Copper-Catalyzed Intramolecular Alkene Carboetherification: Synthesis of Fused-Ring and Bridged-Ring Tetrahydrofurans

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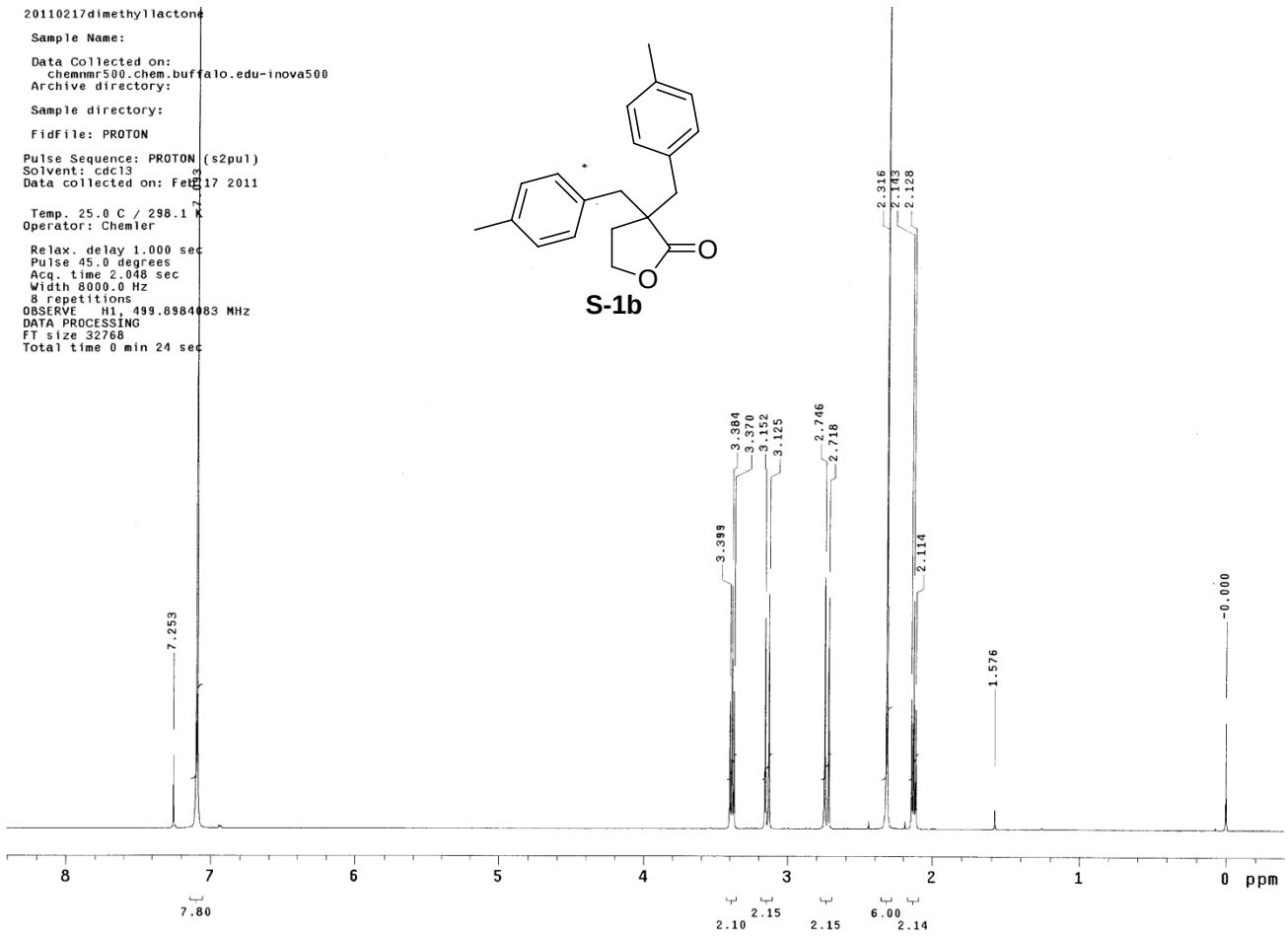
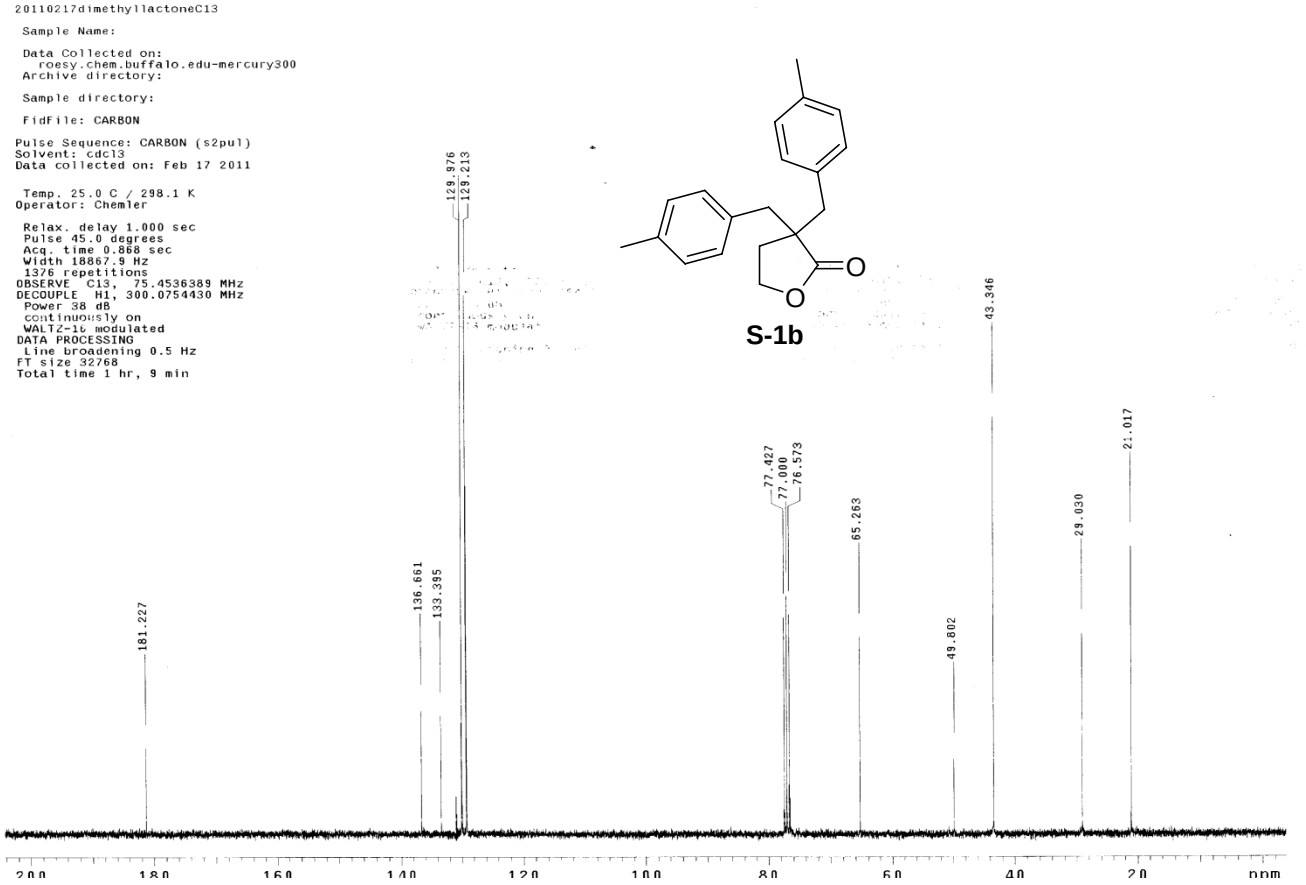
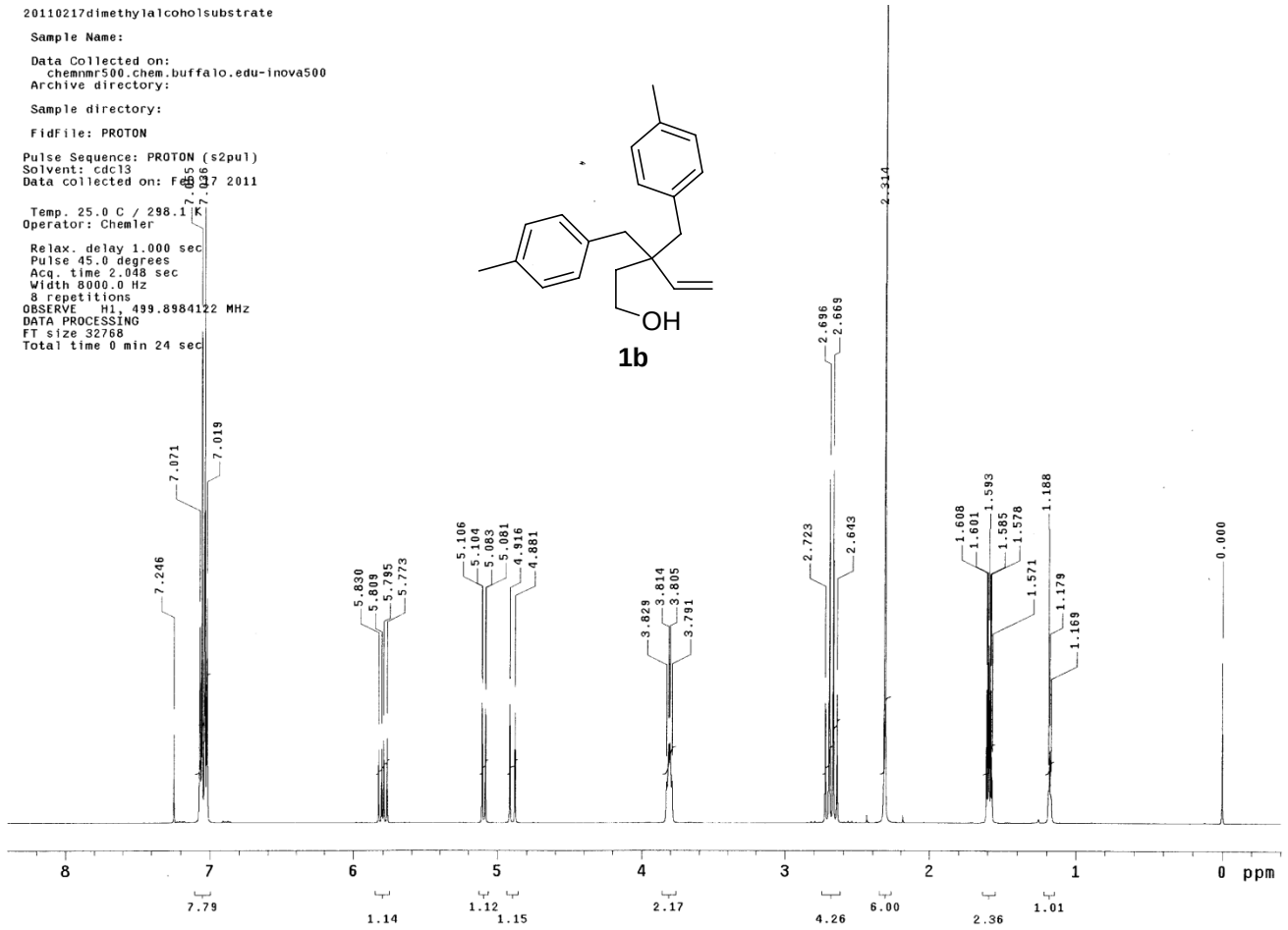
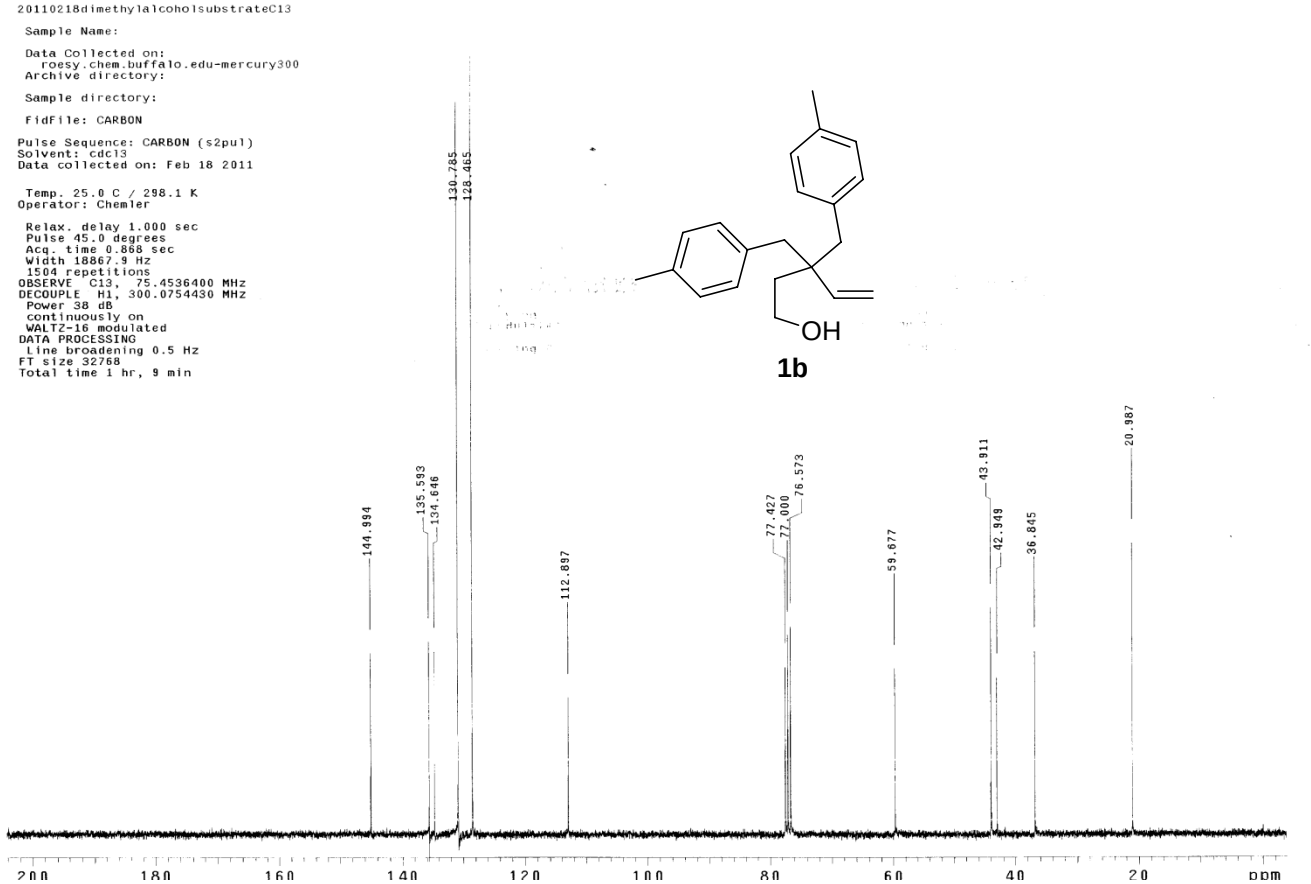
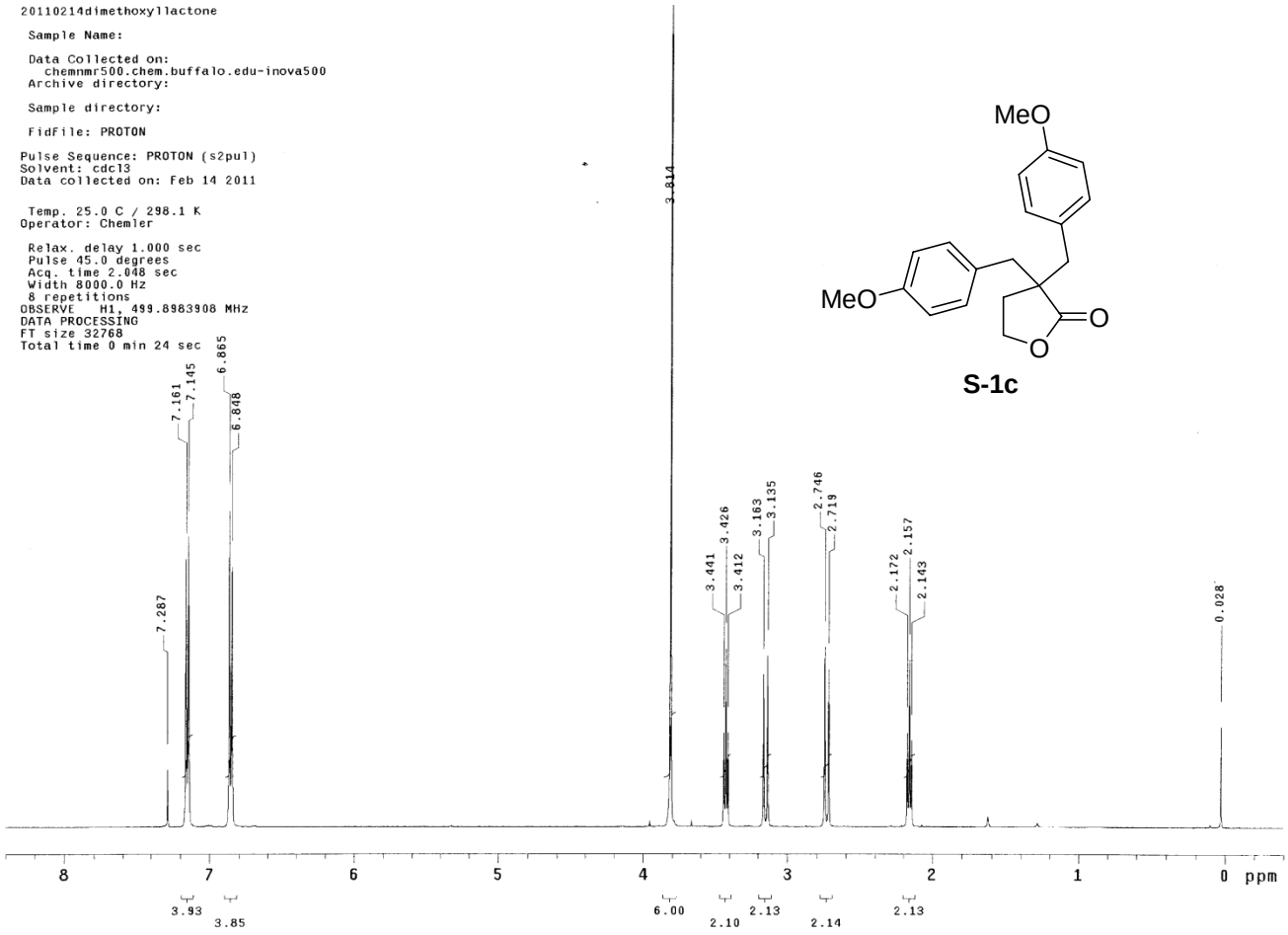
Supporting Information 2: ^{1}H NMR and ^{13}C NMR of substrates and products

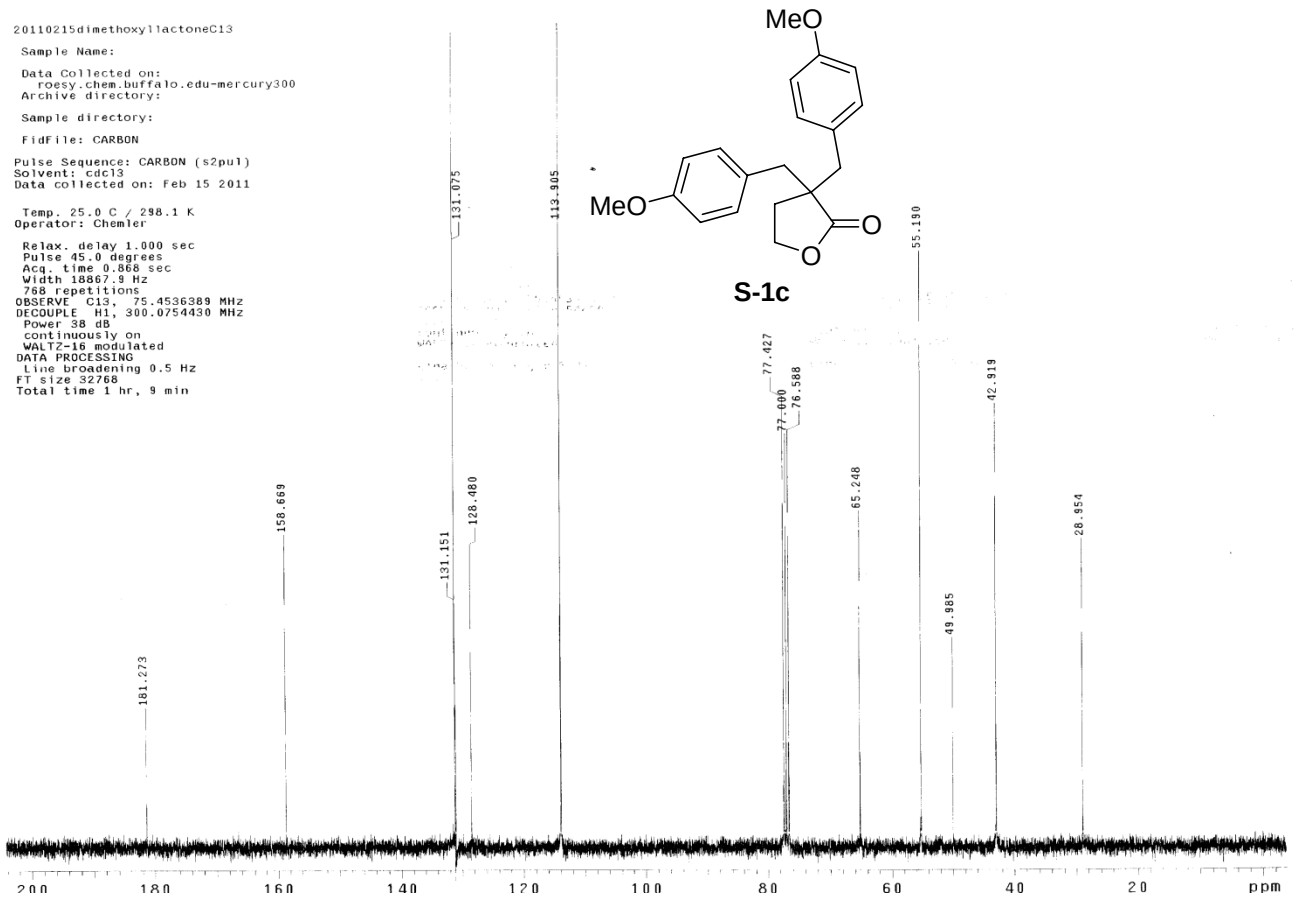

20110217dimethyllactone
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 17 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984083 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
S-1b
7.253
3.399
3.384
3.370
3.152
3.125
2.746
2.718
2.316
2.143
2.128
2.114
1.576
-0.000
8
7
6
5
4
3
2
1
0 ppm
7.80
2.10
2.15
2.15
6.00
2.14

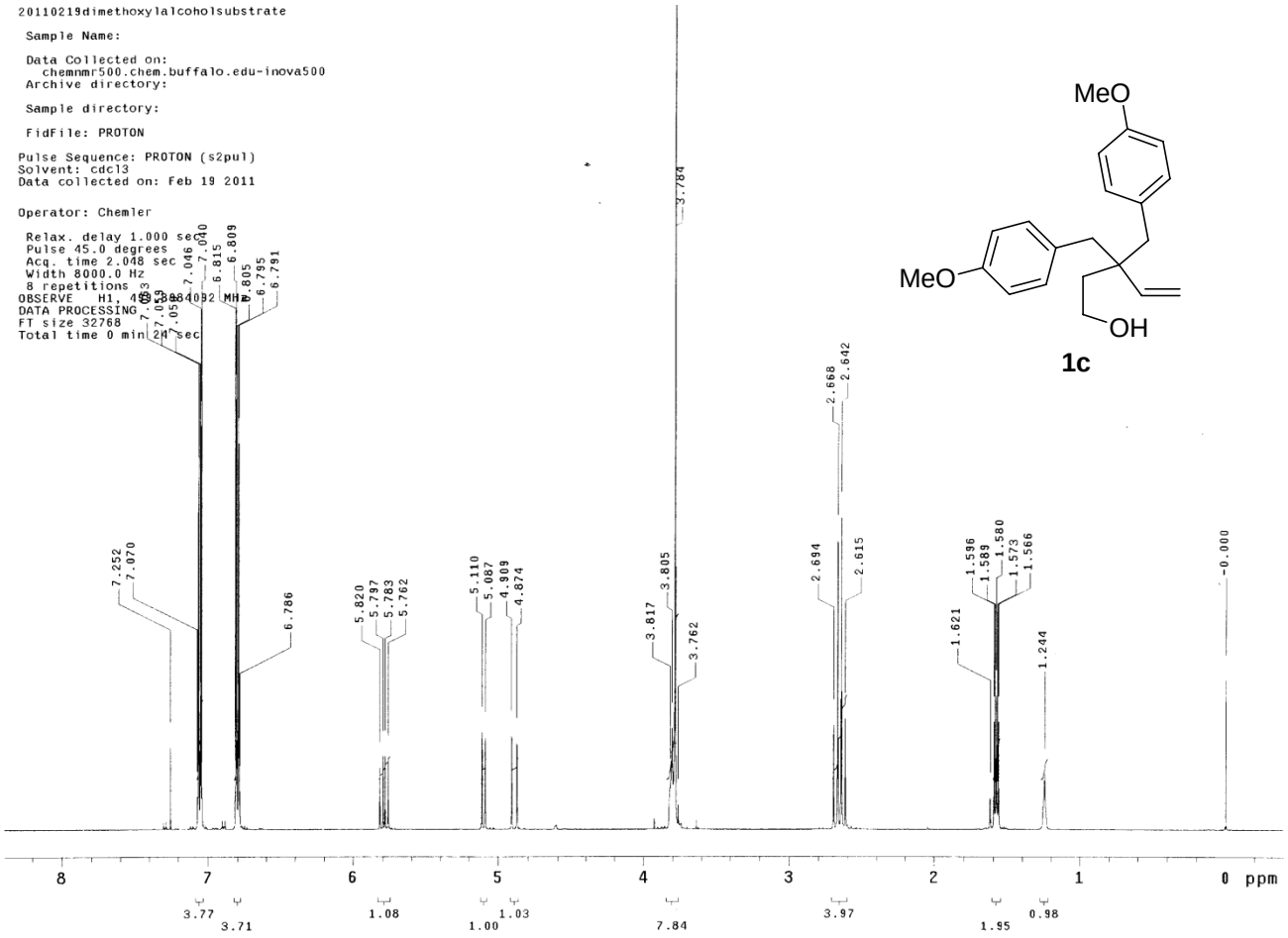

20110217dimethyllactoneC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 17 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
1376 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
S-1b
181.227
136.661
133.395
129.976
129.213
77.427
77.000
76.573
65.263
49.802
43.346
29.030
21.017
200
180
160
140
120
100
80
60
40
20
ppm

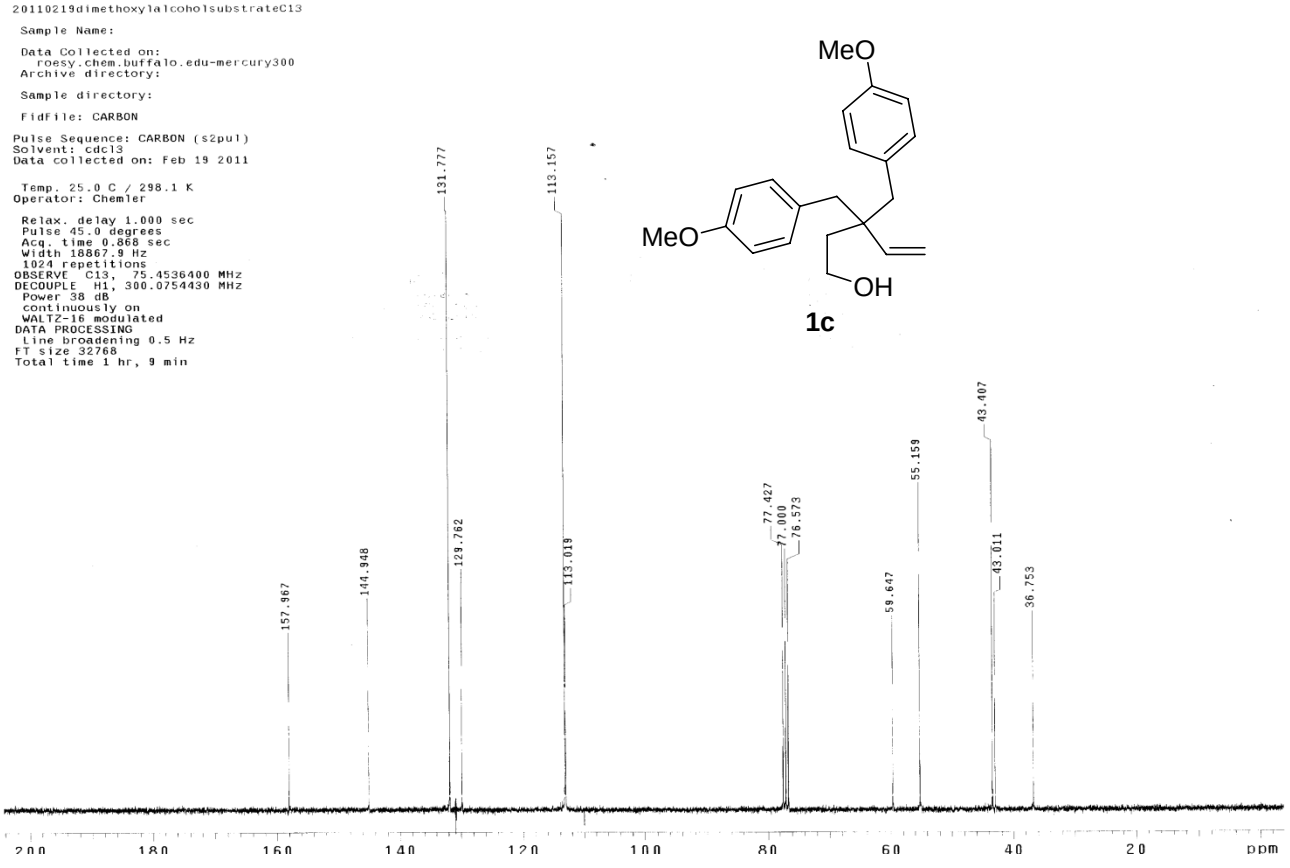

20110217dimethylalcoholsubstrate
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 17 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984122 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OH
1b
7.246
7.071
7.019
5.830
5.809
5.795
5.773
5.106
5.104
5.083
5.081
4.916
4.881
3.829
3.814
3.805
3.791
2.723
2.696
2.669
2.643
2.314
1.608
1.601
1.593
1.585
1.578
1.571
1.188
1.179
1.169
0.000
8
7
6
5
4
3
2
1
0 ppm
7.79
1.14
1.12
1.15
2.17
4.26
6.00
2.36
1.01


20110218dimethylalcoholsubstrateC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 18 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
1504 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
OH
1b
144.994
135.593
134.646
130.785
128.465
112.897
77.427
77.000
76.573
59.677
43.911
42.949
36.845
20.987
200
180
160
140
120
100
80
60
40
20
ppm


20110214dimethoxyllactone
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 14 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8983908 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
MeO
MeO
O
O
S-1c
7.287
7.161
7.145
6.865
6.848
3.814
3.441
3.426
3.412
3.163
3.135
2.746
2.719
2.172
2.157
2.143
0.028
8
7
6
5
4
3
2
1
0 ppm
3.93
3.85
6.00
2.10
2.13
2.14
2.13


20110215dimethoxyllactoneC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 15 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
768 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
MeO
MeO
O
O
S-1c
181.273
158.669
131.151
131.075
128.480
113.905
77.427
77.000
76.588
65.248
55.190
49.985
42.919
28.954
200
180
160
140
120
100
80
60
40
20
ppm


20110219dimethoxylalcoholsubstrate
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8884092 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 2M sec
MeO
MeO
OH
1c
7.252
7.070
6.786
5.820
5.797
5.783
5.762
5.110
5.087
4.909
4.874
3.817
3.805
3.784
3.762
2.694
2.668
2.642
2.615
1.621
1.596
1.589
1.580
1.573
1.566
1.244
0.000
8
7
6
5
4
3
2
1
0 ppm
3.77
3.71
1.08
1.00
1.03
7.84
3.97
1.95
0.98


20110219dimethoxylalcoholsubstrateC13
Sample Name:
Data Collected on:
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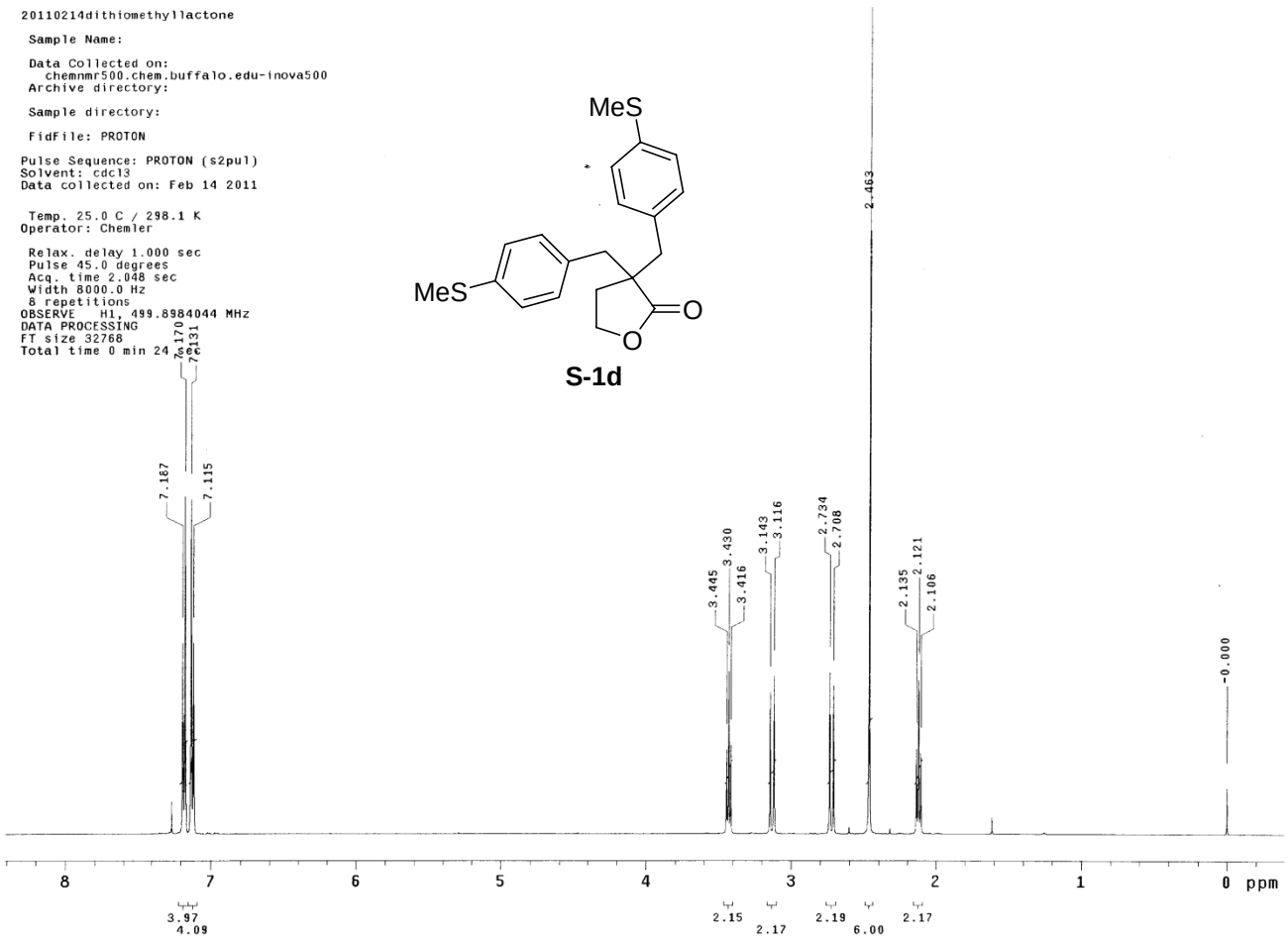
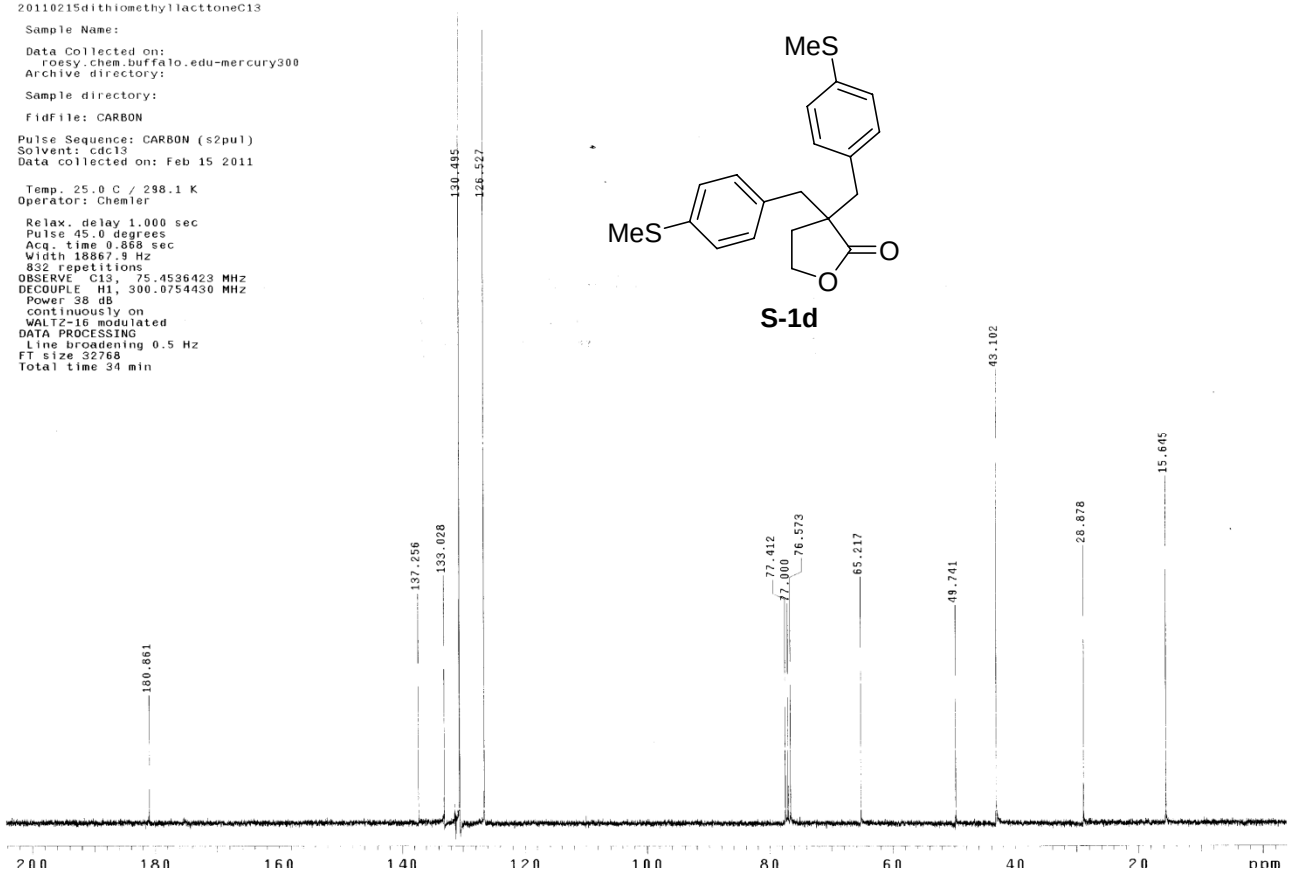
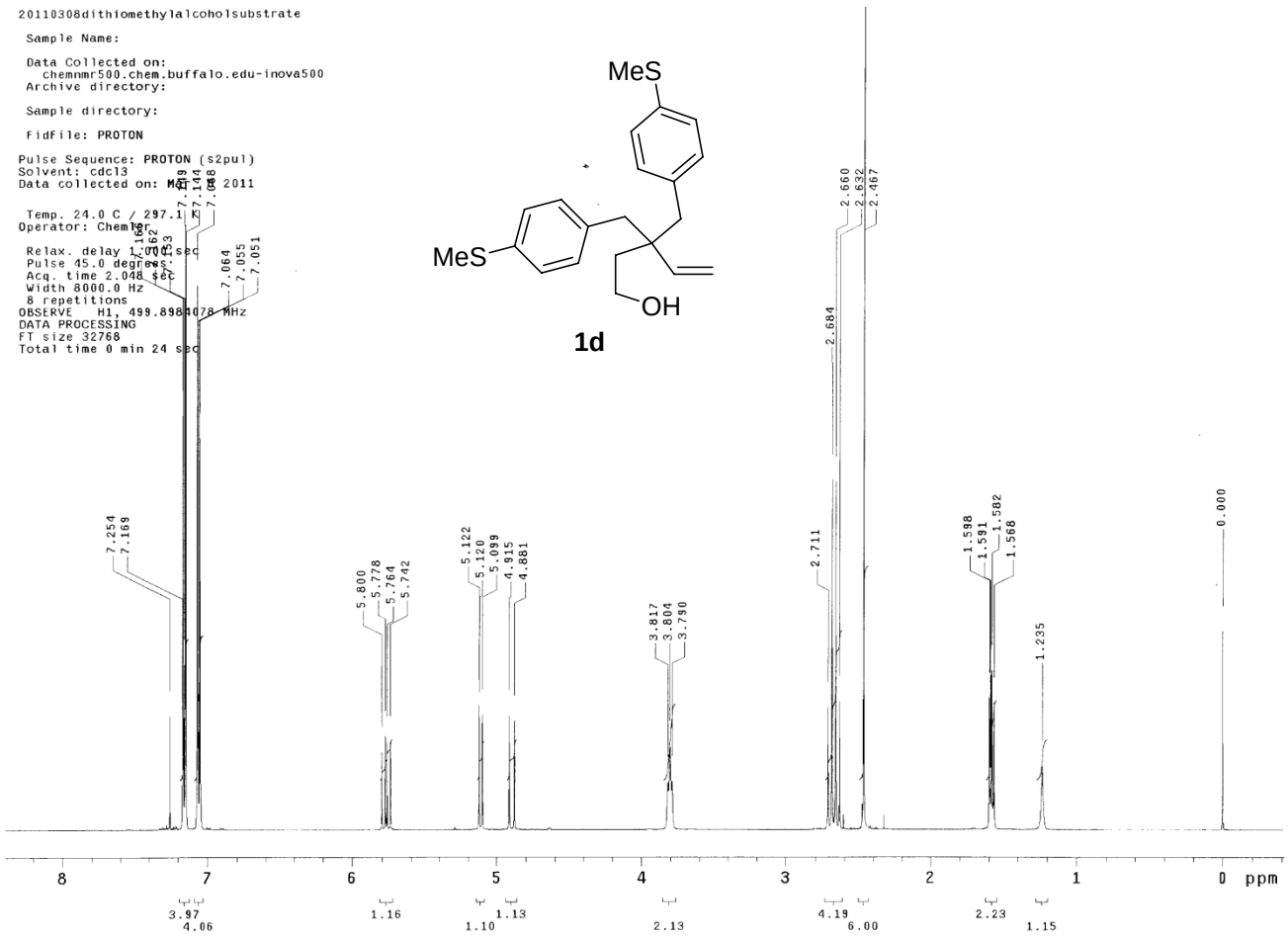
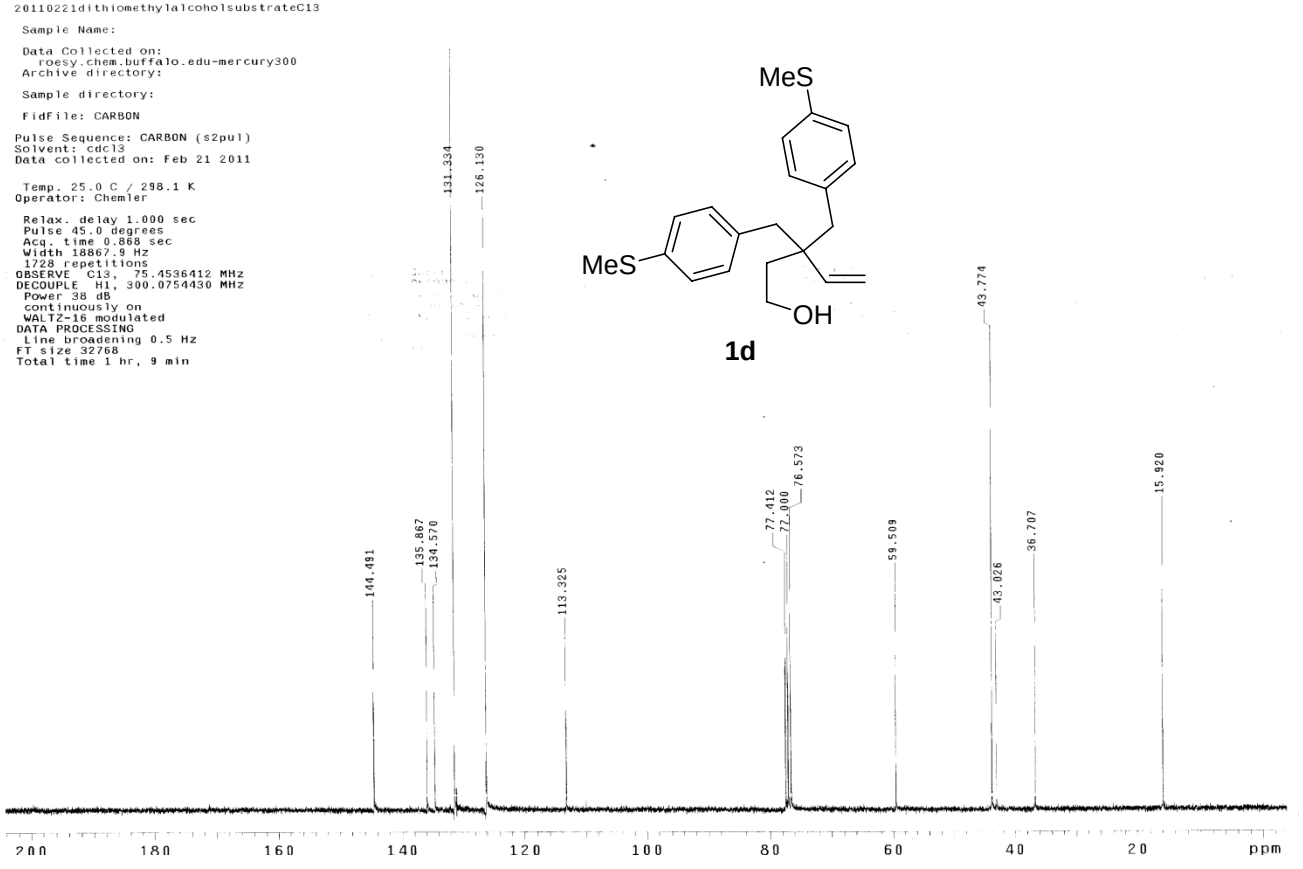
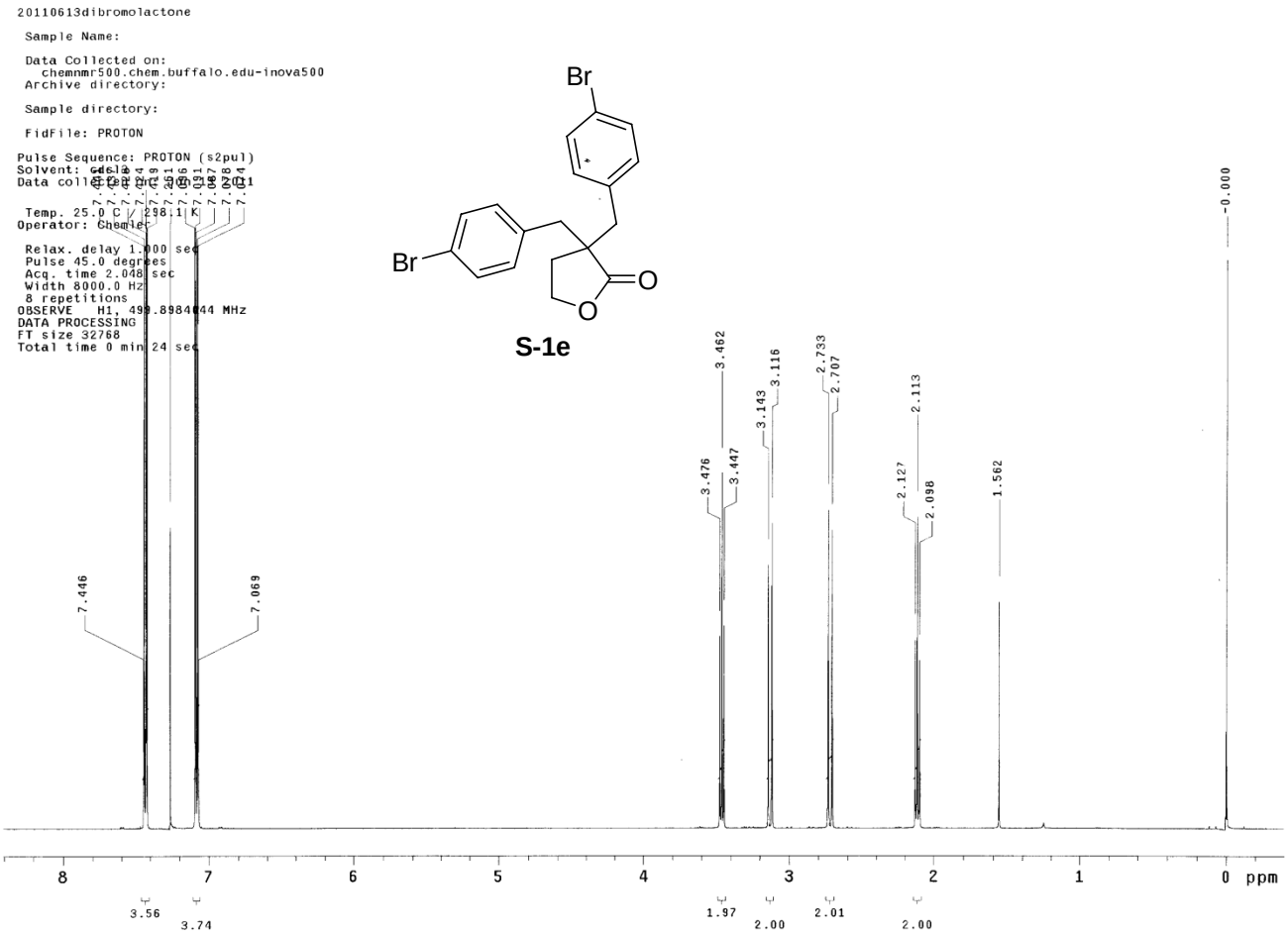
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
1024 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
MeO
MeO
OH
1c
157.367
144.948
131.777
129.762
113.157
113.018
77.427
77.000
76.573
58.647
55.159
43.407
43.011
36.753
200
180
160
140
120
100
80
60
40
20
ppm

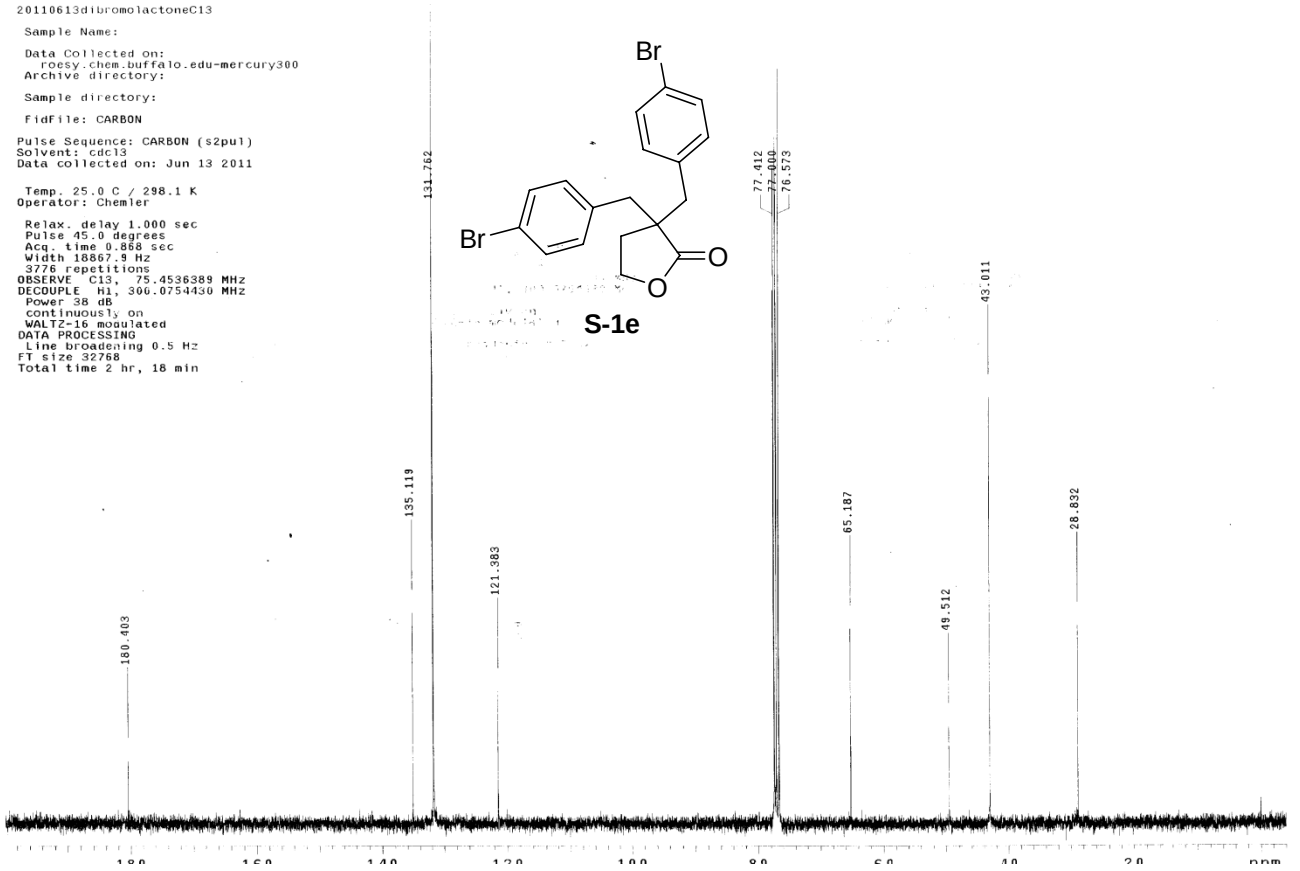

20110214dithiomethyllactone
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 14 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984044 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
MeS
MeS
O
O
S-1d
7.170
7.131
7.167
7.115
3.445
3.430
3.416
3.143
3.116
2.734
2.708
2.463
2.135
2.121
2.106
-0.000
8
7
6
5
4
3
2
1
0 ppm
3.97
4.09
2.15
2.17
2.19
6.00
2.17


