749924	-0.210541	-1.197414
H	1.648378	-0.777540	-3.435116
H	-0.314161	-2.216955	-3.677761
H	-1.099741	-2.400386	-1.315982
C	-0.535436	1.871893	-2.793851
H	-0.488205	2.379129	-3.761027
H	-0.571049	2.643817	-2.020035
H	-1.474953	1.314256	-2.759493
C	1.963046	1.811650	-2.916828

H	1.954193	2.141704	-3.959849
H	2.872825	1.226854	-2.743615
H	1.995957	2.703858	-2.284648
C	1.090411	1.439701	-0.007195
H	0.474539	2.335409	-0.119820
H	2.134812	1.764566	0.000364
C	0.698014	0.718632	1.265081
C	-0.065616	1.348320	2.218700
C	-0.690181	0.584612	3.237173
C	-0.534190	-0.791820	3.298082
O	-0.307284	2.683556	2.135675
C	0.280557	-1.429752	2.356479
C	-1.604532	0.035925	-0.355155
H	-1.608052	1.094246	-0.098598
H	-1.918153	-0.555998	0.513876
H	-2.356379	-0.165151	-1.130196
C	0.876527	-0.692412	1.323568
H	1.626130	-1.163725	0.700181
C	-0.298904	-0.459322	-0.846753
Br	0.443471	0.091798	-5.405587
O	0.436186	-2.754907	2.536440
H	-0.948404	2.915990	2.826050
H	-1.003464	-1.385713	4.072866
O	-1.448035	1.318893	4.068403
C	1.241682	-3.479106	1.616100
H	0.831966	-3.416083	0.603403
H	1.218459	-4.514479	1.954428
H	2.274686	-3.114809	1.622614
C	-2.197407	0.655071	5.082954
H	-2.896888	-0.059706	4.638473
H	-2.745926	1.438319	5.603872
H	-1.528683	0.141744	5.780423

Compound 38:

C	0.145614	-1.329250	0.520556
C	-0.039987	-2.333762	2.734537
C	0.551433	0.138351	2.496340
C	-0.150243	-0.934033	3.348323
C	0.003555	0.114646	1.068130
C	-0.586524	-2.459101	1.284895
C	0.890191	0.828584	-0.018211
C	0.447857	0.189532	-1.295964
C	-0.042379	-1.208156	-0.999813
C	0.350392	0.936754	-2.432884
C	0.575890	2.351508	-2.364275
C	0.873469	3.025405	-1.202046
C	1.013110	2.286580	-0.012268
C	-2.120475	-2.382987	1.218575
C	-0.142067	-3.795860	0.668610
Br	-0.878375	-3.618963	3.964350

H	1.214469	-1.560949	0.659595
C	-1.399275	0.738871	0.995070
O	-0.026230	0.538542	-3.661814
O	1.323431	2.886893	1.103392
O	1.068512	4.347539	-1.036191
C	0.900939	5.212222	-2.159566
C	0.205808	-0.807238	-4.070243
H	1.929845	0.489683	0.169620
H	1.012050	-2.635818	2.725926
H	1.631136	-0.063065	2.479481
H	0.417403	1.120471	2.960526
H	0.302399	-0.947674	4.343214
H	-1.203428	-0.675682	3.498673
H	0.499897	-1.986338	-1.543193
H	-1.096440	-1.288586	-1.293010
H	0.459336	2.892682	-3.298515
H	-2.463769	-2.129782	0.210060
H	-2.551267	-3.354032	1.473429
H	-2.548203	-1.657983	1.913266
H	0.950396	-3.873990	0.613234
H	-0.509762	-4.635449	1.264163
H	-0.546052	-3.908796	-0.343432
H	-1.341917	1.809348	1.220889
H	-1.860510	0.623448	0.008816
H	-2.077268	0.303024	1.726545
H	1.436965	3.843313	0.932525
H	1.077471	6.218867	-1.785788
H	-0.118065	5.135100	-2.552226
H	1.631292	4.973174	-2.939118
H	1.215111	-1.126113	-3.789638
H	-0.537681	-1.488747	-3.649183
H	0.111947	-0.802183	-5.155361

Compound TS39:

C	0.712204	0.996413	-2.637831
C	-0.487926	-1.226481	-3.200763
C	-0.392360	-1.708431	-1.704497
C	0.836183	0.386462	-1.166329
C	0.634797	-0.251899	-3.557792
H	-1.466824	-0.772775	-3.381370
H	0.537561	-2.270383	-1.582955
H	1.692481	-0.293341	-1.240967
H	1.595111	-0.773683	-3.510707
H	-0.429637	-2.121954	-3.824035
H	-1.249560	-2.342182	-1.467820
C	-0.492786	1.930965	-2.794347
H	-0.432007	2.450170	-3.753498
H	-0.498423	2.694770	-2.011606
H	-1.455649	1.412337	-2.768935

C	2.003322	1.782820	-2.893263
H	2.022042	2.137515	-3.927587
H	2.893193	1.165685	-2.727625
H	2.061504	2.658513	-2.241030
C	1.092164	1.360968	-0.007039
H	0.520994	2.286282	-0.111710
H	2.149504	1.641824	0.003137
C	0.677863	0.655759	1.266832
C	-0.142542	1.290347	2.170538
C	-0.736327	0.549570	3.223433
C	-0.510739	-0.810752	3.351964
O	-0.472333	2.594947	1.997048
C	0.344055	-1.454549	2.446239
C	-1.637354	0.067574	-0.398722
H	-1.623460	1.134823	-0.179236
H	-1.857899	-0.477226	0.531604
H	-2.455343	-0.177085	-1.088566
C	0.922594	-0.734576	1.397216
H	1.663537	-1.208519	0.764831
C	-0.367926	-0.448965	-0.948721
Br	0.439715	0.211411	-5.450389
O	0.537082	-2.766686	2.674714
H	-1.046592	2.858619	2.732204
H	-0.952036	-1.395558	4.149592
O	-1.536114	1.291447	4.010152
C	1.394899	-3.487909	1.812456
H	1.022224	-3.471568	0.779735
H	1.393099	-4.513742	2.178475
H	2.416840	-3.092270	1.842957
C	-2.199184	0.665027	5.102352
H	-2.874654	-0.119670	4.745462
H	-2.772937	1.450531	5.591366
H	-1.472355	0.245426	5.805035

Compound 39:

C	-0.785297	-0.405447	-1.099761
C	-2.031384	0.035952	-3.313570
C	-3.107828	0.611287	-1.089240
C	-3.335302	0.130884	-2.528304
C	-1.987342	-0.052815	-0.391205
C	-0.960887	-0.811894	-2.589705
C	0.306915	2.042453	1.424257
C	0.710075	1.020045	0.553652
C	0.146881	0.923239	-0.817550
C	1.665084	0.093052	0.992090
C	2.209368	0.187993	2.277001
C	1.799116	1.216643	3.118402
C	0.837710	2.155784	2.693790
C	-1.478823	-2.271746	-2.555841
C	0.376364	-0.828136	-3.337786
Br	-1.444698	1.869691	-3.769327