20110215dithiomethyllacttoneC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 15 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
832 repetitions
OBSERVE C13, 75.4536423 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 34 min
MeS
MeS
O
O
S-1d
180.861
137.256
133.028
130.495
126.522
77.412
77.000
76.573
65.217
49.741
43.102
28.878
15.645
200
180
160
140
120
100
80
60
40
20
ppm


20110308dithiomethylalcoholsubstrate
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 8 2011
Temp. 24.0 C / 297.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8981078 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
MeS
MeS
OH
1d
7.254
7.169
7.162
7.153
7.119
7.114
7.108
7.064
7.055
7.051
5.800
5.778
5.764
5.742
5.122
5.120
5.089
4.915
4.881
3.817
3.804
3.790
2.711
2.684
2.660
2.632
2.467
1.598
1.591
1.582
1.568
1.235
0.000
8
7
6
5
4
3
2
1
0 ppm
3.97
4.06
1.16
1.10
1.13
2.13
4.19
6.00
2.23
1.15


20110221dithiomethylalcoholsubstrateC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 21 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
1728 repetitions
OBSERVE C13, 75.4536412 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
MeS
MeS
OH
1d
144.491
135.867
134.570
131.334
126.130
113.325
77.412
77.000
76.573
59.509
43.774
43.026
36.707
15.920
200
180
160
140
120
100
80
60
40
20
ppm


20110613dibromolactone
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984044 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 24 sec
Br
Br
O
O
S-1e
7.446
7.069
3.462
3.476
3.447
3.143
3.116
2.733
2.707
2.127
2.113
2.098
1.562
0.000
8
7
6
5
4
3
2
1
0 ppm
3.56
3.74
1.97
2.00
2.01
2.00


20110613dibromolactoneC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 13 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3776 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
Br
Br
O
O
S-1e
180.403
135.119
131.762
121.383
77.412
77.000
76.573
65.187
49.512
43.011
28.832
180
160
140
120
100
80
60
40
20
ppm

20110623dibromoalcoholsubstrate

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

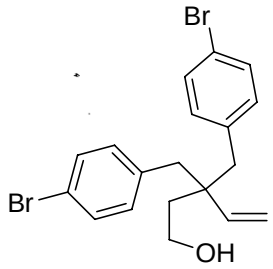
Sample directory:

FidFile: PROTON

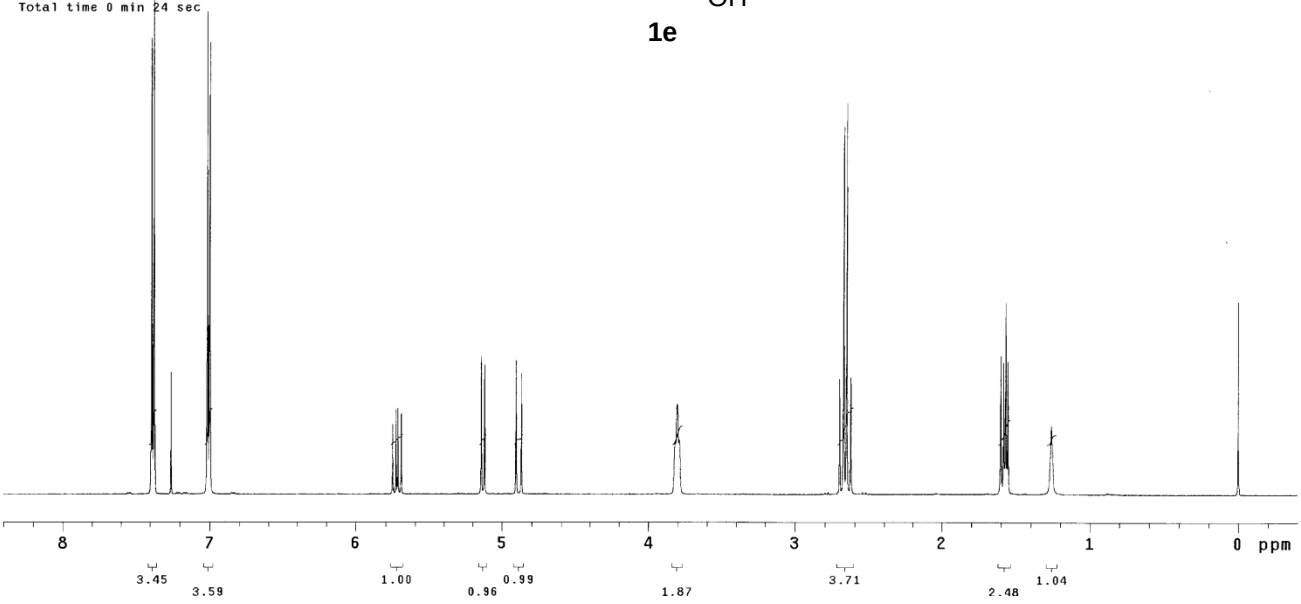
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 23 2011

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984053 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



1e



20110621dibromoalcoholsubstrateC13

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

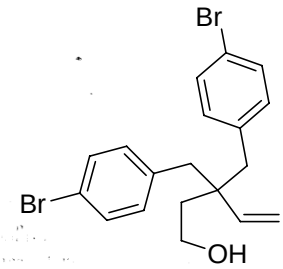
Sample directory:

FidFile: CARBON

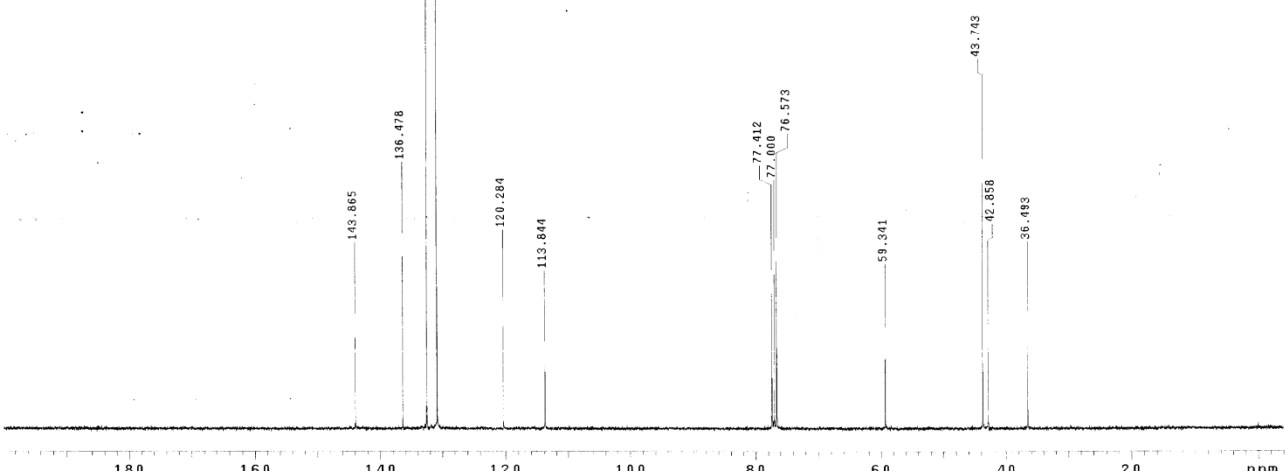
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 21 2011

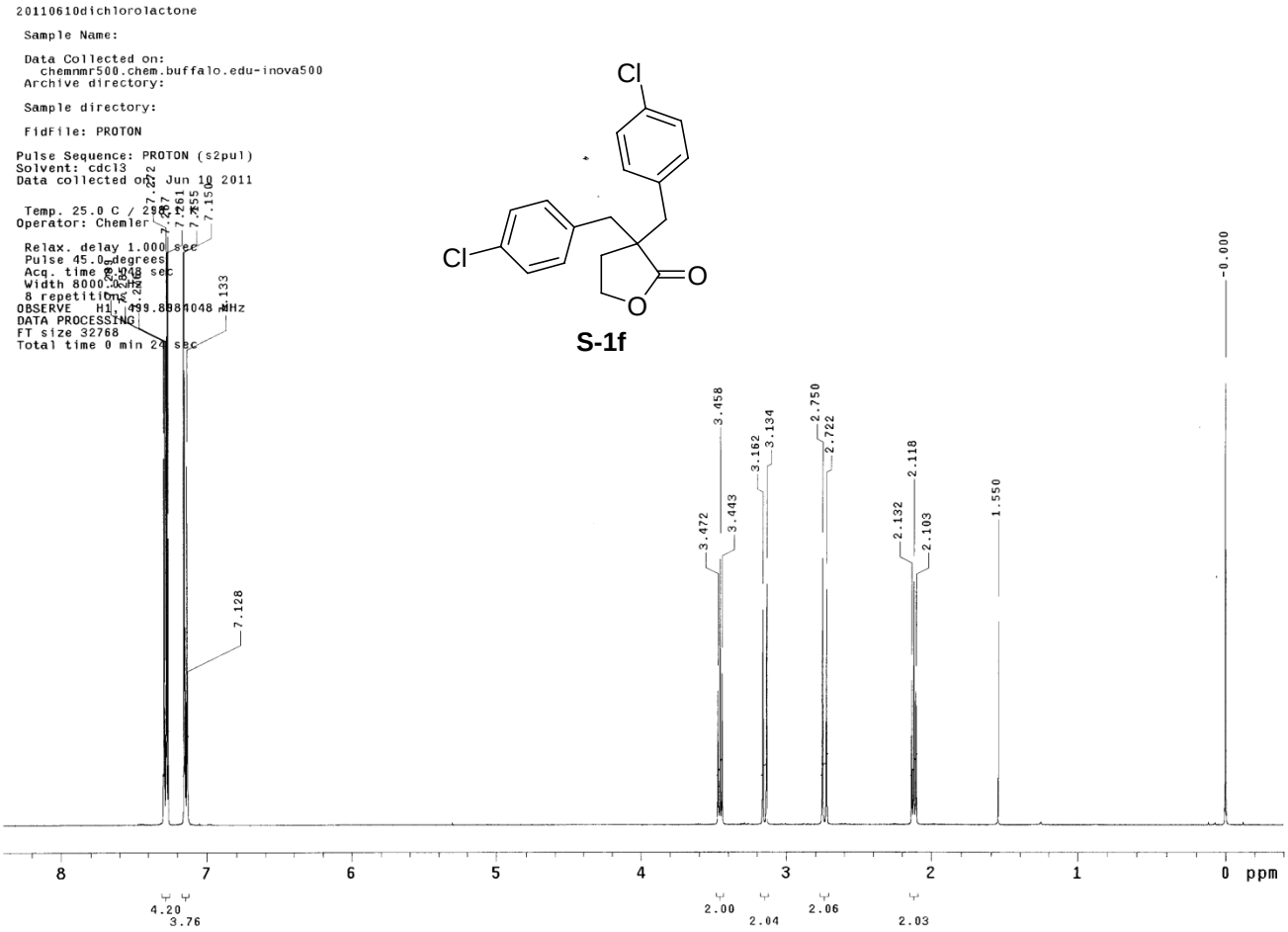
Temp. 25.0 C / 298.1 K
Operator: Chemler

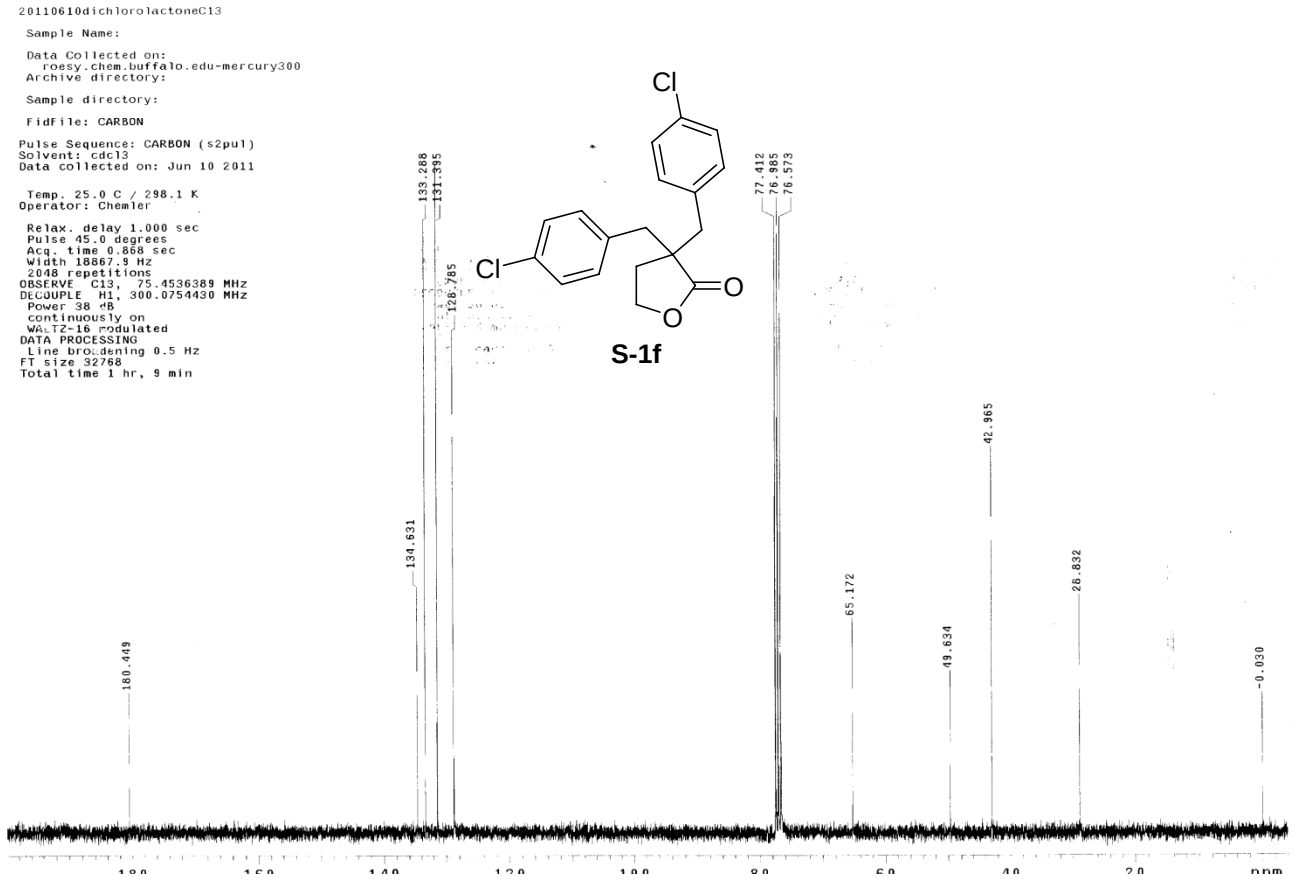
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3552 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min

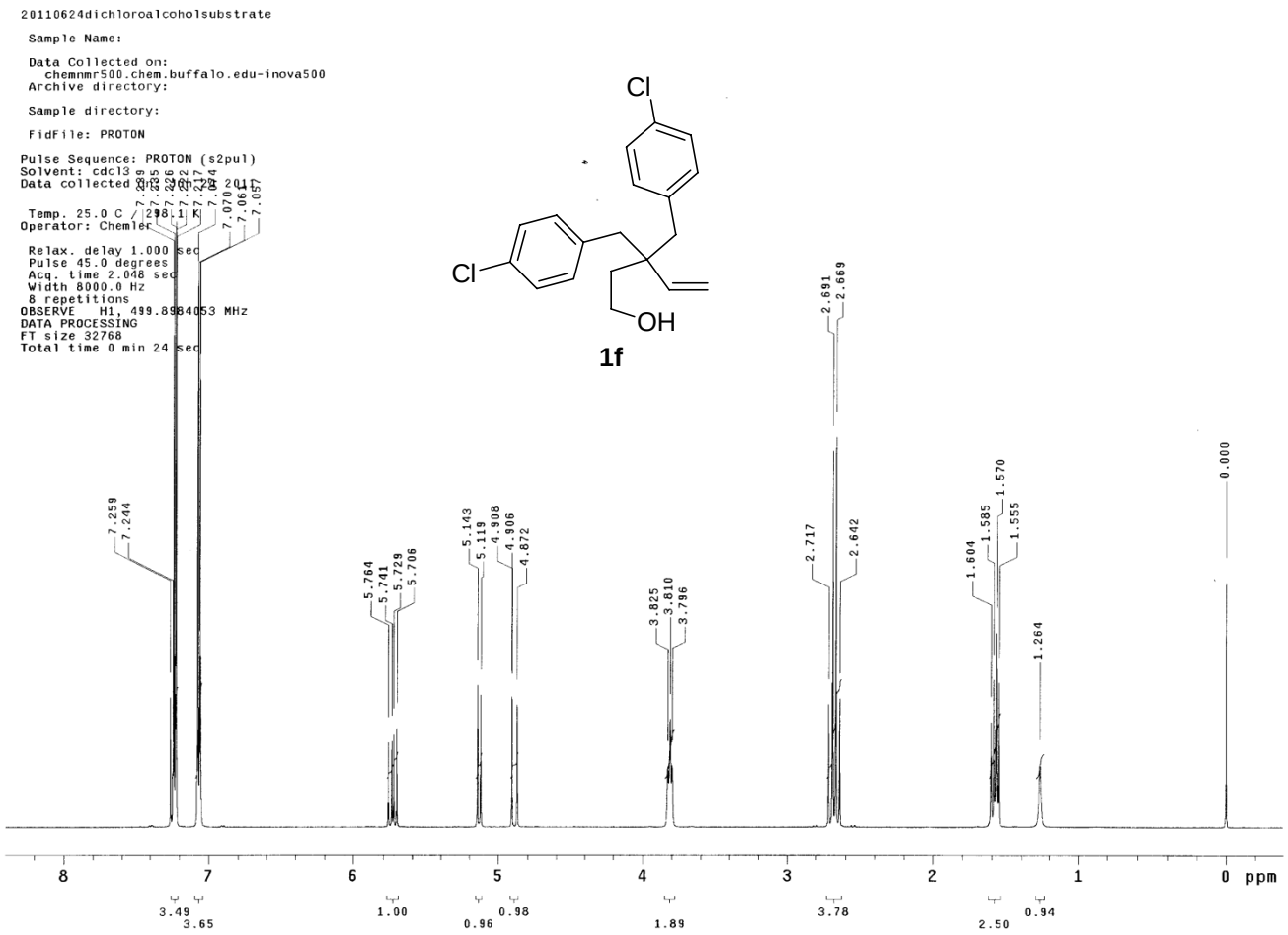


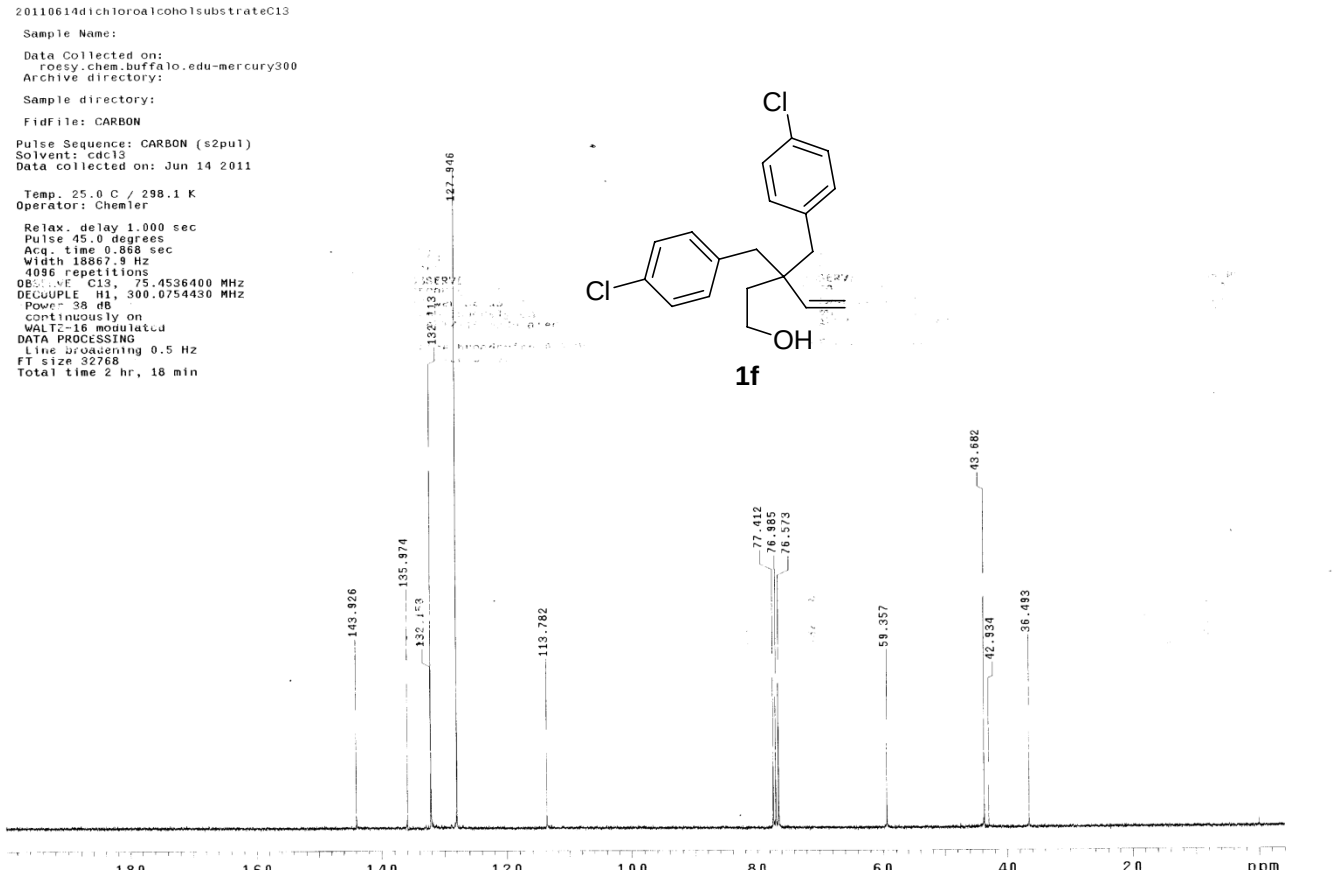
1e

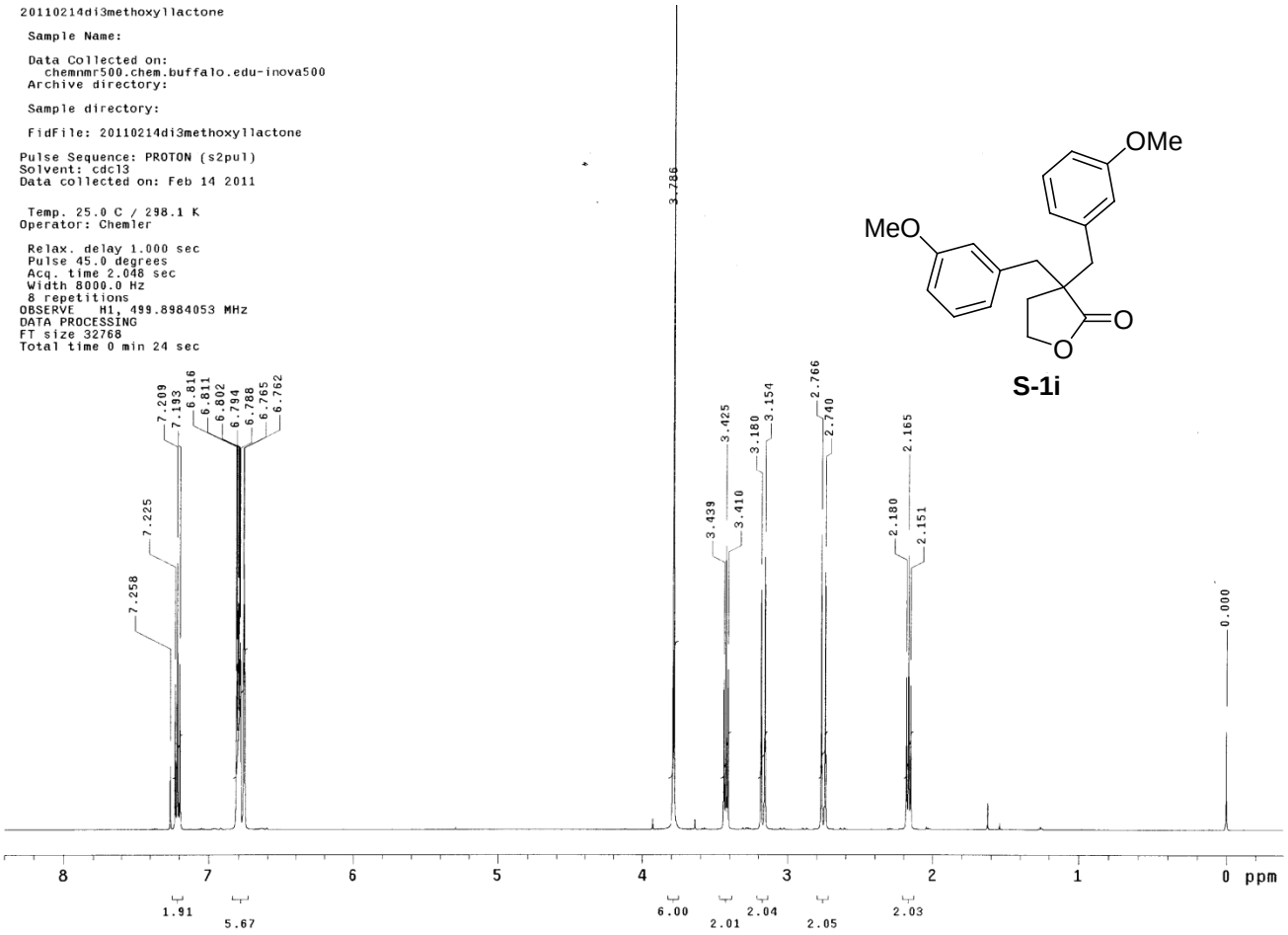


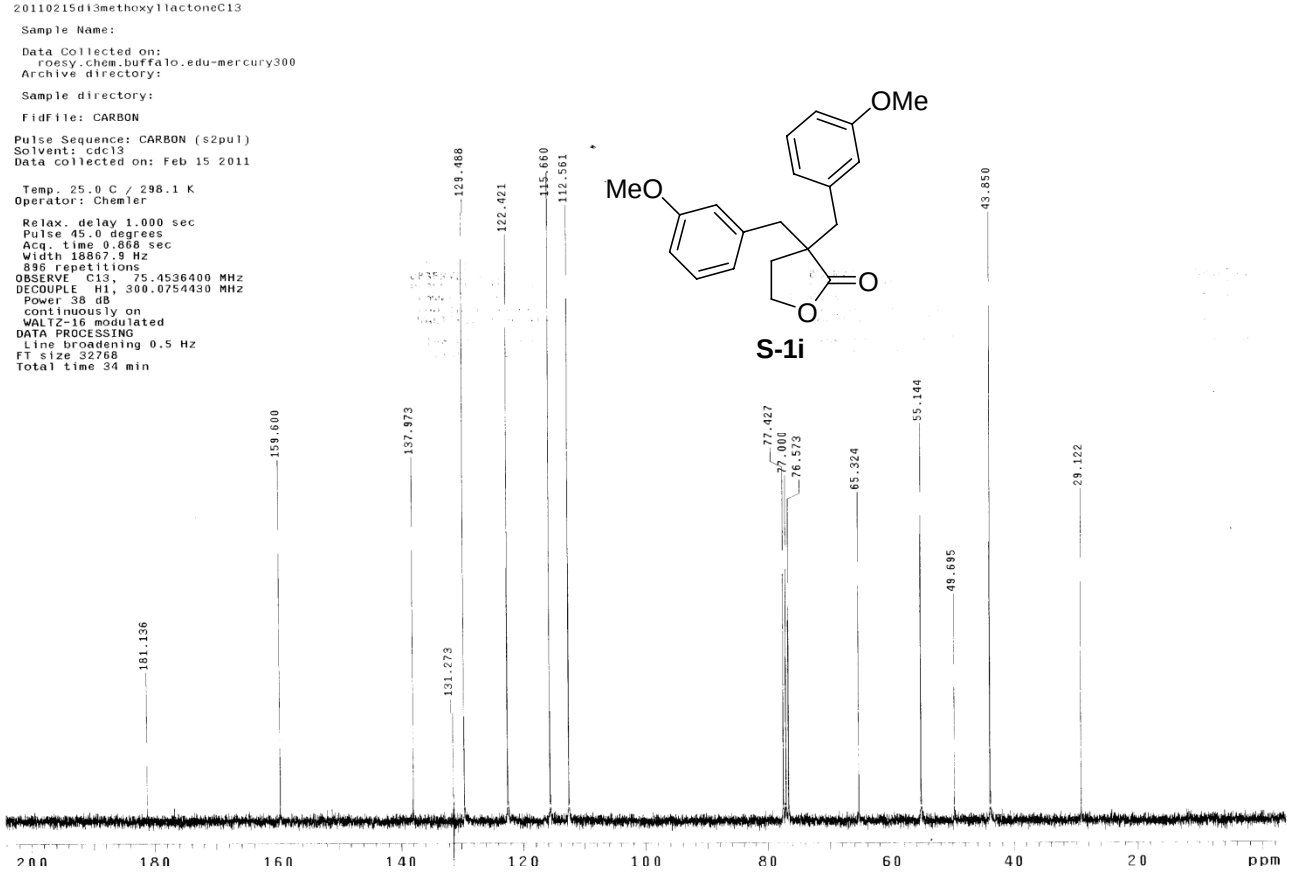

20110610dichlorolactone
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 10 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8881048 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
Cl
Cl
O
O
S-1f
7.272
7.267
7.261
7.255
7.150
7.133
7.128
3.472
3.458
3.443
3.162
3.134
2.750
2.722
2.132
2.118
2.103
1.550
-0.000
8
7
6
5
4
3
2
1
0 ppm
4.20
3.76
2.00
2.04
2.06
2.03

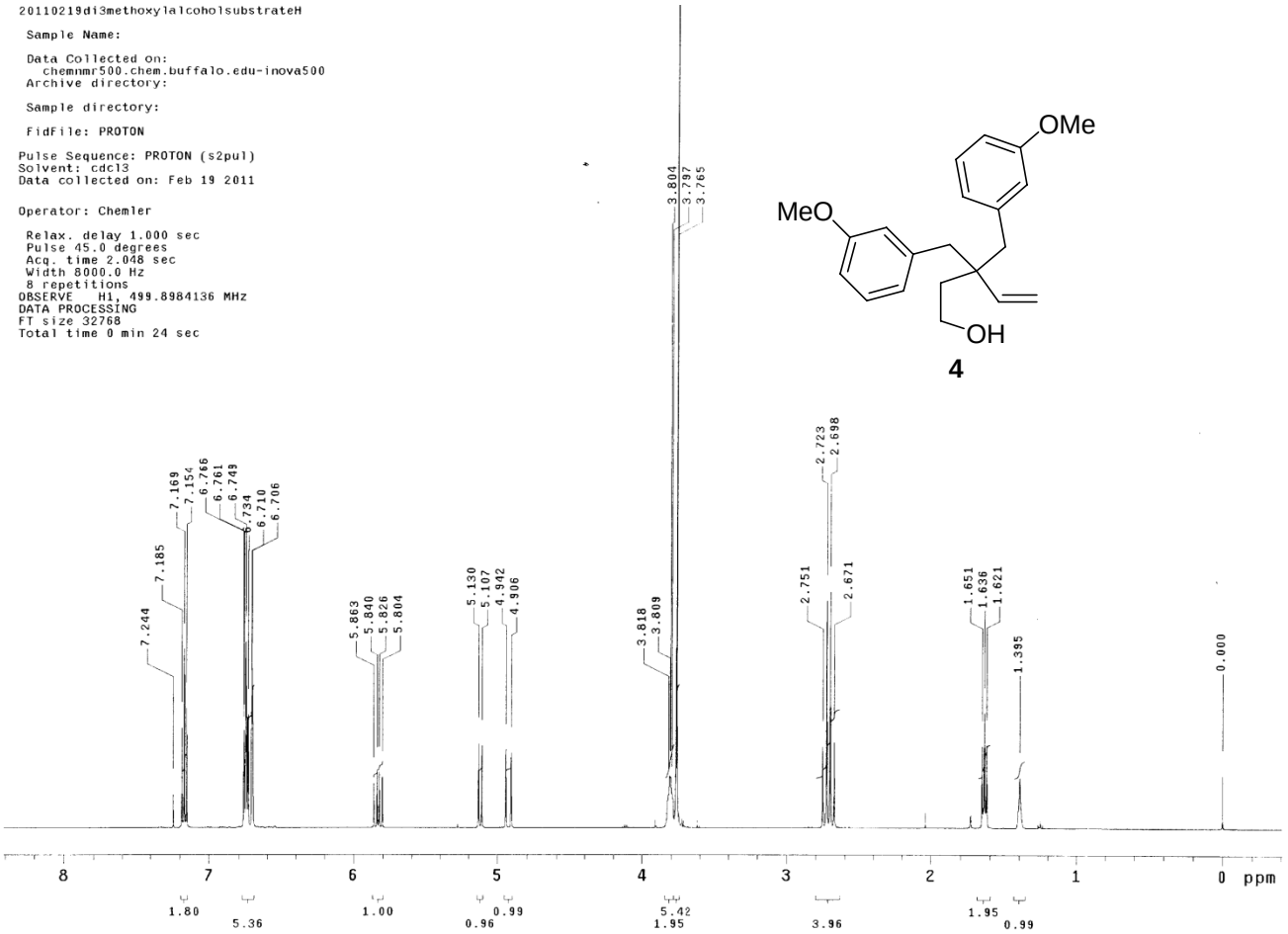

20110610dichlorolactoneC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 10 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2048 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
Cl
Cl
O
O
S-1f
133.288
131.395
128.785
77.412
76.985
76.573
134.631
180.449
65.172
49.634
42.965
28.832
-0.030
180
160
140
120
100
80
60
40
20
ppm

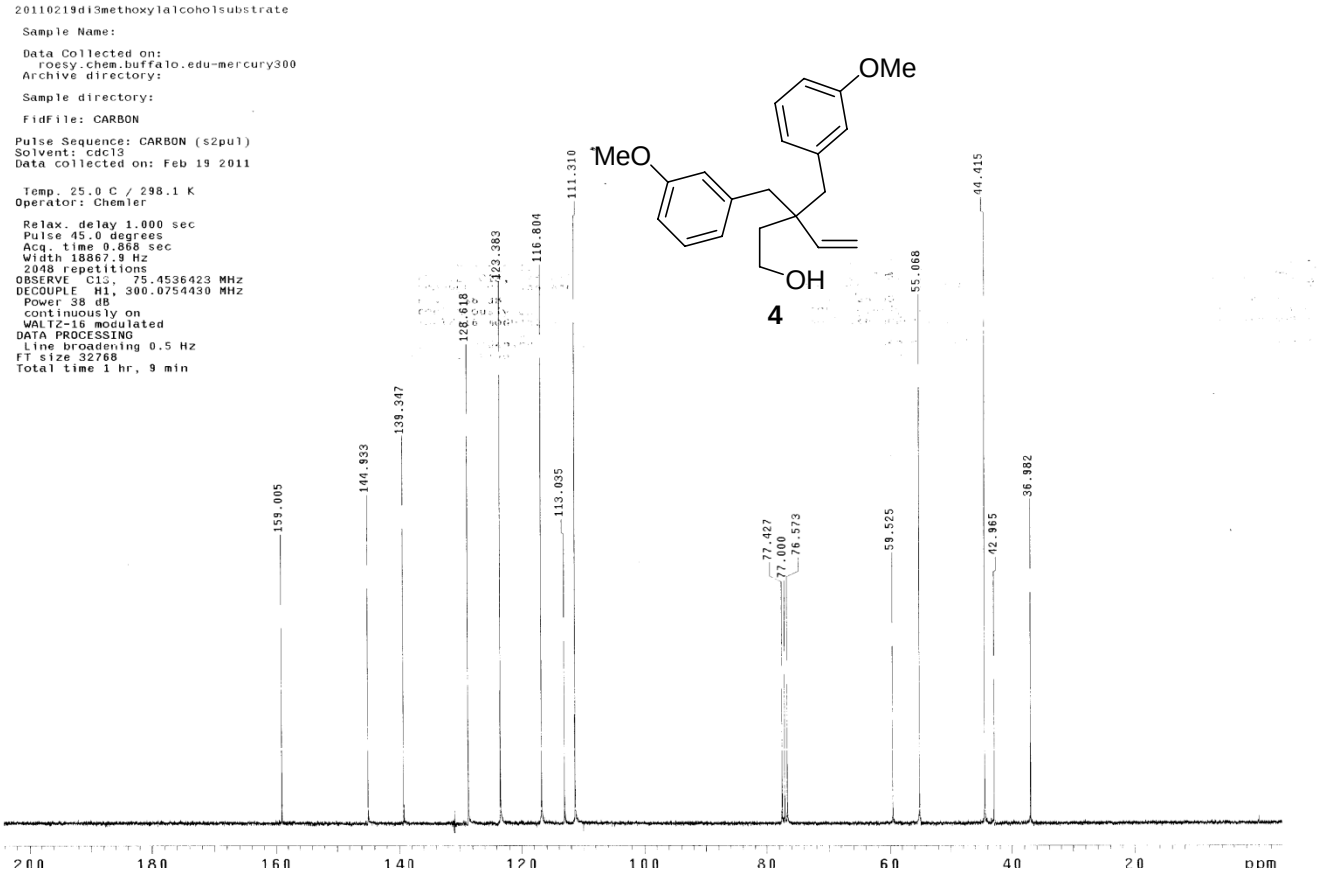

20110624dichloroalcoholsubstrate
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984053 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
Cl
Cl
OH
1f
7.259
7.244
5.764
5.741
5.729
5.706
5.143
5.119
4.908
4.906
4.872
3.825
3.810
3.796
2.691
2.669
2.717
2.642
1.604
1.585
1.570
1.555
1.264
0.000
8
7
6
5
4
3
2
1
0 ppm
3.49
3.65
1.00
0.96
0.98
1.89
3.78
2.50
0.94

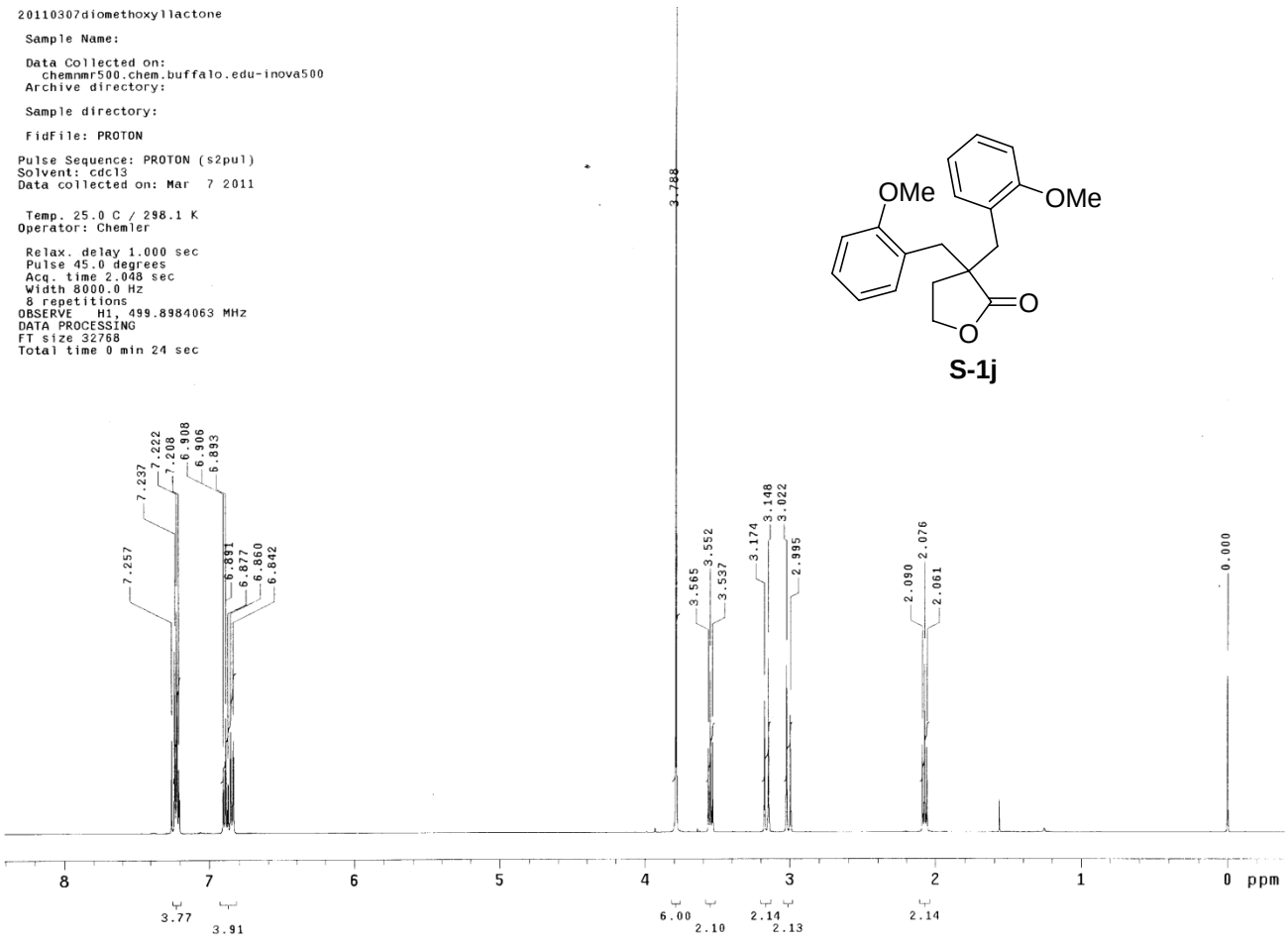

20110614dichloroalcoholsubstrateC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 14 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
4096 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
Cl
Cl
OH
1f
143.926
135.874
132.153
127.946
119.782
77.412
76.985
76.573
59.357
43.682
42.934
36.493
180
160
140
120
100
80
60
40
20
ppm

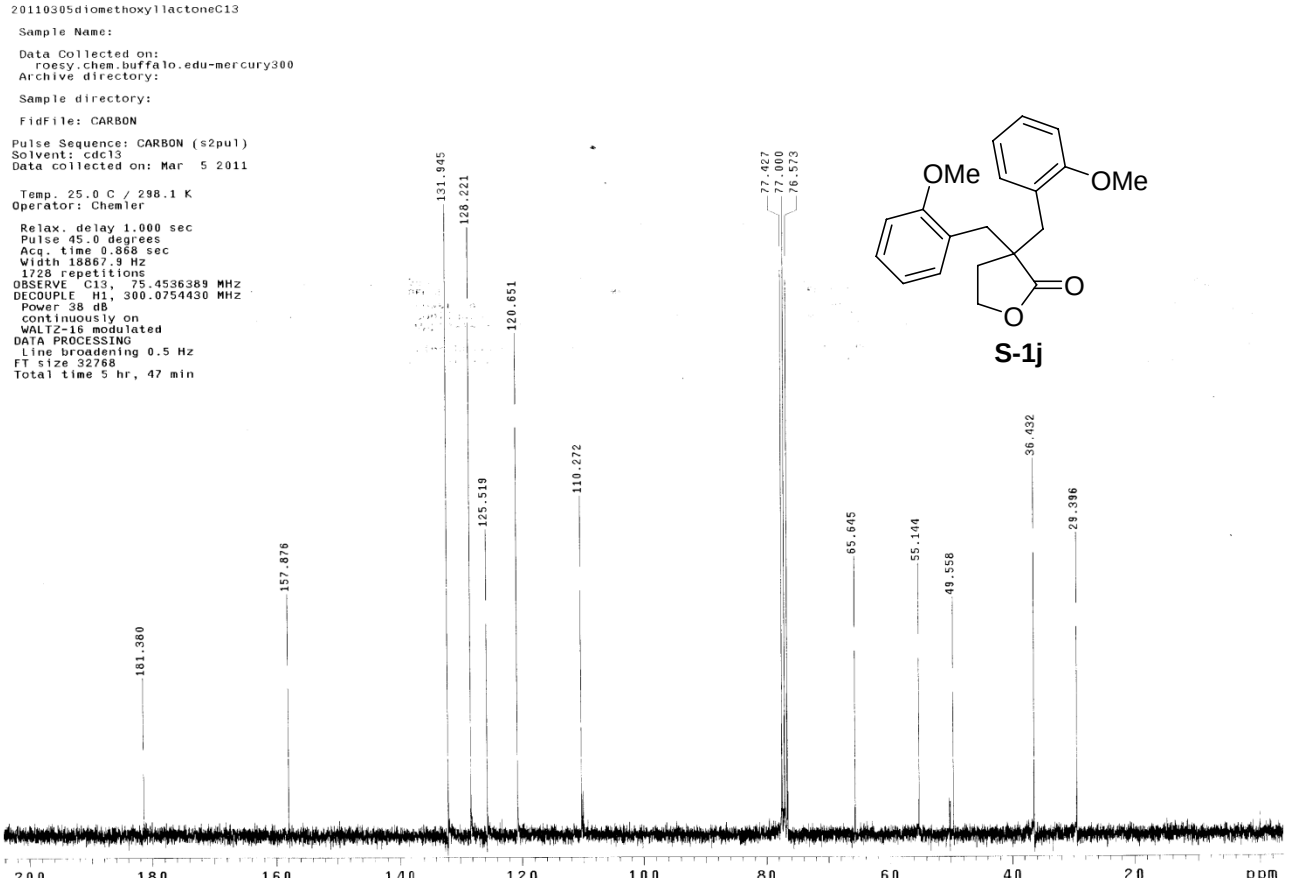

20110214di3methoxyllactone
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: 20110214di3methoxyllactone
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 14 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984053 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
MeO
O
O
S-1i
7.258
7.225
7.209
7.193
6.816
6.811
6.802
6.794
6.788
6.765
6.762
3.786
3.439
3.425
3.410
3.180
3.154
2.766
2.740
2.180
2.165
2.151
0.000
8
7
6
5
4
3
2
1
0 ppm
1.91
5.67
6.00
2.01
2.04
2.05
2.03

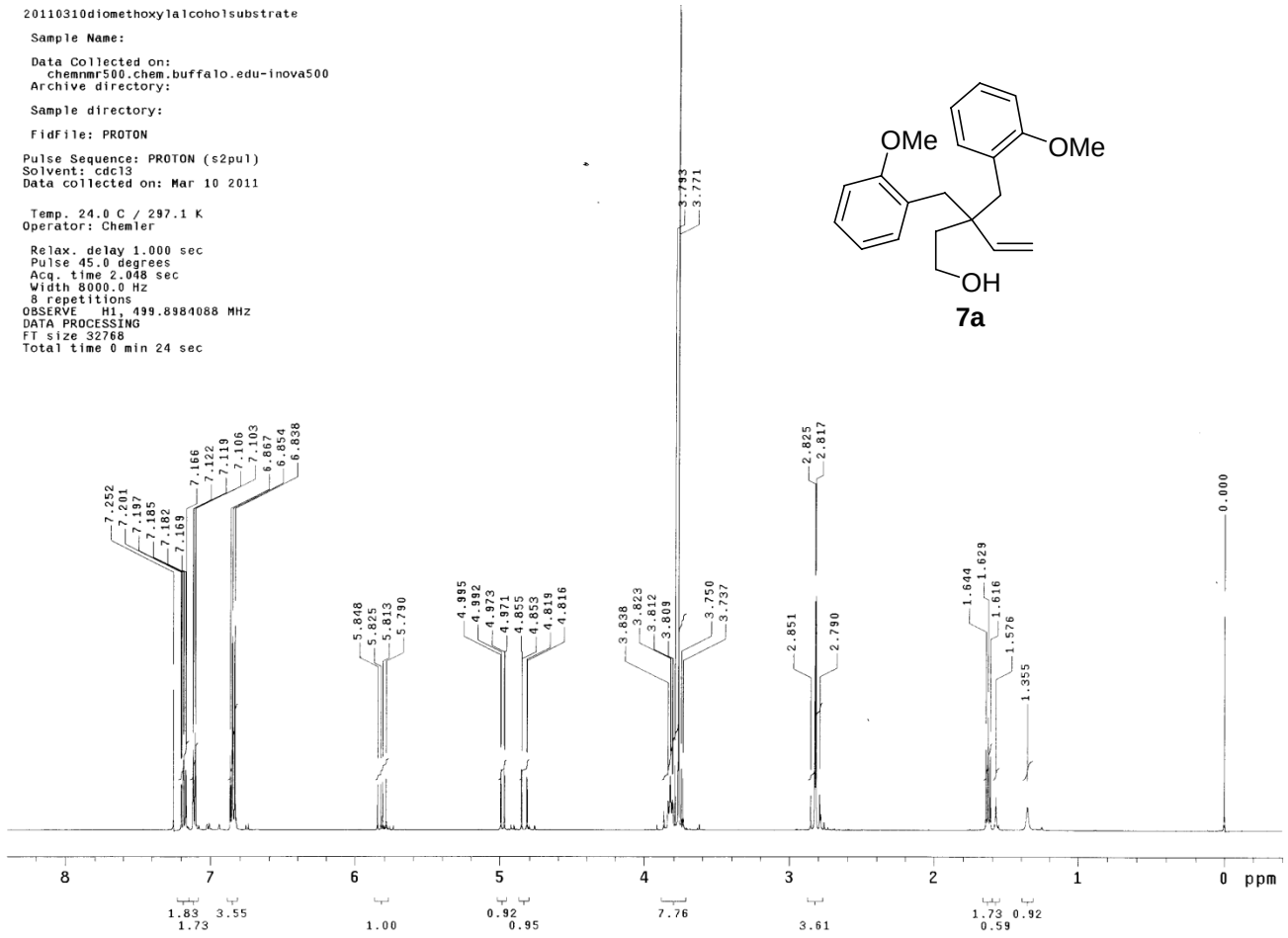

20110215di3methoxyllactoneC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 15 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
896 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 34 min
OMe
MeO
O
O
S-1i
181.136
159.600
137.973
131.273
129.488
122.421
115.660
112.561
77.427
77.000
76.573
65.324
55.144
49.695
43.850
29.122
200
180
160
140
120
100
80
60
40
20
ppm

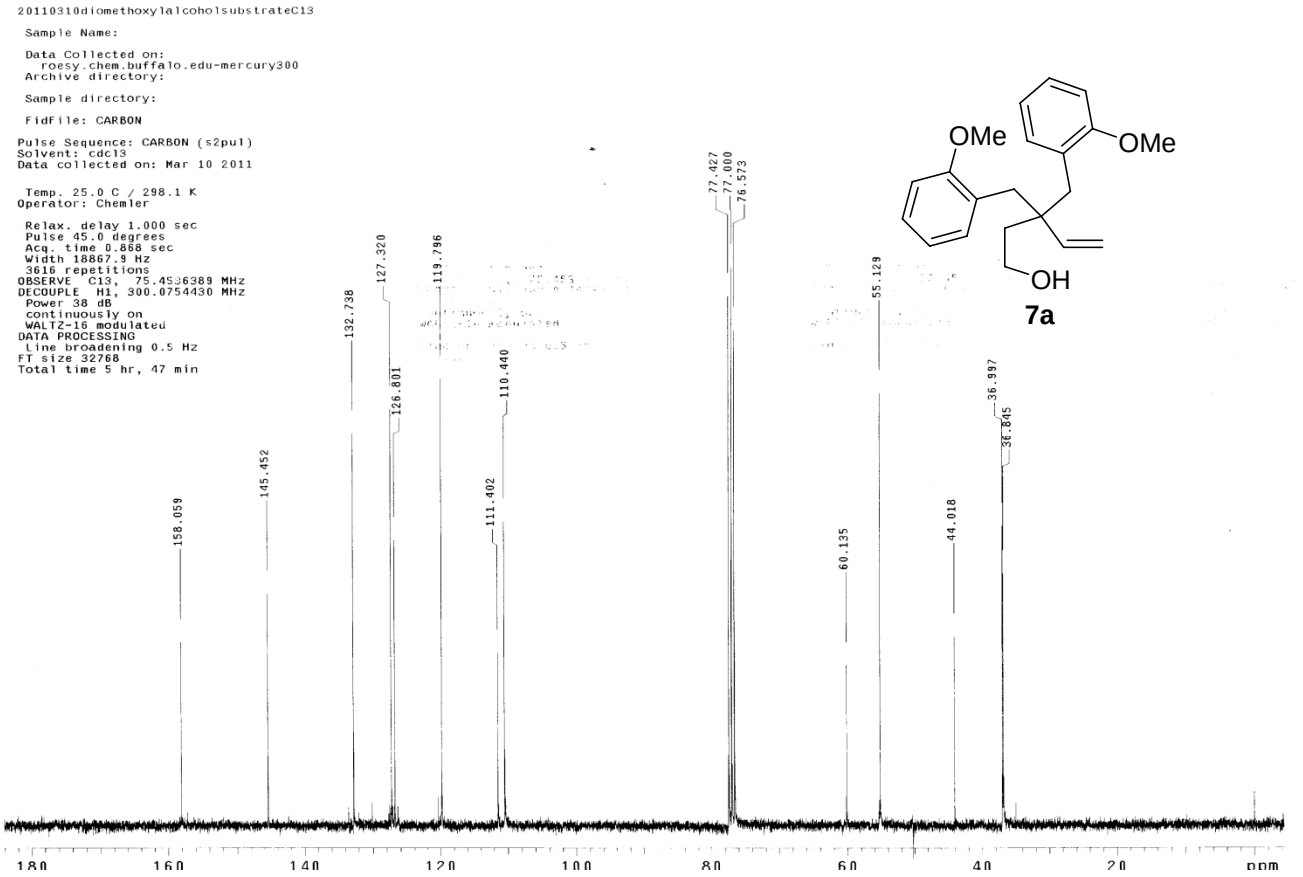

20110219di3methoxylalcoholsubstrateH
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984136 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
MeO
OH
4
7.244
7.185
7.169
7.154
6.766
6.761
6.749
6.734
6.710
6.706
5.863
5.840
5.826
5.804
5.130
5.107
4.942
4.906
3.818
3.809
3.804
3.797
3.765
2.751
2.723
2.698
2.671
1.651
1.636
1.621
1.395
0.000
8
7
6
5
4
3
2
1
0 ppm
1.80
5.36
1.00
0.96
0.99
5.42
1.95
3.96
1.95
0.99

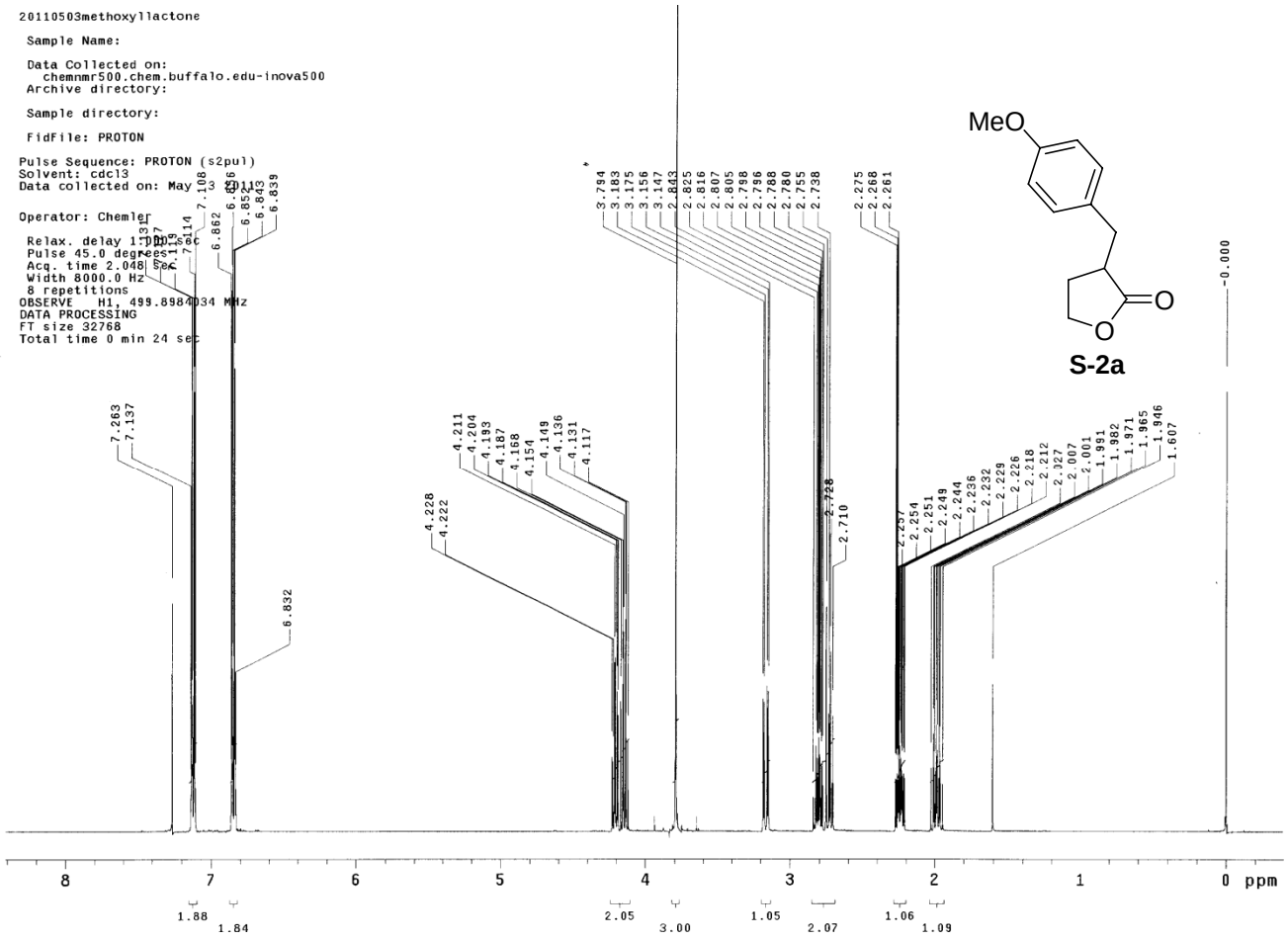

20110219di3methoxylalcoholsubstrate
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 19 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2048 repetitions
OBSERVE C13, 75.4536423 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
OMe
MeO
OH
4
159.005
144.933
139.347
128.618
123.383
116.804
113.035
111.310
77.427
77.000
76.573
59.525
55.068
44.415
42.965
36.382
200
180
160
140
120
100
80
60
40
20
ppm

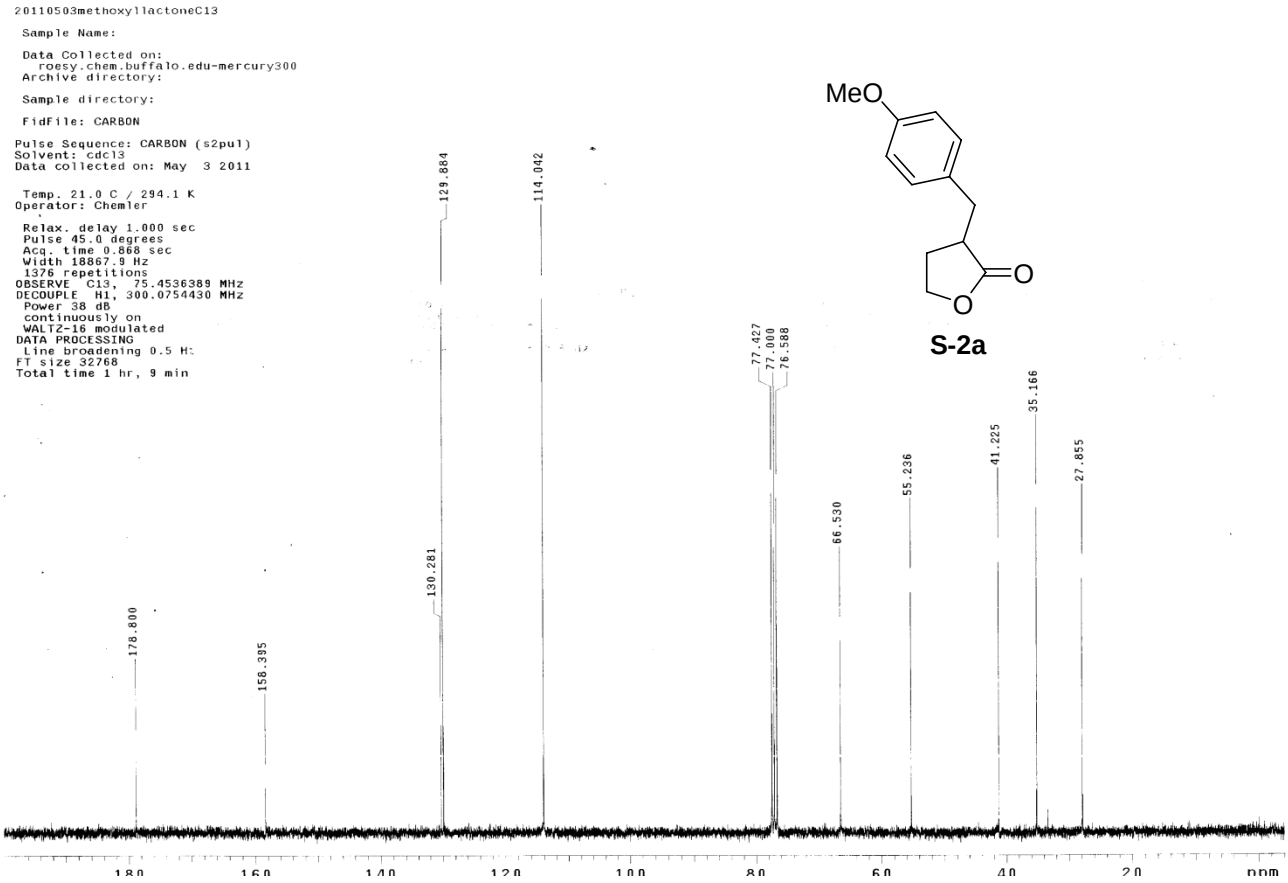

20110307diomethoxyllactone
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 7 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984063 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
OMe
O
O
S-1j
7.257
7.237
7.222
7.208
6.908
6.906
6.893
6.891
6.877
6.860
6.842
3.788
3.565
3.552
3.537
3.174
3.148
3.022
2.995
2.090
2.076
2.061
0.000
8
7
6
5
4
3
2
1
0 ppm
3.77
3.91
6.00
2.10
2.14
2.13
2.14

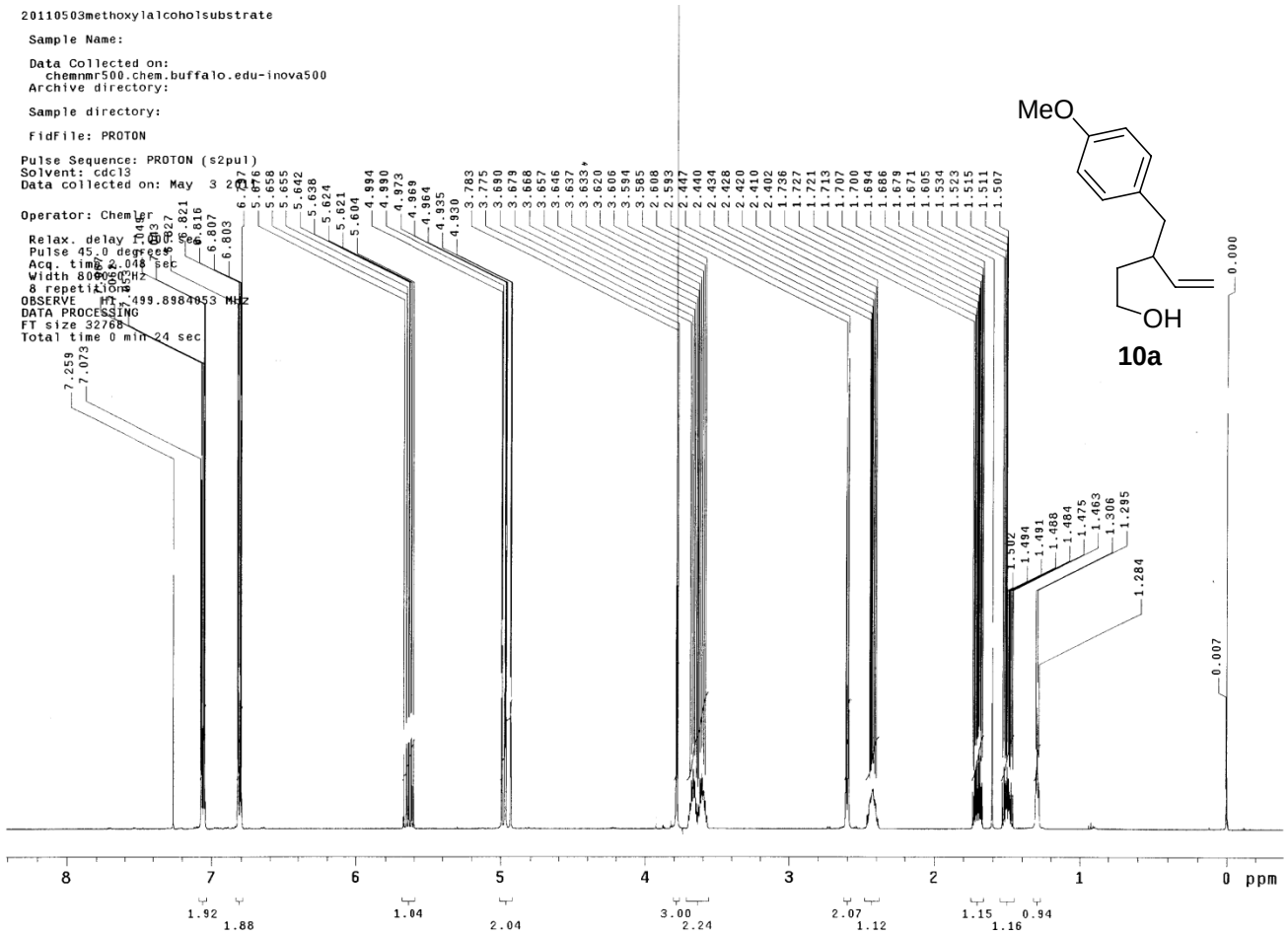

20110305diomethoxyllactoneC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 5 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
1728 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min
OMe
OMe
O
O
S-1j
181.380
157.876
131.945
128.221
125.519
120.651
110.272
77.427
77.000
76.573
65.645
55.144
49.558
36.432
29.396
200
180
160
140
120
100
80
60
40
20
ppm

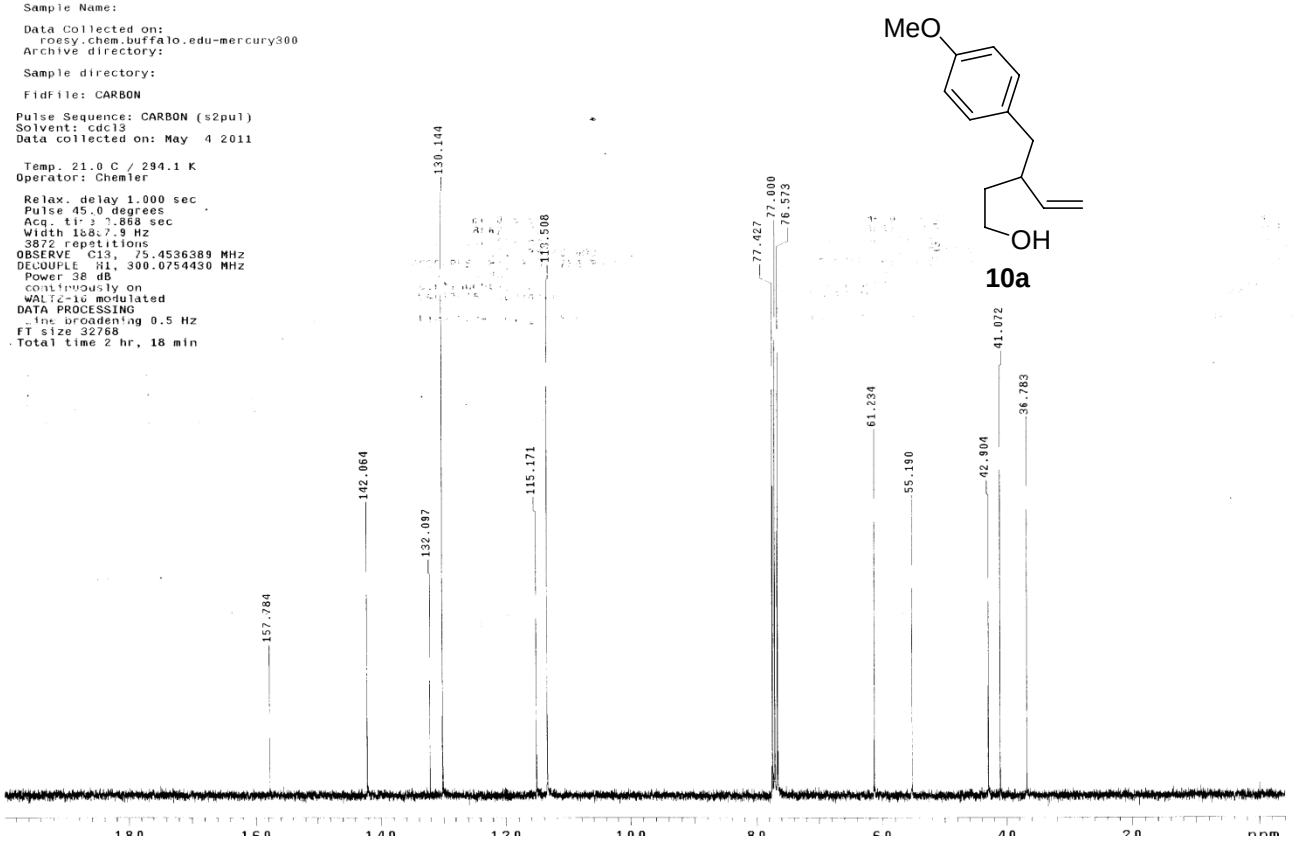

20110310diomethoxylalcoholsubstrate
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 10 2011
Temp. 24.0 C / 297.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984088 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
OMe
OH
7a
7.252
7.201
7.197
7.185
7.182
7.169
7.166
7.122
7.119
7.106
7.103
6.867
6.854
6.838
5.848
5.825
5.813
5.790
4.995
4.992
4.973
4.971
4.855
4.853
4.819
4.816
3.838
3.823
3.812
3.809
3.793
3.771
3.750
3.737
2.851
2.825
2.817
2.790
1.644
1.629
1.616
1.576
1.355
0.000
8
7
6
5
4
3
2
1
0 ppm
1.83
3.55
1.73
1.00
0.92
0.95
7.76
3.61
1.73
0.92
0.59

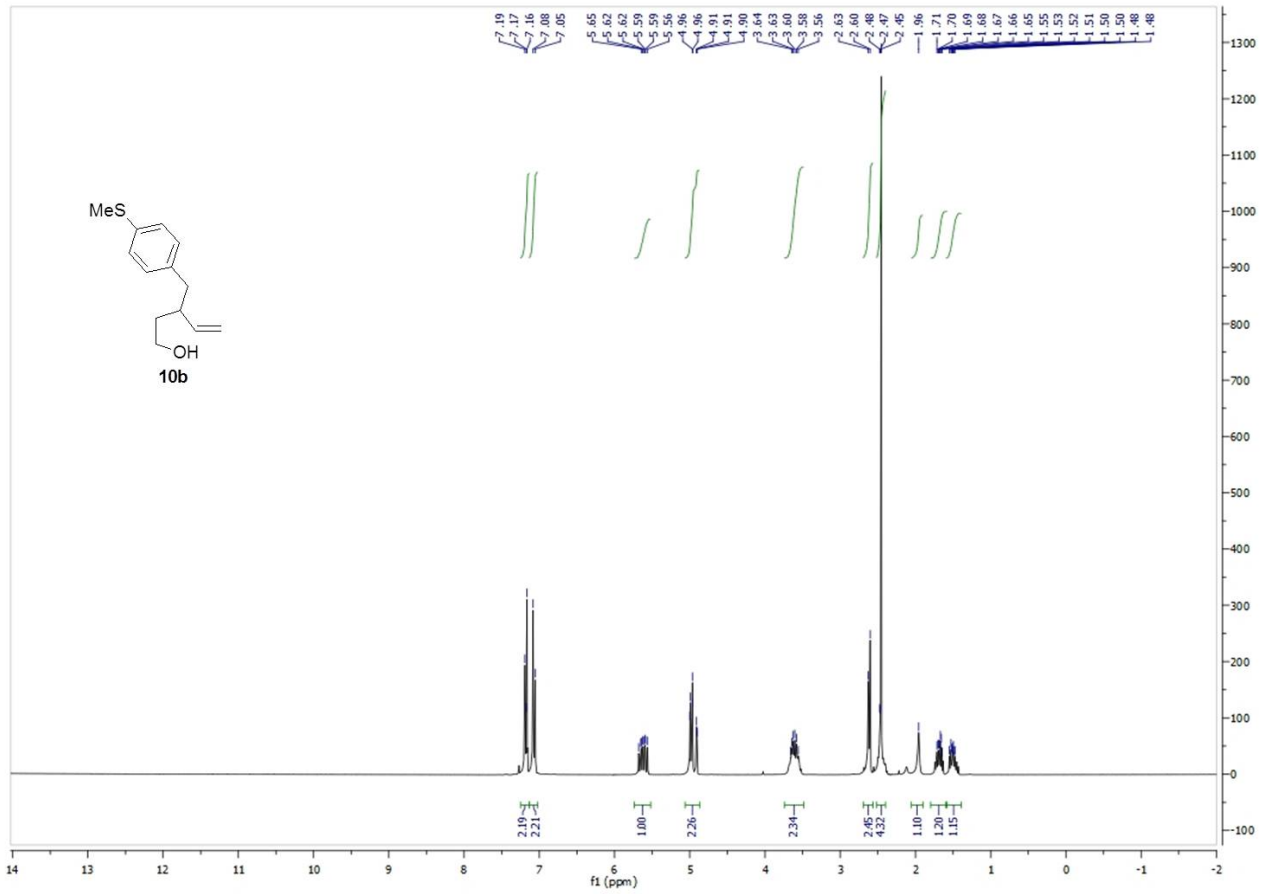

20110310diomethoxylalcoholsubstrateC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 10 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3616 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min
OMe
OMe
OH
7a
158.059
145.452
132.738
127.320
126.801
119.796
111.402
110.440
77.427
77.000
76.573
60.135
55.129
44.018
36.997
36.845
180
160
140
120
100
80
60
40
20
ppm

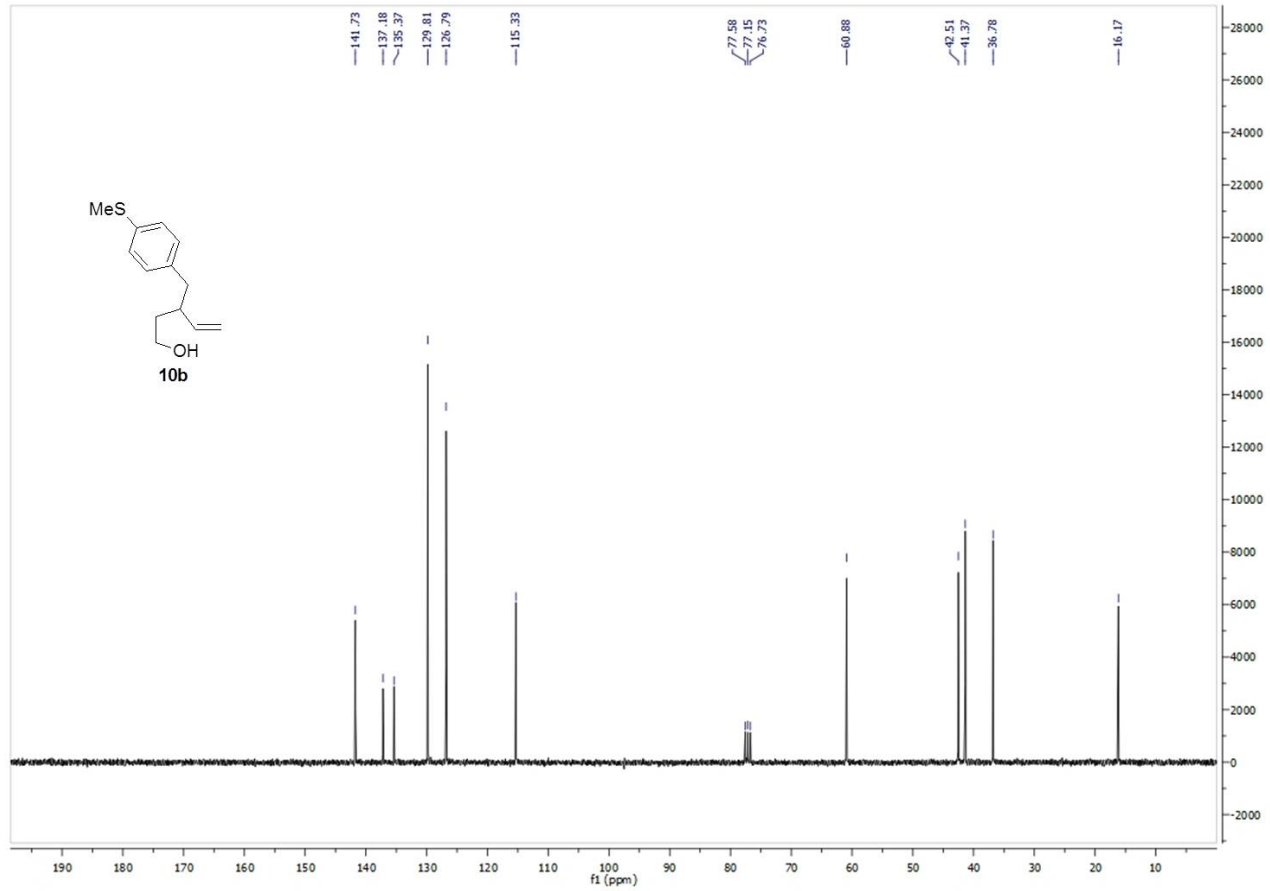

20110503methoxyllactone
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 3 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984034 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
MeO
O
O
S-2a
7.263
7.137
6.862
6.856
6.851
6.843
6.839
6.832
4.228
4.222
4.211
4.204
4.193
4.187
4.168
4.154
4.149
4.136
4.131
4.117
3.794
3.183
3.175
3.156
3.147
3.143
2.825
2.816
2.807
2.805
2.798
2.796
2.788
2.780
2.755
2.738
2.728
2.710
2.275
2.268
2.261
2.257
2.254
2.251
2.249
2.244
2.236
2.232
2.229
2.226
2.218
2.212
2.027
2.007
2.001
1.991
1.982
1.971
1.965
1.946
1.607
0.000
8
7
6
5
4
3
2
1
0 ppm
1.88
1.84
2.05
3.00
1.05
2.07
1.06
1.09

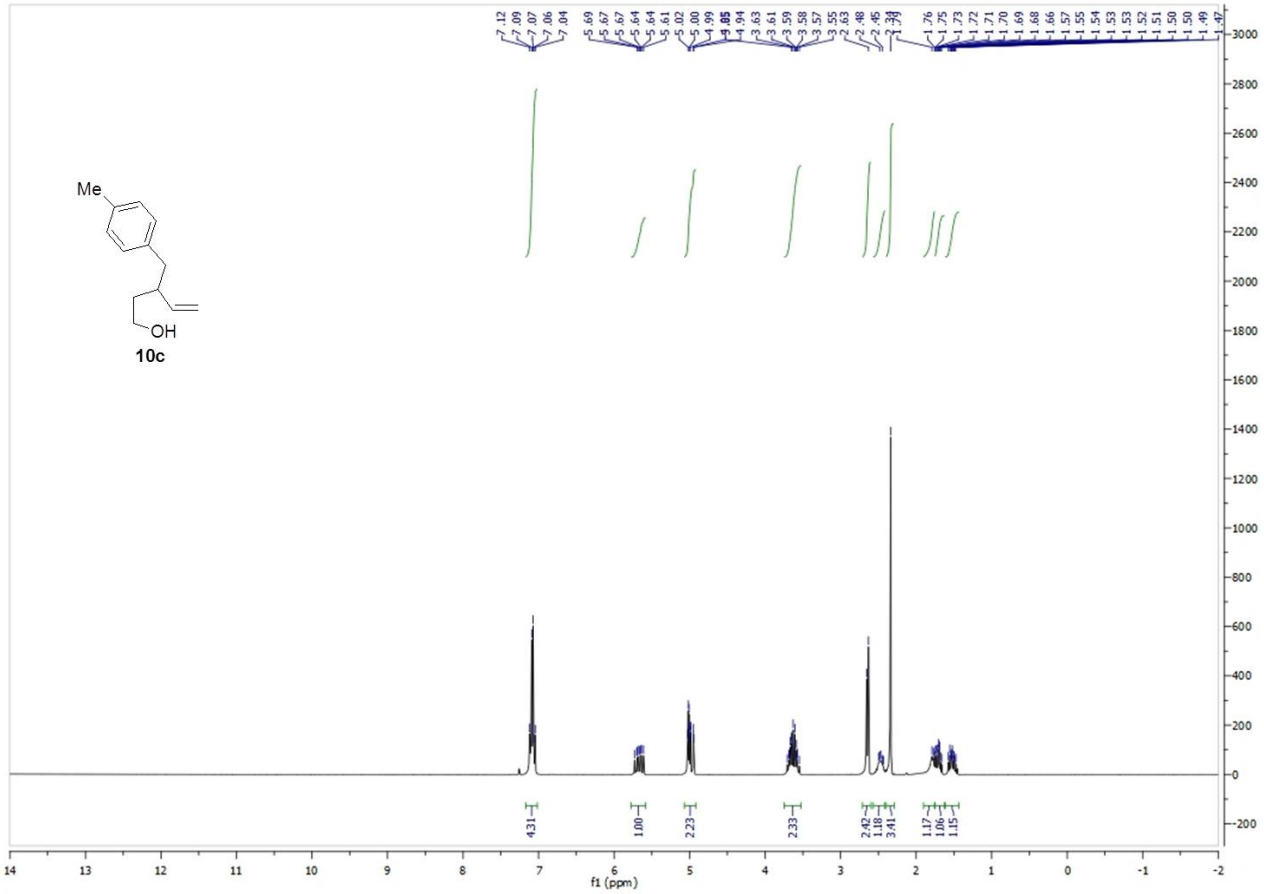

20110503methoxyllactoneC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 3 2011
Temp. 21.0 C / 294.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
1376 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
MeO
O
O
S-2a
178.800
158.395
130.281
129.884
114.042
77.427
77.000
76.588
66.530
55.236
41.225
35.166
27.855
180
160
140
120
100
80
60
40
20
ppm

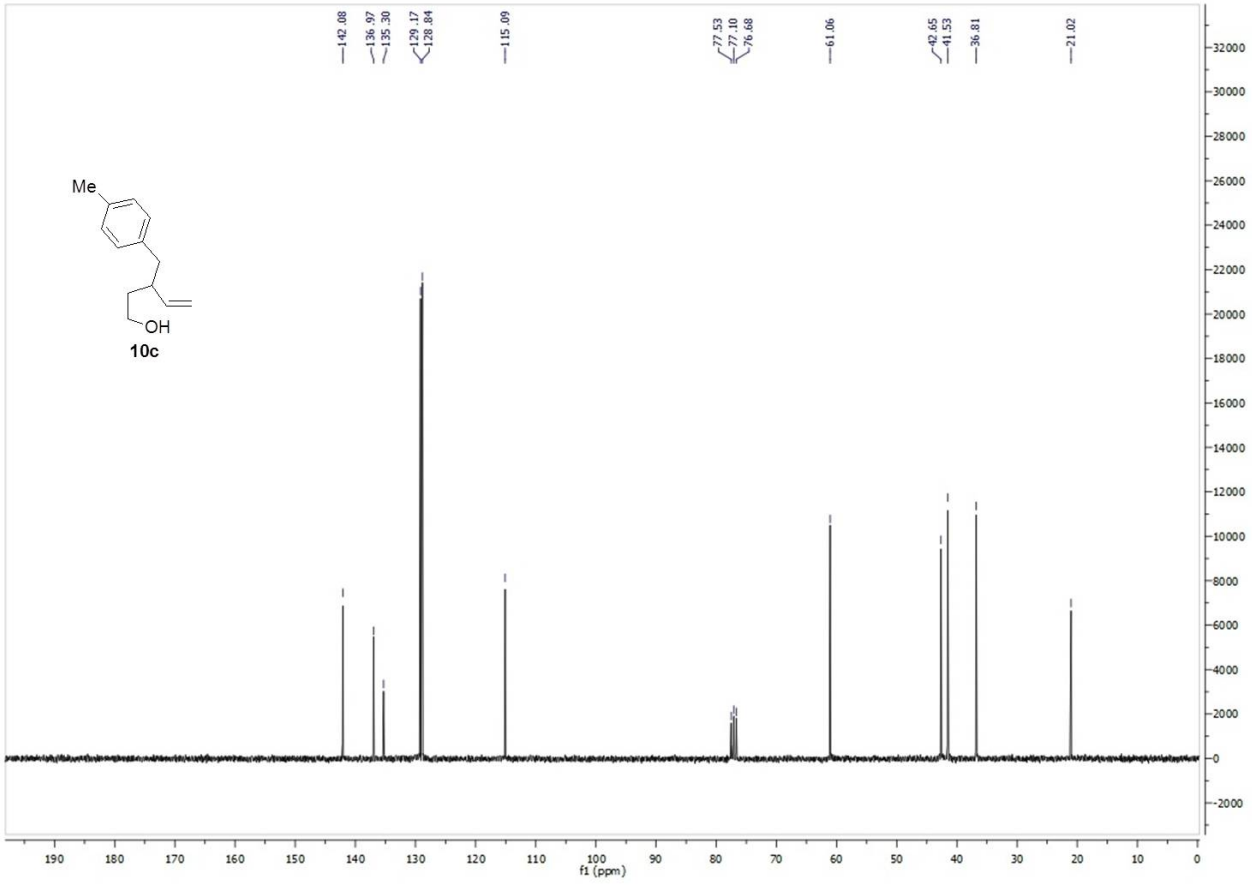

20110503methoxylalcoholsubstrate
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 3 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984053 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
MeO
OH
10a
8
7
6
5
4
3
2
1
0 ppm
1.92
1.88
1.04
2.04
3.00
2.24
2.07
1.12
1.15
0.94
1.16


20110504methoxylalcoholsubstrateC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 4 2011
Temp. 21.0 C / 294.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.868 sec
Width 18867.9 Hz
3872 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
MeO
OH
10a
157.784
142.064
132.097
130.144
115.171
113.508
77.427
77.000
76.573
61.234
55.190
42.904
41.072
36.783
180
160
140
120
100
80
60
40
20
ppm


MeS
OH
10b
f1 (ppm)


MeS
OH
10b
f1 (ppm)


Me
OH
10c
f1 (ppm)


Me
OH
10c
f1 (ppm)

20110809dibenzylphenylsubstrate

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

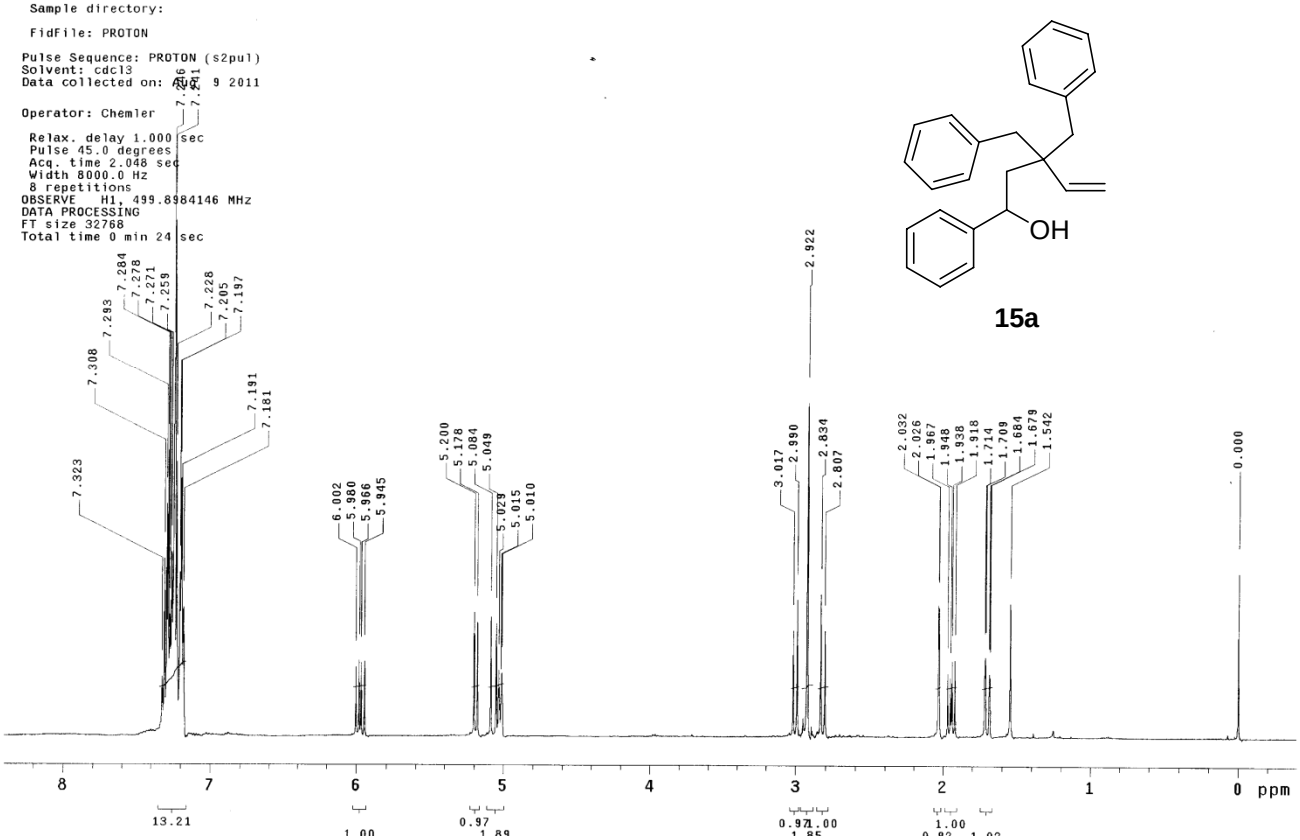
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 9 2011

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984146 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



20110622dibenzylphenylalcoholsubstrateC13

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

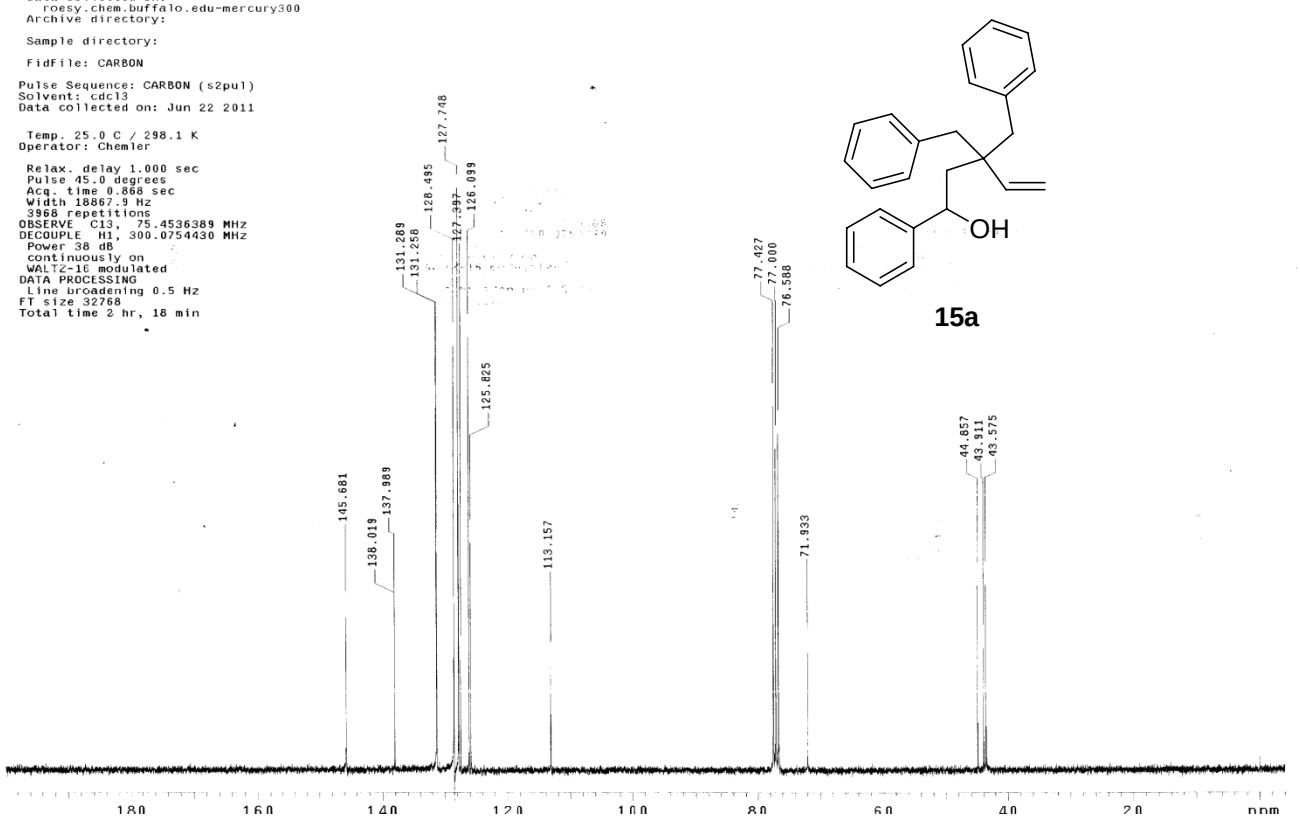
Sample directory:

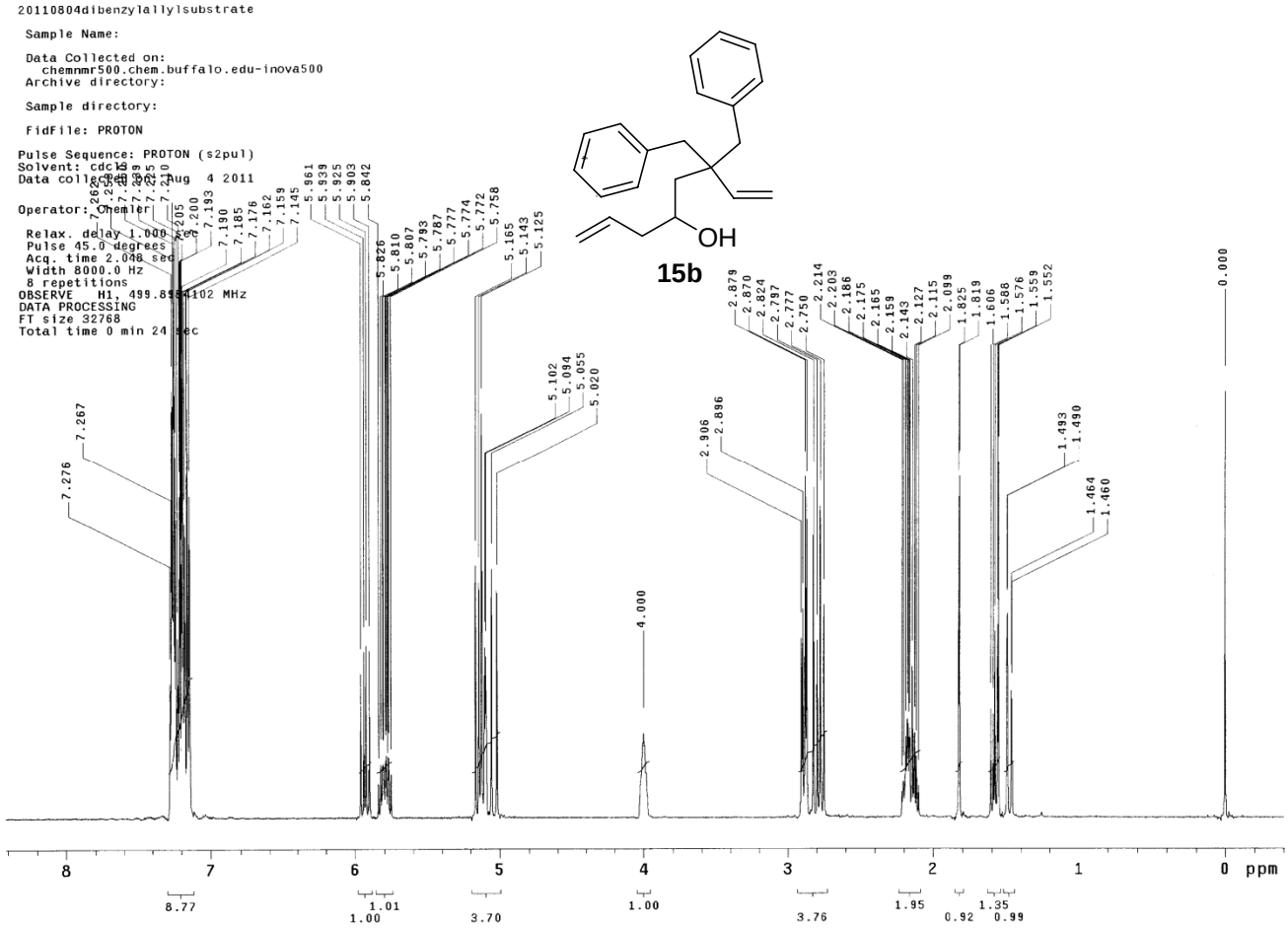
FidFile: CARBON

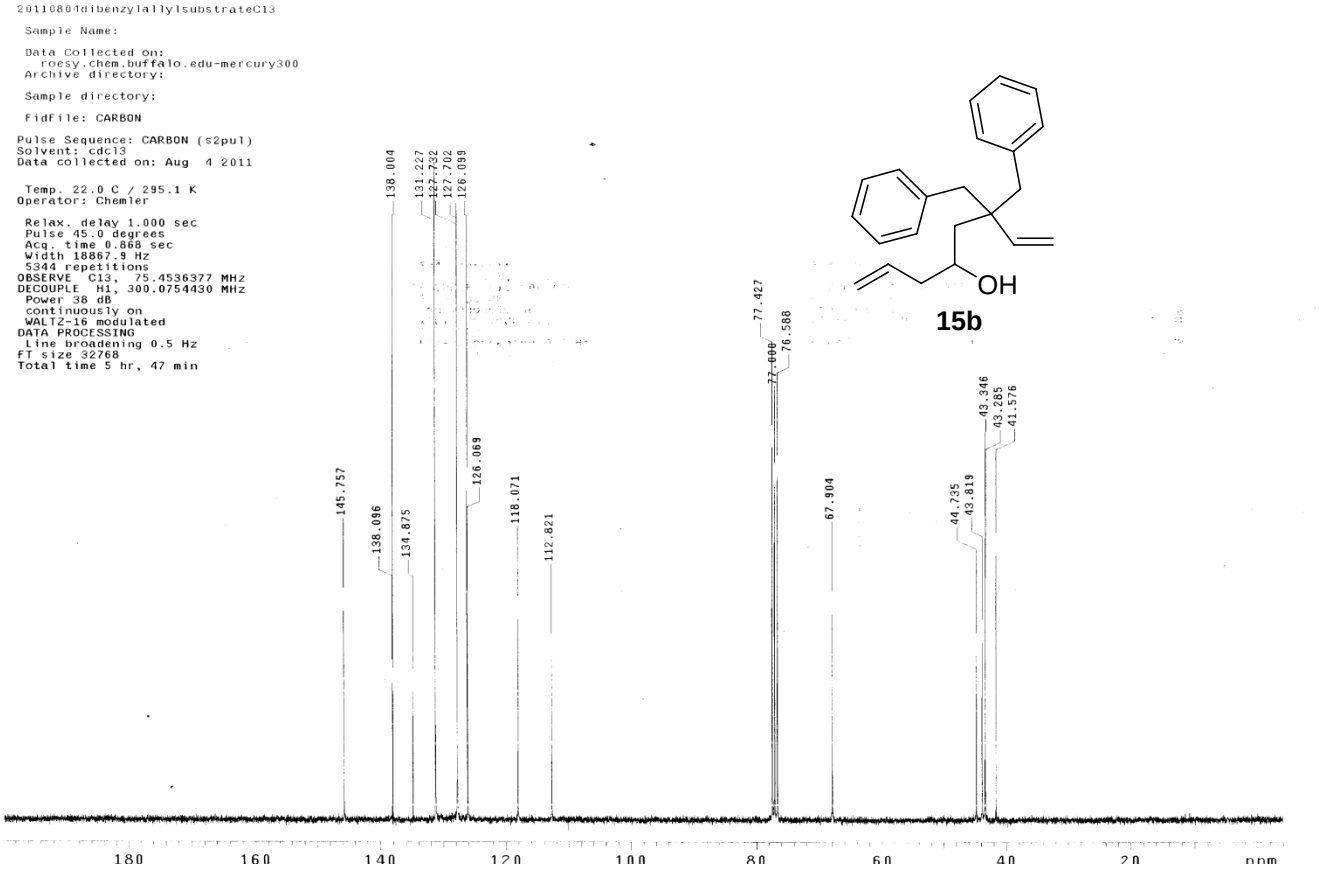
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 22 2011

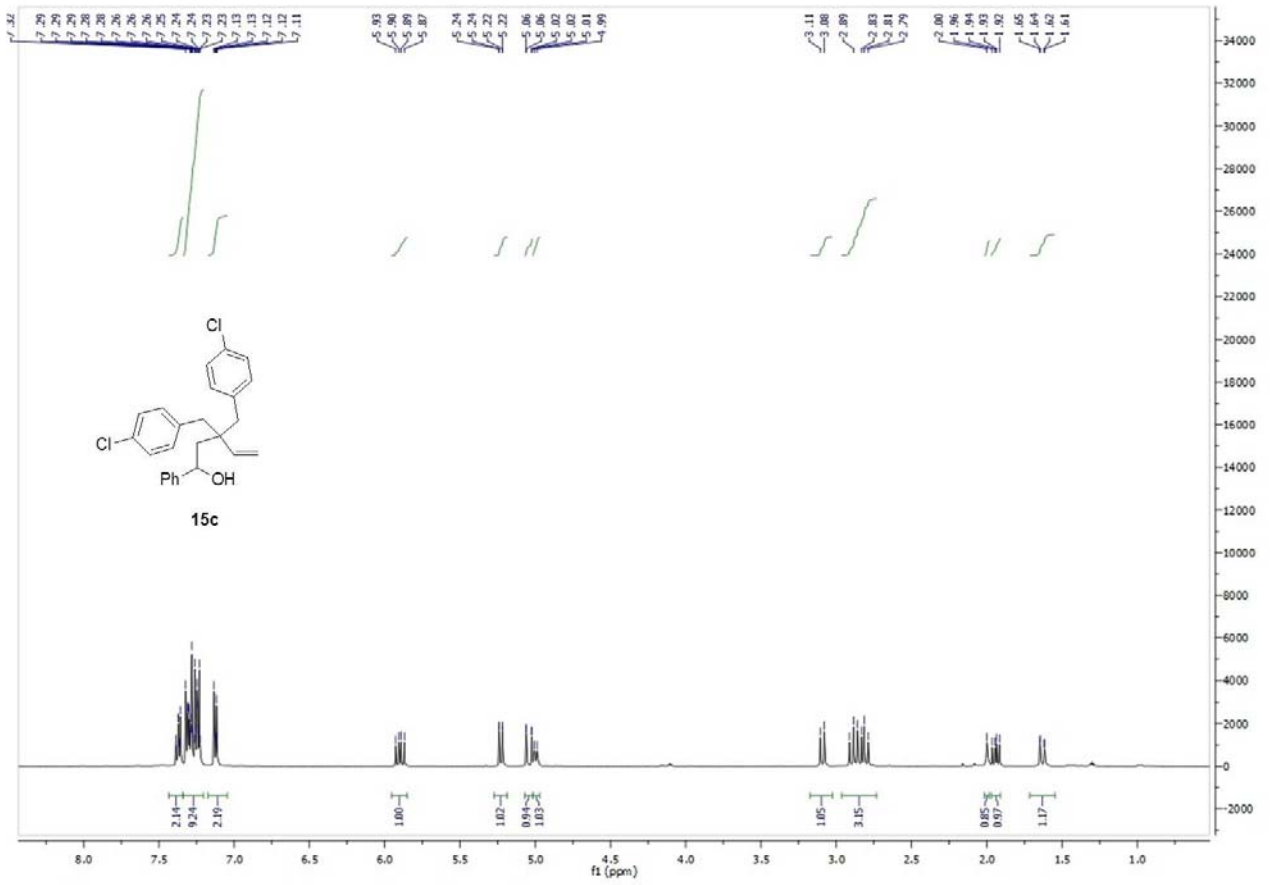
Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3968 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min