H	-0.221229	-1.183461	-0.575141
C	-2.088053	-0.281389	1.055529
O	1.988935	-0.885373	0.102421
O	0.435567	3.148601	3.514534
O	2.244734	1.427342	4.375957
C	3.245747	0.571709	4.902001
C	3.034774	-1.783967	0.431688
H	-0.419818	2.783372	1.103381
H	-2.222275	-0.408943	-4.291293
H	-4.019906	0.566705	-0.486984
H	-2.819633	1.680199	-1.110046
H	-3.810729	-0.855253	-2.510391
H	-4.035206	0.805498	-3.024734
H	0.940222	0.758949	-1.548739
H	-0.386642	1.829429	-1.104017
H	2.947897	-0.525570	2.617595
H	-2.366847	-2.395847	-1.926232
H	-0.701895	-2.932116	-2.157792
H	-1.725938	-2.622118	-3.562633
H	0.764027	0.171138	-3.544177
H	0.253960	-1.333959	-4.300646
H	1.125419	-1.379374	-2.759587
H	-1.113322	-0.386865	1.537638
H	-2.604336	-1.253789	1.148682
H	-2.712243	0.460637	1.561513
H	0.943464	3.083531	4.337100
H	3.460482	0.942281	5.903260
H	4.155174	0.613718	4.292305
H	2.883487	-0.460777	4.964382
H	3.968573	-1.245581	0.626791
H	2.772447	-2.399658	1.300098
H	3.163212	-2.426054	-0.439364

Compound TS40:

C	-2.092367	-1.953477	-0.151553
C	-2.590002	-0.718214	-2.335119
C	-0.819534	0.171838	-0.886042
C	-1.197670	-0.043059	-2.313751
C	-0.812641	-1.061946	0.018678
C	-2.556785	-2.068416	-1.621678
C	0.581706	-1.703739	-0.147056
C	1.451589	-0.470419	-0.097334
C	1.448662	0.343991	-1.256069
C	-1.840873	-3.320270	0.497487
C	-3.254508	-1.293106	0.628080
C	-1.107413	1.488957	-0.267606
C	1.879131	0.077320	1.106596
C	2.354181	1.402338	1.146204
C	2.369259	2.192173	0.000240
C	1.924183	1.661238	-1.217933
H	-0.836145	-0.698017	1.052596

O	1.743901	-0.704448	2.203604
C	2.253801	-0.242925	3.442284
O	2.799167	3.470601	-0.082461
C	3.396724	4.069241	1.059212
O	1.942642	2.387326	-2.342779
H	1.338688	-0.103259	-2.235660
H	-3.346037	-0.078170	-1.868034
H	-2.884224	-0.839845	-3.380157
H	-1.195700	0.894987	-2.872614
H	-0.525048	-0.747322	-2.807741
H	-3.552681	-2.513930	-1.635973
H	0.794523	-2.399003	0.663844
H	0.686887	-2.231051	-1.098712
H	-1.590285	-3.194265	1.556126
H	-1.031091	-3.869886	0.014513
H	-2.744340	-3.935615	0.438281
H	-2.990780	-1.202072	1.686262
H	-4.155328	-1.911462	0.567487
H	-3.519593	-0.295105	0.266505
H	-2.161933	1.461405	0.049199
H	-0.978202	2.320070	-0.962869
H	-0.516174	1.645299	0.640087
H	3.327176	-0.030875	3.375607
H	1.717187	0.649763	3.787236
H	2.091344	-1.054354	4.150727
H	4.264335	3.489172	1.392375
H	3.718891	5.059939	0.742341
H	2.670562	4.165757	1.874162
H	2.355661	3.244518	-2.148335
Br	-1.501797	-3.337394	-2.714658
H	2.690943	1.825713	2.084401

Compound 40:

C	-0.404869	1.866284	-1.891375
C	-0.701566	1.909681	0.961359
C	-0.336510	3.072679	-1.105814
C	-0.610532	0.701208	-1.240762
C	-0.821929	0.627184	0.225373
C	-0.478496	3.097580	0.292565
C	-0.475914	-0.686081	-1.759430
C	0.441201	-1.306774	-0.677139
C	0.009706	-0.644970	0.696463
C	0.612264	-2.855726	-0.714645
C	-0.401790	-3.595641	0.183465
C	-0.490303	-3.005464	1.587618
C	-0.906836	-1.539902	1.558004
C	1.255181	-0.221601	1.486090
H	1.437078	-0.899904	-0.895406
C	0.567415	-3.361173	-2.164988
C	2.018246	-3.229847	-0.182340
Br	-2.237028	-3.681572	-0.582852

O	-0.197612	1.914532	-3.221347
O	-0.104748	4.139002	-1.835993
C	0.046503	5.438245	-1.242669
O	-0.901982	1.804896	2.251141
C	-0.900715	2.971836	3.083417
H	-1.886843	0.366154	0.357355
H	-0.419157	4.038304	0.822255
H	-0.044607	-0.718613	-2.760423
H	-1.455938	-1.177358	-1.793180
H	-0.124013	-4.649734	0.231271
H	0.484446	-3.126765	2.074122
H	-1.204575	-3.575910	2.187162
H	-0.946709	-1.137102	2.576154
H	-1.930844	-1.504411	1.170612
H	1.877774	0.470208	0.906290
H	0.990150	0.255490	2.433368
H	1.871976	-1.090849	1.723735
H	1.360492	-2.888954	-2.755206
H	-0.389024	-3.165272	-2.653136
H	0.733731	-4.443078	-2.190762
H	2.787295	-2.761976	-0.805039
H	2.197475	-2.920746	0.849191
H	2.169063	-4.313060	-0.232294
H	-0.031384	2.827640	-3.495583
H	0.896736	5.438876	-0.556480
H	-0.875456	5.724944	-0.731251
H	0.236433	6.112071	-2.074969
H	0.077430	3.459125	3.047672
H	-1.691612	3.658465	2.769567
H	-1.099601	2.608080	4.088835

Compound 42a:

C	1.043511	0.826682	-0.985328
C	-0.081079	-0.982598	-2.765036
C	1.888150	0.186477	-1.901081
C	-0.336773	0.567784	-0.919183
C	-0.872955	-0.337880	-1.824046
C	1.288713	-0.719637	-2.803130
C	-1.203545	1.247493	0.117176
C	-1.846647	0.256527	1.103867
C	-2.570403	0.962604	2.393536
C	-3.296995	-0.148741	3.171197
C	-2.391520	-1.298890	3.590910
C	-1.637324	-1.894121	2.343665
C	-0.982522	-0.735553	1.727128
C	0.457848	-0.555721	1.886863
C	-3.590714	1.959950	1.834351
C	-1.568031	1.705940	3.285268
O	1.509259	1.719655	-0.058894
C	3.389709	0.448213	-1.929423
C	3.853743	1.102158	-3.239343