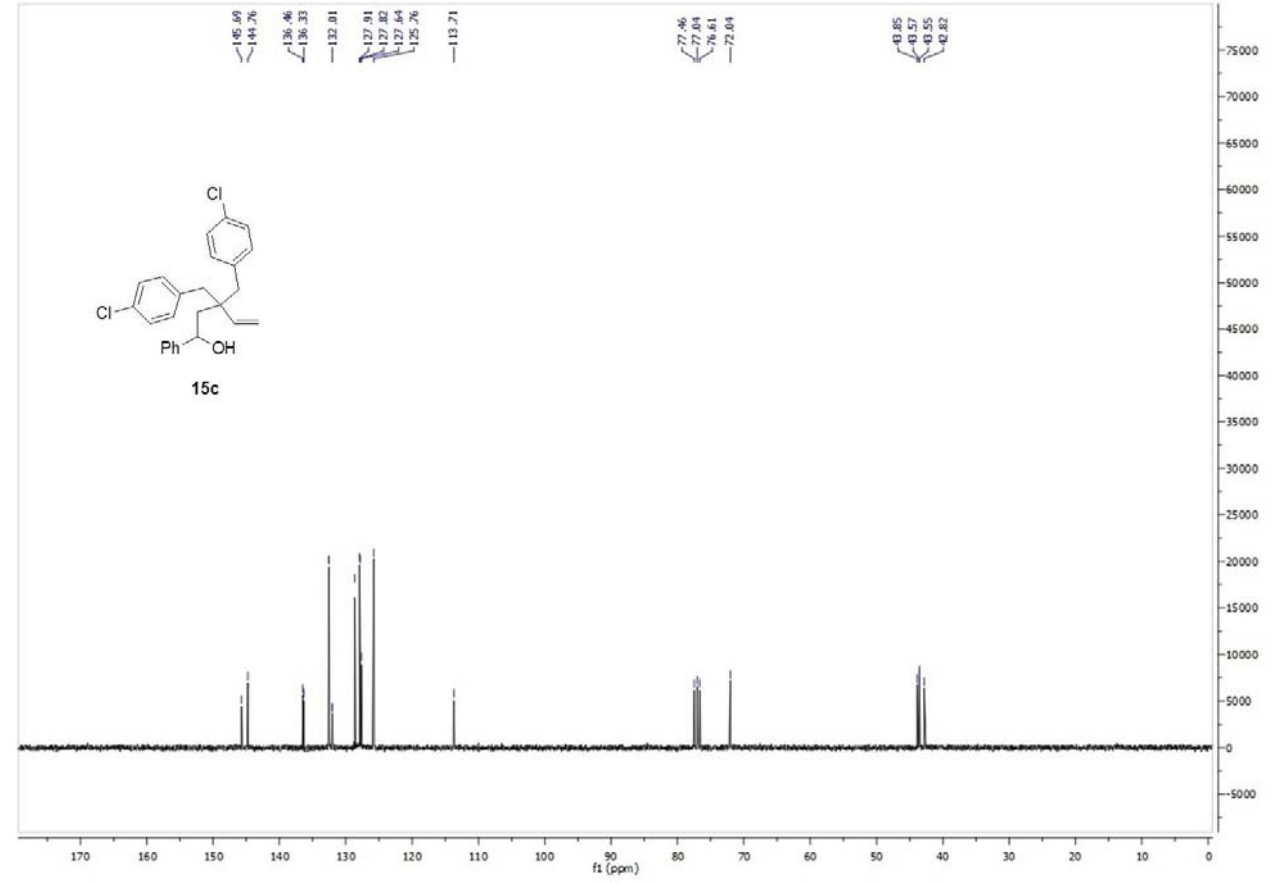



20110804dibenzylallylsubstrate
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OH
15b
ppm

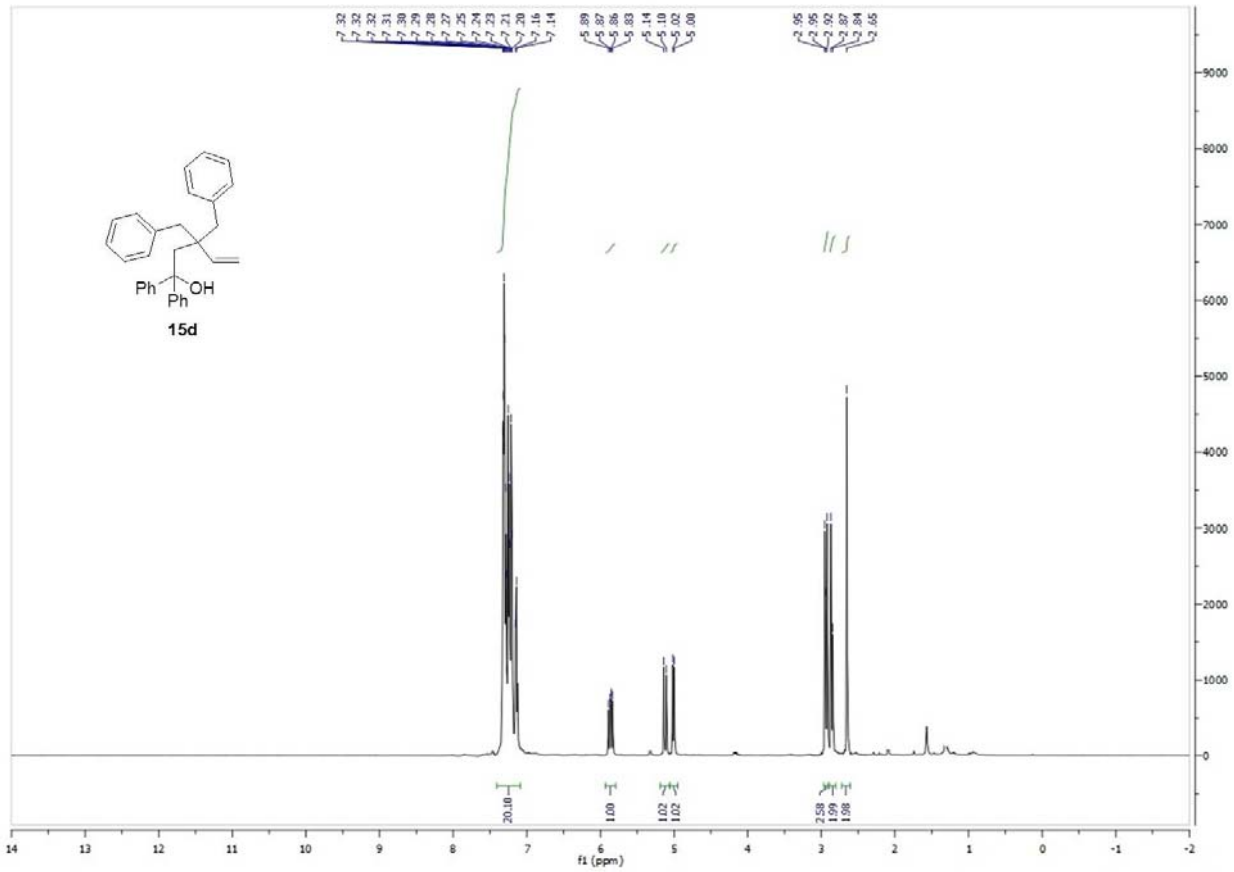

20110804dibenzylallylsubstrateC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 4 2011
Temp. 22.0 C / 295.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
5344 repetitions
OBSERVE C13, 75.4536377 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min
OH
15b
ppm

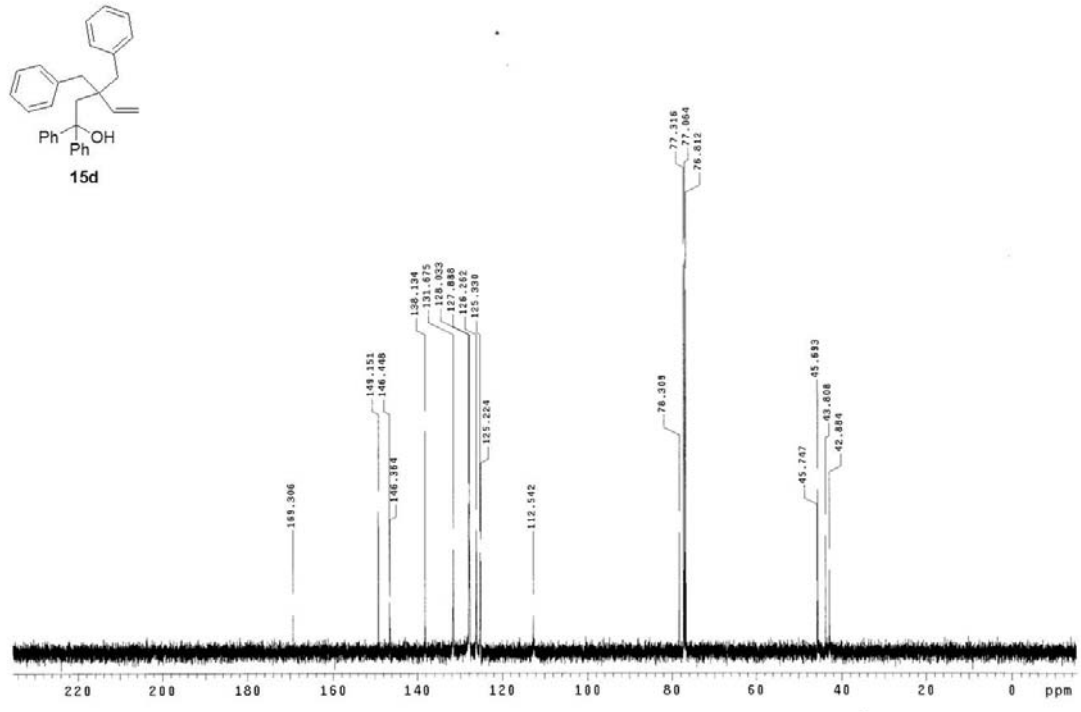


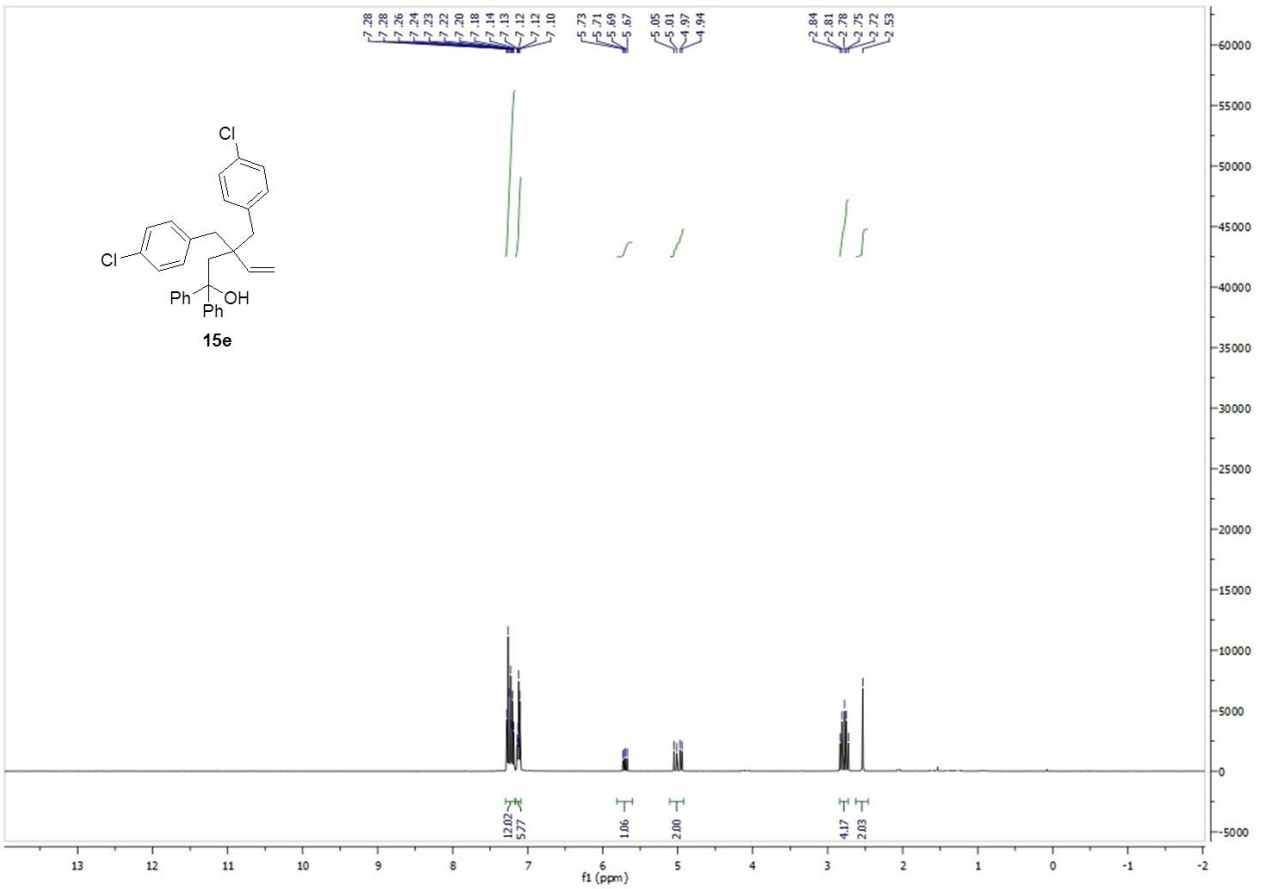
15c

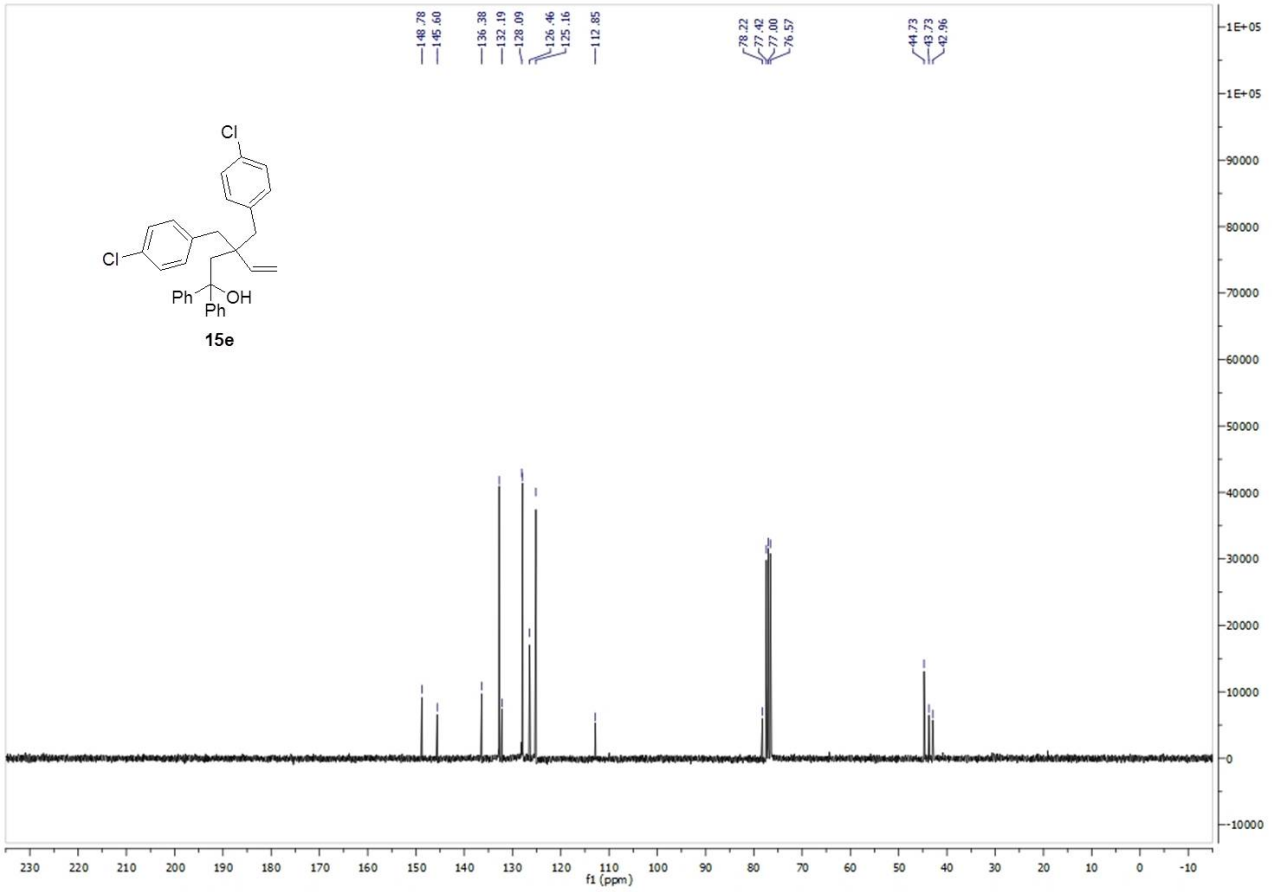


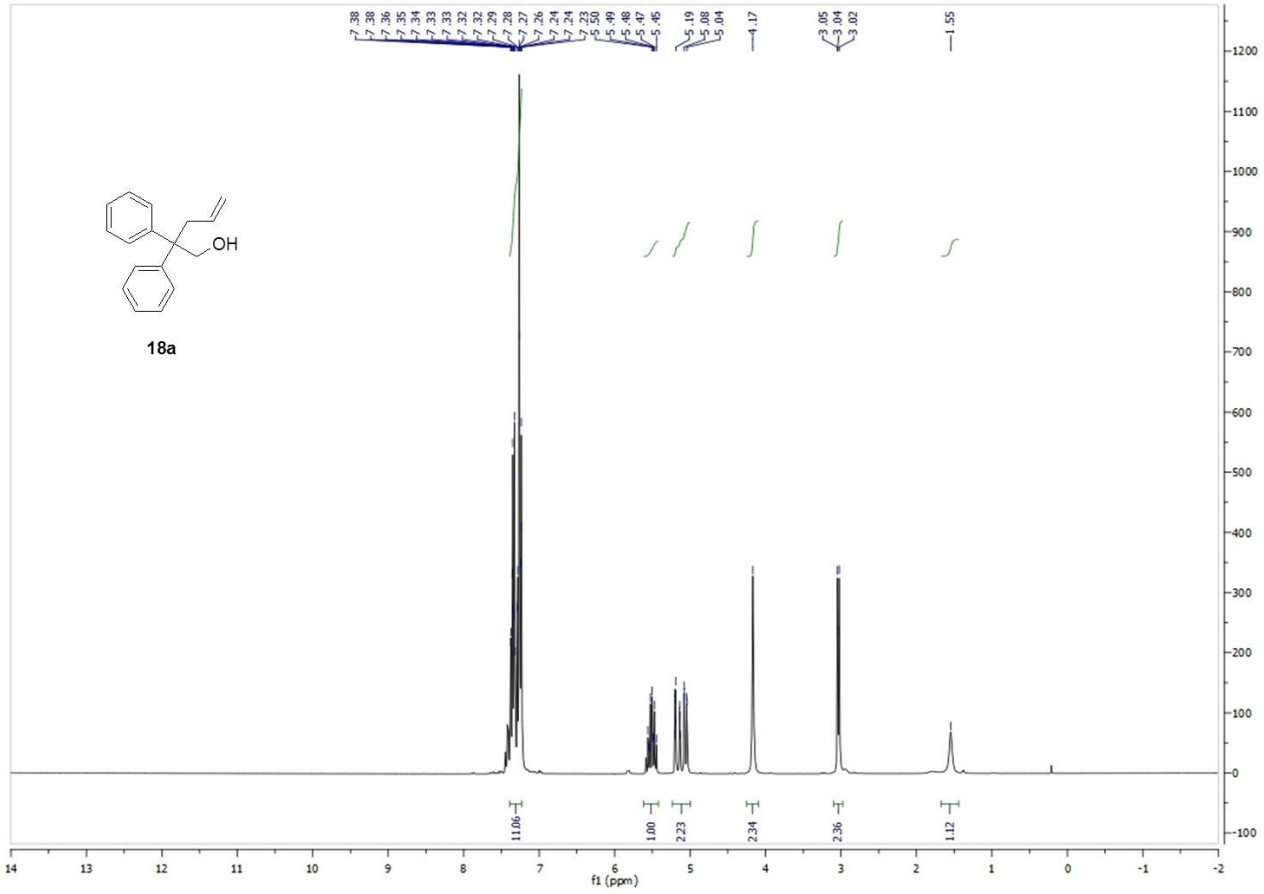
15c


Ph
OH
Ph
15d
f1 (ppm)

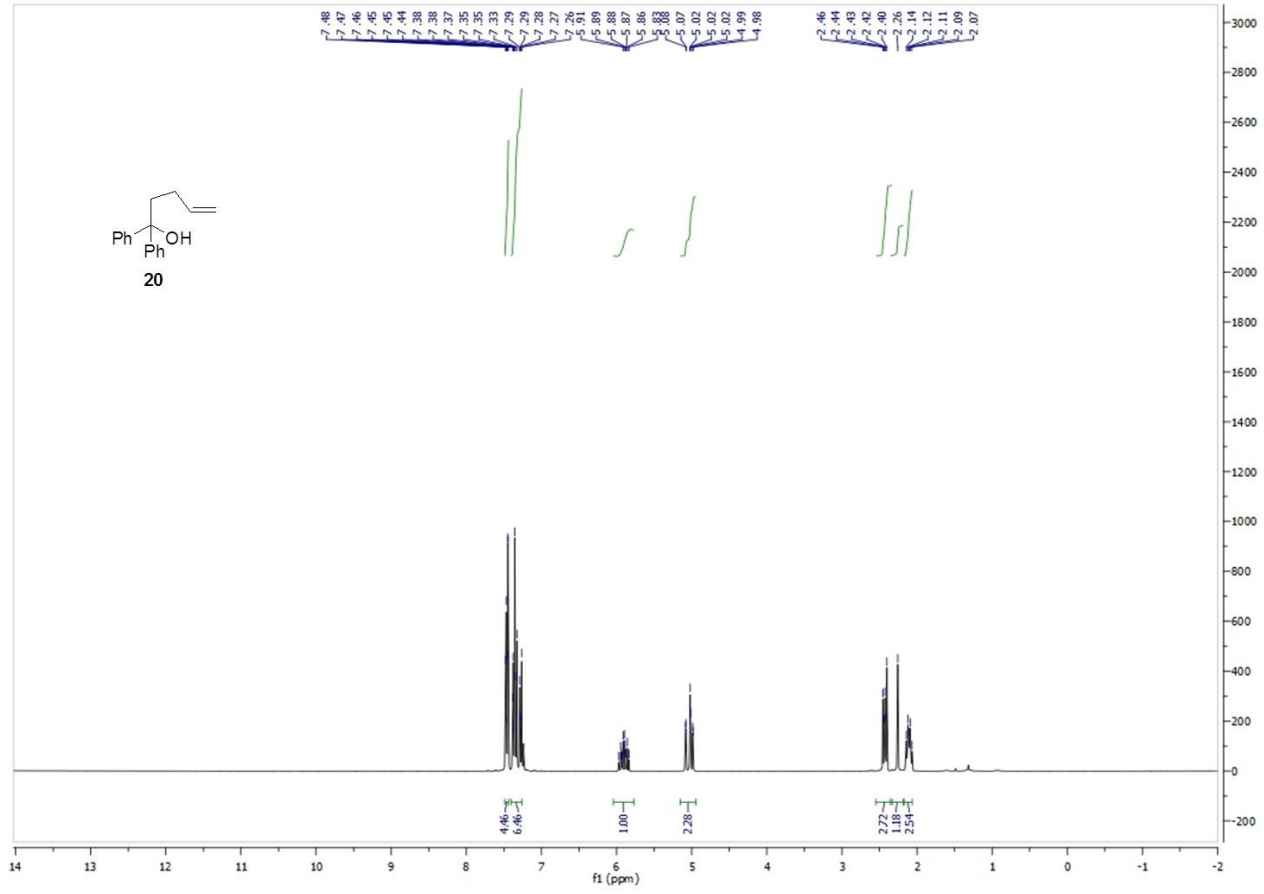

Ph
OH
Ph
15d
ppm


7.28
7.28
7.26
7.24
7.23
7.22
7.20
7.18
7.14
7.13
7.12
7.12
7.10
5.73
5.71
5.69
5.67
5.05
5.01
4.97
4.94
2.84
2.81
2.78
2.75
2.72
2.53
Cl
Cl
Ph
OH
Ph
15e
12.02
5.77
1.06
2.00
4.17
2.03
f1 (ppm)

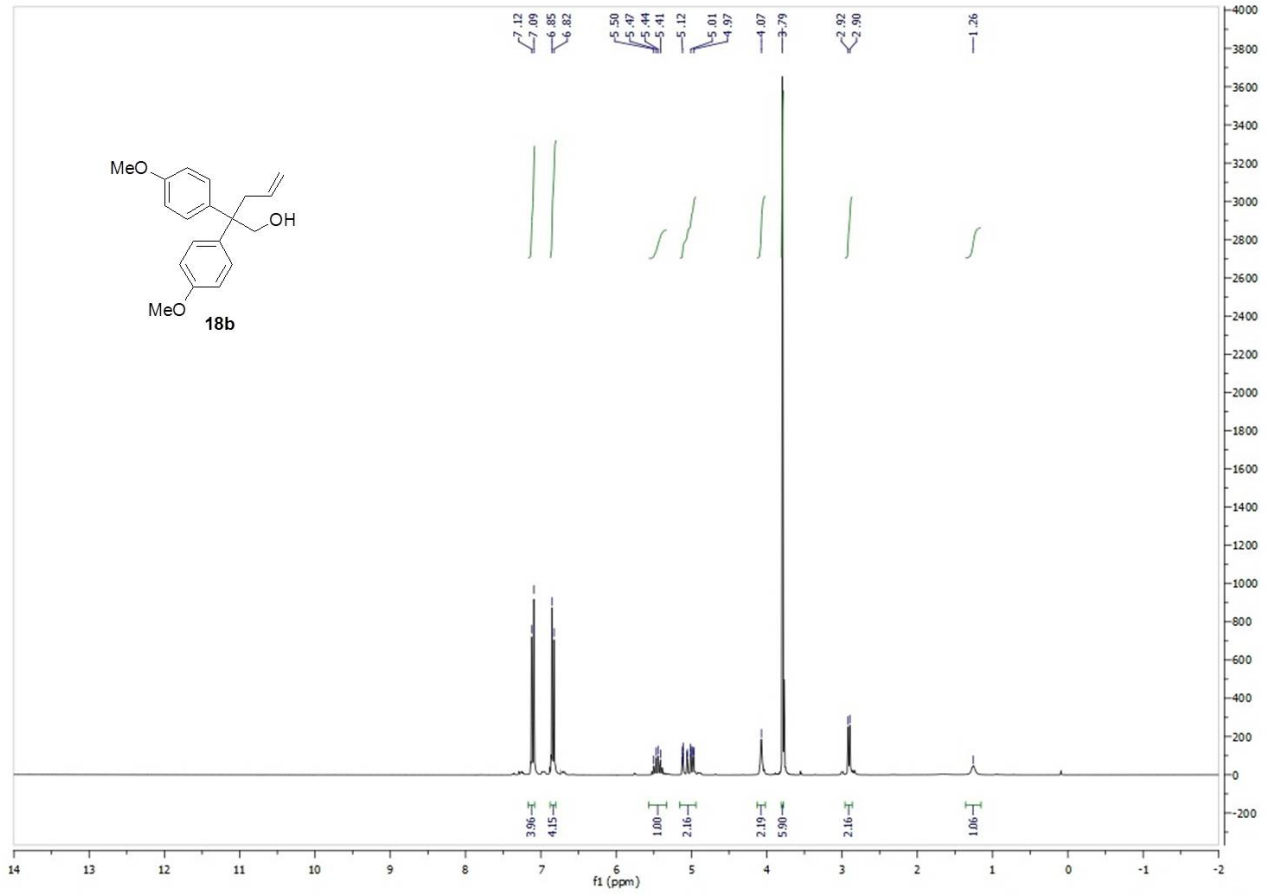

148.78
145.60
136.38
132.19
128.09
126.46
125.16
112.85
78.22
77.42
77.00
76.57
44.73
43.73
42.96
Cl
Cl
Ph
OH
Ph
15e
f1 (ppm)

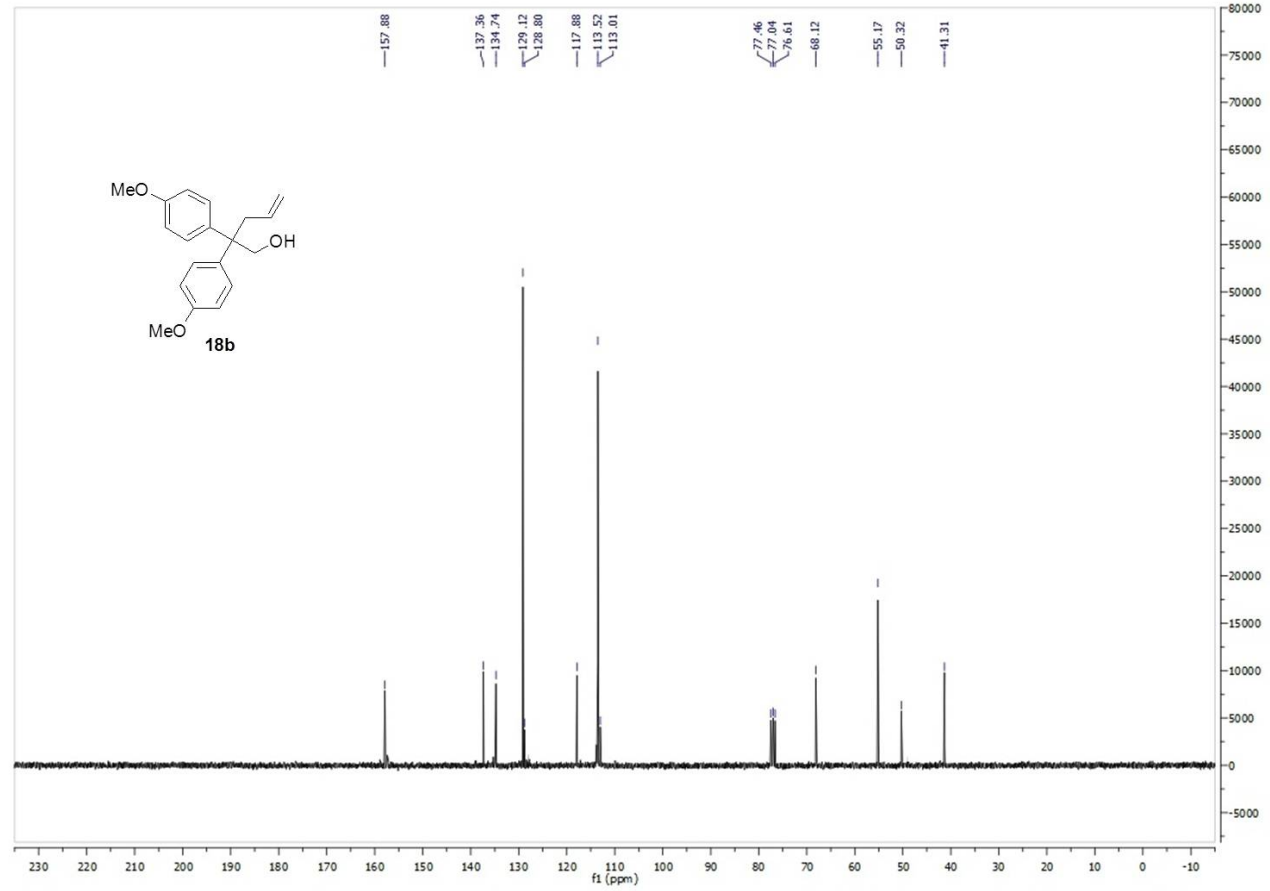

7.38
7.36
7.35
7.34
7.33
7.32
7.29
7.28
7.27
7.26
7.24
7.23
5.50
5.49
5.48
5.47
5.45
5.19
5.08
5.04
4.17
3.05
3.04
3.02
1.55
OH
1106
1.00
2.23
2.34
2.36
1.12
f1 (ppm)

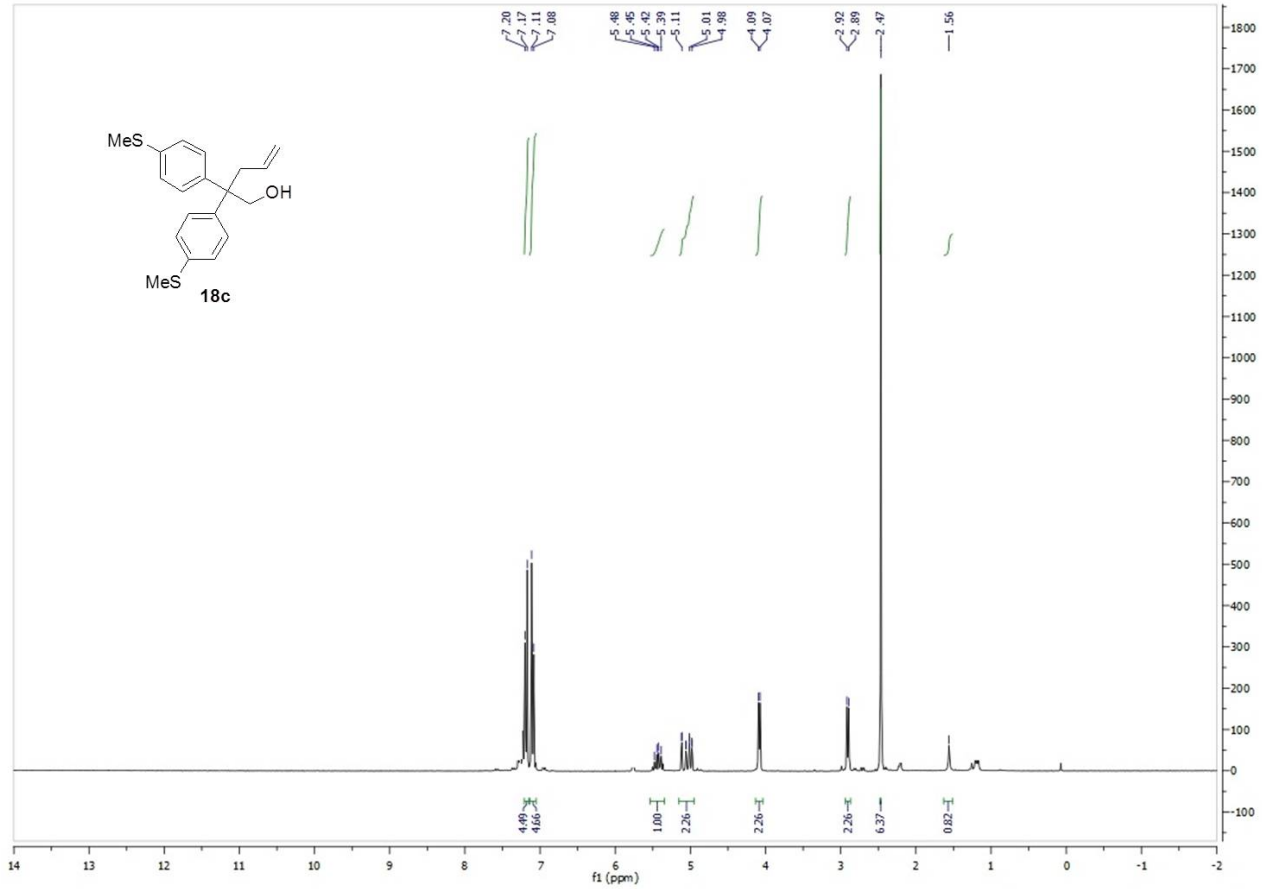
18a

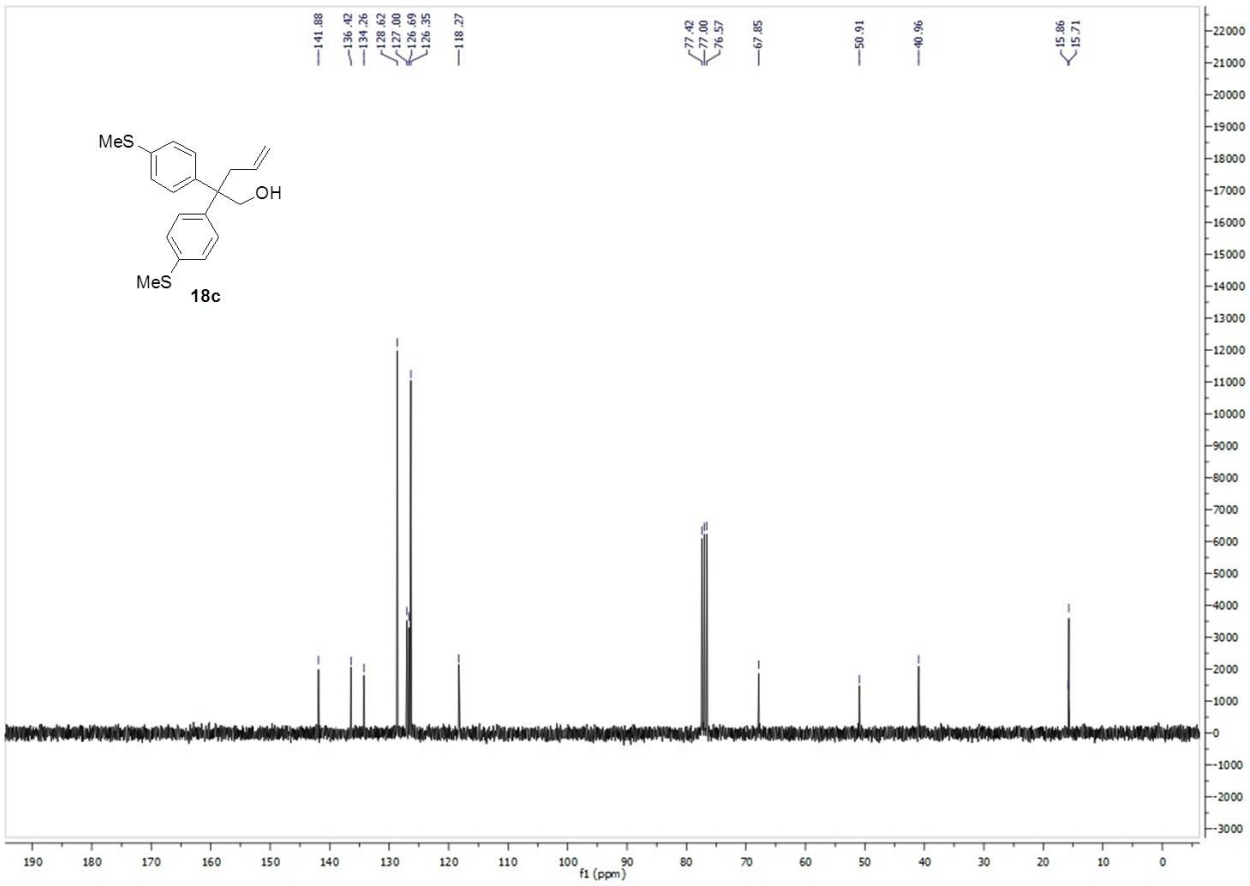

7.48
7.47
7.46
7.45
7.44
7.38
7.37
7.35
7.33
7.29
7.28
7.27
7.26
5.91
5.89
5.88
5.87
5.86
5.83
5.07
5.02
5.02
4.99
4.98
2.46
2.44
2.43
2.42
2.40
2.26
2.14
2.12
2.11
2.09
2.07
Ph
OH
Ph
4.46
6.46
1.00
2.28
2.72
1.18
2.54
f1 (ppm)

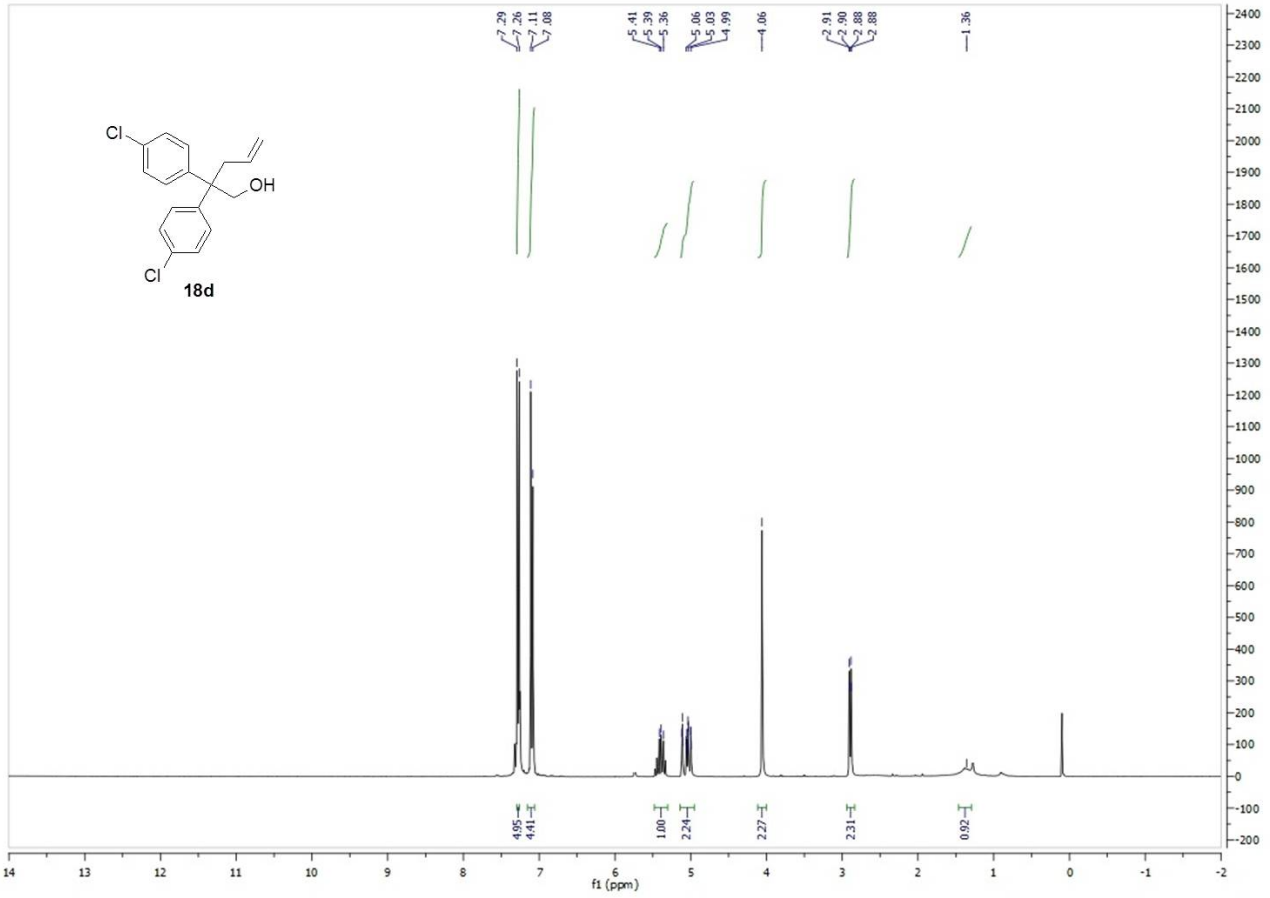
20

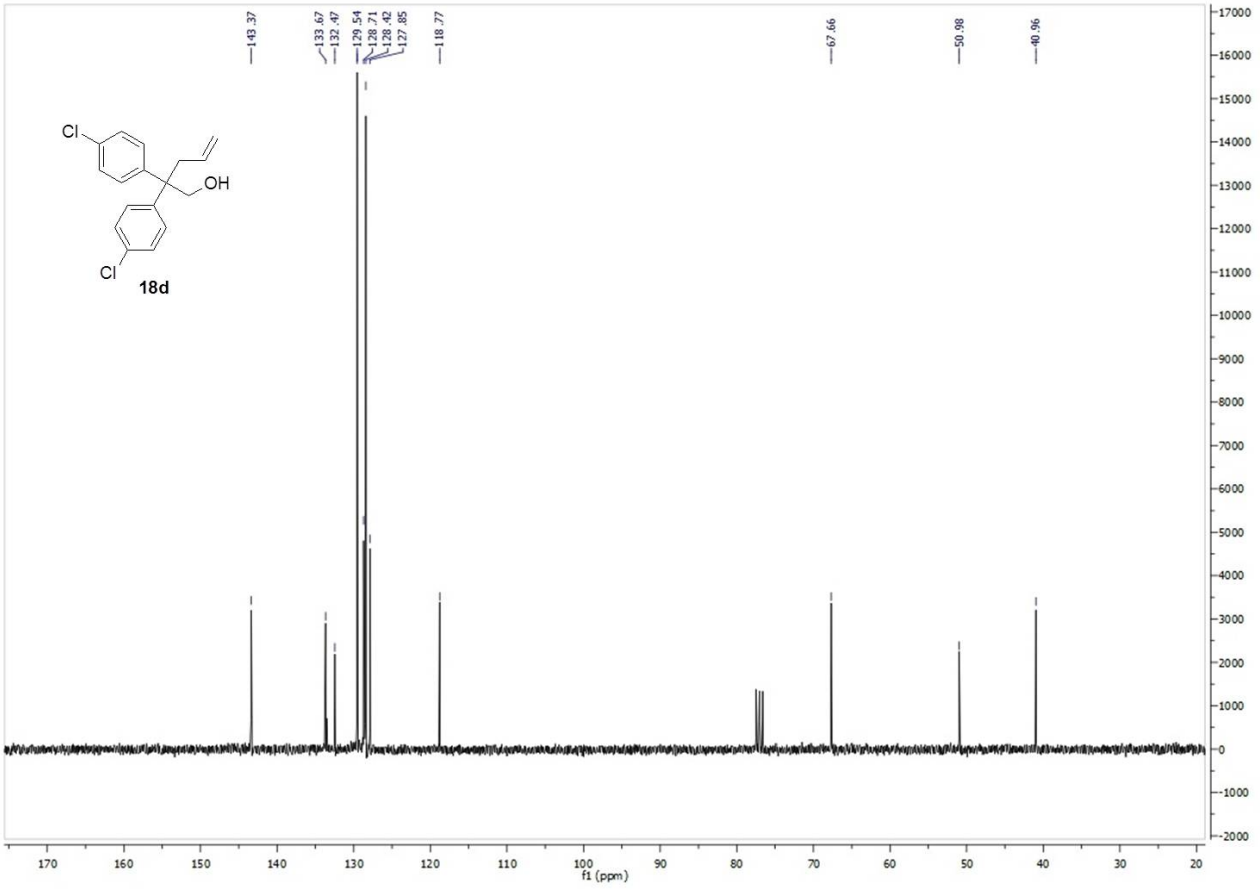

MeO
OH
MeO
18b
7.12
7.09
6.85
6.82
5.50
5.47
5.44
5.41
5.12
5.01
4.97
4.07
3.79
2.92
2.90
1.26
3.96
4.15
1.00
2.16
2.19
5.90
2.16
1.06
f1 (ppm)

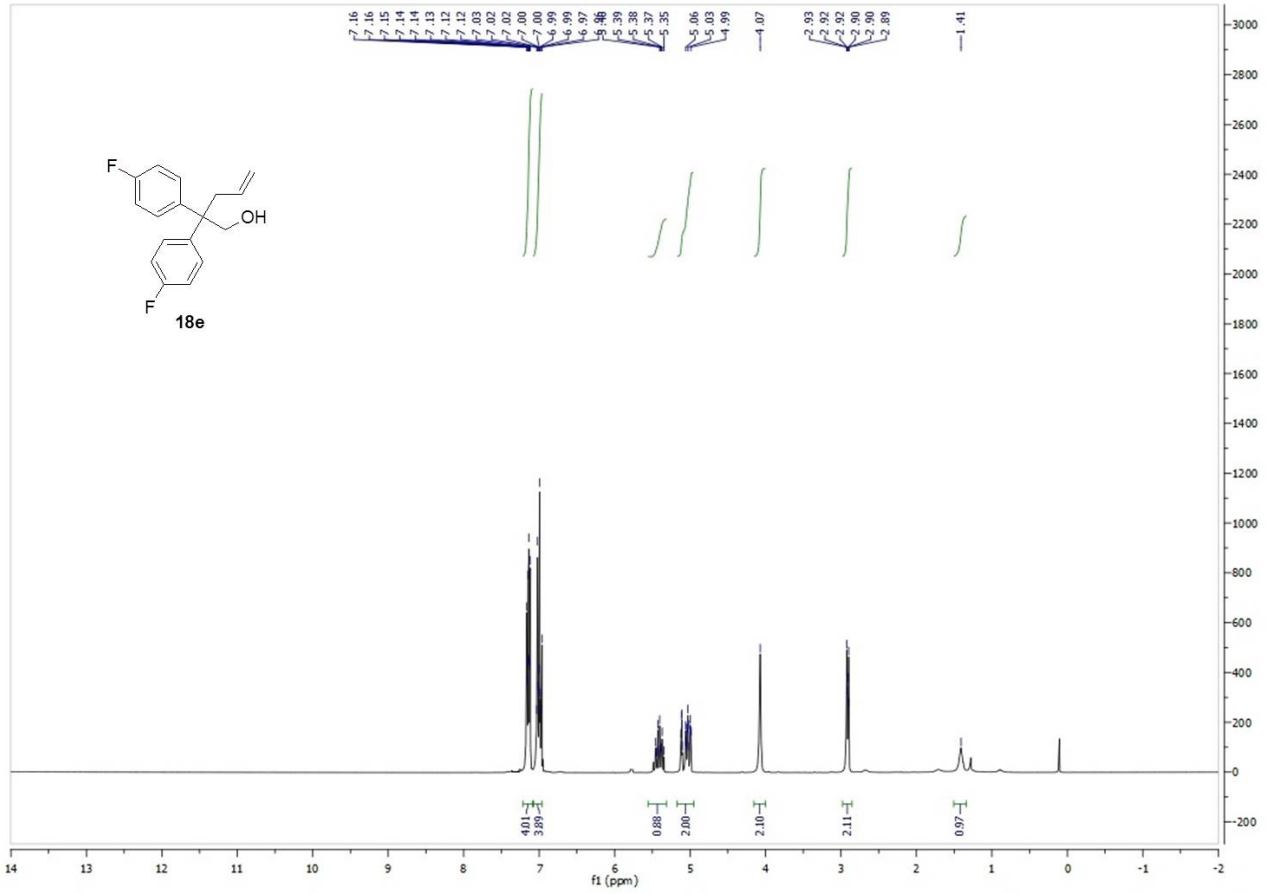

MeO
OH
MeO
18b
157.88
137.36
134.74
129.12
128.80
117.88
113.52
113.01
77.46
77.04
76.61
68.12
55.17
50.32
41.31
f1 (ppm)

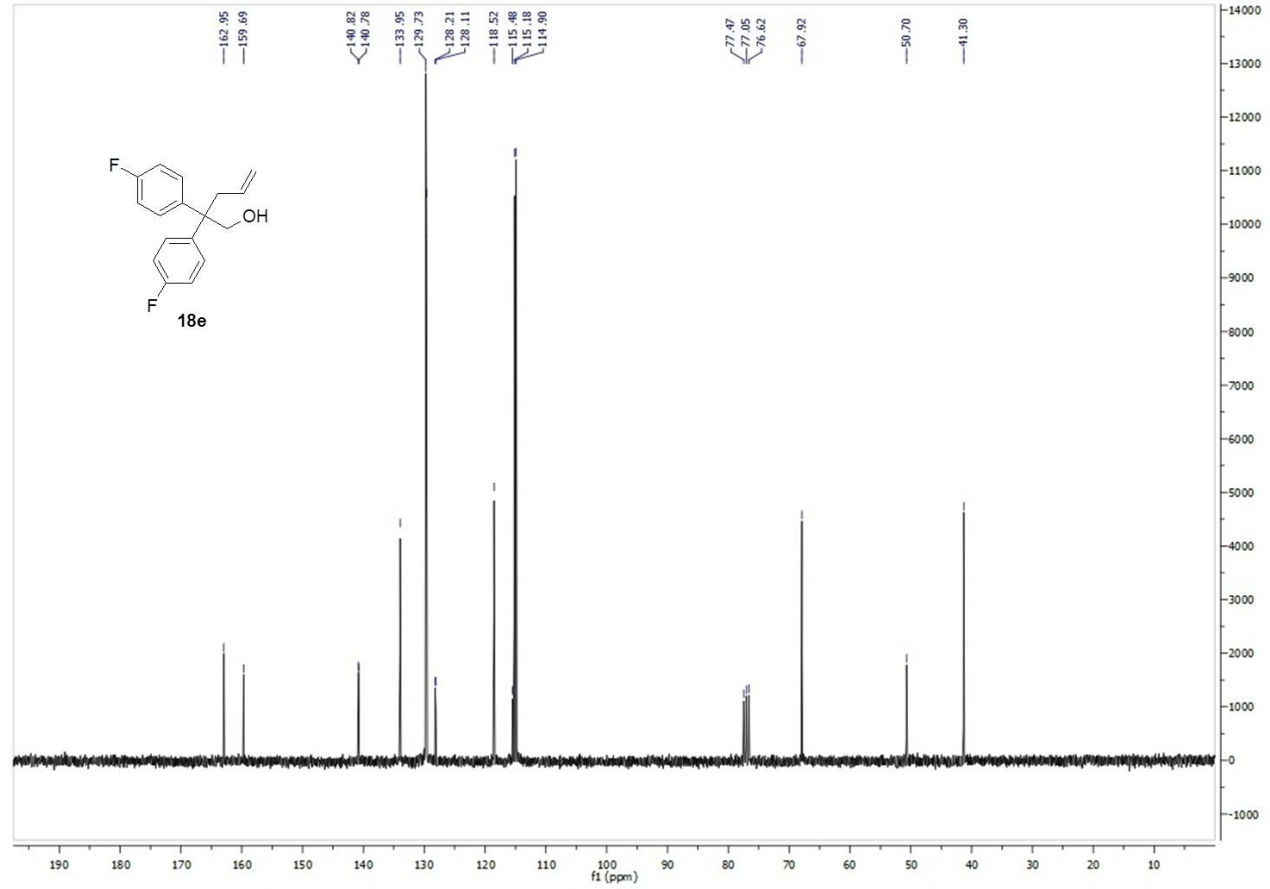

7.20
7.17
7.11
7.08
5.48
5.45
5.42
5.39
5.11
5.01
4.98
4.09
4.07
2.92
2.89
2.47
1.56
MeS
OH
MeS
18c
4.49
4.66
1.00
2.26
2.26
2.26
6.37
0.82
f1 (ppm)