C	4.206208	-0.807741	-1.586938
O	2.123591	-1.310129	-3.686578
C	1.591402	-2.198168	-4.651349
H	-1.942473	-0.537076	-1.813550
H	-2.022825	1.775368	-0.380291
H	-3.749732	0.294856	4.065088
H	-4.122664	-0.535559	2.560902
H	-1.658708	-0.981587	4.339041
H	-2.963839	-2.118896	4.031492
H	-0.929536	-2.662309	2.661389
H	-2.388535	-2.324247	1.674425
H	0.882318	-1.079881	1.007186
H	0.798811	0.477956	1.798953
H	0.846500	-1.060940	2.775293
H	-4.271511	1.487122	1.119122
H	-4.190372	2.351641	2.662639
H	-3.107878	2.811756	1.349221
H	-0.851448	1.046209	3.784416
H	-0.999614	2.453155	2.724843
H	-2.116959	2.239212	4.067641
H	3.633730	1.167389	-1.134585
H	4.912961	1.369558	-3.168003
H	3.284322	2.013704	-3.447036
H	3.728426	0.419946	-4.081908
H	4.085421	-1.575610	-2.353121
H	3.894419	-1.227126	-0.624081
H	5.268979	-0.554609	-1.518646
H	2.439636	-2.519568	-5.254985
H	1.130951	-3.073144	-4.177615
H	0.858585	-1.695533	-5.292688
H	-2.677350	-0.268333	0.617846
H	-0.620926	2.003488	0.645412
H	-0.536801	-1.670955	-3.465008
H	2.412487	1.979709	-0.277023

Compound 42b:

C	0.824943	-0.262224	1.177163
C	-1.584419	-1.061329	2.305980
C	0.841846	-1.340751	2.065233
C	-0.360000	0.418860	0.828693
C	-1.553375	-0.006356	1.405748
C	-0.395669	-1.718536	2.635897
C	-0.309422	1.578725	-0.106468
C	0.096163	1.278742	-1.648018
C	0.113654	2.566046	-2.529346
C	-1.322047	3.058813	-2.782474
C	-2.228833	1.985383	-3.379010
C	-2.190577	0.683033	-2.558758
C	-0.850245	0.273675	-2.096169
C	-0.559844	-1.138686	-1.874916
C	0.798744	2.180238	-3.853350

C	0.936356	3.674101	-1.864264
O	1.939582	0.205782	0.548877
C	2.130413	-2.076933	2.411427
C	2.100422	-3.548552	1.970783
C	2.520572	-1.920370	3.888687
O	-0.348833	-2.748413	3.502583
C	-1.538730	-3.174061	4.144113
H	-2.525836	-1.353231	2.752764
H	-2.477239	0.517645	1.171426
H	0.489980	2.259037	0.194893
H	-1.756026	3.431669	-1.845972
H	-1.284882	3.918587	-3.459980
H	-3.262769	2.336101	-3.426278
H	-1.931047	1.756482	-4.406891
H	-2.732264	0.843940	-1.604251
H	-2.708048	-0.142167	-3.054803
H	0.501877	-1.376474	-1.974507
H	-0.786451	-1.274577	-0.791641
H	-1.193727	-1.821656	-2.442189
H	0.302538	1.340237	-4.355993
H	0.799437	3.028228	-4.545432
H	1.840439	1.888903	-3.681489
H	0.428666	4.110622	-0.998806
H	1.916729	3.304602	-1.542272
H	1.107299	4.482982	-2.581433
H	2.952698	-1.625120	1.837617
H	3.079958	-4.007069	2.138911
H	1.863546	-3.635274	0.904983
H	1.356970	-4.112557	2.536576
H	1.798015	-2.416855	4.538818
H	2.571472	-0.864486	4.172682
H	3.503741	-2.369011	4.062959
H	-1.241808	-3.992724	4.798469
H	-1.975329	-2.367943	4.743881
H	-2.273311	-3.538491	3.417033
H	1.100865	0.852380	-1.575029
H	-1.256225	2.124482	-0.097510
H	2.730030	-0.205449	0.921054

Compound TS43:

C	1.516452	1.411255	-2.788934
C	-0.088064	-0.365558	-3.778649
C	-0.067874	-1.206080	-2.455247
C	1.506047	0.499286	-1.518752
C	1.179649	0.474922	-3.973675
H	-0.981046	0.268313	-3.790341
H	0.751037	-1.928160	-2.514809
H	2.237086	-0.283041	-1.753706
H	2.029793	-0.199861	-4.140387
H	-0.201338	-1.075337	-4.603099
H	-1.014330	-1.736843	-2.327781

H	1.074260	1.070811	-4.886861
C	0.529826	2.584368	-2.710907
H	0.677441	3.240848	-3.573745
H	0.692425	3.190595	-1.813534
H	-0.518059	2.272203	-2.719733
C	2.935488	1.970875	-2.955738
H	3.015582	2.515404	-3.902015
H	3.685811	1.172450	-2.963492
H	3.184744	2.670150	-2.150621
C	1.862570	1.056343	-0.137400
H	1.428890	2.050667	0.012866
H	2.945599	1.150499	-0.009669
C	1.210683	0.070410	0.818424
C	0.457254	0.511303	1.913529
C	-0.494995	-0.300659	2.540332
C	-0.634405	-1.643048	2.081771
O	0.518335	1.817002	2.301015
O	-1.577269	-2.370769	2.698433
C	-1.752667	-3.729738	2.332701
H	-2.567109	-4.097726	2.954688
H	-0.847052	-4.312032	2.534688
H	-2.029542	-3.821334	1.275945
C	-1.390453	0.286684	3.614360
H	-0.987113	1.277471	3.832224
C	-2.815776	0.484804	3.070102
H	-3.432799	0.978637	3.826886
H	-3.284336	-0.471281	2.820510
H	-2.810768	1.120141	2.177301
C	-1.380440	-0.500679	4.934438
H	-1.882297	0.095211	5.703015
H	-0.358059	-0.692386	5.275242
H	-1.901746	-1.454924	4.847939
C	0.177902	-2.138654	1.070812
H	0.133786	-3.177813	0.770531
C	-1.040177	0.467599	-0.832332
H	-0.842092	1.435594	-0.371782
H	-1.498463	-0.188982	-0.078688
H	-1.790462	0.583842	-1.623301
C	1.068513	-1.276914	0.418386
H	1.778582	-1.715035	-0.274326
C	0.169646	-0.189802	-1.400246
H	1.421327	2.148971	2.223629

Compound TS44:

C	-2.192947	-2.487536	-0.484616
C	-2.782572	-1.078946	-2.533645
C	-0.979648	-0.225803	-1.037220
C	-1.428655	-0.348210	-2.480254
C	-0.959129	-1.563551	-0.246236
C	-2.619173	-2.486809	-1.963587
C	0.452620	-2.106131	-0.527594

C	1.180057	-0.794135	-0.375494
C	1.024674	0.152303	-1.411603
C	-1.830723	-3.914243	-0.049219
C	-3.364137	-2.009589	0.394003
C	-1.461654	0.974262	-0.288079
C	1.629038	-0.350699	0.882438
C	1.973754	0.985023	1.105526
C	1.854450	1.912015	0.014292
C	1.413927	1.502150	-1.223065
H	-0.965783	-1.303137	0.819576
O	1.644658	-1.311770	1.834433
C	2.454107	1.456528	2.467281
C	1.514923	2.497745	3.098879
C	3.917807	1.929188	2.426180
O	2.217525	3.172340	0.297669
C	1.988308	4.187840	-0.668010
H	0.994086	-0.206856	-2.431584
H	-3.558904	-0.516112	-2.004594
H	-3.092307	-1.124044	-3.582278
H	-1.472676	0.639249	-2.949015
H	-0.736408	-0.965431	-3.059237
H	-3.554967	-3.047351	-2.062866
H	-1.872815	-3.025291	-2.564283
H	0.772662	-2.859543	0.189376
H	0.558387	-2.507001	-1.540678
H	-1.493300	-3.938441	0.993237
H	-1.042991	-4.345161	-0.675813
H	-2.708250	-4.563756	-0.128872
H	-3.086198	-2.012473	1.453655
H	-4.220676	-2.680626	0.274300
H	-3.710054	-1.001919	0.142933
H	-2.494382	0.772656	0.024499
H	-1.453730	1.881171	-0.895547
H	-0.883888	1.137047	0.627992
H	2.438108	0.600558	3.153723
H	1.834244	2.693762	4.126526
H	0.483195	2.132491	3.130976
H	1.536909	3.439179	2.549068
H	4.024550	2.832551	1.823871
H	4.572152	1.155064	2.013819
H	4.253800	2.151405	3.443292
H	0.926745	4.229466	-0.940015
H	2.279717	5.120214	-0.187188
H	2.599985	4.031559	-1.562973
H	1.381802	2.179951	-2.066297
H	2.043777	-0.991154	2.652318

Compound 46a:

C	1.527838	1.597177	-3.183369
C	-0.390464	0.740286	-4.659580
C	-0.851430	-0.218872	-3.499211

C	1.032088	0.529264	-2.051548
C	1.099838	1.037432	-4.552271
H	-0.987447	1.656917	-4.630731
H	-0.336084	-1.174944	-3.631833
H	1.478907	-0.413018	-2.389234
H	1.670514	0.124089	-4.763047
H	-0.629628	0.232584	-5.597232
H	-1.932956	-0.363838	-3.535769
H	1.376057	1.763993	-5.324467
C	0.951469	2.998869	-2.947190
H	1.386318	3.690101	-3.675803
H	1.203816	3.378484	-1.953296
H	-0.136063	3.051158	-3.058938
C	3.057006	1.655971	-3.101113
H	3.433324	2.253792	-3.937789
H	3.506585	0.659998	-3.169505
H	3.399156	2.133252	-2.179497
C	1.500987	0.844446	-0.621680
H	1.289493	1.883508	-0.363622
H	2.587670	0.720529	-0.602052
C	0.857409	-0.071548	0.394479
C	0.008438	0.434825	1.383561
C	-0.694188	-0.401661	2.267697
C	-0.485800	-1.784921	2.160396
O	-0.198421	1.799441	1.420390
O	-1.138821	-2.616712	3.021962
C	0.660976	2.489514	2.323100
H	0.517893	2.136686	3.349999
H	0.395145	3.545532	2.260474
H	1.713249	2.353086	2.043319
C	-2.017903	-3.569184	2.424750
H	-2.506943	-4.083275	3.252602
H	-1.471204	-4.286297	1.807542
H	-2.773899	-3.059304	1.816106
C	-1.650118	0.194247	3.288936
H	-1.655902	1.272260	3.105992
C	-3.097481	-0.284589	3.106048
H	-3.765531	0.319229	3.728673
H	-3.215507	-1.327999	3.405827
H	-3.424376	-0.179802	2.065277
C	-1.163544	-0.038648	4.726843
H	-1.823867	0.474533	5.433495
H	-0.148078	0.345614	4.872326
H	-1.161500	-1.104580	4.968564
C	0.420290	-2.303966	1.218328
C	-1.388481	1.131007	-1.431623
H	-0.984898	1.927700	-0.803676
H	-1.706456	0.338819	-0.723910
H	-2.281253	1.431069	-1.987186
C	1.058897	-1.448485	0.332286
H	1.741125	-1.887787	-0.391025

C	-0.407546	0.455808	-2.276154
O	0.665127	-3.641610	1.113684
C	1.340545	-4.215839	2.234042
H	2.313273	-3.732428	2.379522
H	1.488008	-5.267921	1.989509
H	0.744346	-4.123993	3.146622

Compound 46b:

C	1.023238	-0.302532	0.936346
C	-1.414385	-1.116775	2.025997
C	1.020859	-1.351574	1.874861
C	-0.148114	0.389853	0.613792
C	-1.364962	-0.024353	1.172757
C	-0.212328	-1.768224	2.390287
C	-0.099693	1.582224	-0.284250
C	0.093592	1.305974	-1.864481
C	0.208939	2.617488	-2.702143
C	-1.154350	3.329329	-2.756455
C	-2.277971	2.435659	-3.276167
C	-2.340013	1.089361	-2.530016
C	-1.033547	0.471040	-2.241310
C	-0.902496	-0.982996	-2.162761
C	0.663415	2.197297	-4.111982
C	1.266519	3.554066	-2.109614
O	2.183294	0.159908	0.358624
C	2.811165	-0.704166	-0.578529
C	2.328044	-1.965321	2.355272
C	2.503634	-3.412310	1.872730
C	2.509300	-1.857150	3.877333
O	-0.231712	-2.845192	3.209845
C	-0.823423	-2.709838	4.503591
H	-2.269315	0.527330	0.936510
H	0.787500	2.173237	-0.052311
H	-1.412281	3.709181	-1.759981
H	-1.066446	4.210037	-3.401394
H	-3.245280	2.933910	-3.175201
H	-2.144153	2.230882	-4.342790
H	-2.755739	1.256615	-1.515521
H	-3.015686	0.374347	-3.006689
H	-0.036645	-1.317271	-2.747976
H	-0.631809	-1.208264	-1.110491
H	-1.799071	-1.535012	-2.444779
H	-0.012517	1.465795	-4.573213
H	0.712034	3.067231	-4.774366
H	1.661514	1.746863	-4.080751
H	0.933290	4.026574	-1.180893
H	2.204186	3.022590	-1.910045
H	1.485216	4.356198	-2.821237
H	3.357978	-1.516943	-0.092853
H	3.515593	-0.088794	-1.141381
H	2.076408	-1.145608	-1.265397