141.88
136.42
134.26
128.62
127.00
126.69
126.35
118.27
77.42
77.00
76.57
67.85
50.91
40.96
15.86
15.71
MeS
OH
MeS
18c
f1 (ppm)


7.29
7.26
7.11
7.08
5.41
5.39
5.36
5.06
5.03
4.99
4.06
2.91
2.90
2.88
2.88
1.36
Cl
OH
Cl
18d
4.95
4.41
1.00
2.24
2.27
2.31
0.92
f1 (ppm)


143.37
133.67
132.47
129.54
128.71
128.42
127.85
118.77
67.66
50.98
40.96
Cl
OH
Cl
18d
f1 (ppm)


F
OH
F
18e
f1 (ppm)


F
OH
F
18e
f1 (ppm)

20110519methoxylalkynealcohol

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

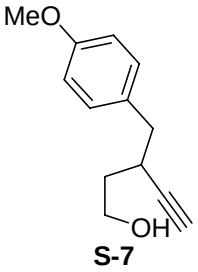
Sample directory:

FidFile: 20110519methoxylalkynealcohol

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 19 2011

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984058 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



S-7

20110519methoxylalkynealcoholC13

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

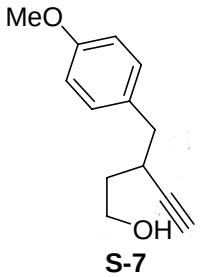
Sample directory:

FidFile: CARBON

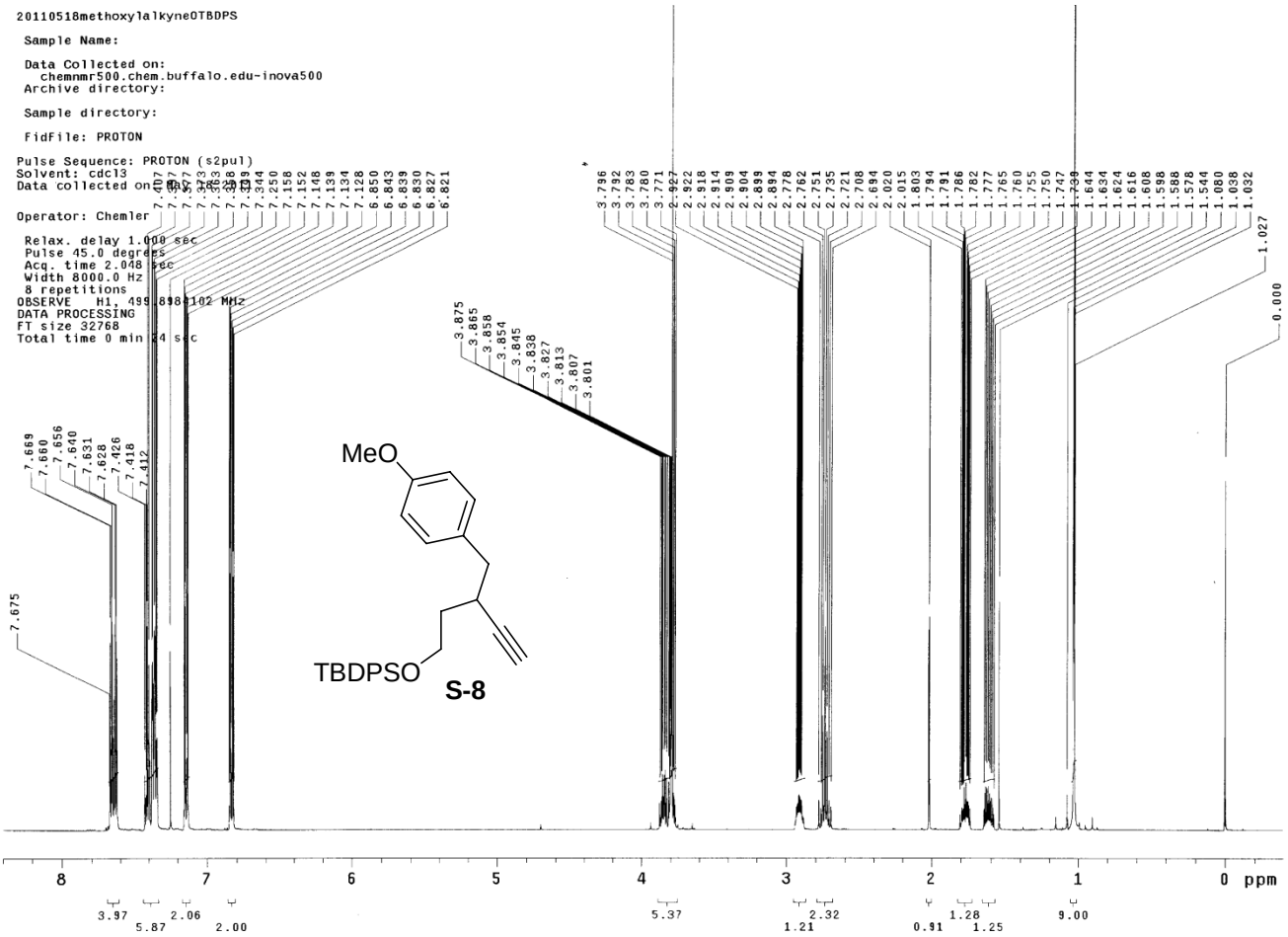
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 19 2011

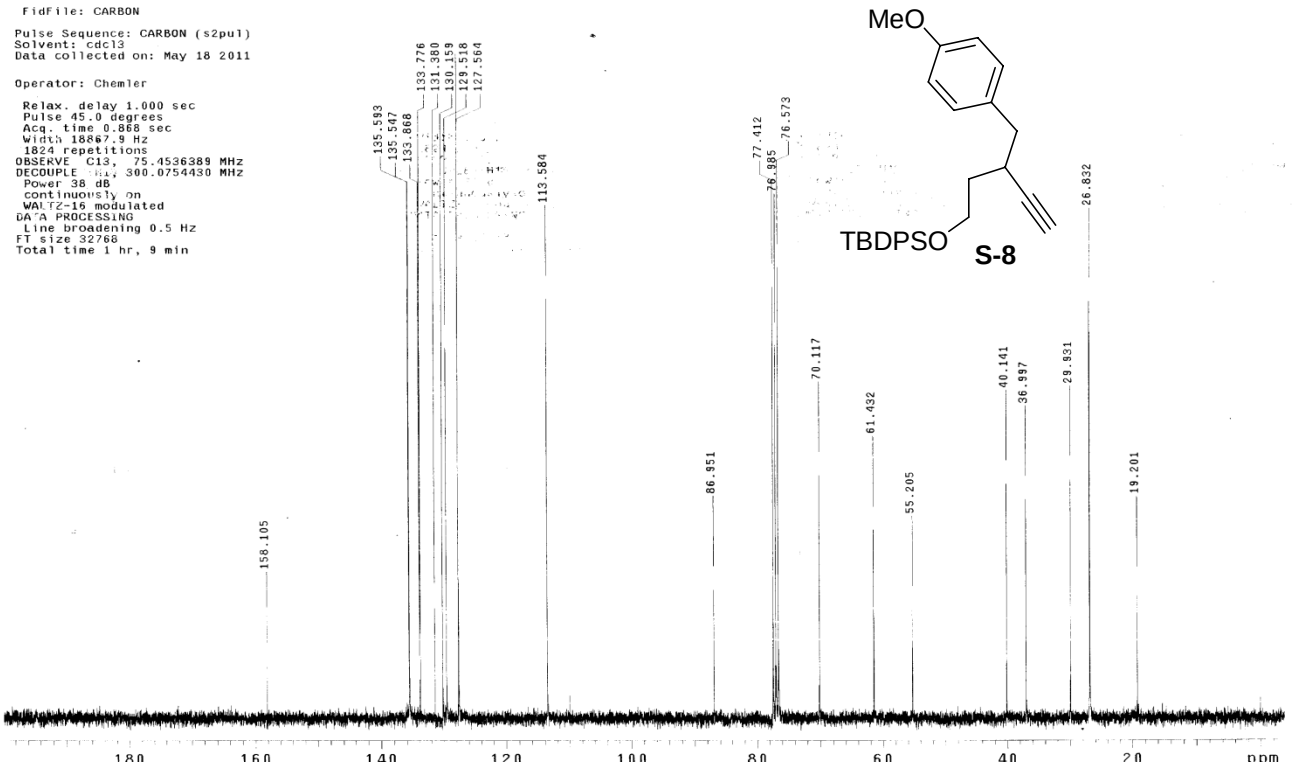
Temp. 4.0 C / 277.1 K
Operator: Chemler

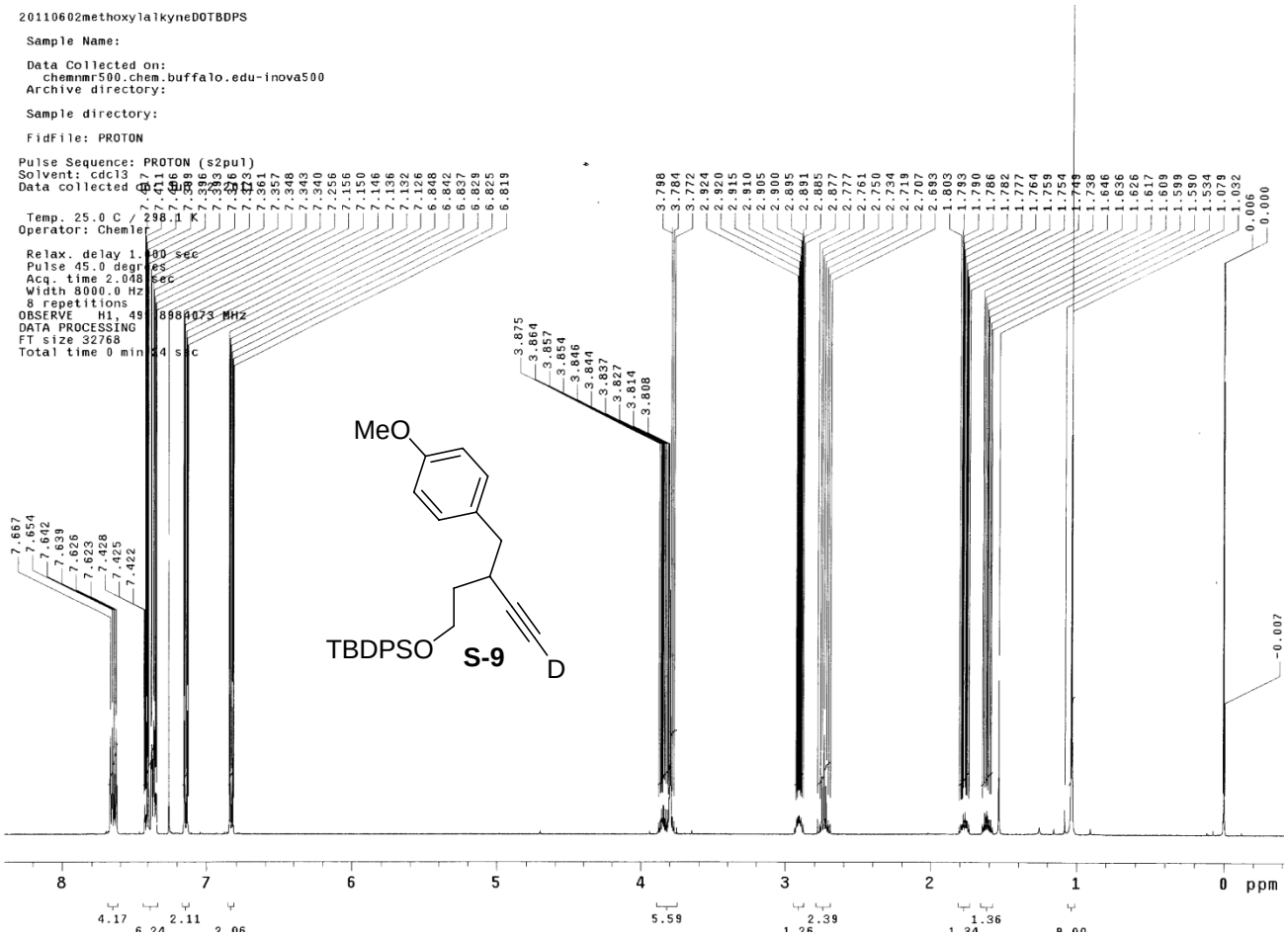
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.568 sec
Width 18867.9 Hz
2048 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min

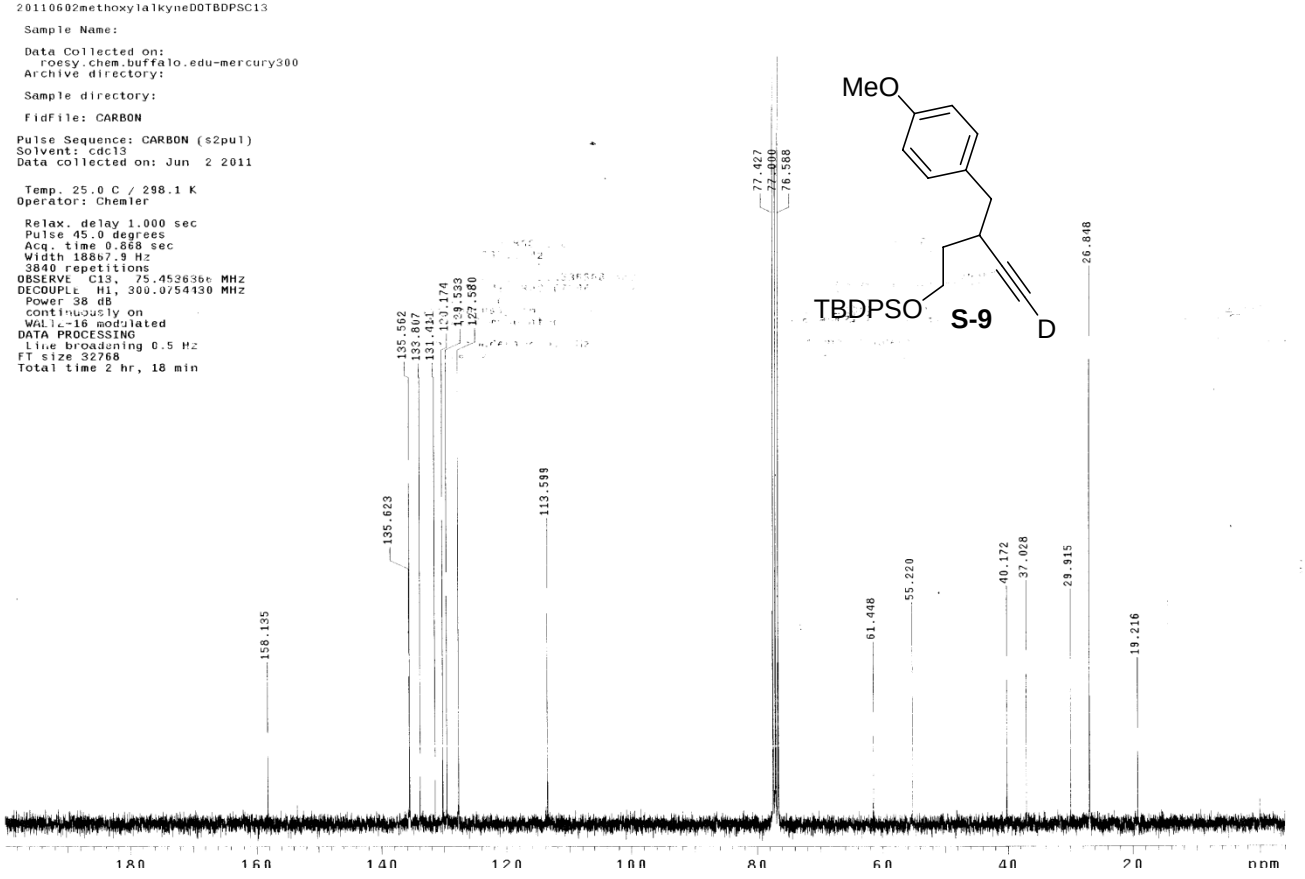


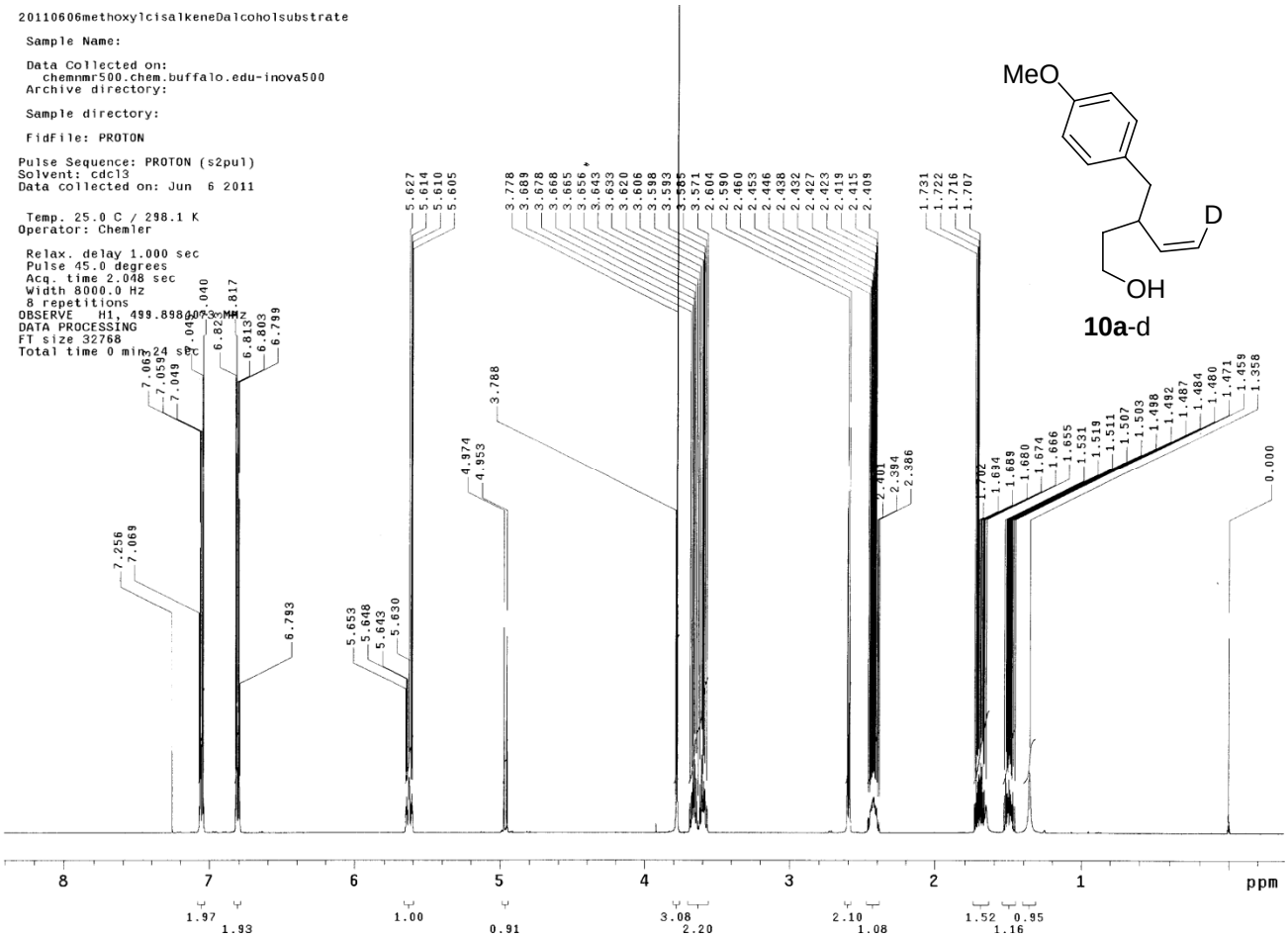
S-7

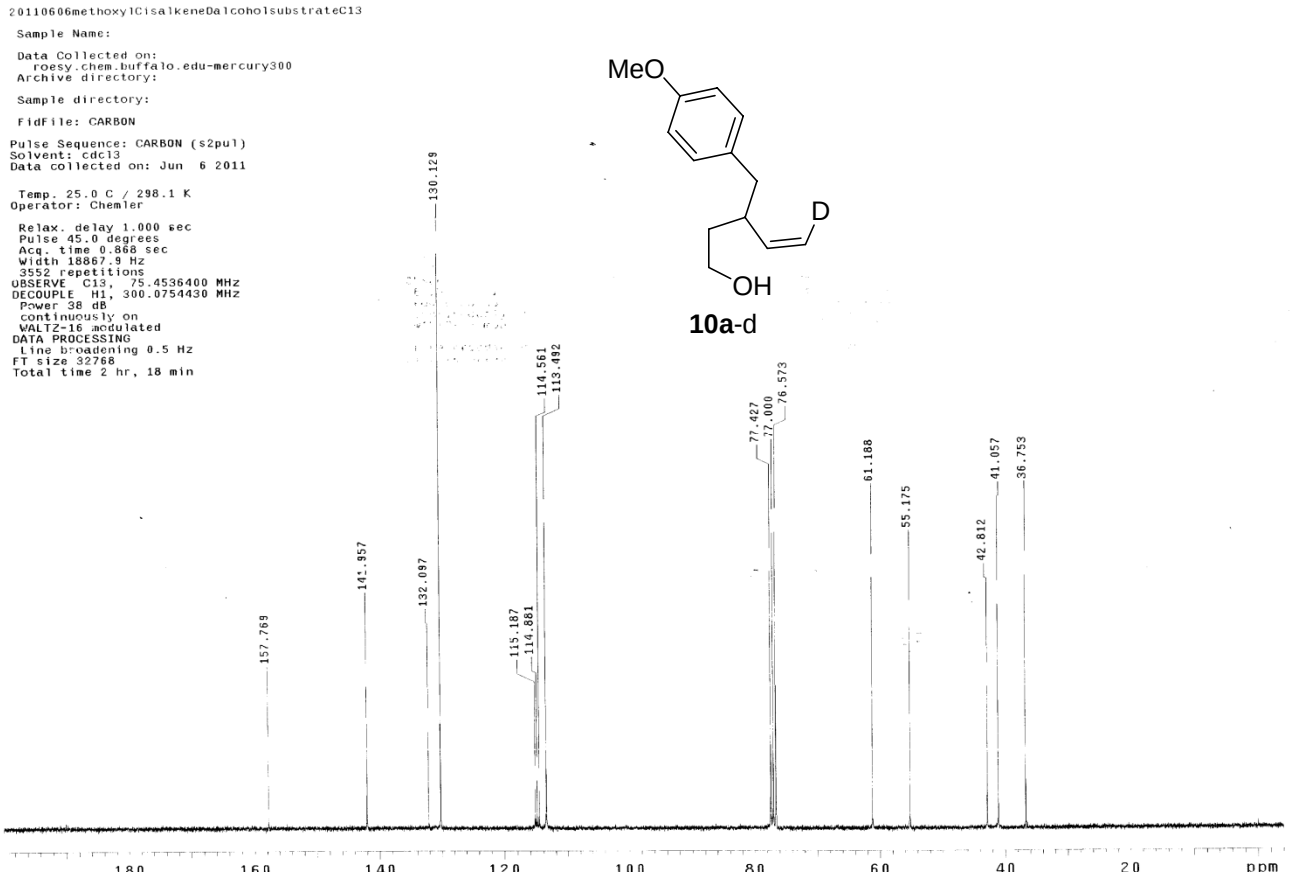

20110518methoxylalkyneOTBDPS
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on:
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8881102 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 24 sec
MeO
TBDPSO
S-8
ppm

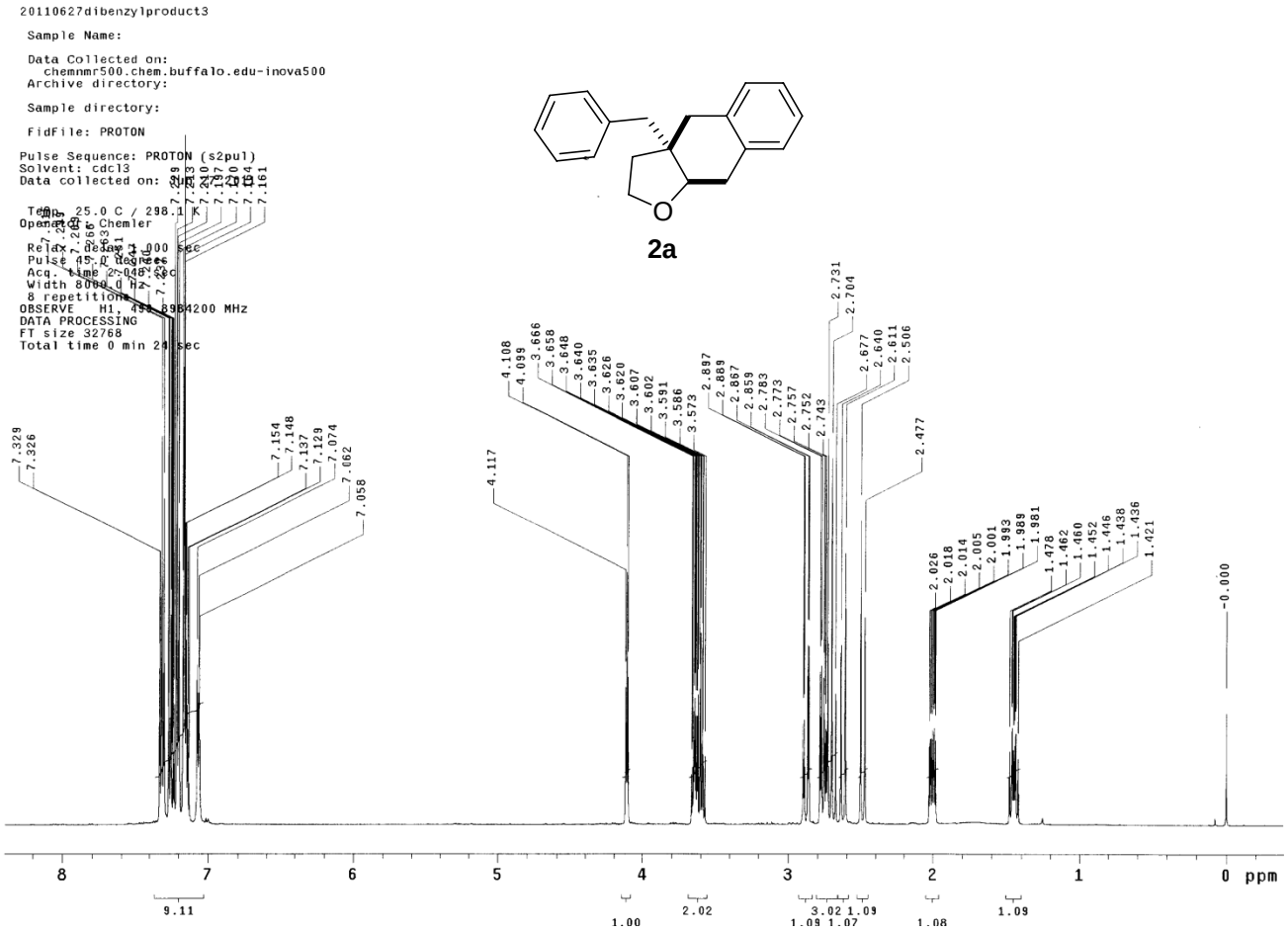

20110518methoxylalkyneOTBDPSC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 18 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
1824 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 1 hr, 9 min
MeO
TBDPSO
S-8
ppm

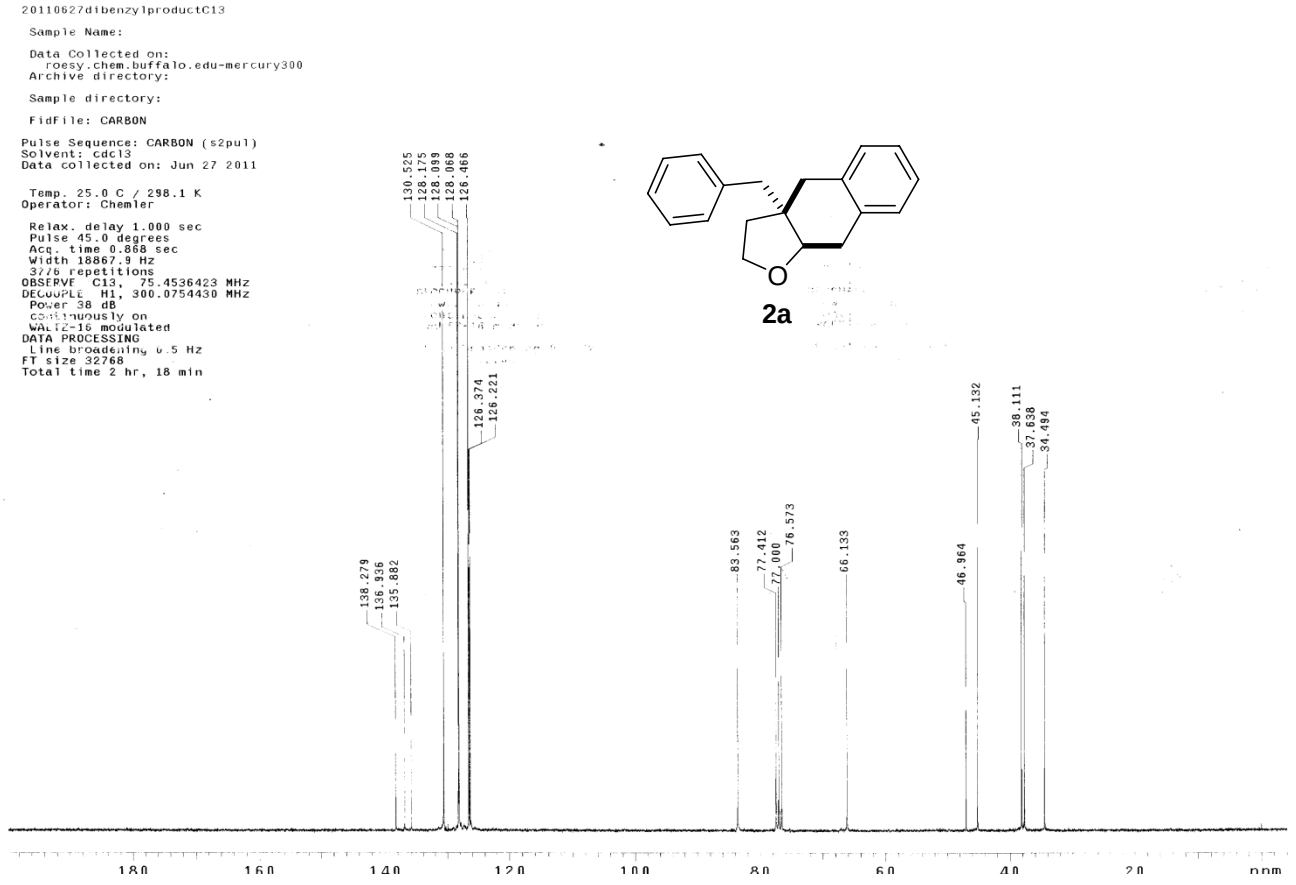

20110602methoxylalkyneDOTBDPS
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
DATA PROCESSING
FT size 32768
MeO
TBDPSO
S-9
D
ppm

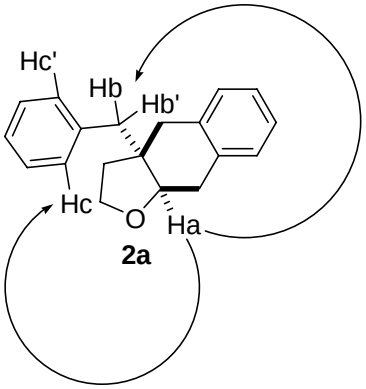

20110602methoxylalkyneDOTBDPSC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 2 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3840 repetitions
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
MeO
TBDPSO
S-9
D
ppm


20110606methoxylcisalkeneDalcoholsubstrate
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 6 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8980073 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 24 sec
MeO
D
OH
10a-d
ppm
1.97
1.93
1.00
0.91
3.08
2.20
2.10
1.08
1.52
0.95
1.16


20110606methoxylCisalkeneDalcoholsubstrateC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 6 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3552 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
MeO
D
OH
10a-d
ppm

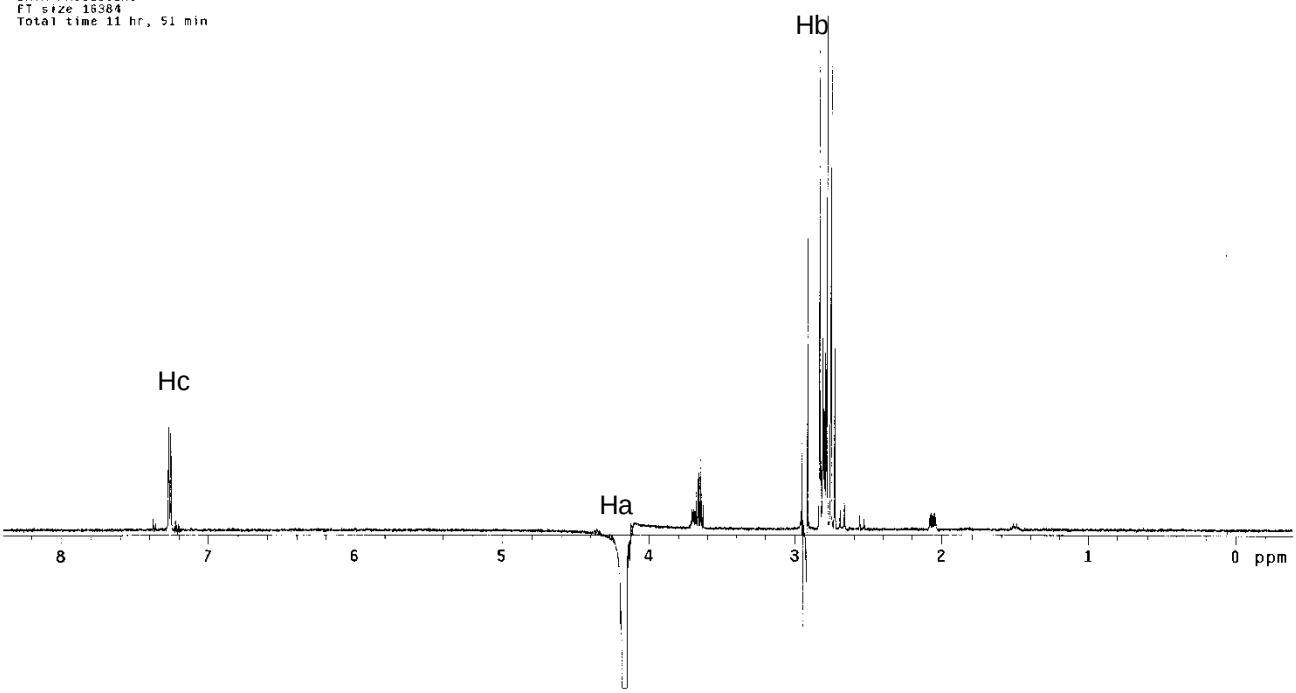

20110627dibenzylproduct3
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 27 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984200 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
2a
ppm
9.11
1.00
2.02
3.02
1.09
1.07
1.08
1.09

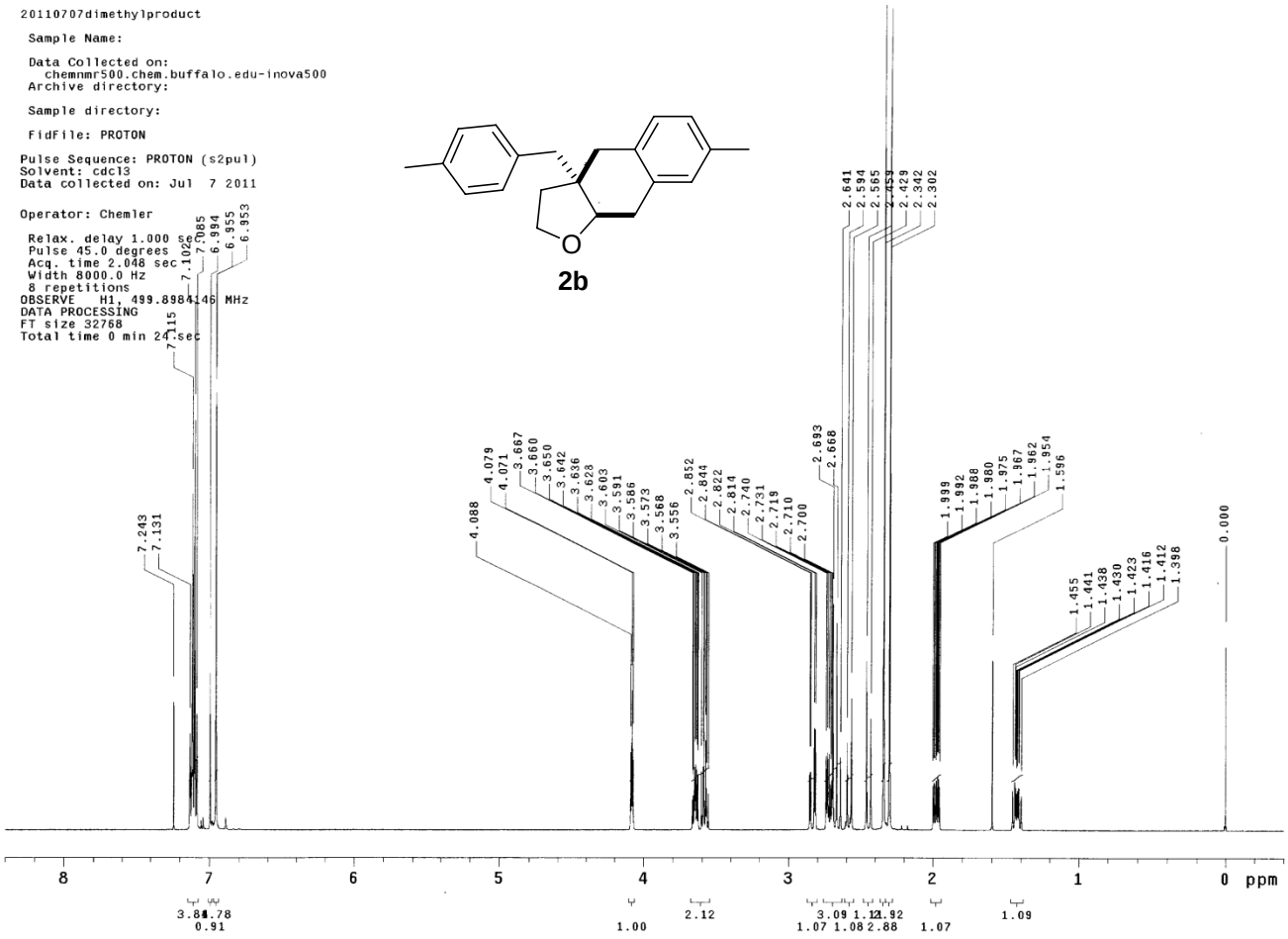

20110627dibenzylproductC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 27 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3776 repetitions
OBSERVE C13, 75.4536423 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
2a
ppm

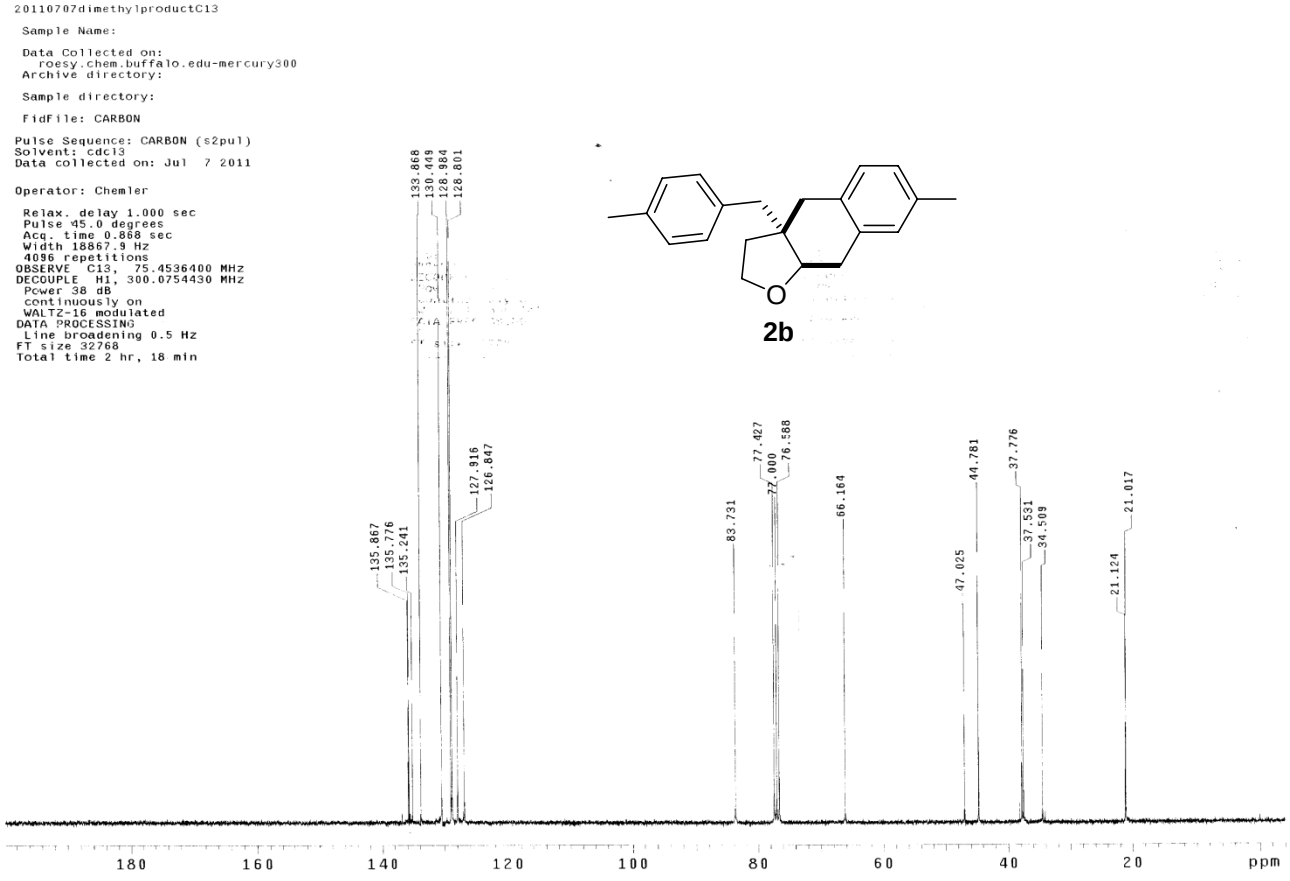


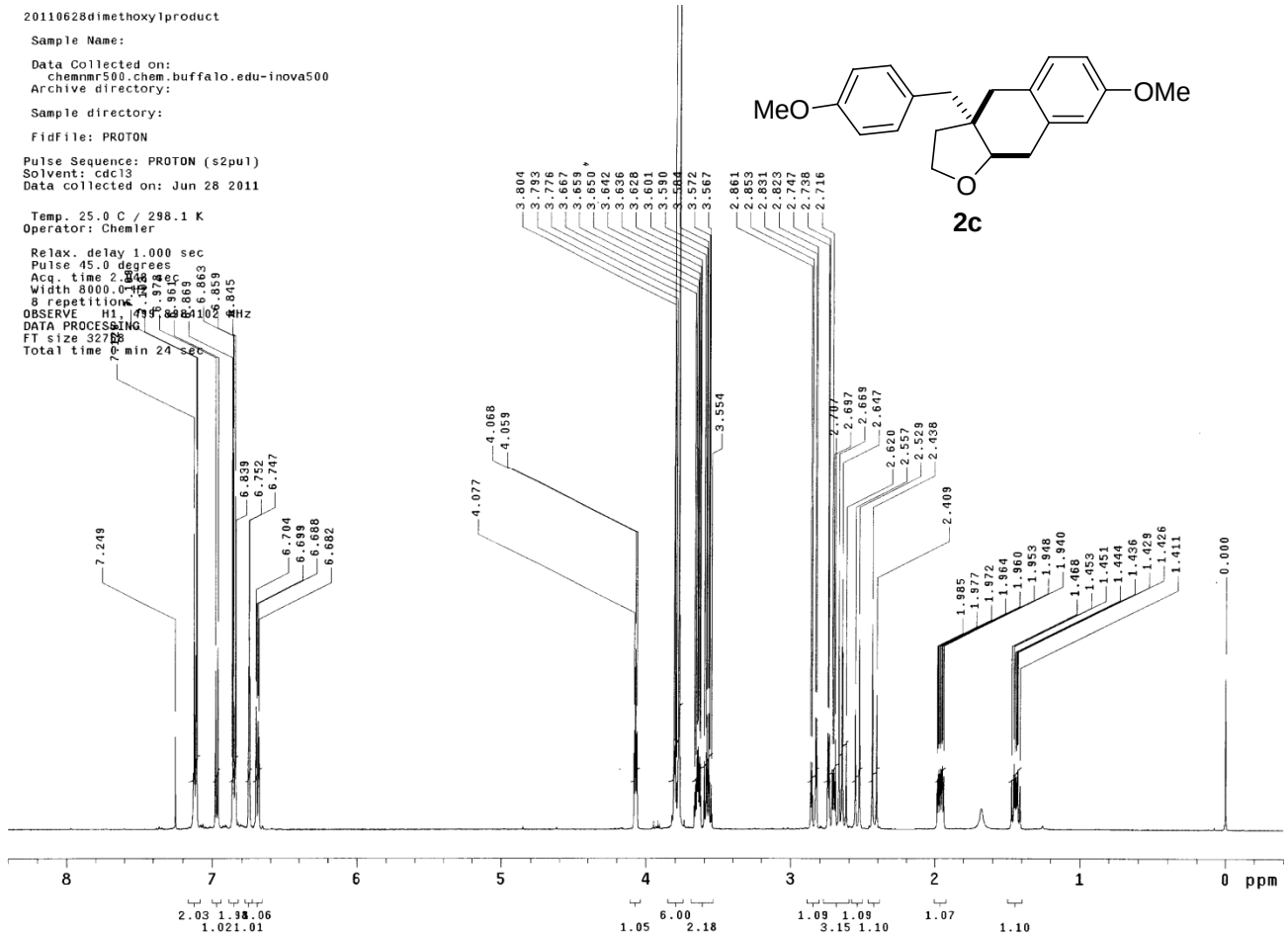
2a

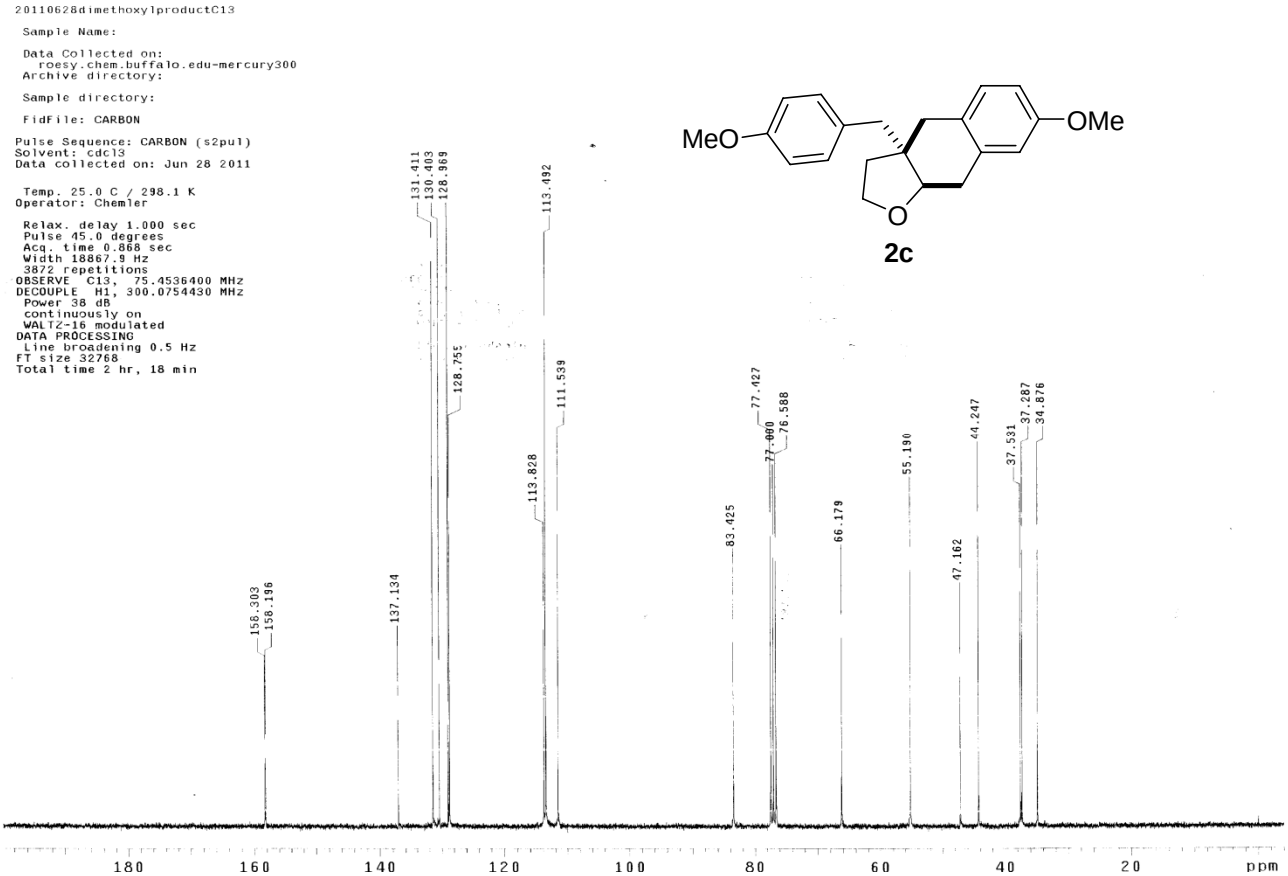
```
20110627dibenzylnoe1d

 Sample Name:

 Data Collected on:
   chemmmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 FidFile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jun 27 2011

 Temp. 25.0 C / 298.1 K
Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 1.866 sec
 Width 4389.8 Hz
 11264 repetitions
OBSERVE    H1, 499.8983908 MHz
DATA PROCESSING
FT size 16384
Total time 11 hr, 51 min
```