H	3.126519	-1.356534	1.922789
H	3.488290	-3.790251	2.166593
H	2.422941	-3.488410	0.782395
H	1.740815	-4.059111	2.313364
H	1.859754	-2.551290	4.413055
H	2.305360	-0.840819	4.229138
H	3.544566	-2.100922	4.136450
H	-0.382151	-3.499686	5.112975
H	-0.577730	-1.735610	4.939388
H	-1.905681	-2.834349	4.456925
H	1.026675	0.739762	-1.927681
H	-0.984930	2.208406	-0.148505
O	-2.548842	-1.627005	2.553247
C	-3.771385	-0.975898	2.279103
H	-3.764875	0.058534	2.644030
H	-4.537219	-1.540968	2.809282
H	-3.995888	-0.986514	1.204487

Compound TS47:

C	1.330451	1.641819	-3.118892
C	-0.139073	-0.218486	-4.157996
C	-0.114543	-1.059076	-2.829206
C	1.329392	0.729895	-1.839967
C	1.086663	0.687615	-4.311111
H	-1.064823	0.365130	-4.198611
H	0.745191	-1.733156	-2.858640
H	2.109105	-0.009482	-2.055217
H	1.977235	0.059984	-4.446445
H	-0.187458	-0.937280	-4.980714
H	-1.034037	-1.640072	-2.730037
H	0.980461	1.276464	-5.228872
C	0.281880	2.760658	-3.073292
H	0.420630	3.422900	-3.933367
H	0.386161	3.373905	-2.172479
H	-0.747853	2.393981	-3.112781
C	2.724178	2.273000	-3.236725
H	2.809222	2.816423	-4.183312
H	3.513765	1.513764	-3.213101
H	2.908166	2.987104	-2.427515
C	1.619930	1.321063	-0.456246
H	1.133607	2.287431	-0.297478
H	2.694361	1.474348	-0.316606
C	1.031430	0.311196	0.511030
C	0.251033	0.710905	1.590842
C	-0.593497	-0.188824	2.271365
C	-0.618578	-1.537762	1.857053
O	0.187081	2.046240	1.884204
O	-1.429365	-2.407429	2.516370
C	1.203220	2.503748	2.772809
H	1.127908	1.998932	3.742835
H	1.039165	3.573434	2.903268

H	2.201125	2.330935	2.351530
C	-2.432487	-3.047220	1.725752
H	-3.046863	-3.613773	2.425283
H	-1.990525	-3.720225	0.985622
H	-3.052830	-2.296835	1.221263
C	-1.461414	0.314815	3.408300
H	-1.313074	1.396863	3.439133
C	-2.962780	0.078148	3.187300
H	-3.531086	0.663691	3.916296
H	-3.230301	-0.971707	3.321837
H	-3.276060	0.398333	2.187463
C	-0.989573	-0.264651	4.752129
H	-1.570130	0.178360	5.567315
H	0.067871	-0.044412	4.932910
H	-1.125757	-1.348860	4.783041
C	0.225877	-1.978176	0.831267
C	-1.217526	0.544122	-1.215640
H	-1.083909	1.518260	-0.745687
H	-1.631998	-0.150510	-0.471426
H	-1.968275	0.614715	-2.012237
C	1.013178	-1.050231	0.139394
H	1.733419	-1.462782	-0.558084
C	0.033427	-0.024910	-1.785792
O	0.289179	-3.271573	0.428708
C	0.749941	-4.212945	1.407049
H	1.767526	-3.957484	1.720269
H	0.751016	-5.181082	0.907280
H	0.091021	-4.239244	2.278557

Compound 47:

C	-1.303758	0.101695	-1.453141
C	0.169520	-0.980108	0.222887
C	-2.293513	-0.912788	0.584087
C	-1.027429	-1.319895	1.017693
C	-2.448746	-0.271652	-0.657017
C	-0.050327	-0.167356	-1.002248
C	1.256035	0.443581	-1.440983
C	2.234923	-0.017859	-0.350632
C	1.363975	-0.219942	0.918861
C	2.174541	-1.026536	1.937590
C	3.523575	-0.336104	2.206374
C	4.337573	-0.083250	0.930070
C	3.585656	0.701184	-0.172661
O	-1.573121	0.830146	-2.560679
C	-0.827625	0.577533	-3.748551
C	-3.847883	0.045284	-1.128472
C	-4.162976	-0.662458	-2.459803
C	-4.112480	1.561143	-1.205101
O	-3.384402	-1.198305	1.354055
C	-3.765270	-0.143140	2.239746
H	2.521670	-1.043667	-0.634594

C	0.786083	1.055593	1.555326
H	0.576759	-1.957630	-0.092846
C	4.368492	0.586065	-1.490791
C	3.484700	2.192786	0.183398
H	1.142378	1.534564	-1.483039
H	1.570511	0.121548	-2.438232
H	1.620212	-1.149594	2.873355
H	2.357583	-2.033740	1.538968
H	3.359145	0.606361	2.741670
H	4.109708	-0.963175	2.885861
H	5.262446	0.447825	1.183657
H	4.643083	-1.053498	0.513671
H	0.073189	1.195476	-3.789284
H	-0.559887	-0.481742	-3.820953
H	-1.481950	0.846847	-4.578388
H	-4.525799	-0.373857	-0.382399
H	-5.229649	-0.543951	-2.671250
H	-3.952250	-1.734723	-2.401807
H	-3.601135	-0.233862	-3.290878
H	-5.174130	1.720049	-1.415349
H	-3.879090	2.061535	-0.259573
H	-3.527104	2.030838	-1.996438
H	-4.608614	-0.520931	2.817342
H	-2.939813	0.119920	2.912848
H	-4.071629	0.748138	1.682024
H	1.541935	1.610310	2.108313
H	0.004259	0.790966	2.276214
H	0.350747	1.736968	0.817154
H	5.395457	0.941560	-1.356522
H	4.418702	-0.451708	-1.841427
H	3.912232	1.192902	-2.281698
H	3.170969	2.371933	1.213291
H	2.791954	2.726437	-0.477039
H	4.467158	2.661351	0.065108
O	-0.750122	-2.037148	2.072202
C	-1.713096	-2.772003	2.858080
H	-2.383257	-3.335029	2.210647
H	-2.277343	-2.094824	3.498486
H	-1.102769	-3.440066	3.462816

Compound TS48:

C	0.016493	-1.299577	0.974969
C	-0.021274	-0.691501	-1.343539
C	1.957385	-1.712581	-0.392652
C	1.276315	-1.178134	-1.497327
C	1.319992	-1.817326	0.854505
C	-0.651413	-0.711210	-0.098223
C	-1.945497	0.033581	0.138095
C	-2.057909	1.277966	-0.775843
C	-0.728137	1.849518	-1.091471
C	0.100301	2.337721	0.018489