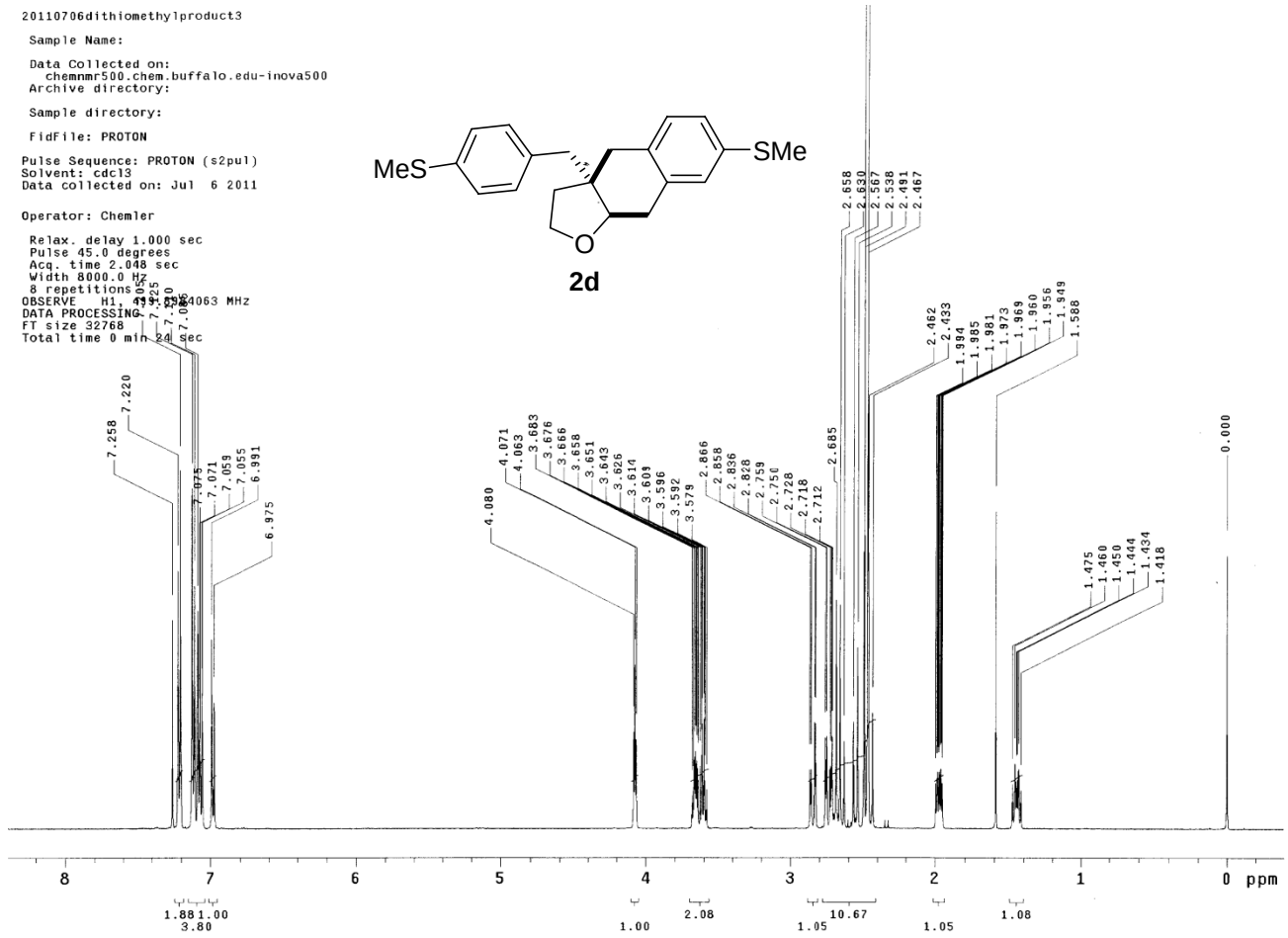


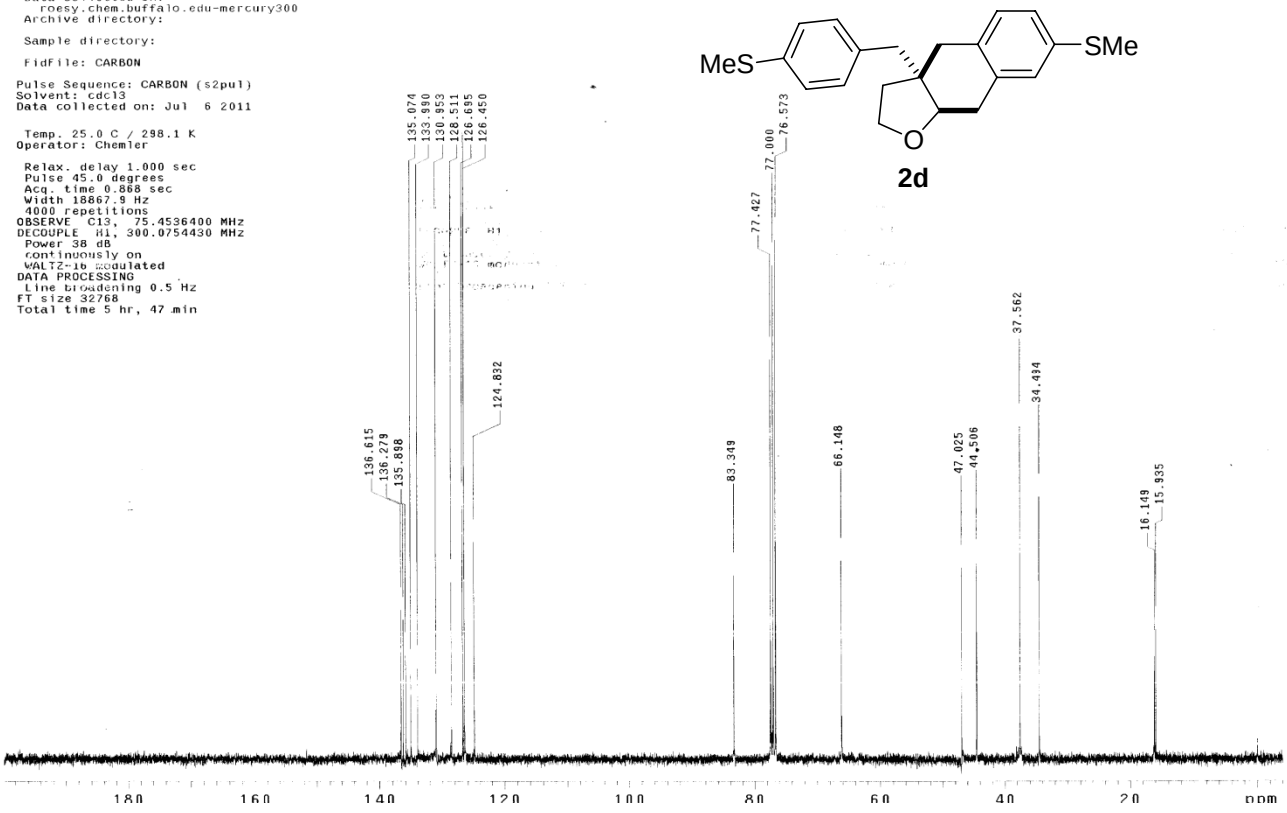

20110707dimethylproduct
Sample Name:
Data Collected on:
chemmmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 7 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984146 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
2b
ppm
3.84
0.91
1.00
2.12
3.09
1.07
1.08
2.88
1.07
1.09


20110707dimethylproductC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 7 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
4096 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
2b
ppm


20110628dimethoxylproduct
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 28 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.648 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8811102 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
MeO
OMe
O
2c
ppm


20110628dimethoxylproductC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 28 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3872 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
MeO
OMe
O
2c
ppm


20110706dithiomethylproduct3
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 6 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8704063 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 24 sec
MeS
SMe
O
2d
ppm
1.88 1.00 3.80
1.00
2.08
10.67 1.05
1.05
1.08


20110706dithiomethylproductC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 6 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
4000 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min
MeS
SMe
O
2d
ppm

20110705dibromoproduct

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

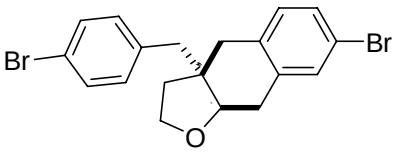
Sample directory:

FidFile: PROTON

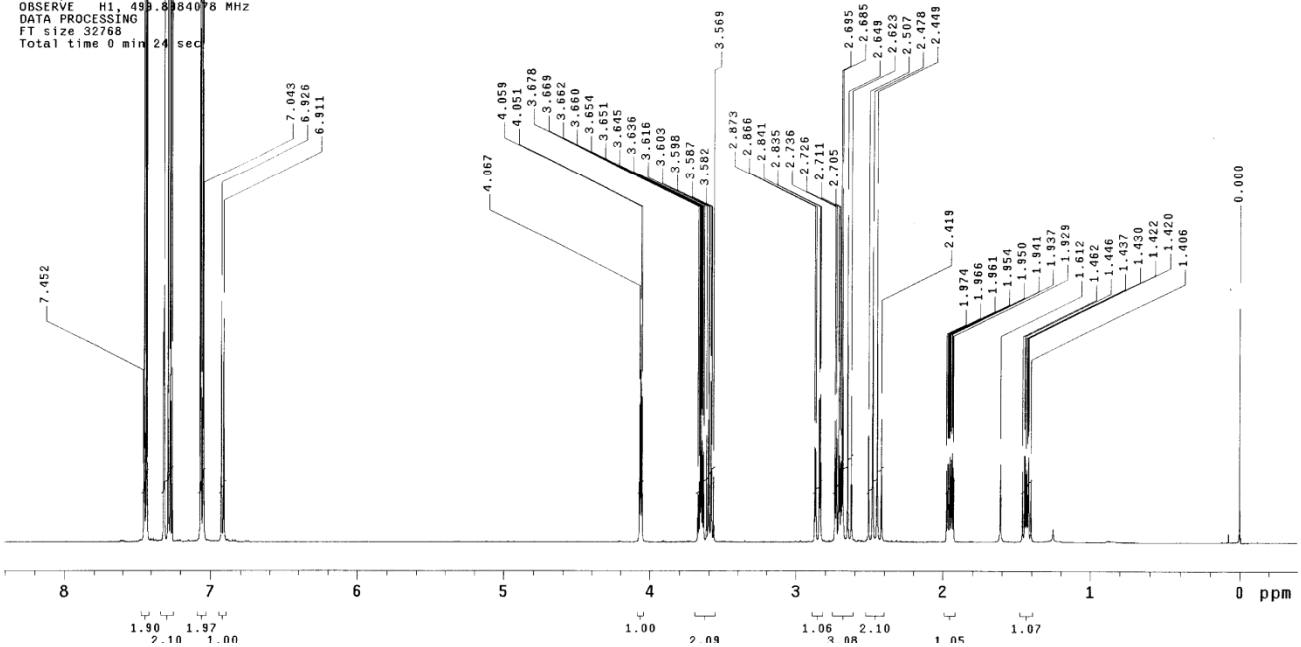
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2011

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8884078 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



2e



20110705dibromoproductC13

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

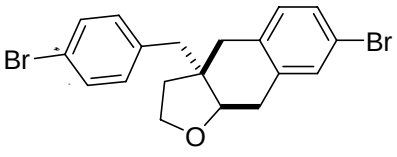
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 5 2011

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2016 repetitions
OBSERVE C13, 75.4536412 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min



2e

20110704dichloroproduct

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

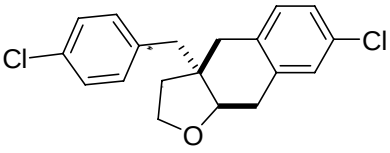
Sample directory:

FidFile: PROTON

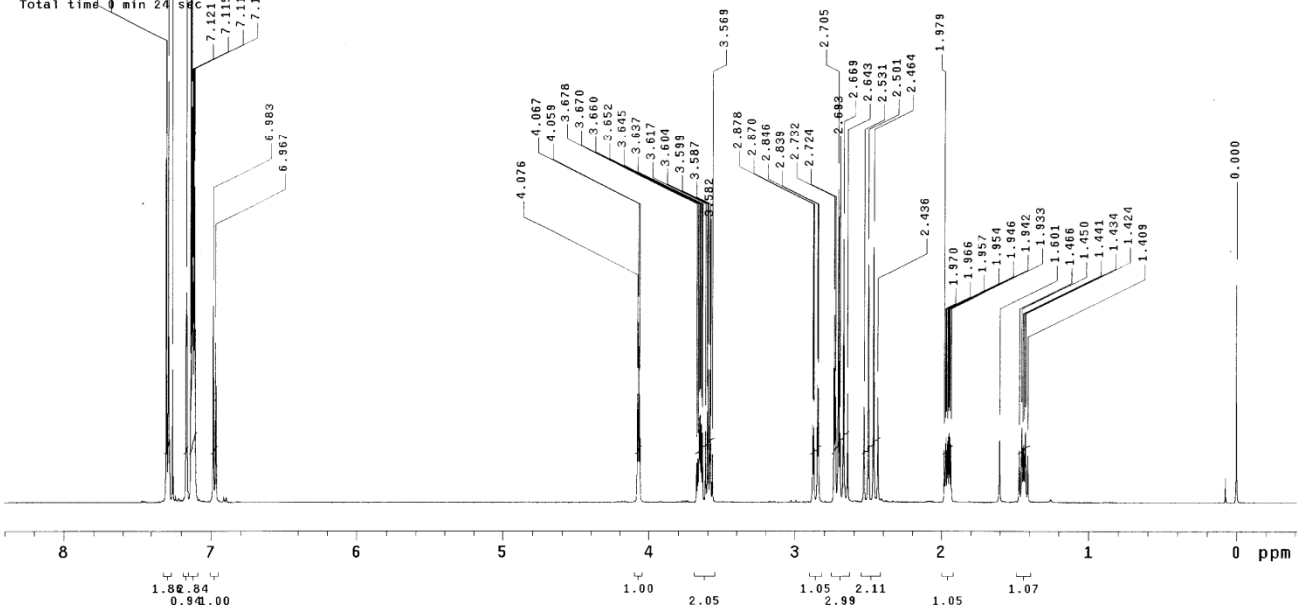
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 4 2011

Operator: Chemler

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE cwH1, 499.8984078 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



2f



20110704dichloroproductC13

Sample Name:

Data Collected On:
roesy.chem.buffalo.edu-mercury300
Archive directory:

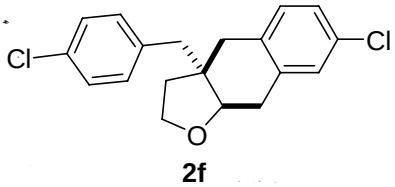
Sample directory:

FidFile: CARBON

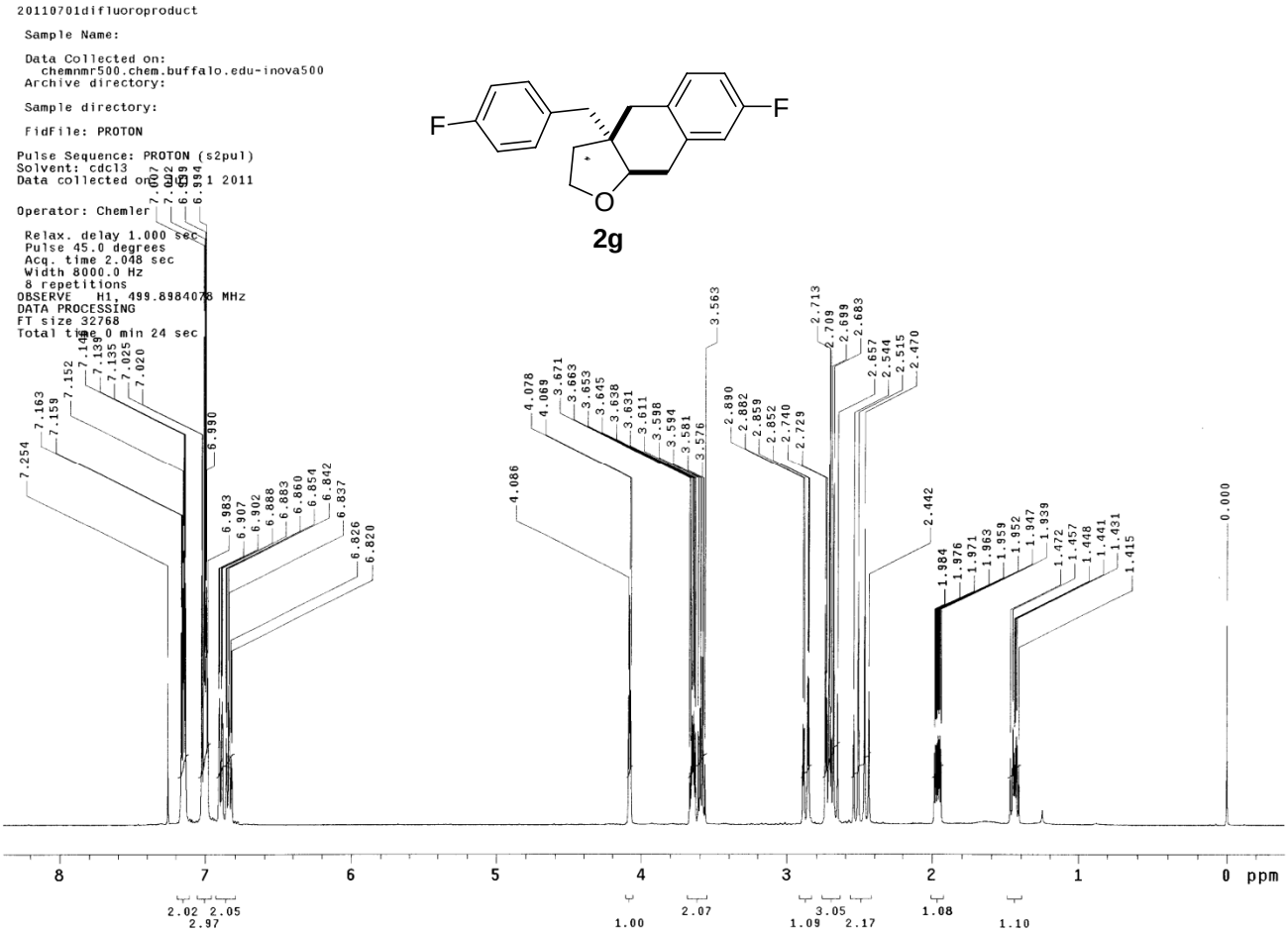
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 4 2011

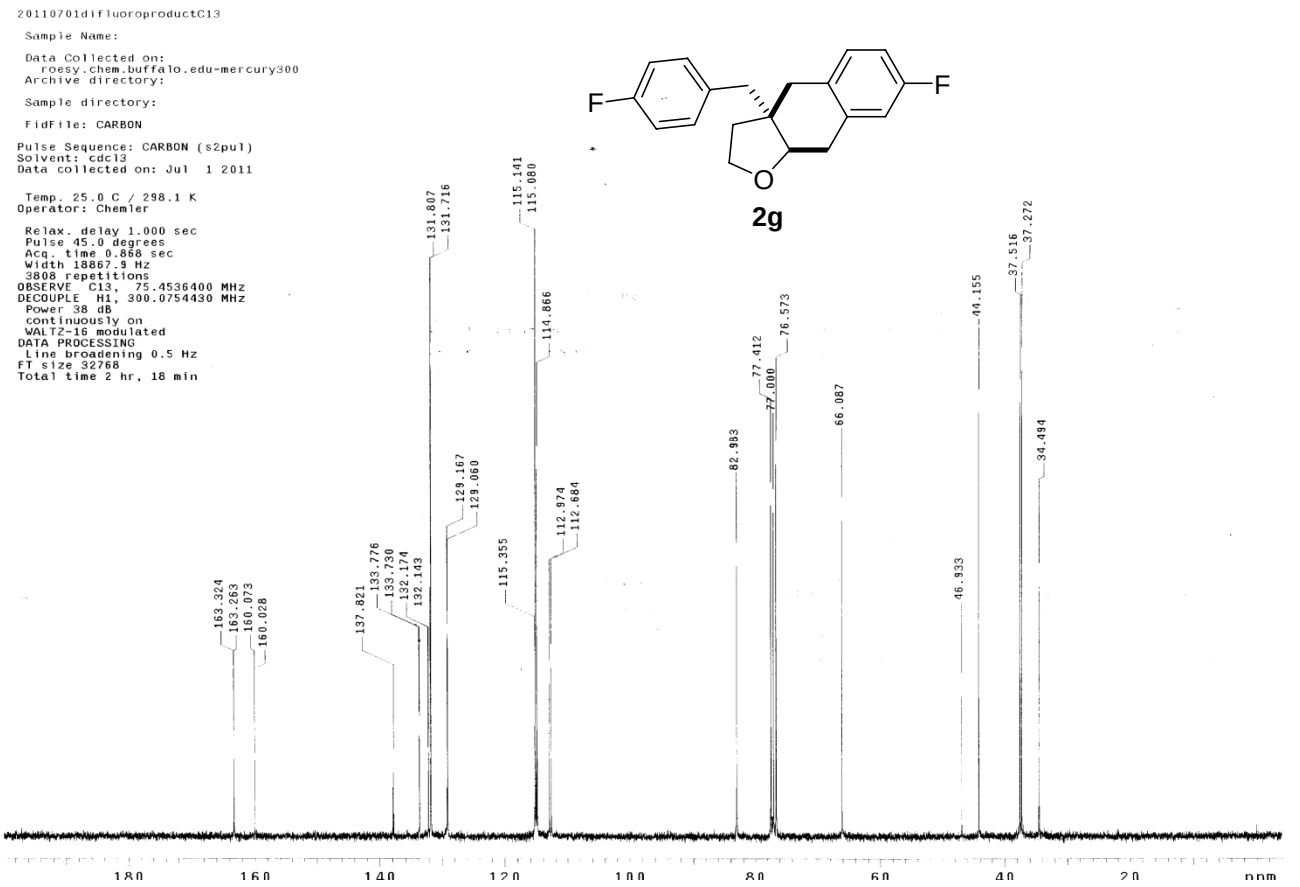
Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3392 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min



2f


20110701difluoroproduct
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 1 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984078 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
F
F
O
2g
ppm
2.02 2.05
2.97
1.00
2.07
3.05
1.09 2.17
1.08
1.10


20110701difluoroproductC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 1 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3808 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
F
F
O
2g
ppm

20110702ditrifuloroproduct

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

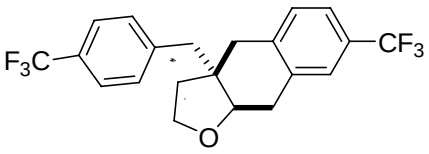
Sample directory:

FidFile: PROTON

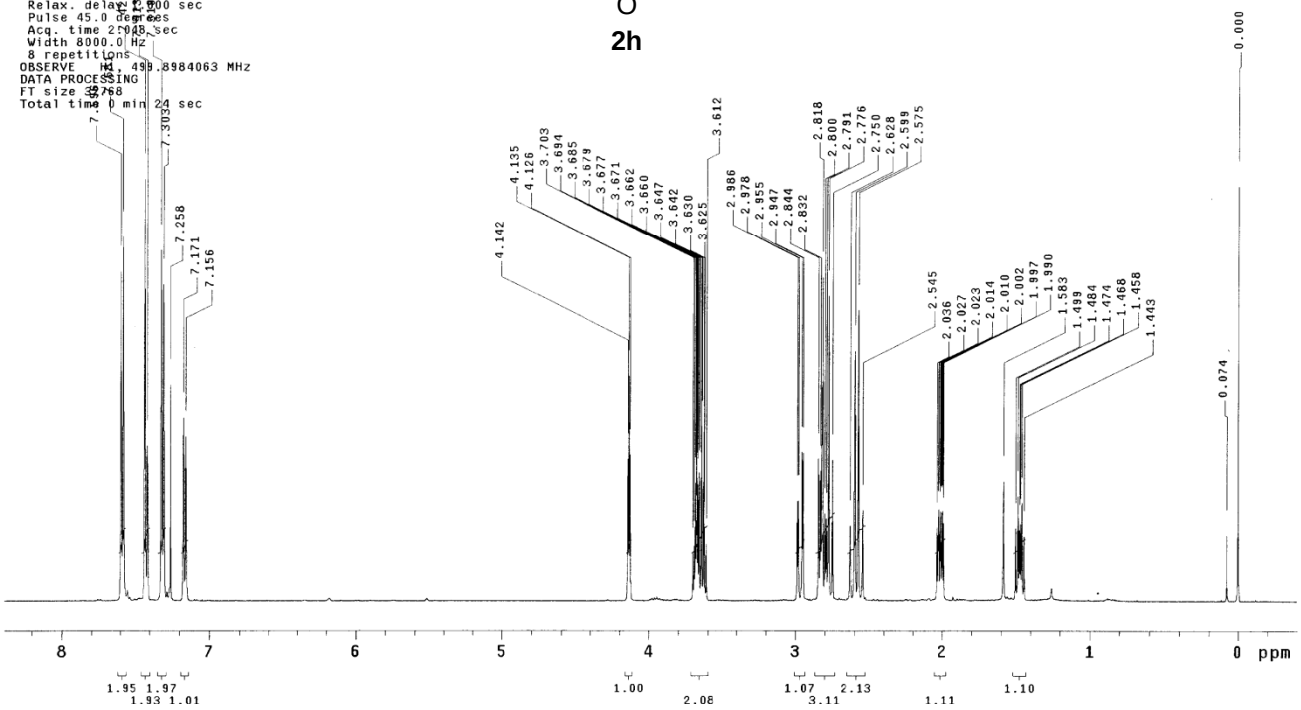
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 2 2011

Operator: Chemler

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984063 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



2h



20110702ditrifluoroproductC13

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

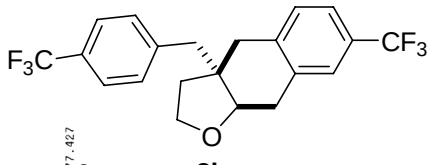
Sample directory:

FidFile: CARBON

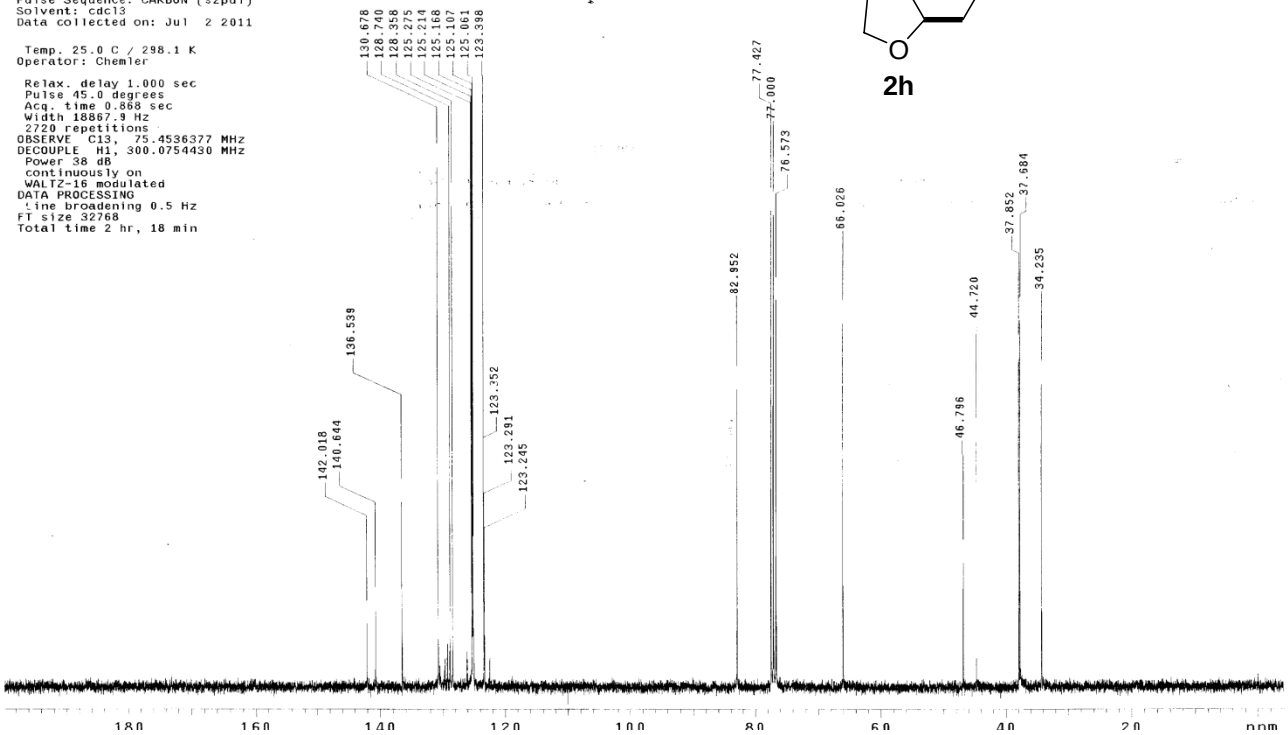
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 2 2011

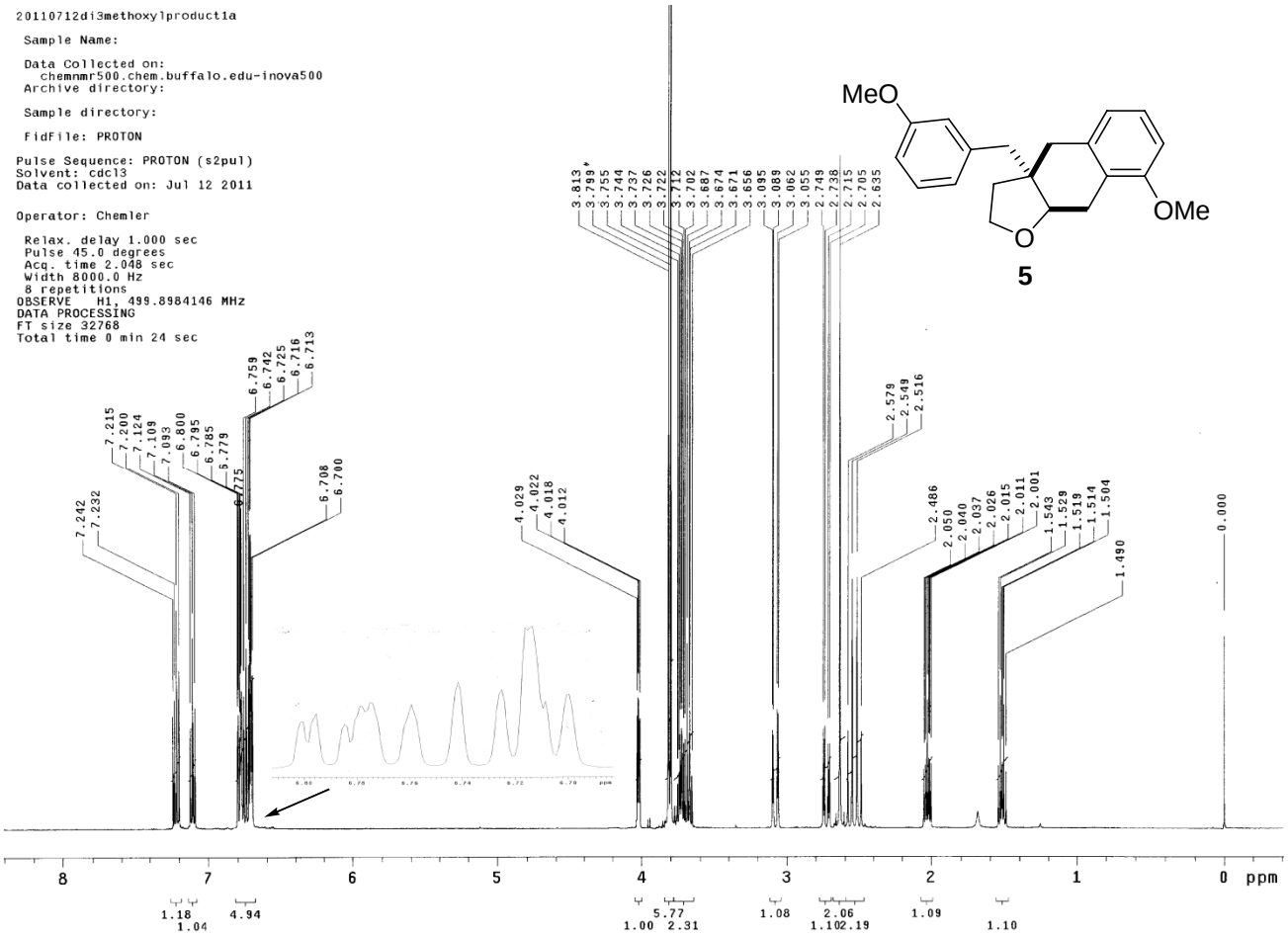
Temp. 25.0 C / 298.1 K
Operator: Chemler

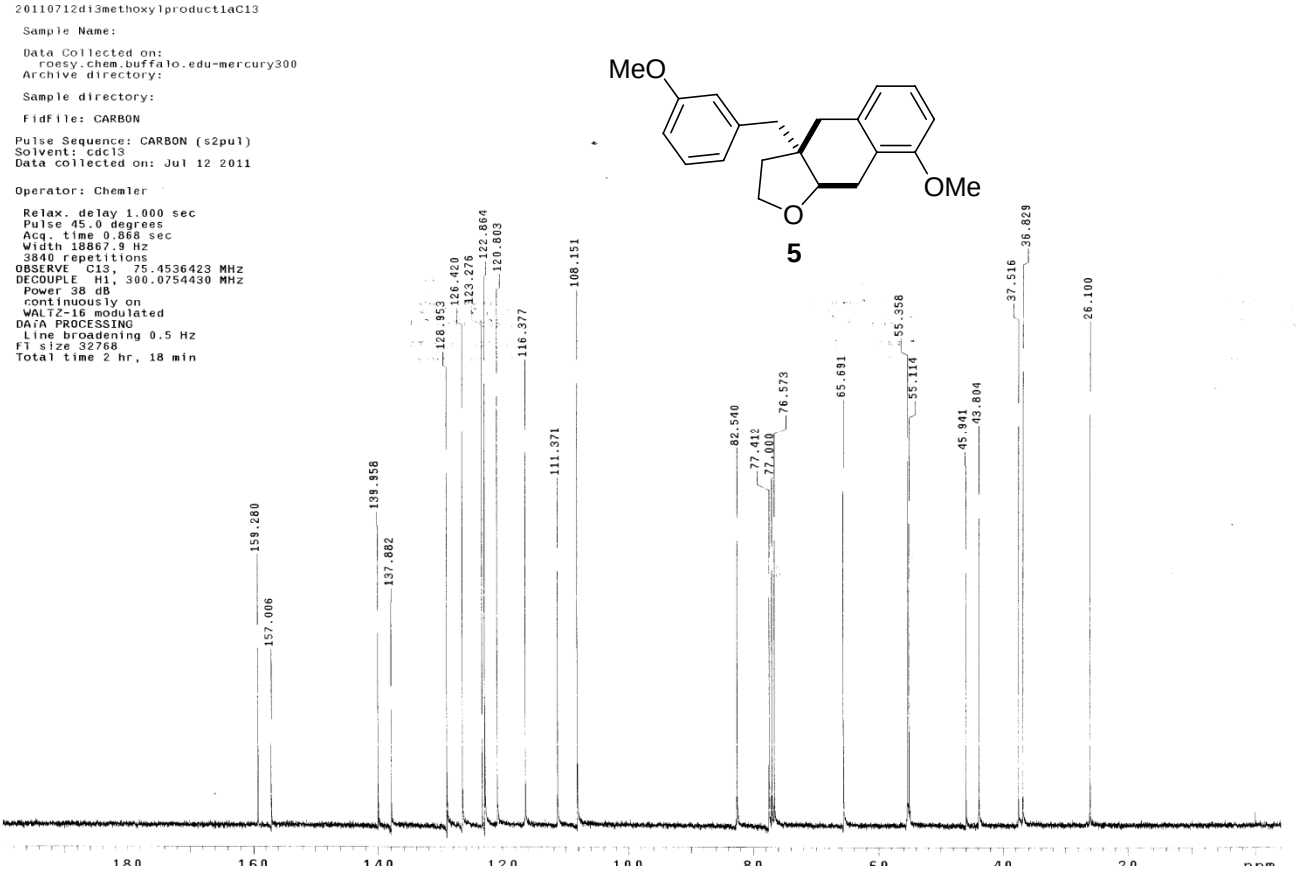
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2720 repetitions
OBSERVE C13, 75.4536377 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min

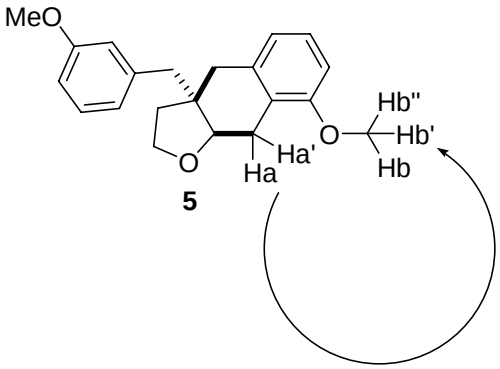


2h



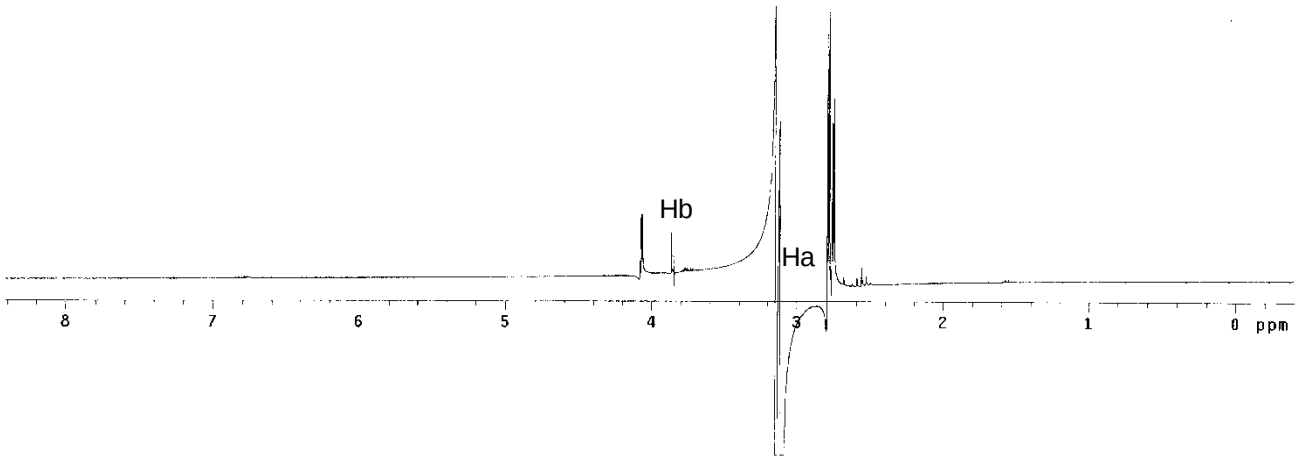

20110712di3methoxylproduct1a
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 12 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984146 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
MeO
OMe
O
5
ppm
1.18
1.04
4.94
5.77
1.00
2.31
1.08
2.06
1.10
2.19
1.09
1.10

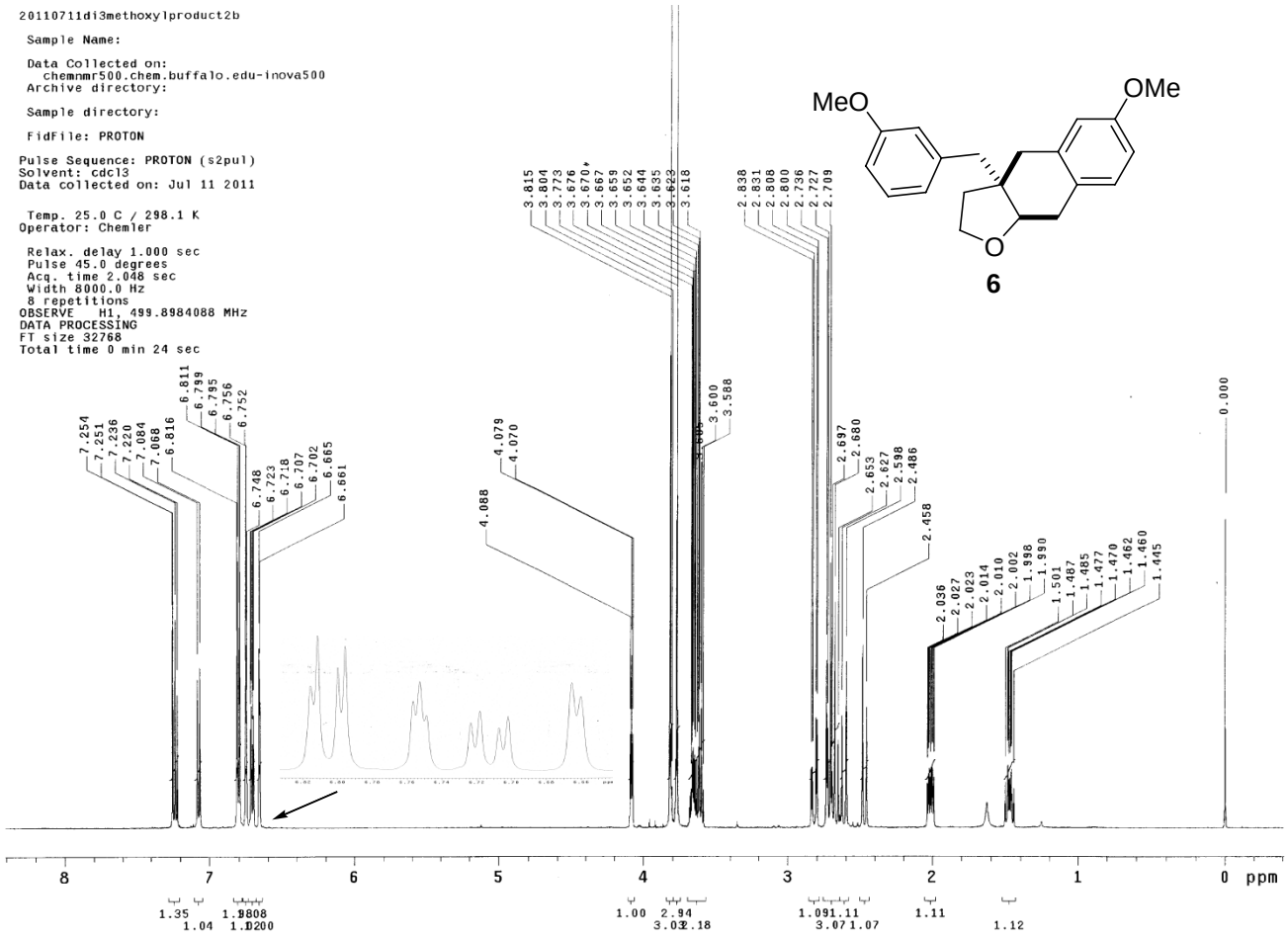

20110712di3methoxylproduct1aC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 12 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3840 repetitions
OBSERVE C13, 75.4536423 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
MeO
OMe
O
5
ppm

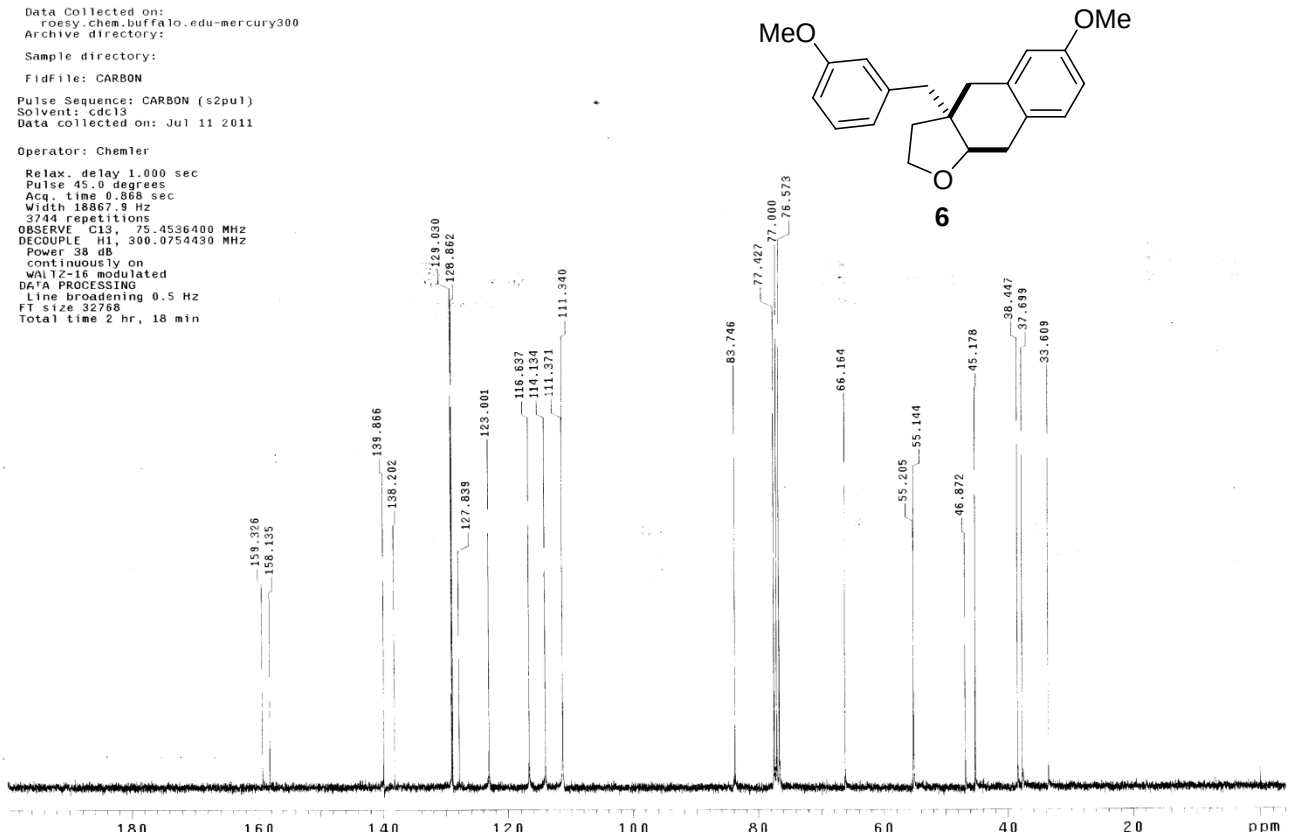


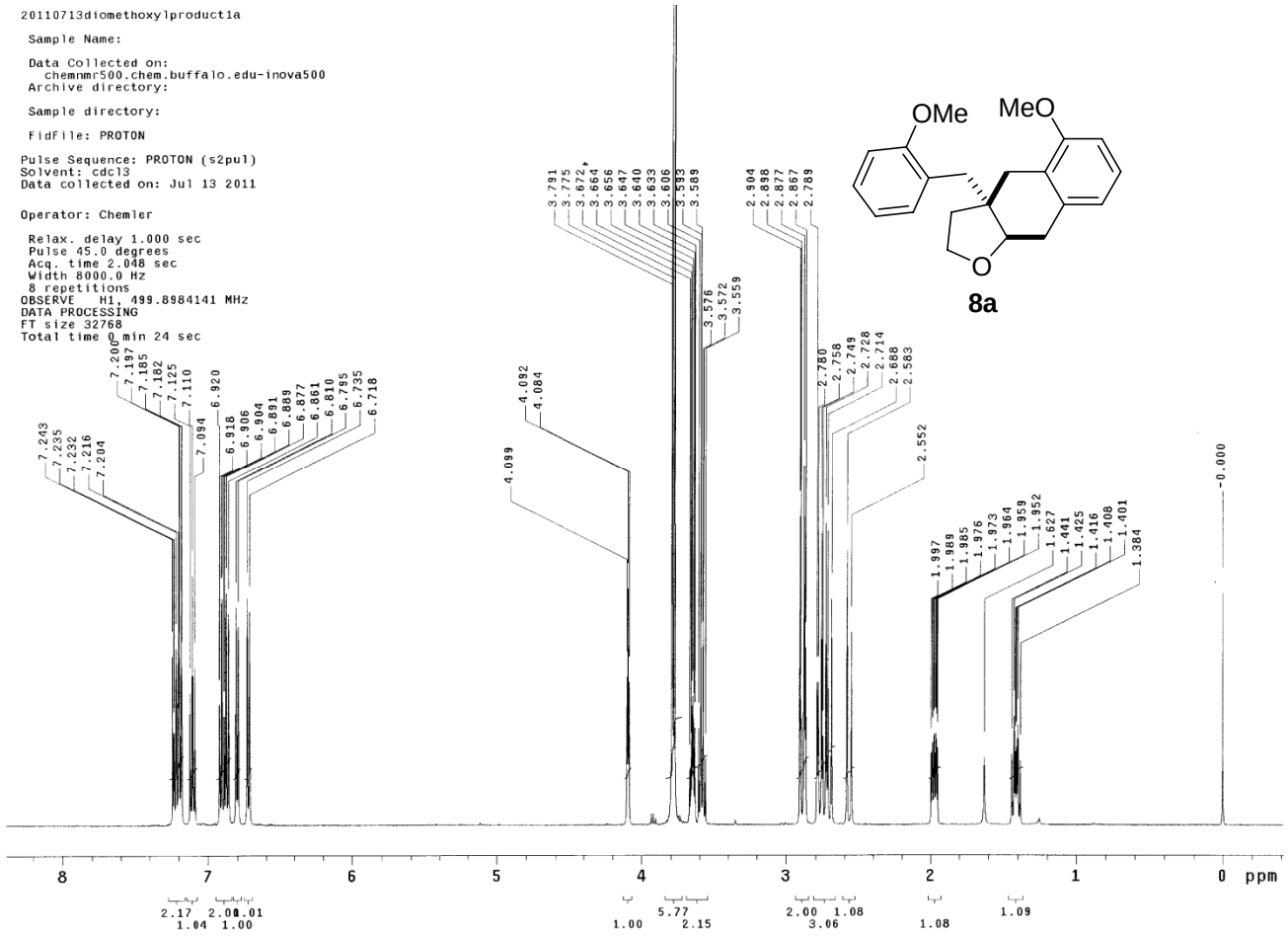
5

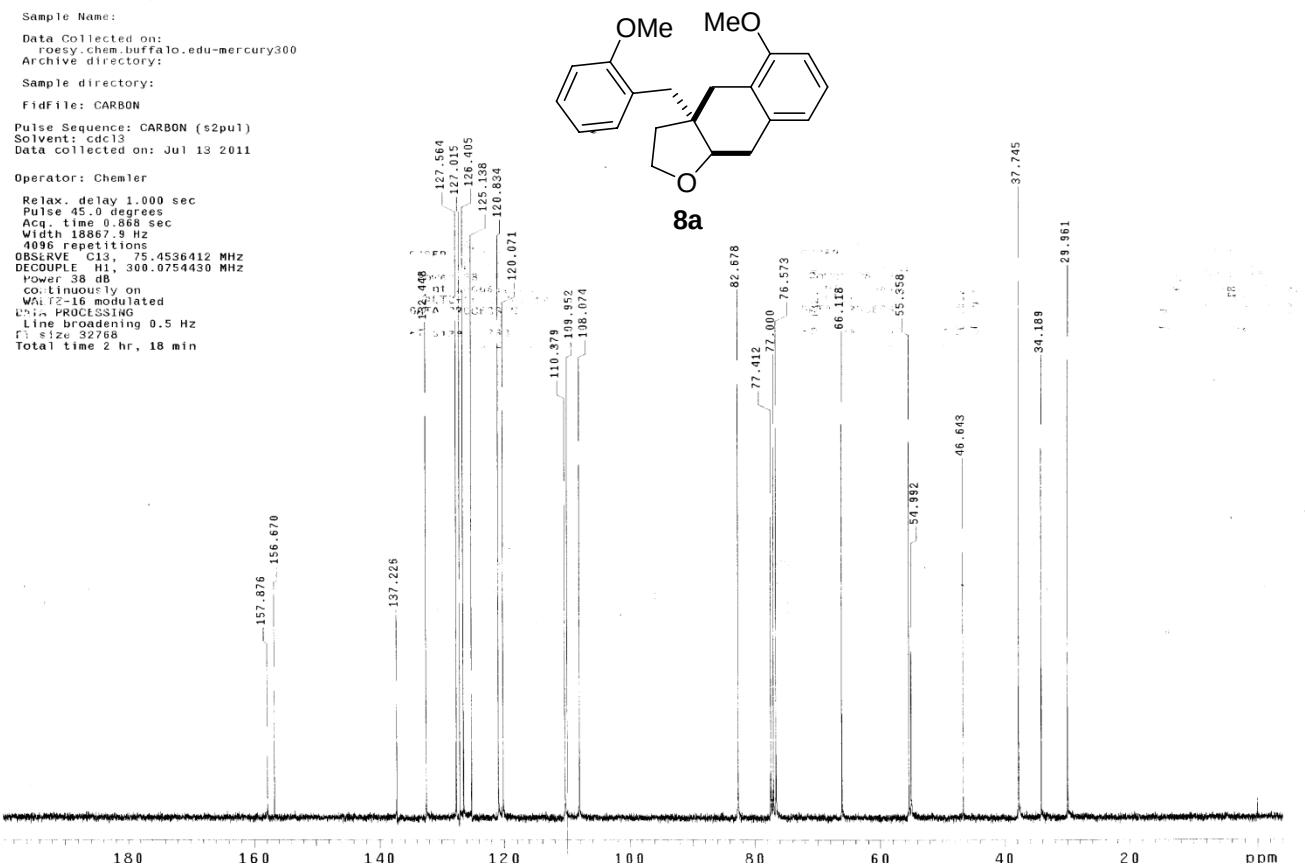
```
20110712di3methoxylproduct1aNOE
  Selective band center: 3.13 (ppm); width: 35.0 (Hz)

 Sample Name:

 Data Collected on:
   chemnmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 FidFile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jul 12 2011

Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 1.859 sec
 Width 4406.3 Hz
 10752 repetitions
OBSERVE   N1, 499.8983908 MHz
DATA PROCESSING
FT size 16384
Total time 10 hr, 54 min
```