C	-0.710292	3.538481	0.624513
C	-2.111656	3.095947	1.030605
C	-2.915912	2.464265	-0.121099
O	-0.601213	-1.290240	2.201353
C	-1.425251	-2.426697	2.440893
C	1.987087	-2.461759	2.057257
C	3.276147	-1.754340	2.497738
C	2.221974	-3.961892	1.821327
O	3.225703	-2.194731	-0.530692
C	4.226359	-1.222784	-0.831331
C	-0.367900	2.256518	-2.465541
H	-0.544786	-0.390874	-2.246345
C	-4.229287	1.873205	0.406281
C	-3.259077	3.510361	-1.192934
H	-2.822739	-0.598754	-0.033480
H	0.209326	1.581172	0.800388
H	1.086095	2.666055	-0.317281
H	-0.140742	3.890182	1.488537
H	-0.740604	4.364355	-0.093423
H	-2.036348	2.390263	1.866438
H	-2.669198	3.959709	1.409068
H	-0.833417	-3.349466	2.423051
H	-1.860315	-2.291909	3.431574
H	-2.224429	-2.500969	1.692523
H	1.278794	-2.358698	2.883190
H	3.586573	-2.140332	3.473964
H	3.124553	-0.674359	2.598860
H	4.092921	-1.932660	1.794881
H	2.602905	-4.425845	2.736796
H	1.293412	-4.472890	1.544845
H	2.952081	-4.123447	1.024081
H	4.242022	-0.441358	-0.062839
H	5.175577	-1.758994	-0.820810
H	4.062266	-0.772885	-1.814596
H	0.633766	1.881947	-2.709635
H	-0.287712	3.354116	-2.490031
H	-1.084759	1.926750	-3.218533
H	-4.069430	1.158677	1.217889
H	-4.855928	2.681294	0.797196
H	-4.789259	1.374144	-0.391638
H	-3.900359	4.284109	-0.759416
H	-2.384075	4.017143	-1.611316
H	-3.809113	3.054189	-2.022615
H	-1.972933	0.317316	1.192718
H	-2.557988	1.003136	-1.709693
O	1.850664	-1.067649	-2.726848
C	2.146229	-2.305266	-3.383315
H	2.813328	-2.924267	-2.778005
H	2.632040	-2.038405	-4.321763
H	1.218641	-2.850323	-3.589791

Compound 48:

C	-0.012301	1.710623	1.014681
C	-0.323648	-0.459263	-0.151892
C	0.187191	-0.378231	2.299901
C	-0.214690	-1.104988	1.169562
C	0.229608	1.020998	2.257029
C	-0.229896	1.020972	-0.131553
C	0.002966	1.559825	-1.512509
C	0.379171	0.310942	-2.346565
C	0.786199	-0.755163	-1.274353
C	0.832782	-2.183326	-1.829171
C	-0.295488	-2.552025	-2.787731
C	-0.385224	-1.520468	-3.910834
C	-0.703504	-0.104003	-3.397308
O	0.186026	3.056811	0.965897
C	-1.007867	3.838698	0.966631
C	0.519698	1.839068	3.489111
C	1.856971	1.484361	4.159311
C	-0.658879	1.743414	4.478963
O	0.329553	-1.013069	3.487410
C	1.412299	-1.942698	3.583578
H	1.282950	0.519834	-2.930411
C	2.176298	-0.439007	-0.694621
H	-1.281969	-0.749704	-0.601517
C	-2.163363	-0.069738	-2.900817
C	-0.597639	0.886033	-4.569419
H	0.808316	2.299122	-1.467308
H	-0.868505	2.091657	-1.906651
H	1.772943	-2.256301	-2.391314
H	0.942051	-2.900097	-1.006727
H	-0.099371	-3.544797	-3.205503
H	-1.258518	-2.628231	-2.267986
H	0.572322	-1.501598	-4.449605
H	-1.146077	-1.817735	-4.641247
H	-1.648121	3.576446	0.116511
H	-1.564560	3.698017	1.900491
H	-0.691288	4.877646	0.881442
H	0.590634	2.874922	3.151783
H	2.098382	2.262111	4.889456
H	2.674354	1.446493	3.432120
H	1.805083	0.531412	4.688124
H	-0.468122	2.415062	5.321028
H	-1.601671	2.047591	4.012890
H	-0.769931	0.726971	4.863303
H	1.447777	-2.246039	4.629403
H	1.239075	-2.819362	2.954522
H	2.356241	-1.459142	3.309400
H	2.922558	-0.487383	-1.492873
H	2.459861	-1.178471	0.062354
H	2.244068	0.553807	-0.241520
H	-2.444109	0.894293	-2.465940

H	-2.403168	-0.849627	-2.171040
H	-2.832007	-0.237069	-3.751195
H	-0.824086	1.912120	-4.257380
H	0.407850	0.880738	-5.003995
H	-1.304845	0.620611	-5.362024
O	-0.520777	-2.362352	1.394155
C	-1.385531	-3.133120	0.548720
H	-1.770523	-3.922547	1.191552
H	-0.833879	-3.566044	-0.283268
H	-2.213673	-2.519000	0.184949

Compound 50a:

C	-0.949492	1.110428	-0.623490
C	0.654380	-0.146786	-2.514392
C	-0.307795	1.902846	-1.593541
C	-0.756604	-0.273604	-0.551026
C	0.046122	-0.883463	-1.510725
C	0.494068	1.248832	-2.542211
C	-1.404719	-1.092915	0.542202
C	-0.374645	-1.778891	1.456518
C	-1.016991	-2.486116	2.786122
C	0.118765	-3.253939	3.485613
C	1.325936	-2.391748	3.830365
C	1.861073	-1.650538	2.548406
C	0.687727	-0.953296	2.012856
C	0.570570	0.492633	2.178221
C	-2.082006	-3.470330	2.290620
C	-1.666230	-1.465980	3.729934
O	-1.754691	1.646299	0.349338
C	-0.507513	3.413128	-1.636198
C	-1.362524	3.832100	-2.841128
C	0.801824	4.213775	-1.568010
O	1.070155	1.989805	-3.531014
C	2.496572	1.963709	-3.589119
H	0.185569	-1.961531	-1.520435
H	-2.008611	-1.886821	0.092786
H	-0.279948	-3.695471	4.405877
H	0.435201	-4.089718	2.848849
H	1.087096	-1.653859	4.602174
H	2.153345	-2.996039	4.210208
H	2.673515	-0.971807	2.815167
H	2.218912	-2.412421	1.849104
H	1.031105	0.892470	1.252191
H	-0.454352	0.869882	2.170675
H	1.160102	0.869397	3.018032
H	-1.679817	-4.162803	1.543955
H	-2.438446	-4.061431	3.140690
H	-2.947189	-2.957016	1.864082
H	-0.953394	-0.771203	4.185394
H	-2.432876	-0.873549	3.223208
H	-2.161343	-2.002601	4.545252

H	-1.058415	3.707029	-0.732221
H	-1.552701	4.910003	-2.814895
H	-2.327076	3.313962	-2.843761
H	-0.844625	3.596324	-3.774118
H	1.347404	4.158283	-2.510958
H	1.451596	3.849822	-0.764649
H	0.578891	5.267125	-1.370917
H	2.773464	2.648004	-4.391481
H	2.920939	2.320688	-2.643349
H	2.869215	0.960138	-3.805485
H	0.086545	-2.623298	0.930988
H	-2.087414	-0.465792	1.117098
O	1.412518	-0.803778	-3.441885
C	0.837973	-0.847680	-4.748062
H	-0.136246	-1.349263	-4.719550
H	1.528430	-1.424804	-5.363742
H	0.720615	0.158001	-5.163370
H	-2.053961	2.523806	0.083806

Compound 50b:

C	0.667499	-0.182563	1.209286
C	-1.782575	-1.124874	2.116906
C	0.640647	-1.372058	1.958804
C	-0.501641	0.501329	0.866422
C	-1.726733	0.010383	1.317517
C	-0.602619	-1.837439	2.408681
C	-0.436919	1.682172	-0.054106
C	0.017609	1.341634	-1.550746
C	0.055607	2.590683	-2.486277
C	-1.375025	3.078873	-2.772686
C	-2.275591	1.991876	-3.354696
C	-2.227866	0.690081	-2.531584
C	-0.902216	0.310820	-2.021456
C	-0.532985	-1.097508	-1.888733
C	0.754691	2.150773	-3.785090
C	0.876964	3.715791	-1.849017
O	1.855256	0.305625	0.706667
C	2.581782	1.126077	1.618770
C	1.931605	-2.117571	2.254872
C	1.932148	-3.544681	1.687556
C	2.270716	-2.110494	3.752839
O	-0.637363	-2.942076	3.194602
C	-1.433342	-4.041912	2.755778
H	-2.645523	0.548531	1.087747
H	0.326529	2.387579	0.278209
H	-1.820122	3.478448	-1.853061
H	-1.327863	3.919169	-3.473600
H	-3.312091	2.334048	-3.404987
H	-1.977237	1.754694	-4.380587
H	-2.793449	0.832930	-1.586966

H	-2.713601	-0.149016	-3.036913
H	0.300961	-1.271671	-2.589216
H	-0.093436	-1.272511	-0.893577
H	-1.342315	-1.796389	-2.101147
H	0.253552	1.302112	-4.269213
H	0.777874	2.973616	-4.506365
H	1.789291	1.850448	-3.587367
H	0.360679	4.184446	-1.005699
H	1.850363	3.350228	-1.501972
H	1.063371	4.499157	-2.590295
H	1.981356	1.988313	1.935267
H	3.470413	1.468409	1.087061
H	2.882721	0.559833	2.506007
H	2.723008	-1.576371	1.728138
H	2.937425	-3.970524	1.767166
H	1.647986	-3.553066	0.629180
H	1.249200	-4.194900	2.237807
H	1.528468	-2.673885	4.323009
H	2.301851	-1.090814	4.151862
H	3.252398	-2.567417	3.914852
H	-1.136616	-4.886714	3.378150
H	-2.497969	-3.840563	2.884690
H	-1.219553	-4.273982	1.705492
H	1.021480	0.918994	-1.432119
H	-1.395246	2.208032	-0.080612
O	-2.940004	-1.598722	2.638362
H	-3.653550	-0.967382	2.486389

Compound TS51:

C	0.043376	-1.379821	-1.062408
C	-0.056804	-1.114203	1.334561
C	2.009298	-1.791976	0.268566
C	1.268252	-1.540347	1.429909
C	1.400662	-1.773525	-0.992780
C	-0.678076	-1.023974	0.069425
C	-1.982783	-0.257091	-0.039084
C	-1.866042	0.868423	0.996264
C	-0.444452	1.315184	1.105575
C	-0.099872	1.969201	2.378622
C	-0.966583	3.284666	2.341224
C	-2.456596	3.007545	2.123012
C	-2.770807	2.154483	0.872661
O	-0.536094	-1.201462	-2.291448
C	-1.365299	-2.280654	-2.714167
C	2.123856	-2.191211	-2.258841
C	2.414112	-3.701439	-2.224842
C	3.397740	-1.391276	-2.562124
O	3.319159	-2.162138	0.440875
C	4.206075	-1.069220	0.705013
H	-2.143090	0.457562	1.973298

C	0.406207	1.619511	-0.074049
H	-0.618900	-1.032364	2.258181
C	-4.233156	1.692469	0.909270
C	-2.532039	2.946232	-0.419370
H	-2.860892	-0.875561	0.170088
H	-2.088858	0.120815	-1.059388
H	-0.410386	1.373205	3.240585
H	0.959975	2.219217	2.462278
H	-0.805740	3.787462	3.298844
H	-0.573065	3.951442	1.566956
H	-2.857214	2.496697	3.008195
H	-2.987297	3.963282	2.049537
H	-2.190655	-2.442398	-2.010035
H	-1.763384	-1.999597	-3.689303
H	-0.784016	-3.205421	-2.805881
H	1.426060	-1.998154	-3.076981
H	2.857236	-4.013641	-3.175643
H	1.498433	-4.281894	-2.071027
H	3.115587	-3.946300	-1.422078
H	3.708896	-1.588546	-3.592334
H	3.231612	-0.312351	-2.466887
H	4.222874	-1.685479	-1.908951
H	5.203218	-1.501875	0.788570
H	4.186704	-0.346238	-0.116389
H	3.944482	-0.562742	1.641955
H	1.328798	1.024653	-0.021759
H	0.721151	2.669060	-0.020726
H	-0.078807	1.422652	-1.029691
H	-4.439013	1.073514	1.789479
H	-4.896842	2.562333	0.947112
H	-4.492169	1.117614	0.014448
H	-3.276093	3.744931	-0.497214
H	-1.547203	3.419913	-0.465038
H	-2.642602	2.314323	-1.306364
O	1.816017	-1.697538	2.648395
H	2.635051	-2.207958	2.541906

Compound 51:

C	-0.635374	-3.224628	-1.598378
C	-0.316824	-4.165021	0.802210
C	-0.150256	-1.675803	0.483370
C	0.368380	-2.873645	1.283643
C	0.049140	-1.968170	-1.028680
C	-0.165308	-4.400485	-0.707107
C	-0.125205	-0.610206	-1.727899
C	0.292716	0.375522	-0.664498
C	0.733498	-0.373608	0.547065
C	-2.169296	-3.156349	-1.657816
C	-0.119691	-3.446288	-3.029635
C	-1.573193	-1.289024	0.920026
C	0.083345	1.717689	-0.630957