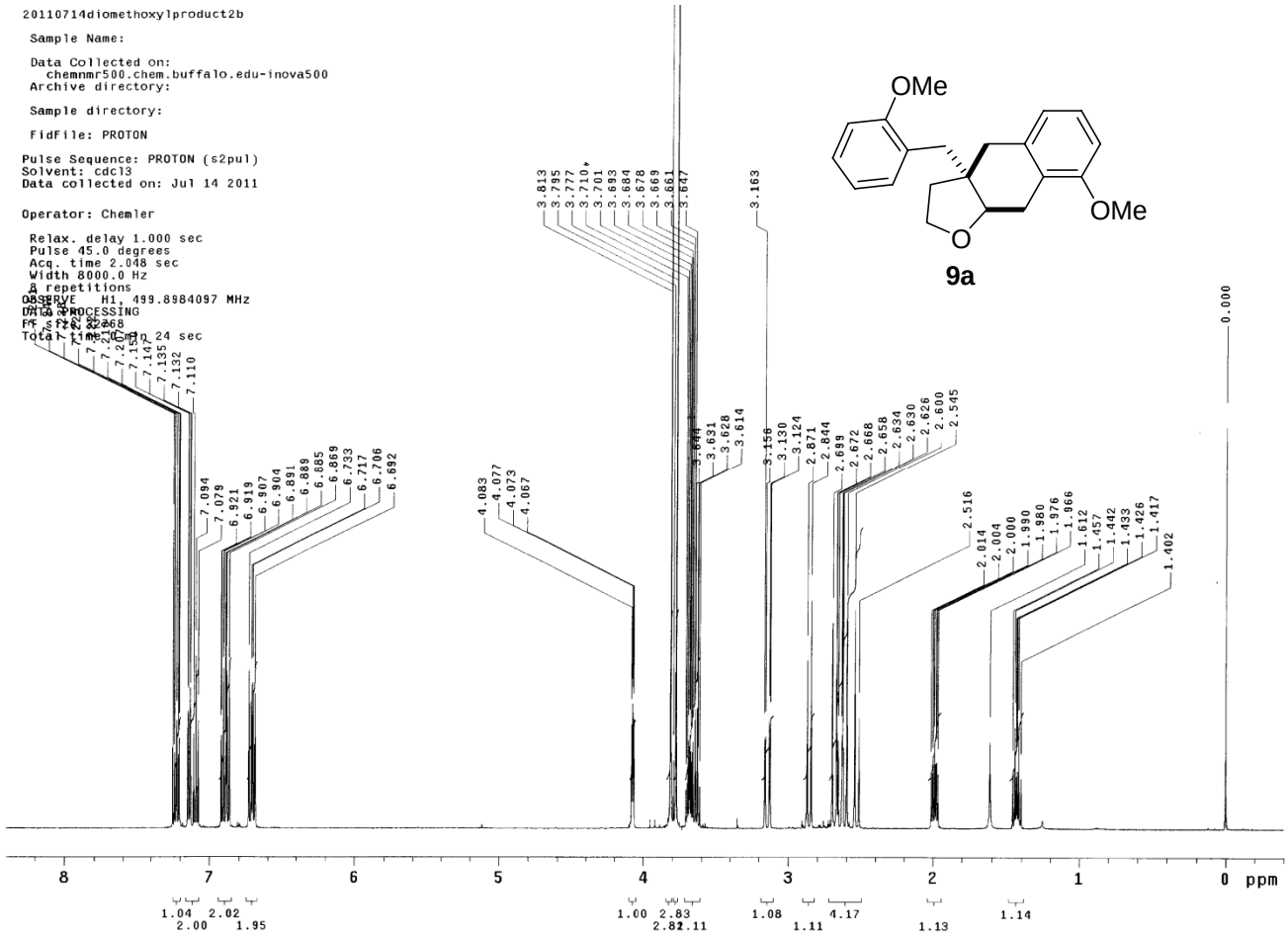


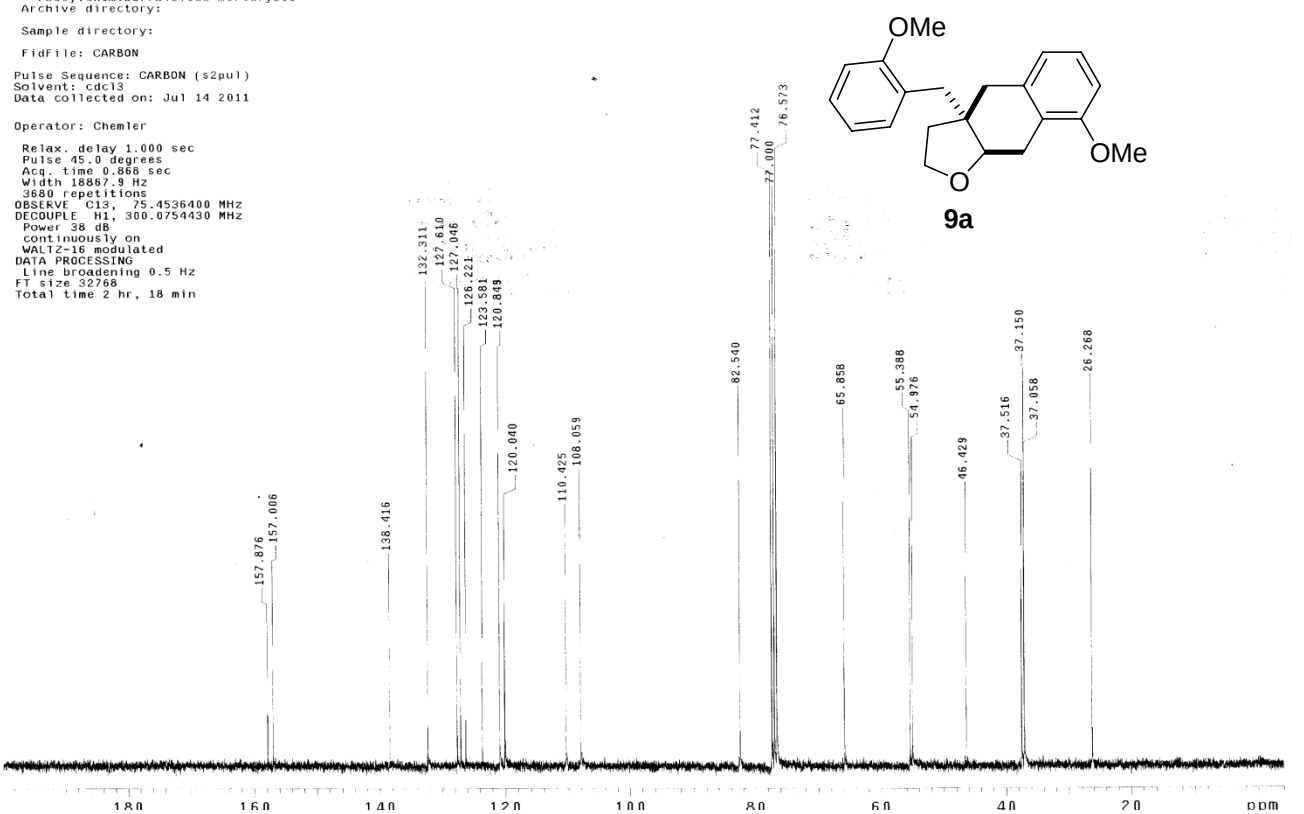

20110711di3methoxylproduct2b
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 11 2011
Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984088 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
MeO
OMe
O
6
ppm

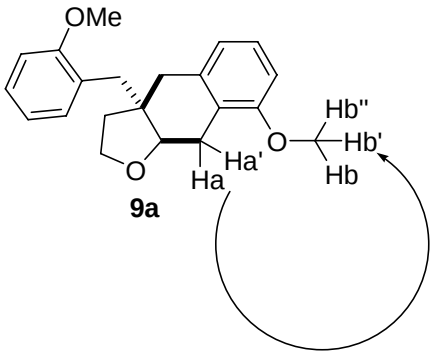

20110711di3methoxylproduct2bC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 11 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3744 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
MeO
OMe
O
6
ppm


20110713diomethoxylproduct1a
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 13 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984141 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
MeO
O
8a
ppm
2.17 2.00 1.01
1.04 1.00
1.00 5.77 2.15
2.00 1.08
3.06
1.08
1.09


20110713diomethoxylproduct1aC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 13 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
4096 repetitions
OBSERVE C13, 75.4536412 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
OMe
MeO
O
8a
ppm

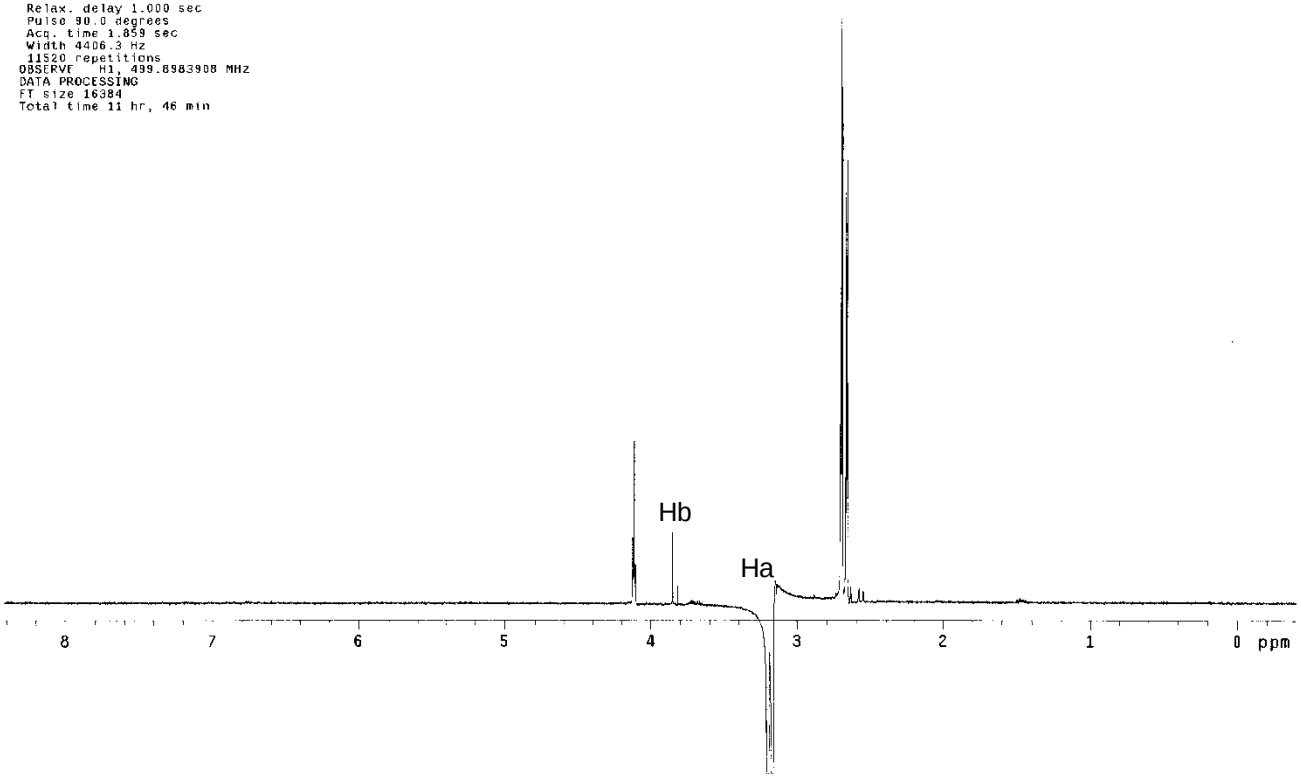

20110714diomethoxylproduct2b
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984097 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 24 sec
OMe
OMe
O
9a
ppm

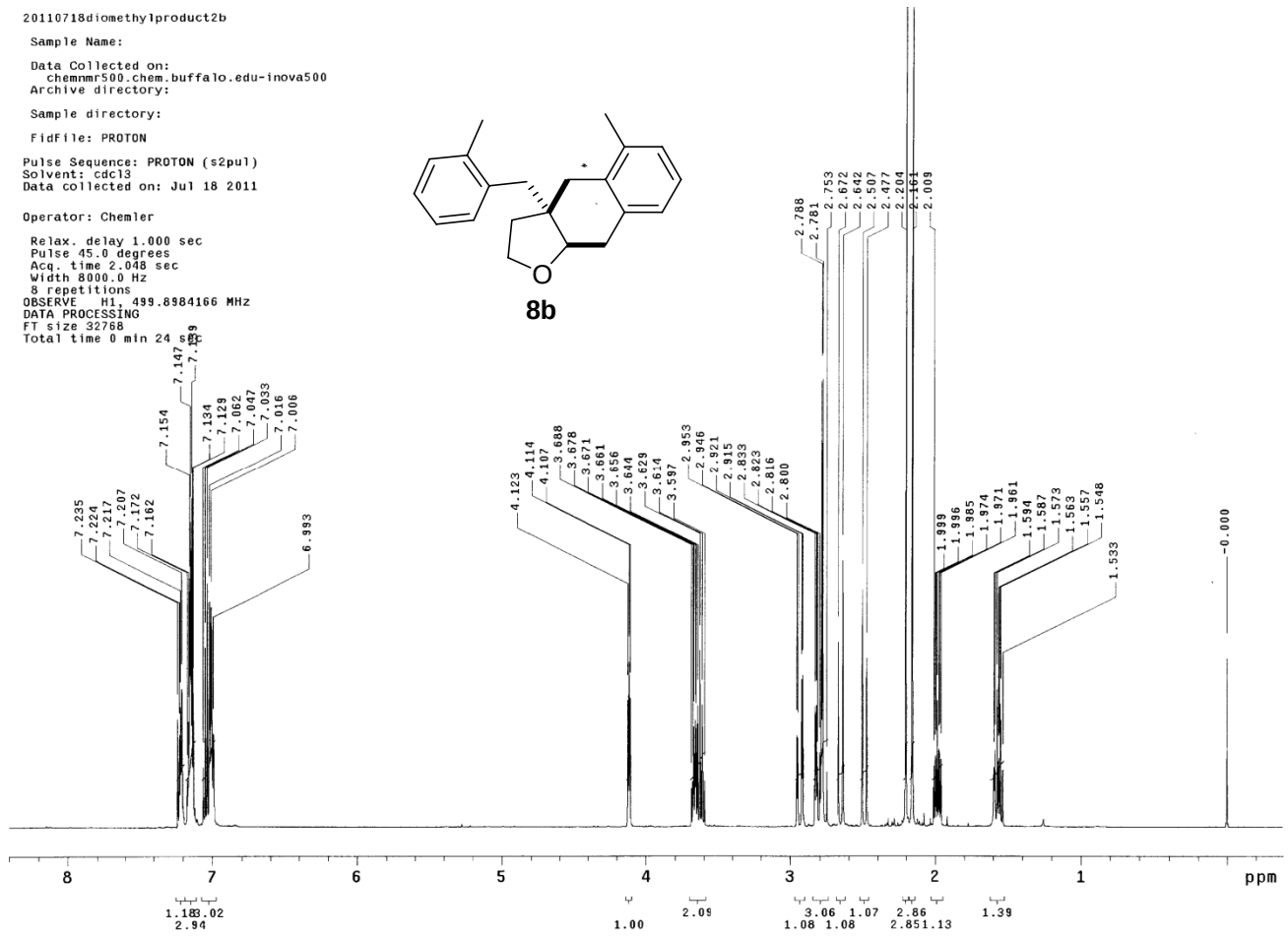

20110714diomethoxylproduct2bC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3680 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
OMe
OMe
O
9a
ppm

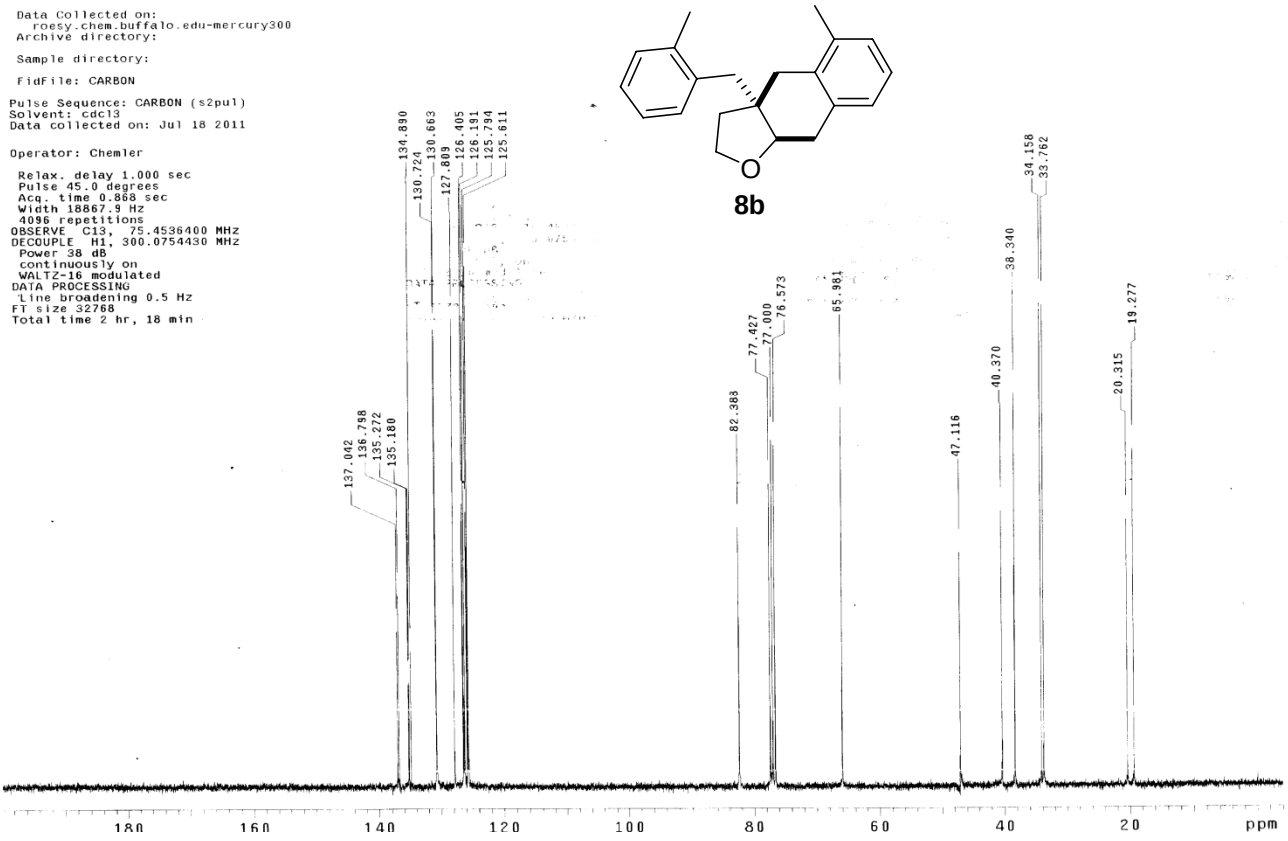


9a

```
20110714diomethoxylproduct2bNOE
  Selective band center: 3.18 (ppm); width: 30.8 (Hz)

 Sample Name:

 Data Collected on:
   chemmmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 FidFile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jul 14 2011

Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 1.859 sec
 Width 4406.3 Hz
 11520 repetitions
OBSERVE   H1, 499.8983908 MHz
DATA PROCESSING
FT size 16384
Total time 11 hr, 46 min
```




20110718diomethylproduct2b
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984166 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
8b
ppm
1.18 3.02 2.94 1.00 2.09 3.06 1.07 1.08 1.08 2.86 2.85 1.13 1.39


20110718diomethylproduct2bC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 18 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
4096 repetitions
OBSERVE C13, 75.4536400 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
8b
ppm

20110725diomethylproduct1a

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

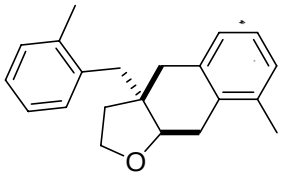
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 25 2011

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984078 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



9b

20110725diomethylproduct1aC13

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

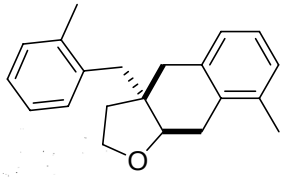
Sample directory:

FidFile: CARBON

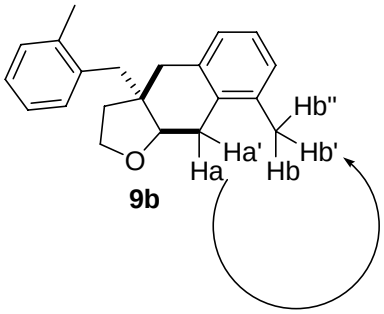
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 26 2011

Temp. 22.0 C / 295.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
7776 repetitions
OBSERVE C13, 75.4536377 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min

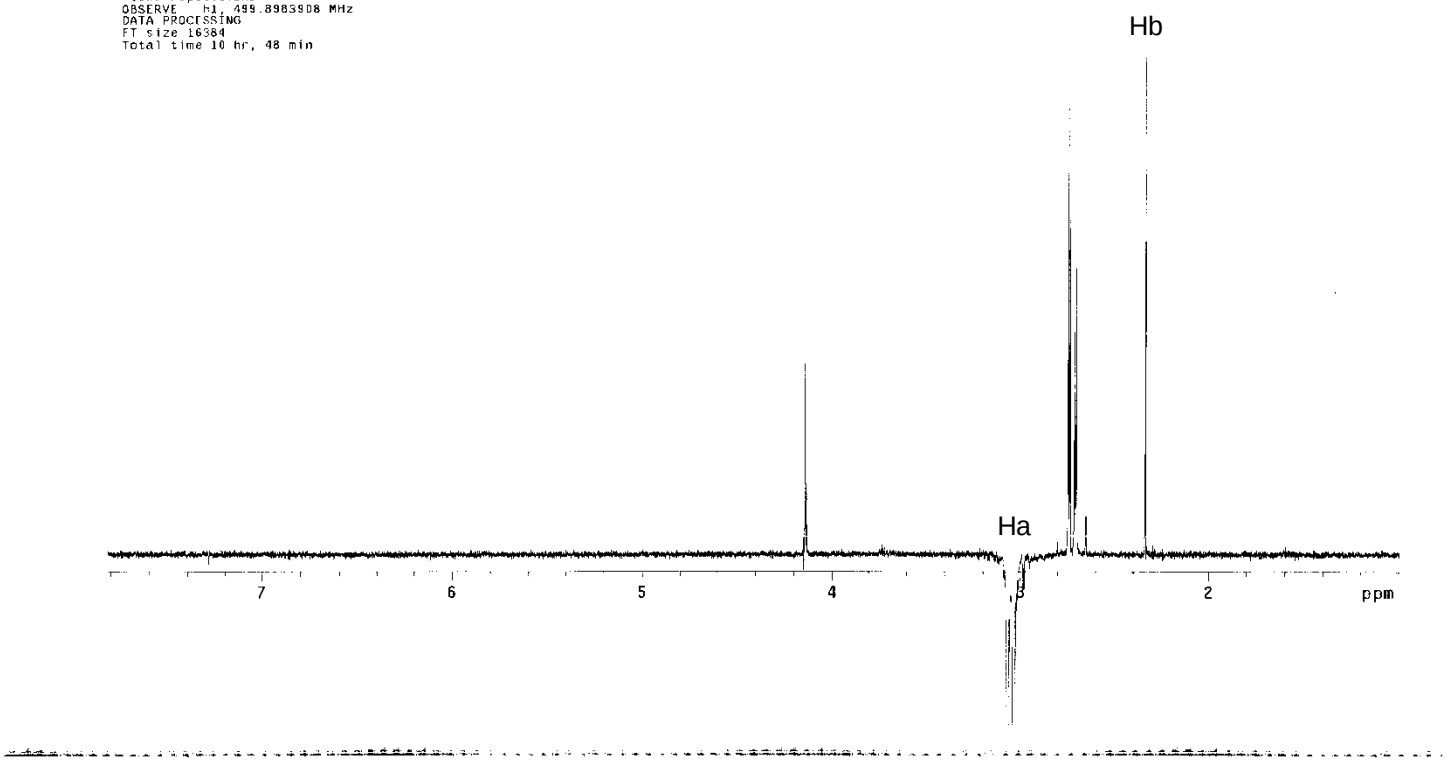


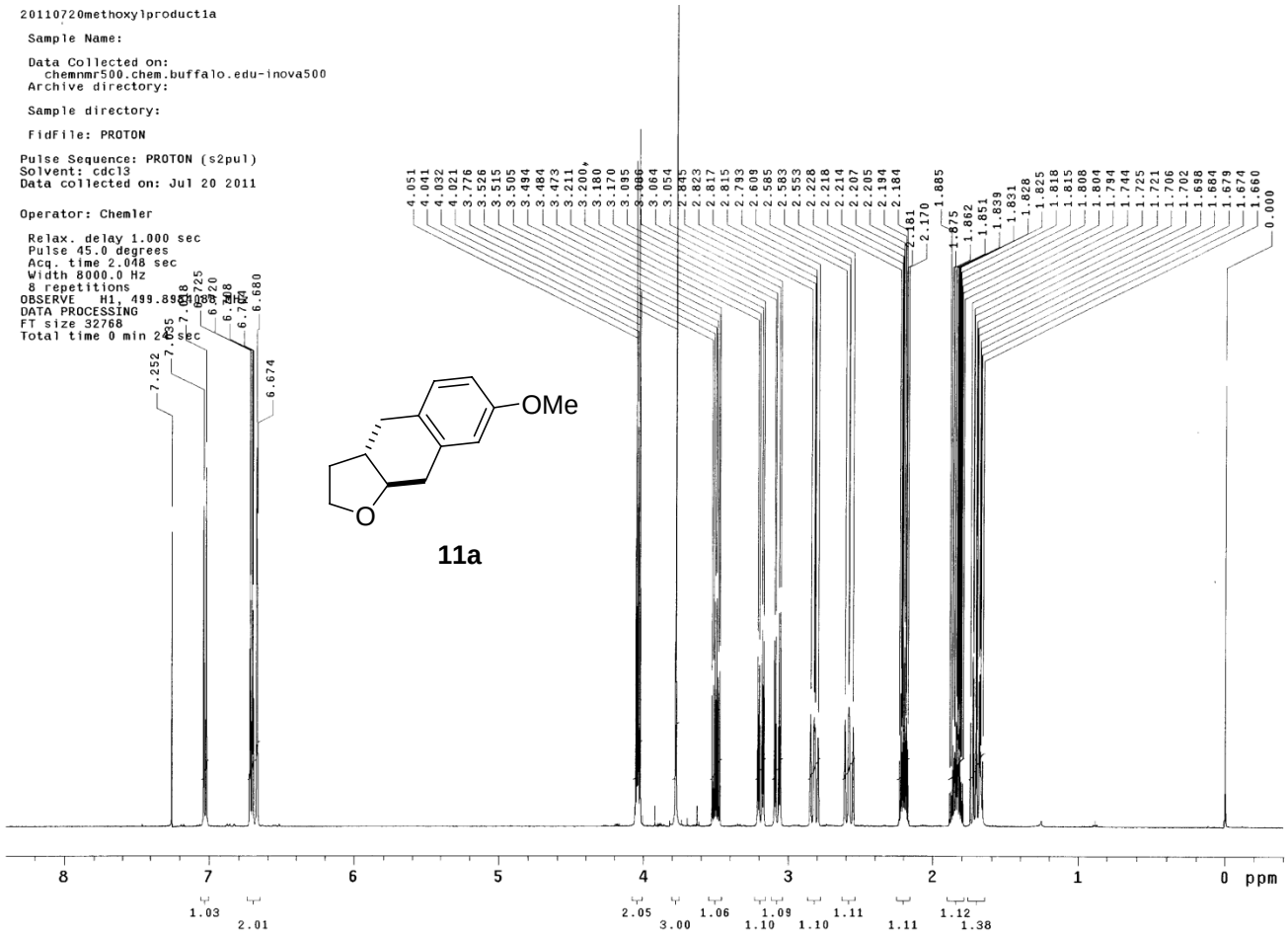
9b

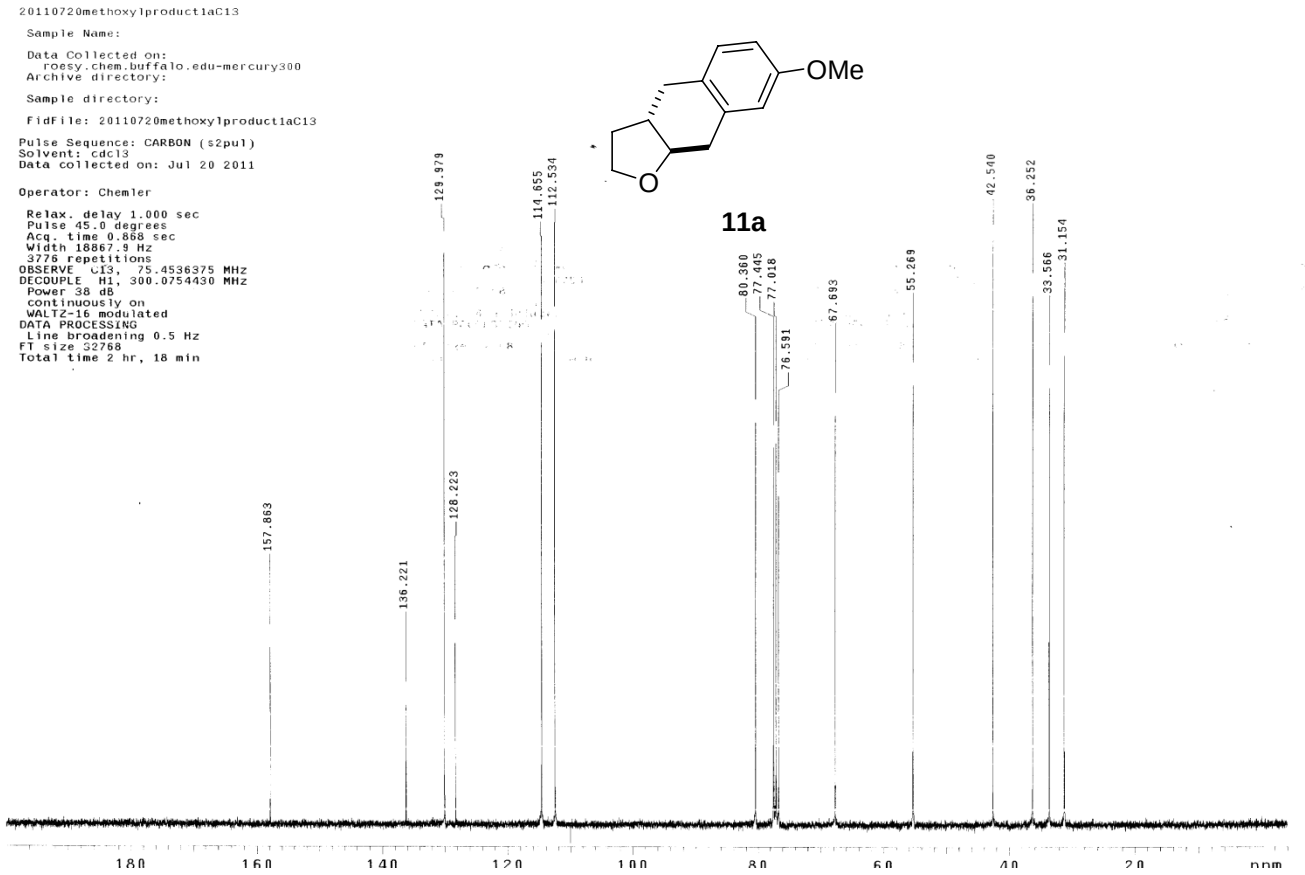


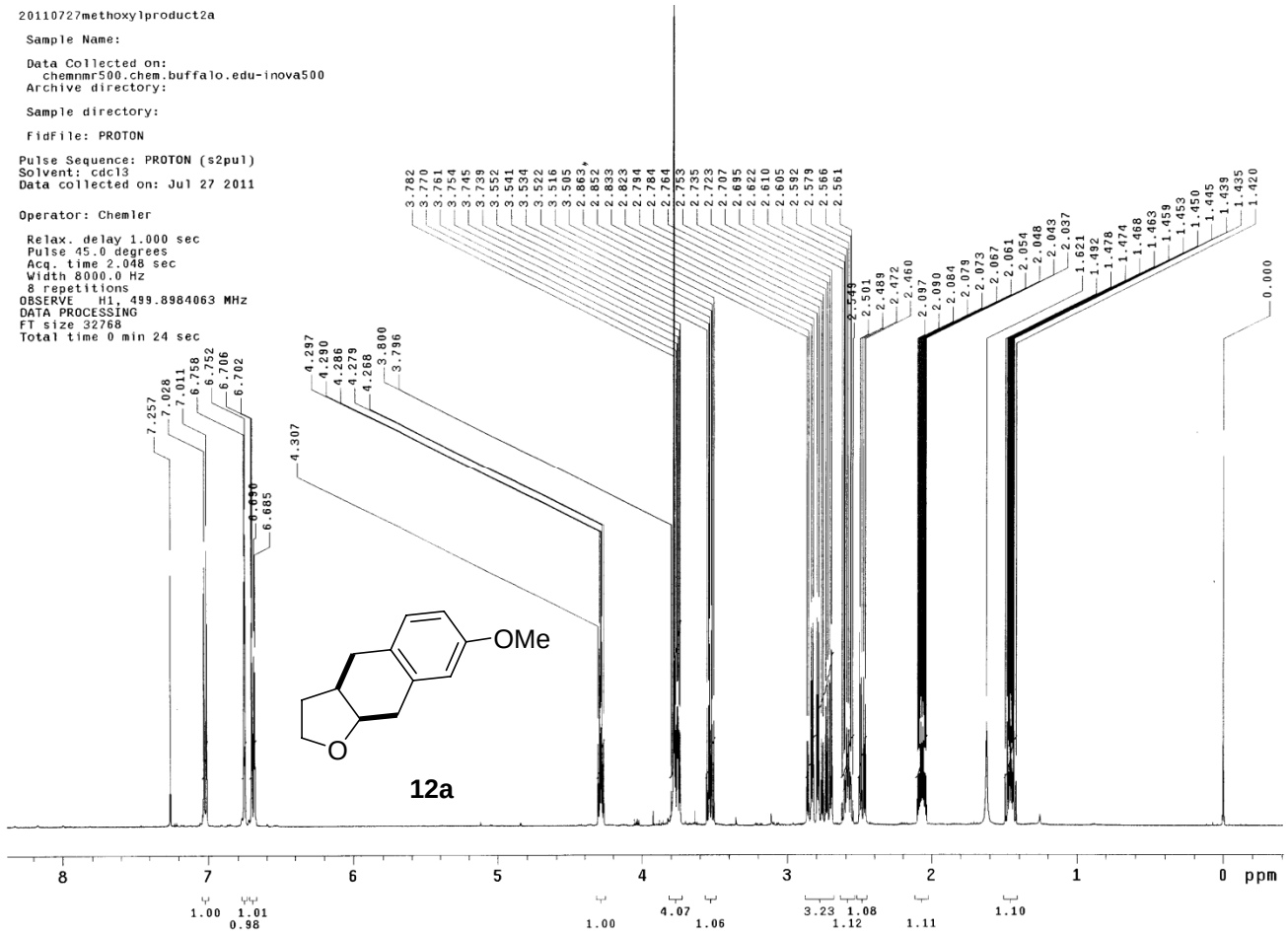
9b

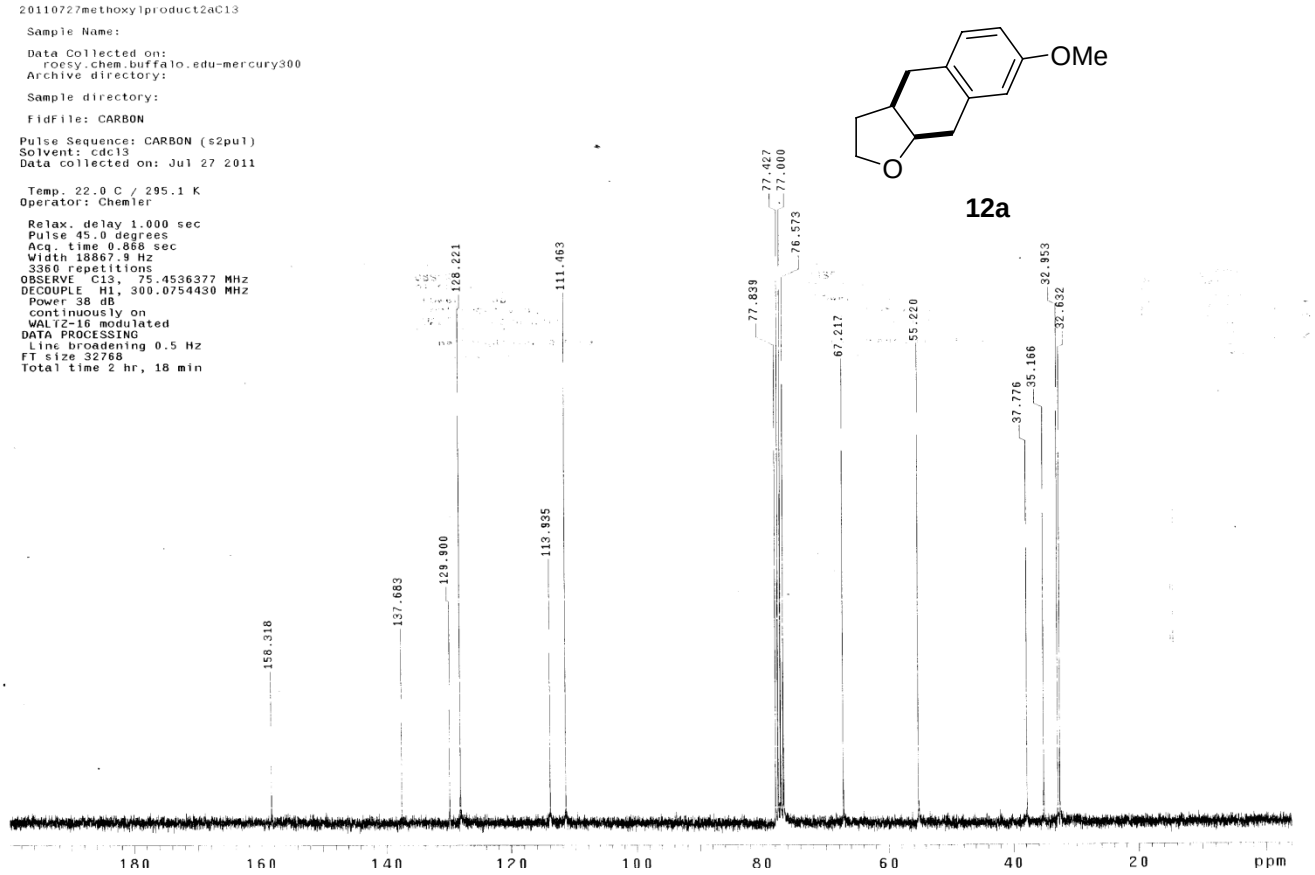
```
20110725diomethylproductNOF

 Sample NAme:

 Data Collected on:
   chemmmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 Fidfile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jul 25 2011

Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 2.402 sec
 Width 3410.1 Hz
 9152 repetitions
OBSERVE   h1, 499.8985908 MHz
DATA PROCESSING
FT size 16384
Total time 10 hr, 48 min
```

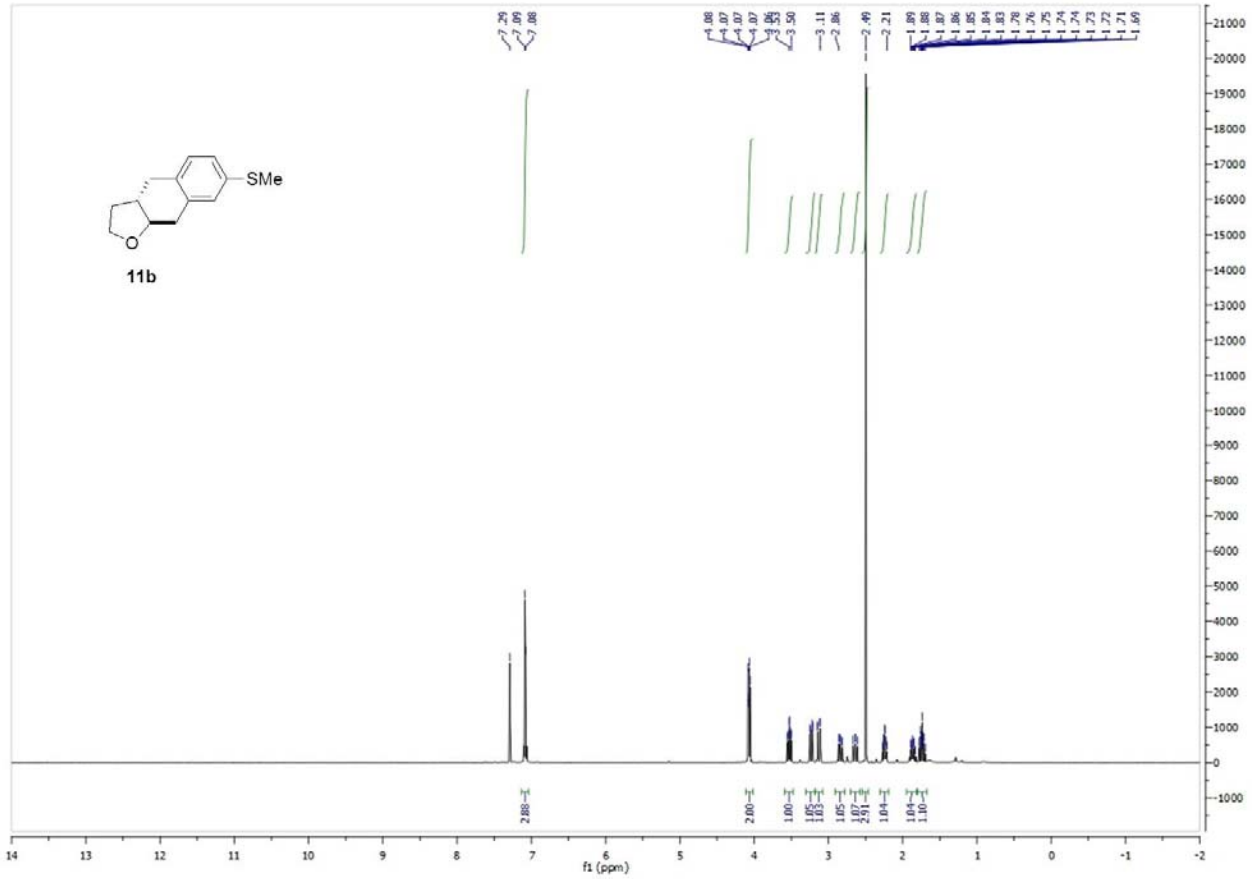


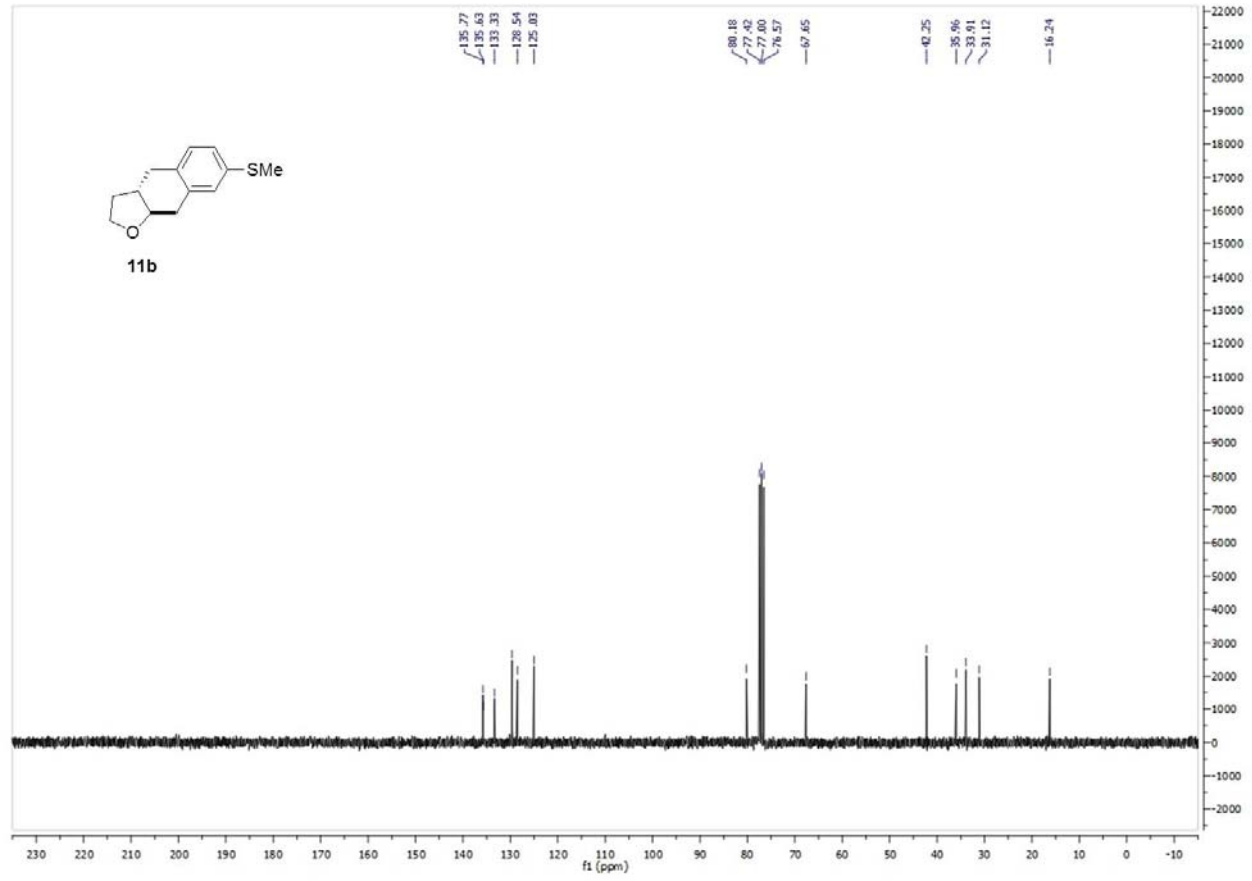

20110720methoxylproduct1a
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8900038 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
11a
ppm

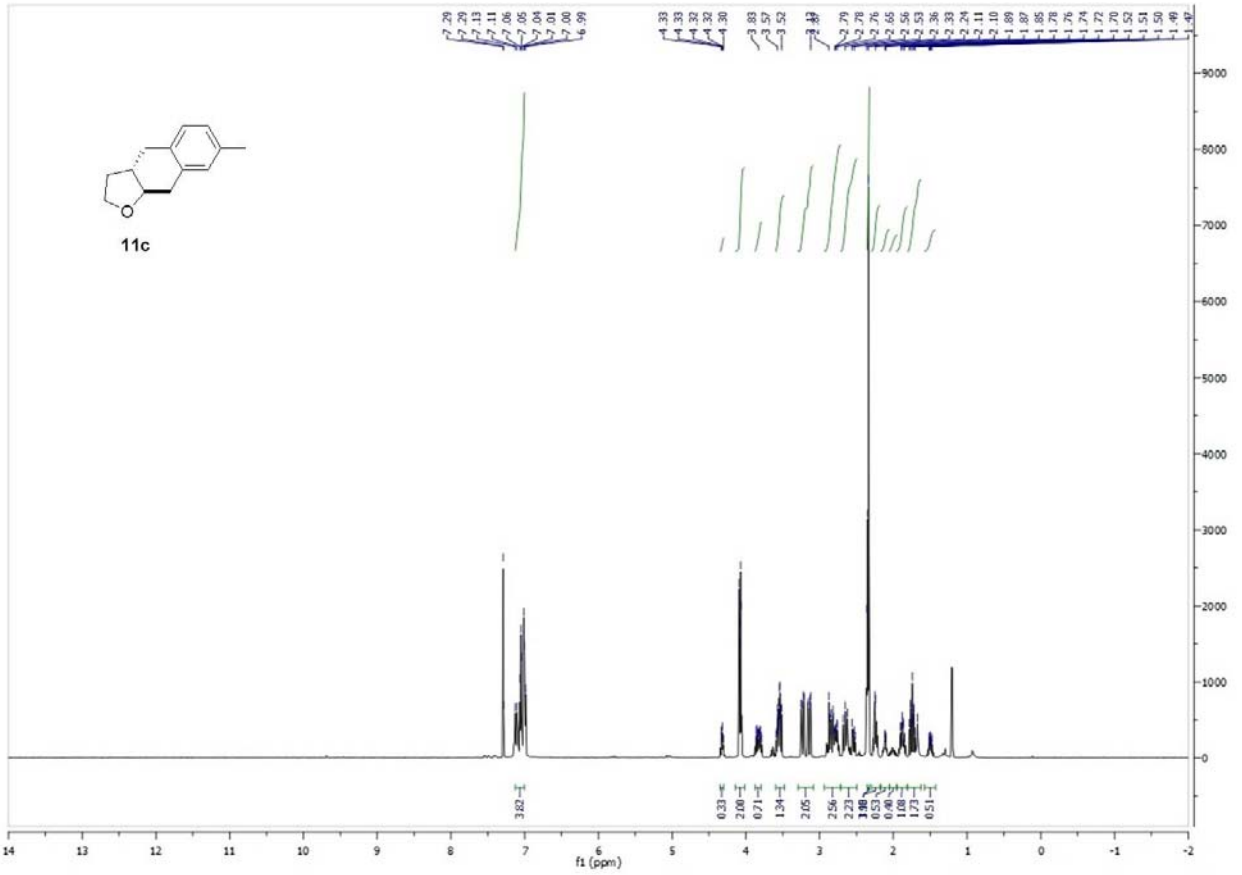

20110720methoxylproduct1aC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: 20110720methoxylproduct1aC13
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3776 repetitions
OBSERVE C13, 75.4536375 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
OMe
11a
ppm

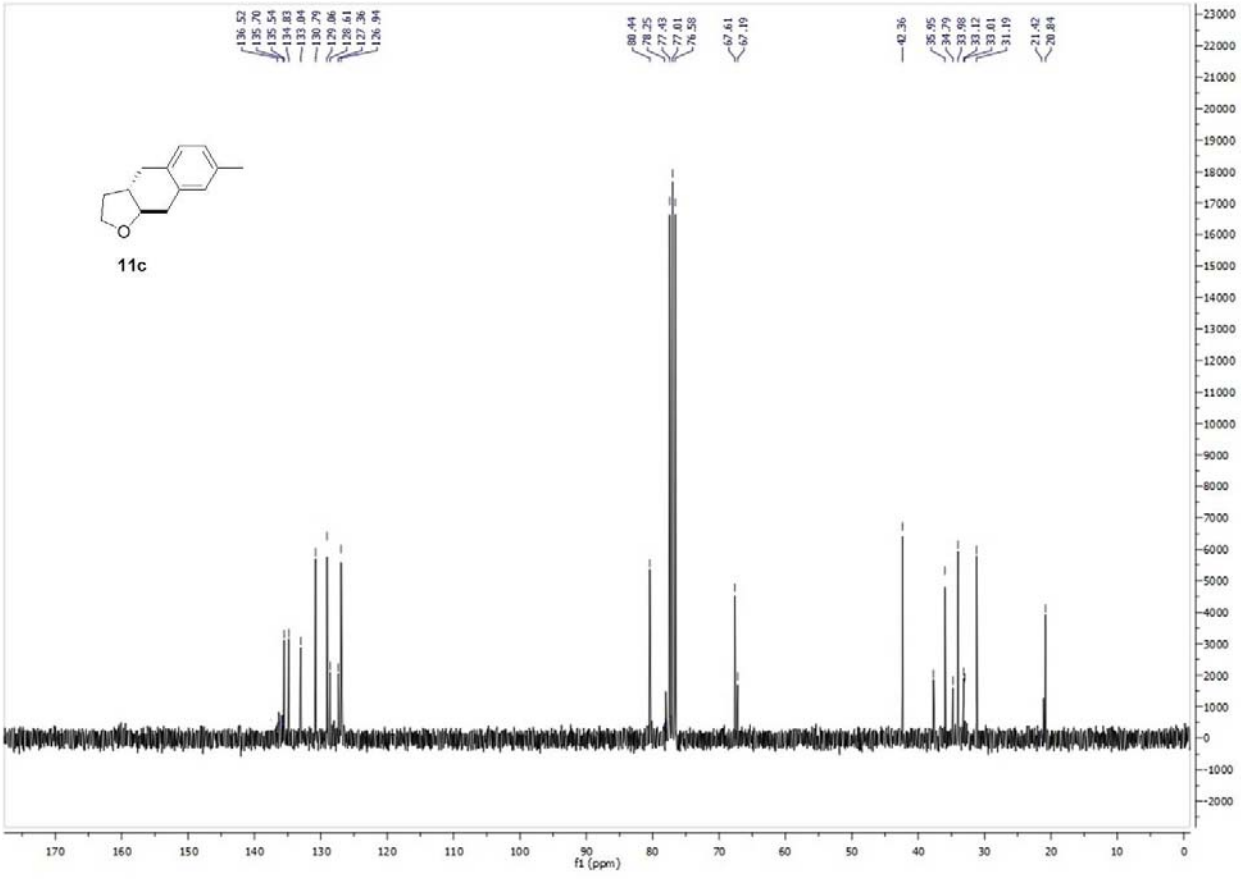

20110727methoxylproduct2a
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984063 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
O
12a
ppm