C	0.193512	2.461795	0.613112
C	0.594487	1.799145	1.774481
C	0.788830	0.416194	1.776687
H	1.124303	-2.198226	-1.109994
O	-0.362949	2.447059	-1.679645
C	0.191129	2.216618	-2.972412
C	-0.179450	3.922977	0.558554
C	1.005211	4.736272	-0.009483
C	-0.743920	4.542955	1.840874
O	0.731470	2.380417	3.007968
C	1.997651	3.015231	3.242697
O	1.068073	-0.202119	2.895528
H	1.776303	-0.707833	0.386293
H	0.116072	-5.013268	1.341816
H	-1.377630	-4.149159	1.078107
H	1.453362	-2.967159	1.136529
H	0.201676	-2.732721	2.356443
H	0.894600	-4.594123	-0.924906
H	-0.708954	-5.308538	-0.992852
H	0.470784	-0.541011	-2.642785
H	-1.166240	-0.406583	-2.009974
H	-2.521020	-2.229457	-2.125040
H	-2.545345	-3.985738	-2.265634
H	-2.644443	-3.239762	-0.678814
H	0.975964	-3.433809	-3.071125
H	-0.455435	-4.417018	-3.409161
H	-0.497379	-2.678360	-3.714902
H	-1.552461	-0.863727	1.929538
H	-2.035933	-0.556026	0.251509
H	-2.231931	-2.154749	0.964300
H	1.251270	1.952235	-2.897641
H	-0.352462	1.431712	-3.504185
H	0.083548	3.155908	-3.515226
H	-0.964872	3.975278	-0.201248
H	1.865623	4.730248	0.666141
H	0.687724	5.774541	-0.138888
H	1.326680	4.355918	-0.982437
H	0.020361	4.755616	2.590397
H	-1.504785	3.907349	2.300795
H	-1.216300	5.493245	1.575569
H	2.823925	2.320854	3.052254
H	1.993387	3.313484	4.290664
H	2.110909	3.899800	2.611865
H	1.042721	0.464550	3.612888

Compound TS52:

C	-1.755091	-1.892140	-2.177150
C	-3.361839	0.076981	-2.447932
C	-1.535660	0.275007	-0.829032
C	-2.324580	1.050978	-1.822998
C	-0.812304	-0.964616	-1.324764

C	-2.625423	-1.065718	-3.140688
C	0.503375	-0.472257	-1.967235
C	0.994897	0.497899	-0.915150
C	0.356950	1.756307	-0.870158
C	-0.892223	-2.881193	-2.970829
C	-2.648971	-2.698801	-1.218484
C	-1.896492	0.347972	0.603149
C	1.712378	0.064689	0.186537
C	1.826920	0.842729	1.371690
C	1.154321	2.068191	1.405295
C	0.475039	2.548165	0.276567
H	-0.505258	-1.543657	-0.446115
O	2.237910	-1.202685	0.180097
C	3.497578	-1.314271	-0.480397
C	2.613926	0.252103	2.529719
C	1.750007	-0.762136	3.301268
C	3.288731	1.256561	3.470552
O	1.177301	2.933848	2.470194
C	0.138594	2.726598	3.428056
O	-0.082687	3.764411	0.289460
H	-0.025138	2.227558	-1.766279
H	-4.061552	-0.289393	-1.689753
H	-3.950592	0.655560	-3.165395
H	-2.795157	1.924915	-1.367578
H	-1.700711	1.382590	-2.656057
H	-3.344897	-1.733949	-3.626122
H	-2.000081	-0.651123	-3.942859
H	1.181126	-1.309345	-2.127613
H	0.334679	0.026141	-2.927488
H	-0.228589	-3.450696	-2.310469
H	-0.280535	-2.376758	-3.725508
H	-1.535899	-3.597451	-3.491368
H	-2.043651	-3.312399	-0.542933
H	-3.297512	-3.372498	-1.787262
H	-3.301543	-2.070193	-0.602899
H	-2.667539	-0.421875	0.769672
H	-2.304995	1.318030	0.891051
H	-1.049132	0.071174	1.240618
H	3.413720	-1.045554	-1.540364
H	4.247416	-0.667539	-0.010613
H	3.802384	-2.356755	-0.387846
H	3.414890	-0.330419	2.065324
H	2.352471	-1.242676	4.078063
H	1.369965	-1.541718	2.634996
H	0.900912	-0.276298	3.794144
H	2.584366	1.733938	4.154820
H	3.810257	2.044227	2.920283
H	4.025705	0.721313	4.077200
H	0.242542	1.752068	3.914155
H	0.247046	3.516295	4.171904
H	-0.849917	2.795656	2.956680

H	0.222560	4.212207	1.097844

Compound 52:

C	0.697070	-2.992896	-1.649864
C	-0.812912	-4.193146	0.038336
C	-0.206735	-1.755491	0.540748
C	-1.276923	-2.864027	0.626953
C	0.411058	-1.655567	-0.905030
C	-0.443307	-4.005173	-1.432378
C	-0.503339	-0.654978	-1.652962
C	-0.716702	0.359312	-0.582142
C	-0.942433	-0.346367	0.698971
C	0.846426	-2.720853	-3.155694
C	2.031934	-3.594043	-1.170958
C	0.869718	-1.941110	1.613032
C	-0.512438	1.697644	-0.646852
C	-0.404432	2.497438	0.558075
C	-0.460419	1.859041	1.799011
C	-0.754989	0.495056	1.889736
H	1.376286	-1.140652	-0.797259
O	-0.279650	2.328744	-1.829767
C	-1.404357	2.429288	-2.704710
C	-0.186249	3.977548	0.371113
C	1.306201	4.246071	0.071680
C	-0.726774	4.894729	1.473279
O	-0.372500	2.486801	3.014323
C	0.961633	2.647713	3.521165
O	-0.984750	-0.034830	3.062991
H	-2.025815	-0.566841	0.742104
H	0.031089	-4.600307	0.606542
H	-1.621511	-4.925283	0.129111
H	-1.591827	-2.975593	1.671726
H	-2.168239	-2.553227	0.062721
H	-0.153881	-4.962434	-1.880584
H	-1.338403	-3.671077	-1.977255
H	-0.034954	-0.223771	-2.538465
H	-1.449626	-1.124105	-1.954832
H	1.630113	-1.979528	-3.352626
H	-0.085969	-2.364828	-3.606252
H	1.126387	-3.642710	-3.675406
H	2.850411	-2.875253	-1.289609
H	2.277870	-4.477179	-1.769945
H	2.016829	-3.911942	-0.126198
H	1.386276	-2.892135	1.479602
H	0.438114	-1.946078	2.617233
H	1.625159	-1.148368	1.559208
H	-1.770314	1.439213	-2.996852
H	-2.215462	2.992782	-2.229482
H	-1.052940	2.962690	-3.587213
H	-0.720054	4.221861	-0.552961
H	1.434807	5.311526	-0.138033

H	1.646392	3.681789	-0.799450
H	1.941787	3.992612	0.925156
H	-0.102223	4.899239	2.368338
H	-1.744056	4.625685	1.769533
H	-0.748527	5.916237	1.082779
H	1.525398	3.356186	2.909752
H	0.852665	3.043002	4.530712
H	1.486816	1.686105	3.547433
H	-0.957725	0.691481	3.721417