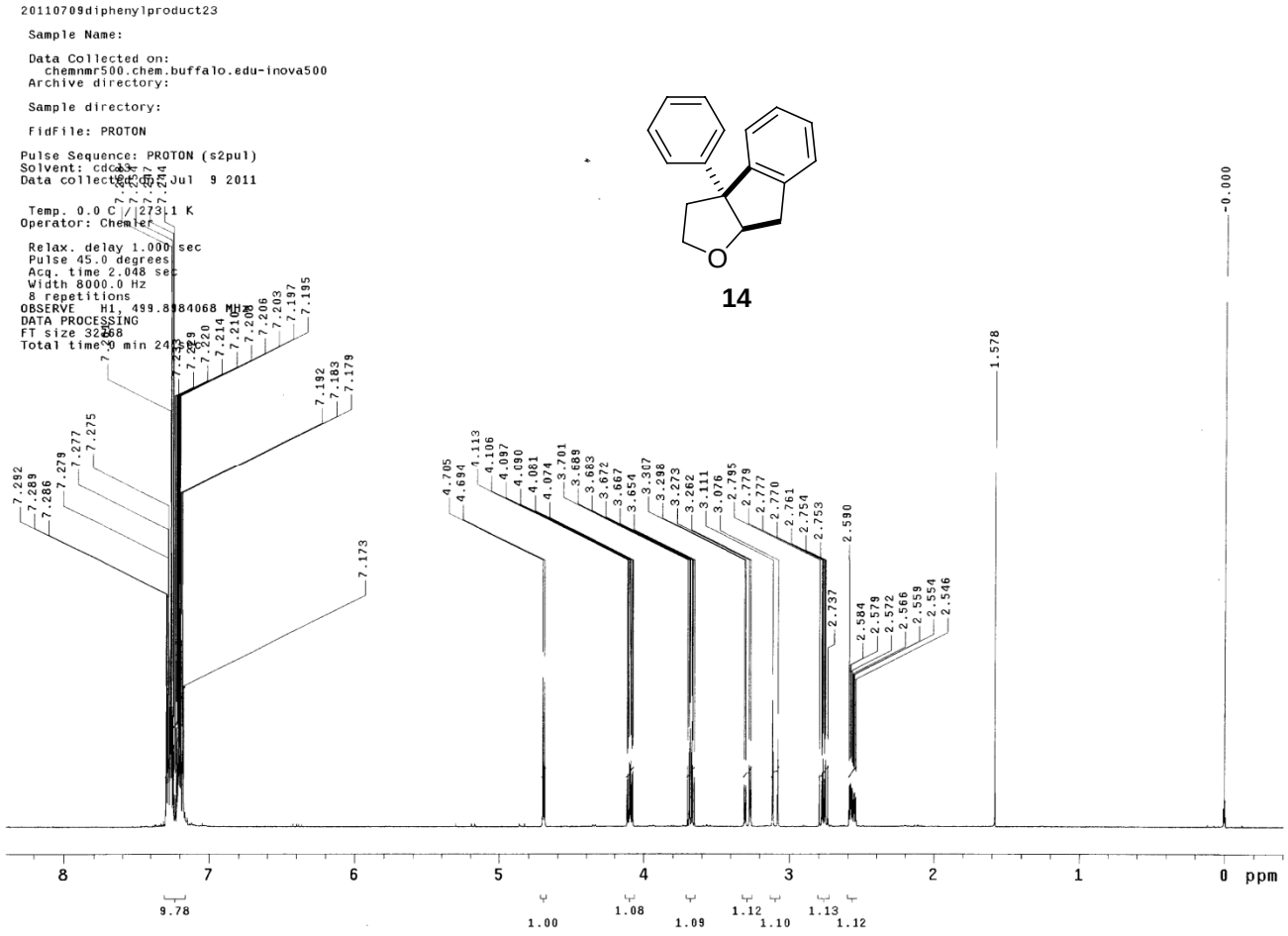

20110727methoxylproduct2aC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2011
Temp. 22.0 C / 295.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3360 repetitions
OBSERVE C13, 75.4536377 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
OMe
O
12a
ppm

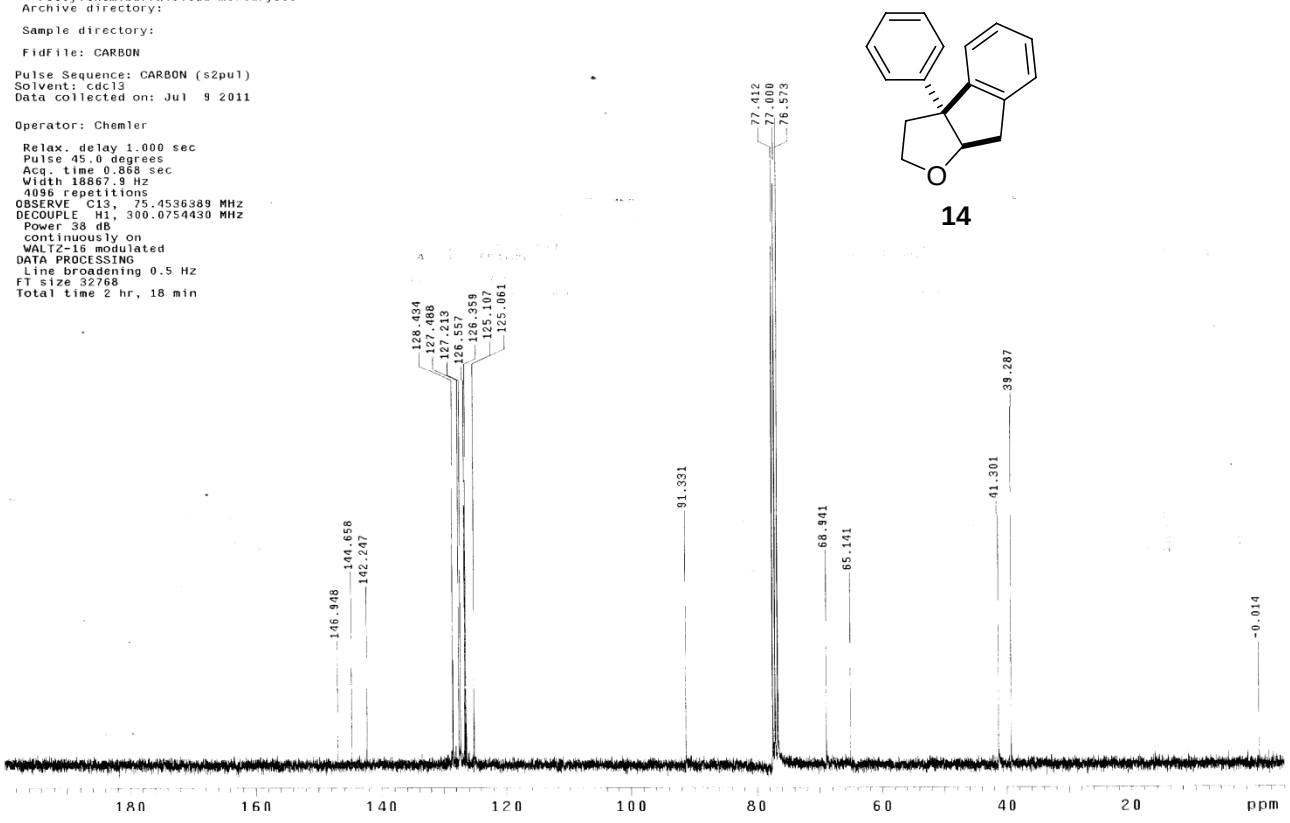

SMe
11b
f1 (ppm)

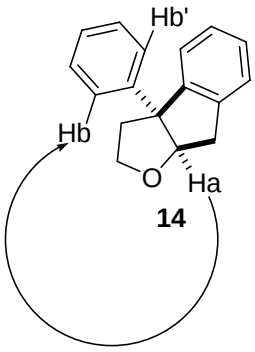

SMe
11b
f1 (ppm)


11c
f1 (ppm)


11c
f1 (ppm)

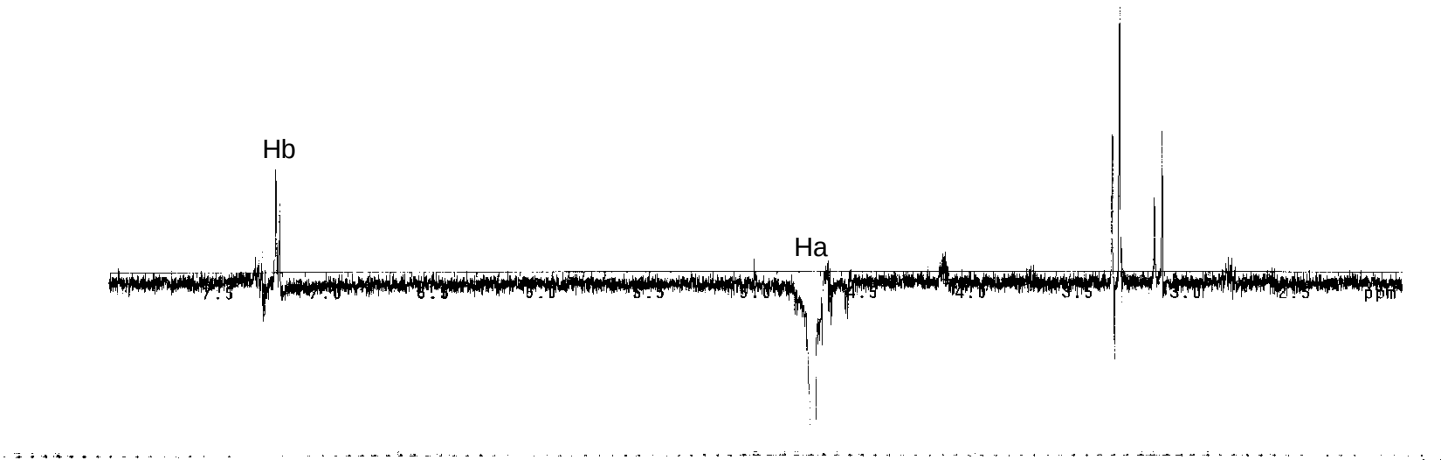

20110709diphenylproduct23
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 9 2011
Temp. 0.0 C / 273.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984068 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
14
ppm
9.78
1.00
1.08
1.09
1.12
1.10
1.13
1.12

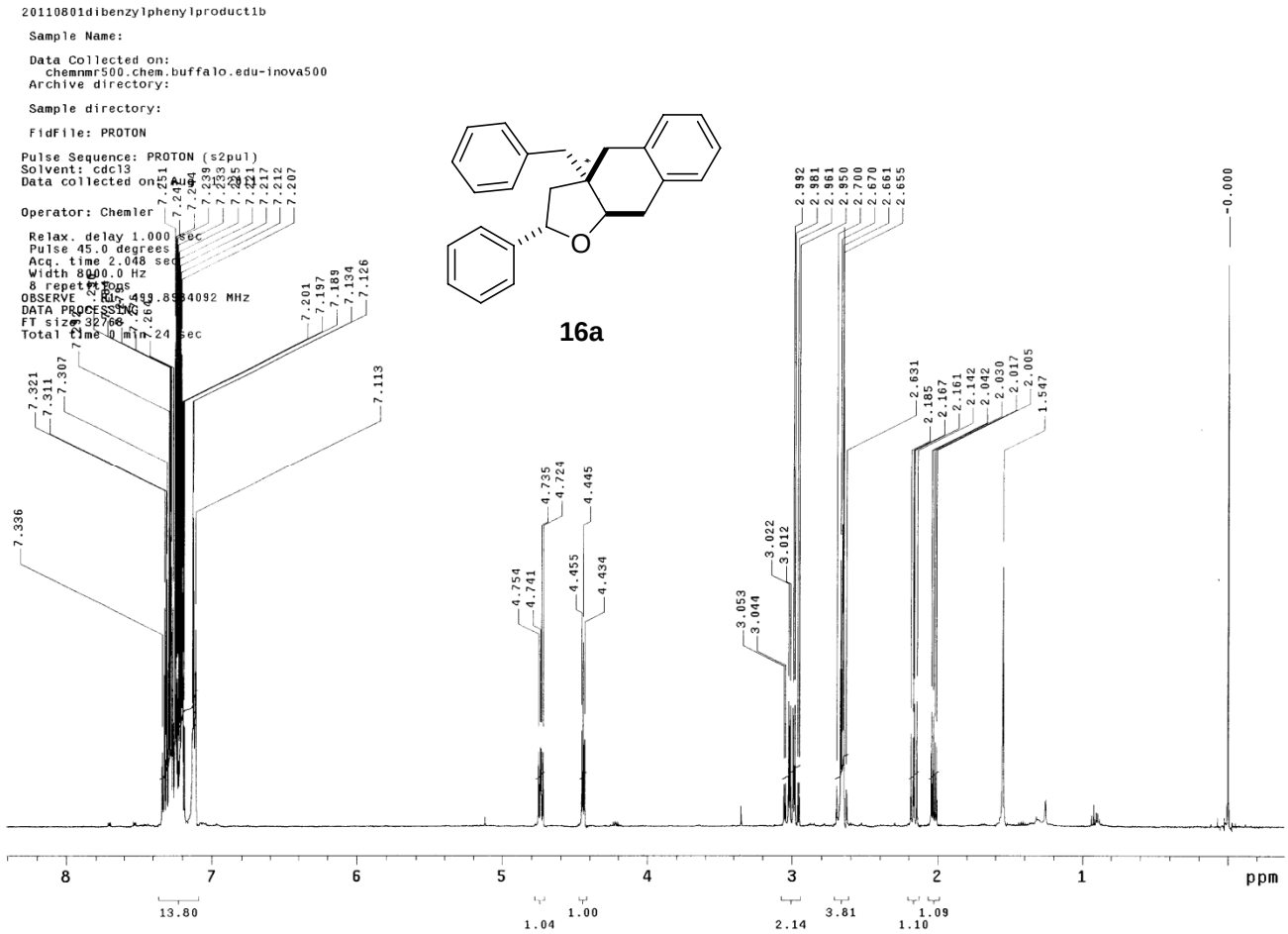

20110709diphenylproductC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 9 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
4096 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
14
ppm

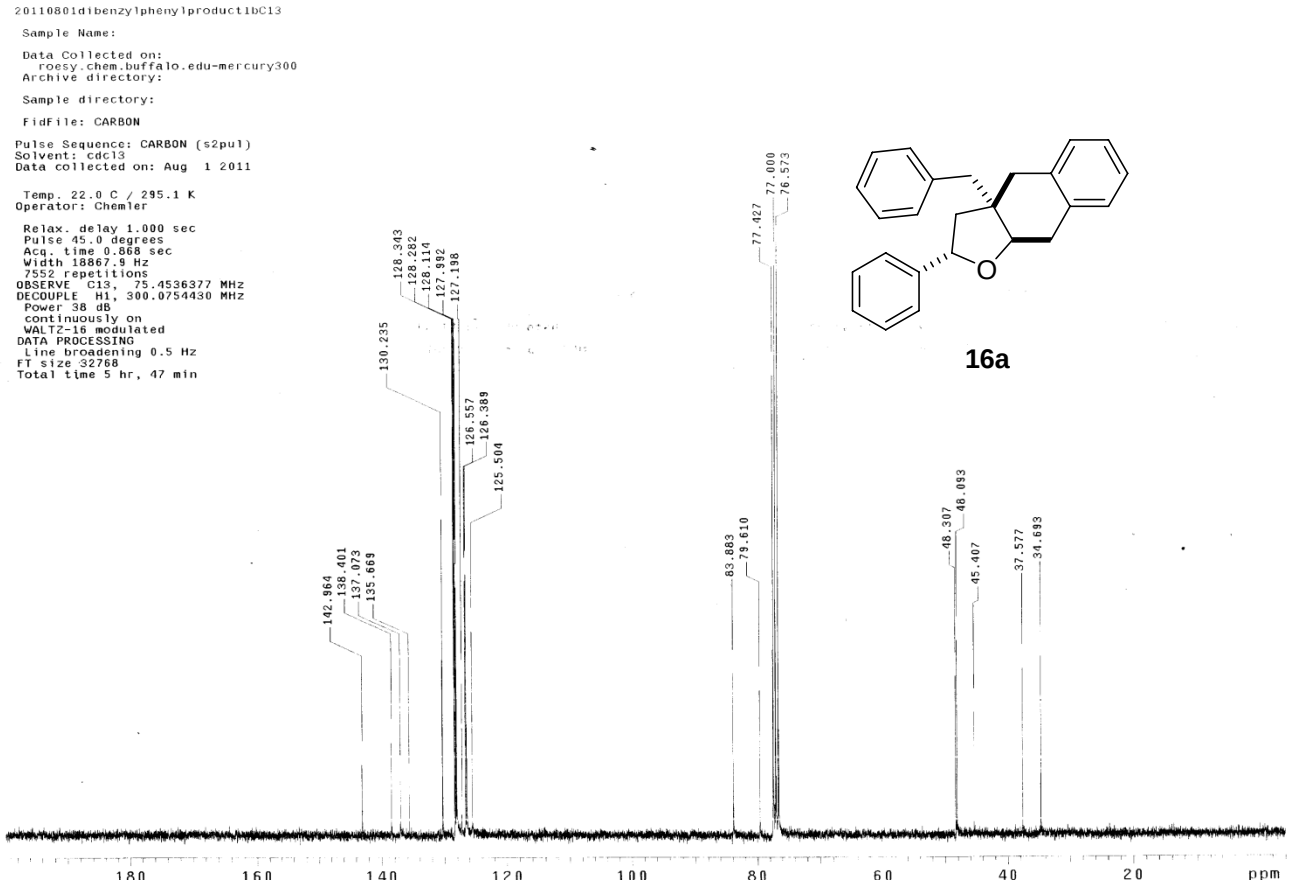


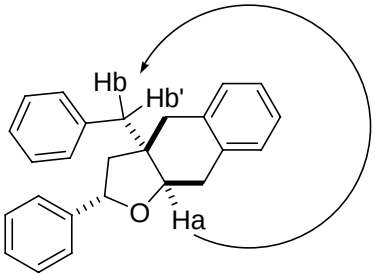
14

```
20110721diphenylproductNOE

 Sample Name:

 Data Collected on:
   chemnmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 FidFile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jul 21 2011

Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 2.730 sec
 Width 3001.2 Hz
 9216 repetitions
OBSERVE    H1, 499.8983908 MHz
DATA PROCESSING
FT size 16384
Total time 11 hr, 36 min
```



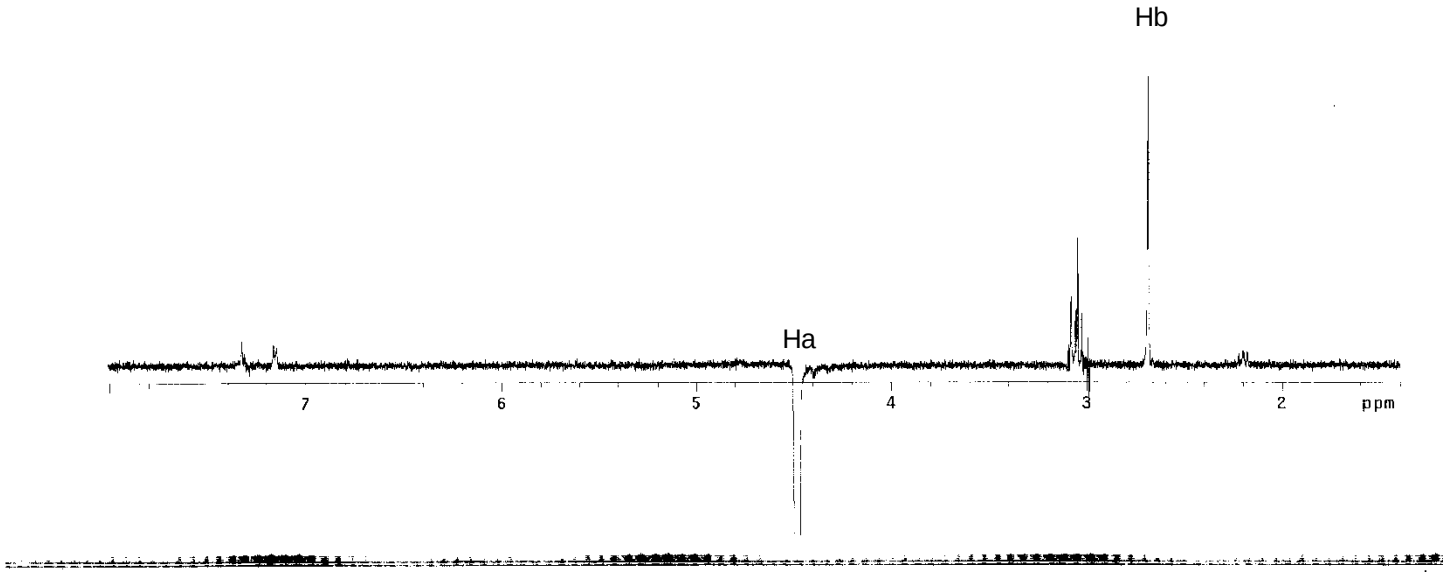

20110801dibenzylphenylproduct1b
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on:
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984092 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 24 sec
16a
ppm
13.80
1.04
1.00
2.14
3.81
1.10
1.09


20110801dibenzylphenylproduct1bC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 1 2011
Temp. 22.0 C / 295.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
7552 repetitions
OBSERVE C13, 75.4536377 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min
16a
ppm



16a

```
20110801dibenzylphenylproduct1bNOE

 Sample Name:

 Data Collected on:
   chemmmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 FidFile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Aug  1 2011

Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 2.479 sec
 Width 3304.7 Hz
 9856 repetitions
OBSERVE    H1, 499.8983908 MHz
DATA PROCESSING
FT size 16384
Total time 12 hr, 7 min
```



20110805dibenzylphenylproduct2b

Sample Name:

Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

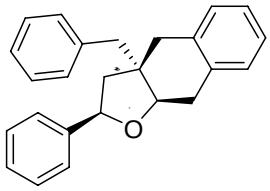
Sample directory:

FidFile: PROTON

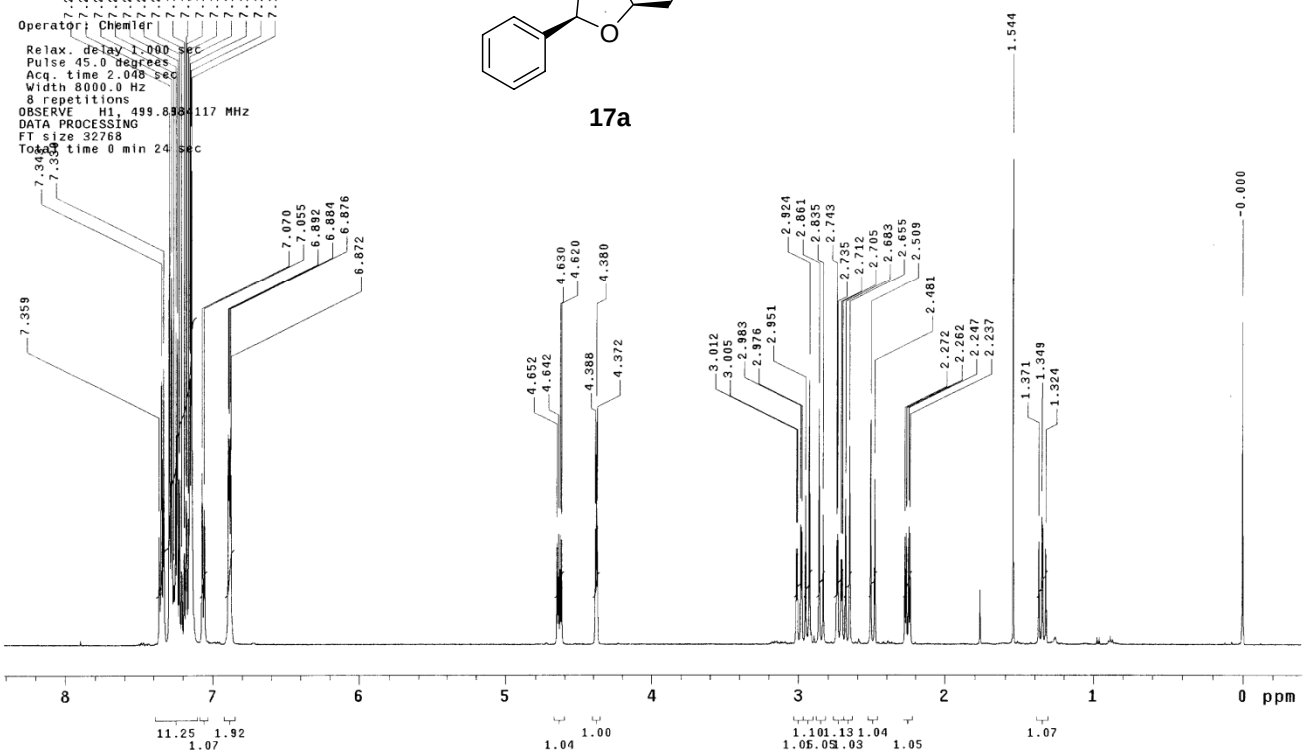
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 5 2011

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8384117 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



17a



20110805dibenzylphenylproduct2bC13

Sample Name:

Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

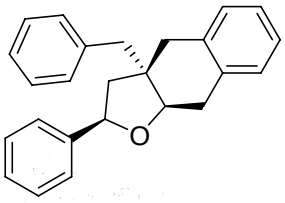
Sample directory:

FidFile: CARBON

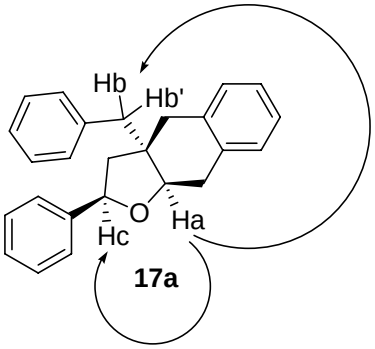
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 5 2011

Temp. 22.0 C / 295.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
7456 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min

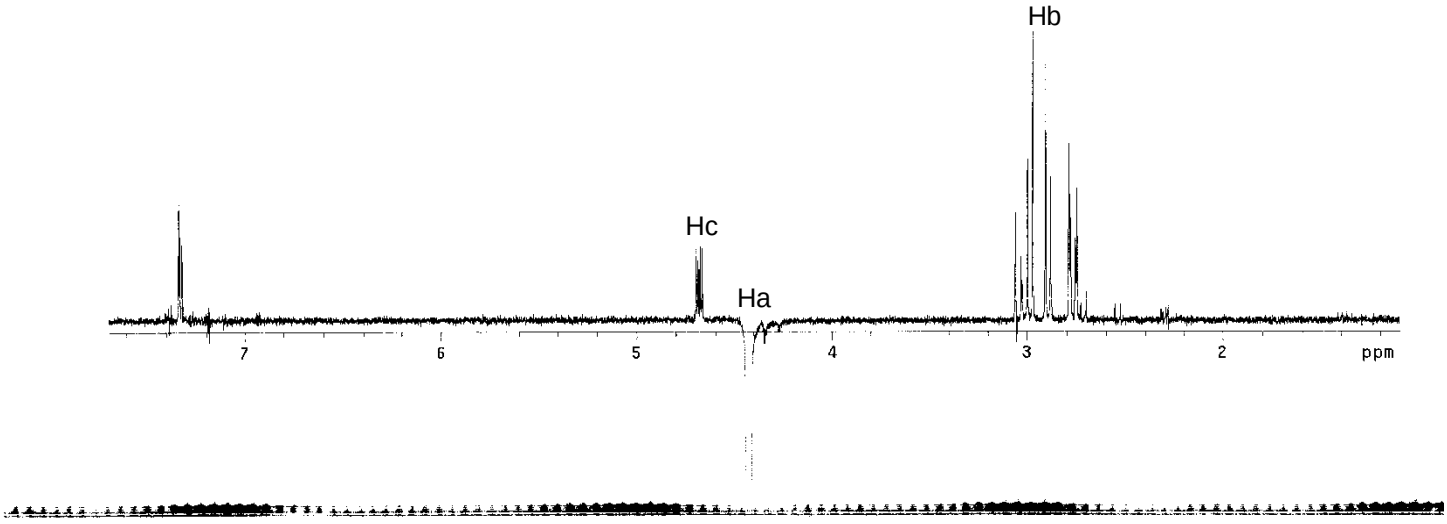


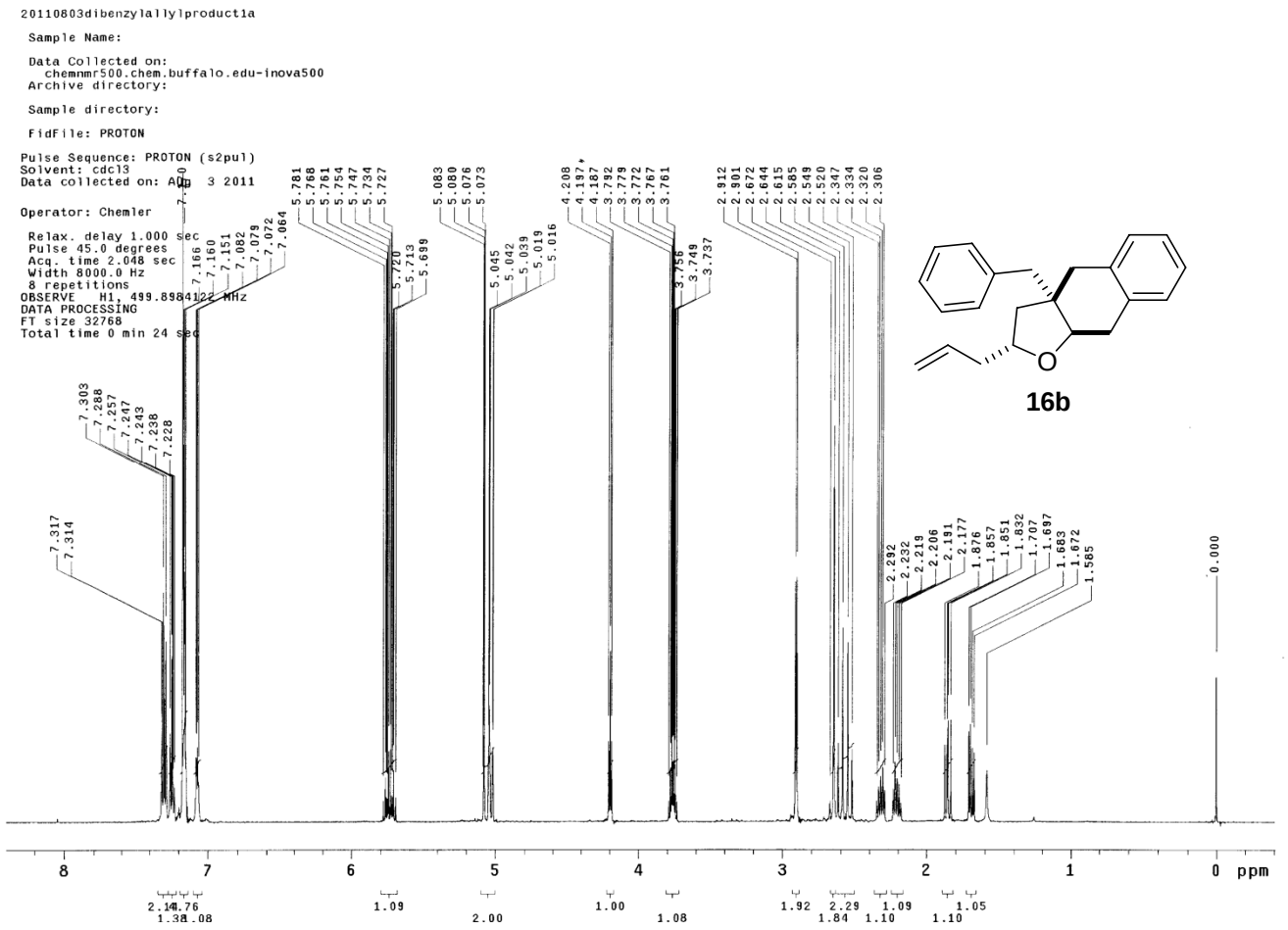
17a

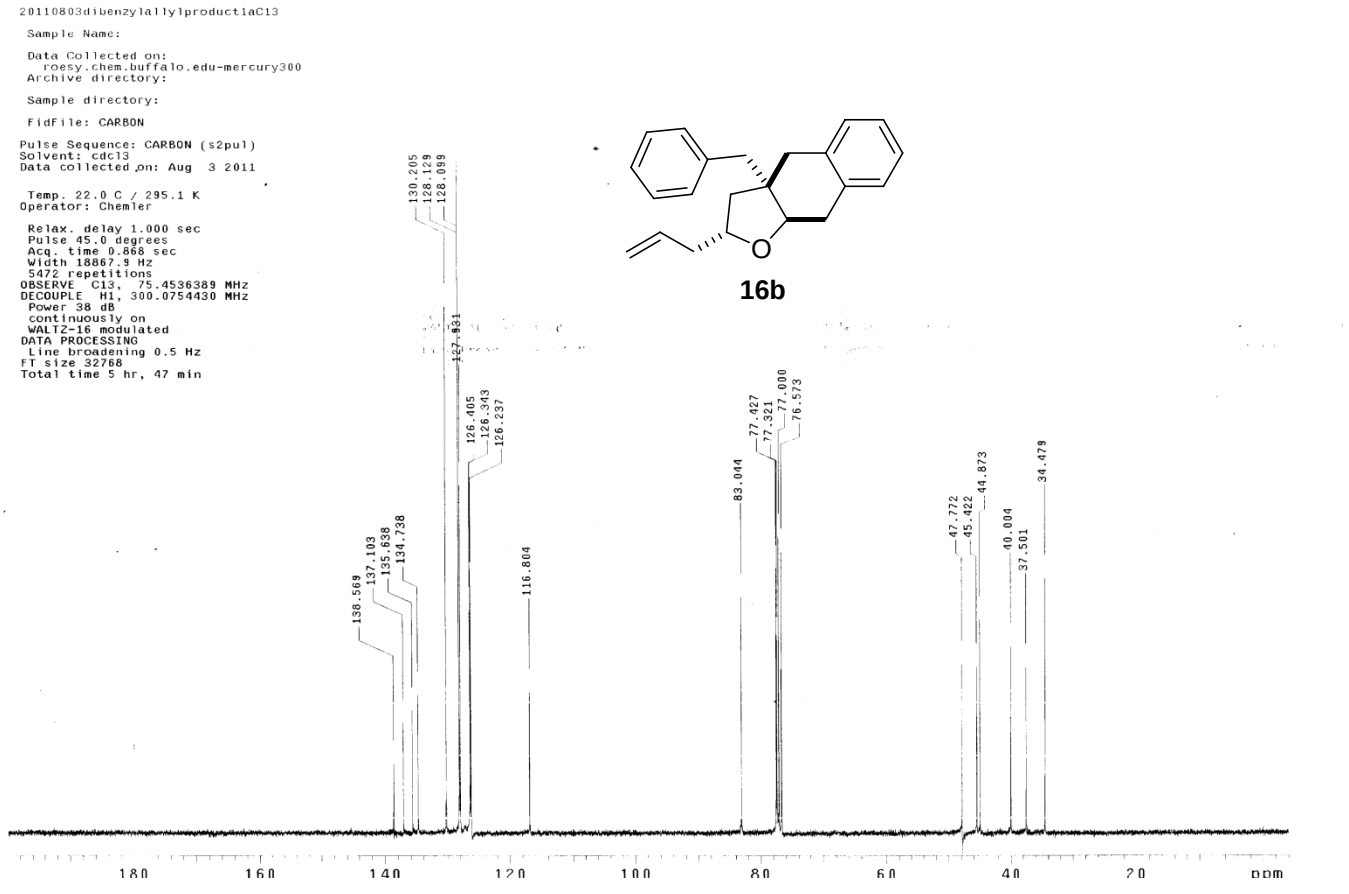


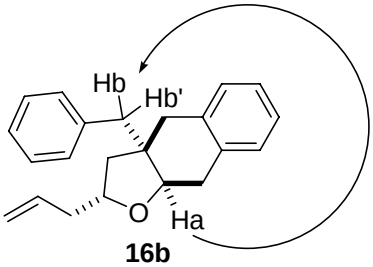
17a

```
20110802dibenzylphenylproduct2NOE

 Sample Name:

 Data Collected on:
   chemnmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 FidFile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Aug  2 2011

Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 2.486 sec
 Width 3295.4 Hz
 8960 repetitions
OBSERVE   H1, 499.8983908 MHz
DATA PROCESSING
FT size 16384
Total time 10 hr, 58 min
```



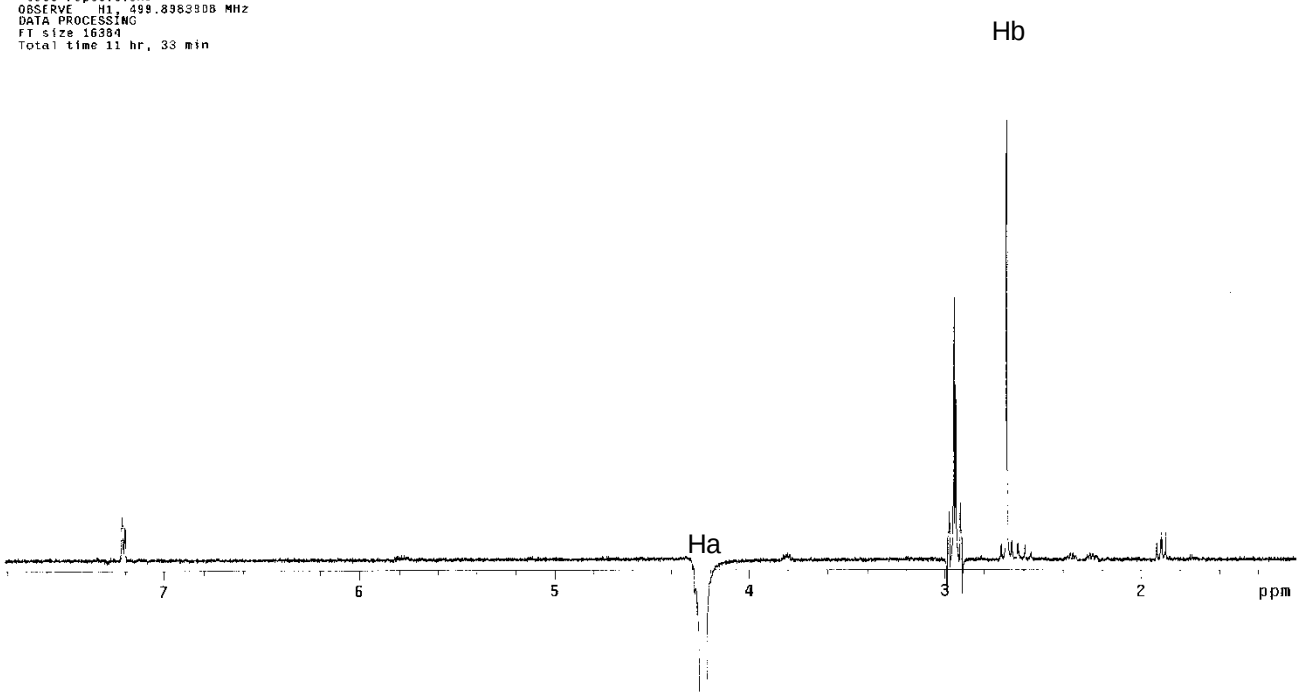

20110803dibenzylallylproduct1a
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 3 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984122 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
16b
ppm

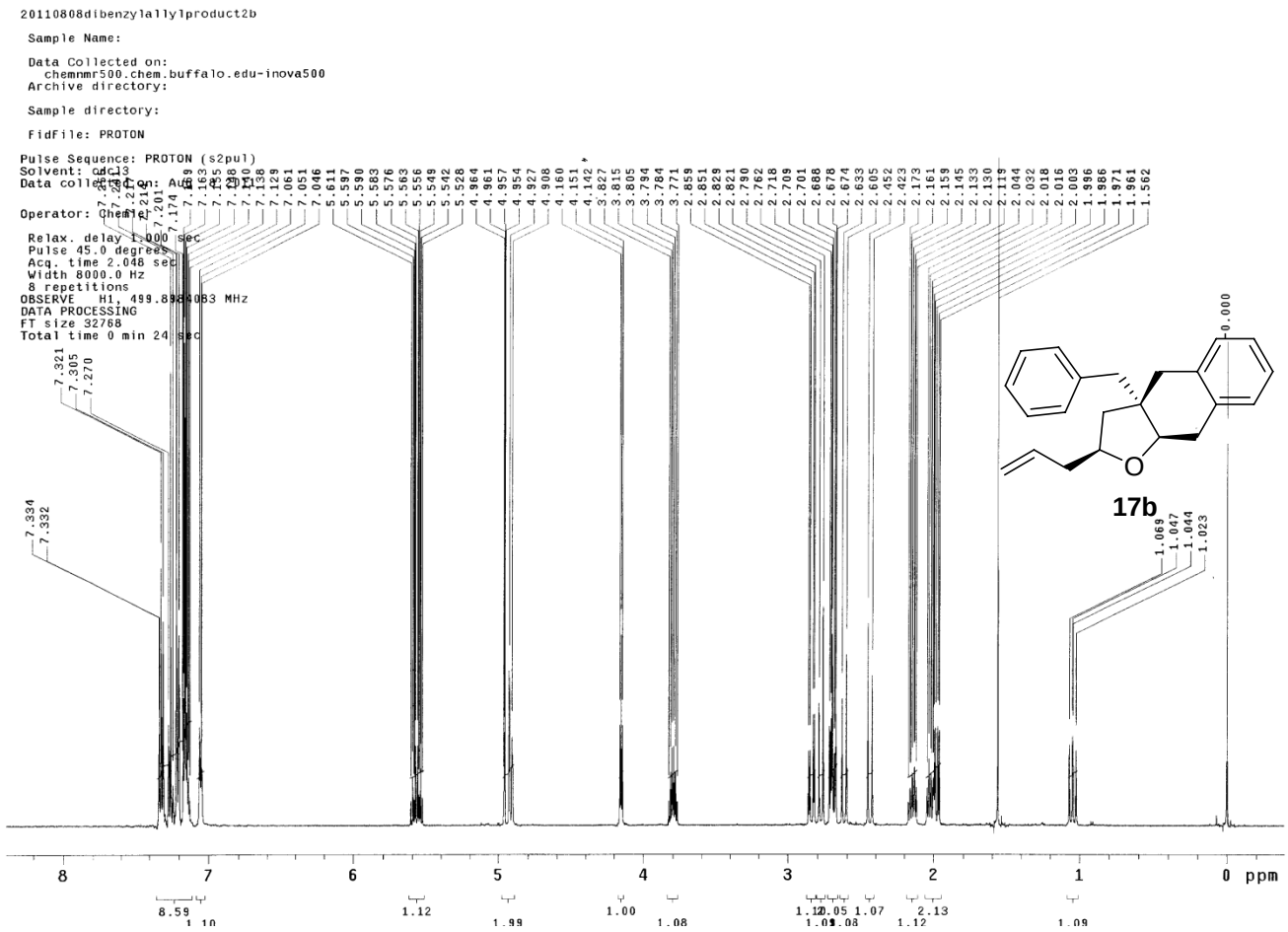

20110803dibenzylallylproduct1aC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 3 2011
Temp. 22.0 C / 295.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
5472 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min
16b
ppm

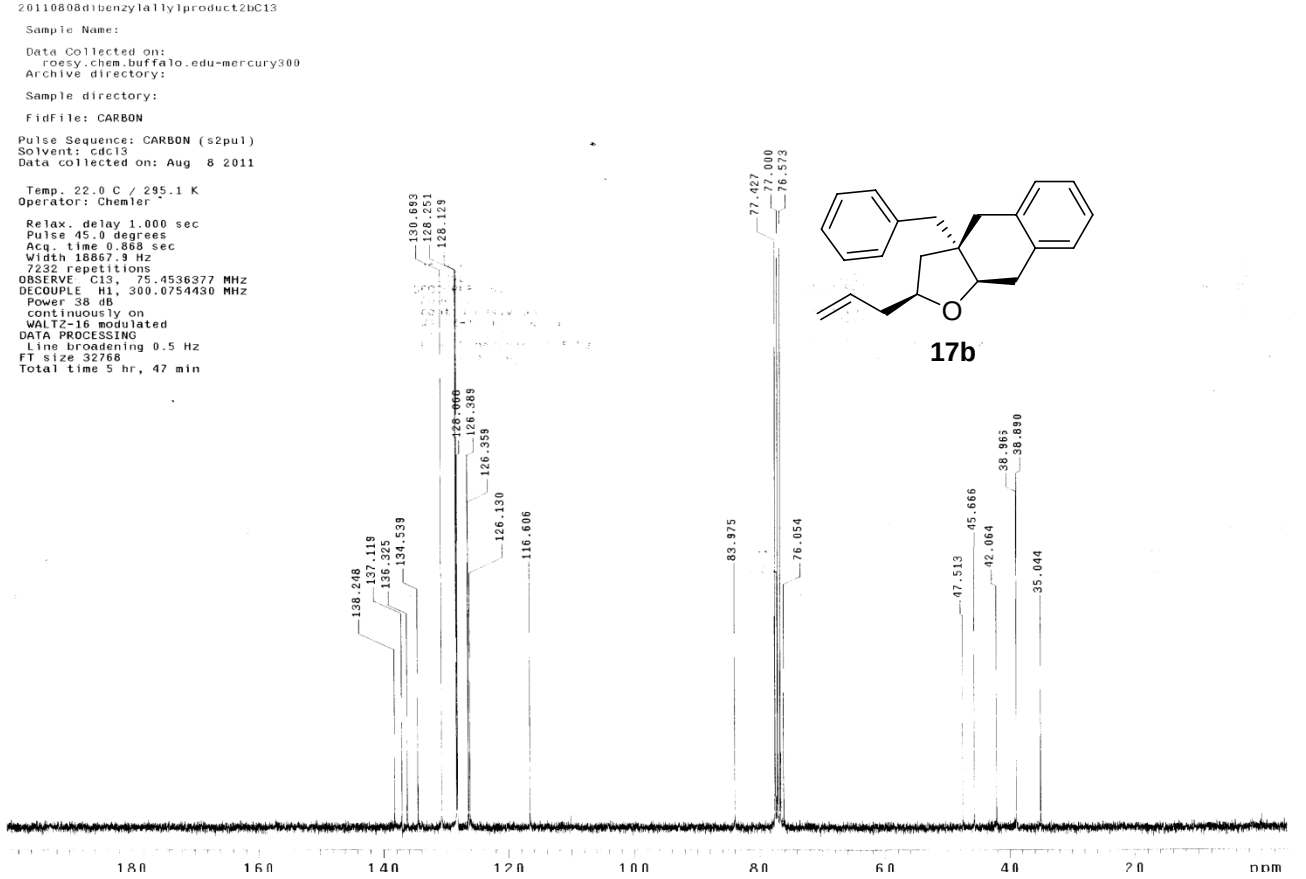


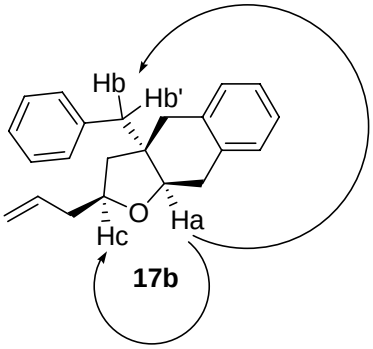
16b

```
20110803dibenzylallylproductlaNOE

 Sample Name:

 Data Collected on:
   chemnmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 FidFile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Aug  3 2011

Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 2.479 sec
 Width 3304.7 Hz
 9600 repetitions
OBSERVE   H1, 499.8883908 MHz
DATA PROCESSING
FT size 16384
Total time 11 hr, 33 min
```



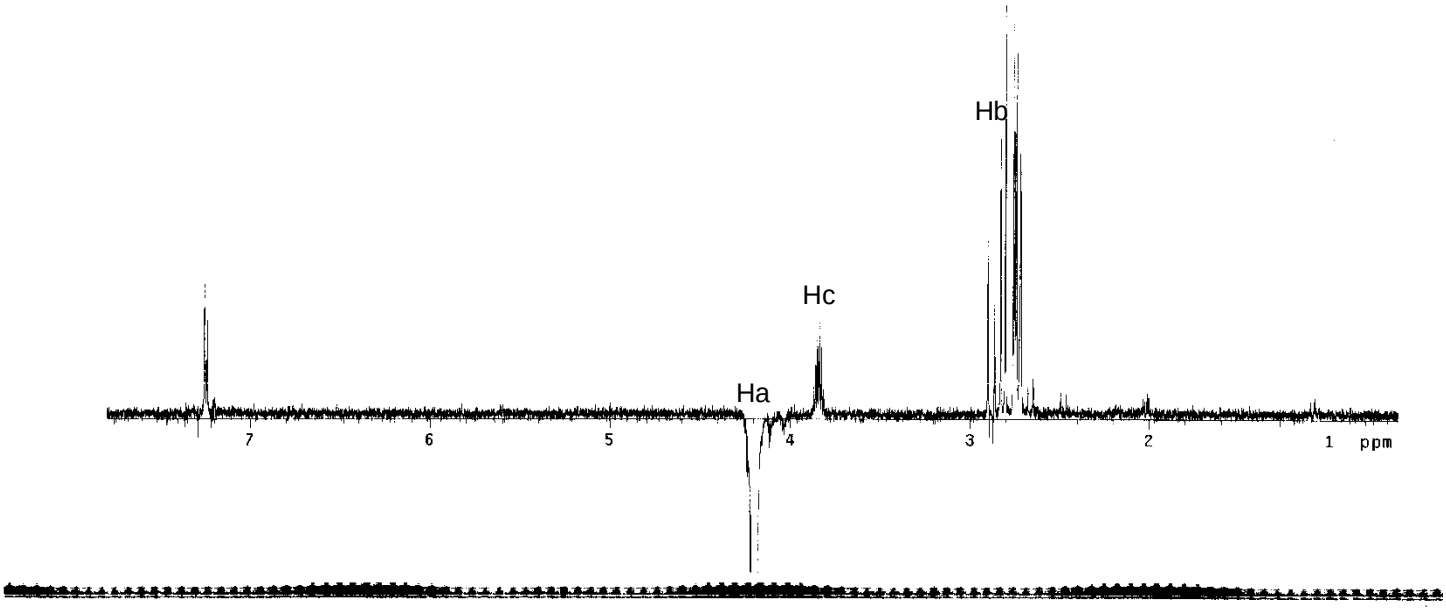

20110808dibenzylallylproduct2b
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 8 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984083 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
17b
8.59
1.10
1.12
1.99
1.00
1.08
1.12
1.05
1.08
1.07
2.13
1.12
1.09
ppm

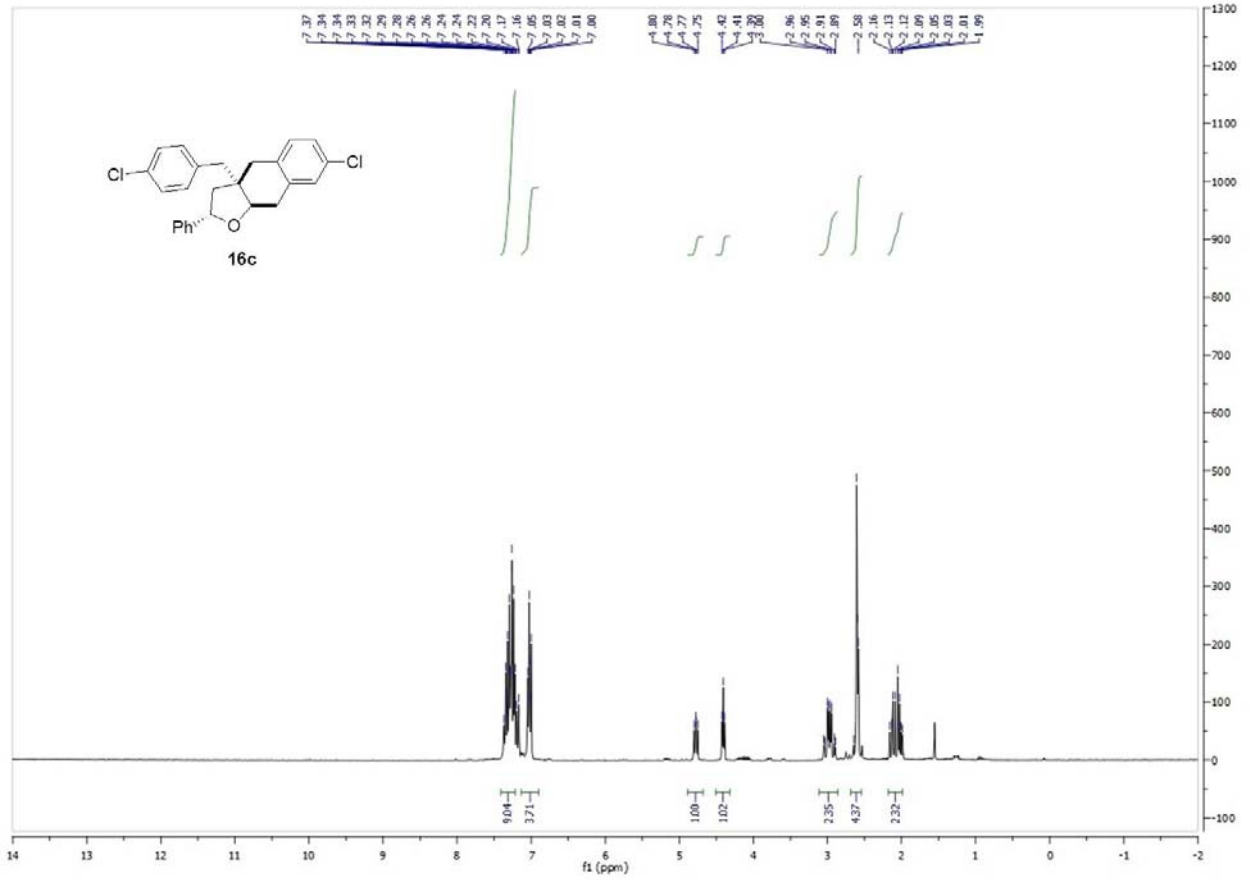

20110808dibenzylallylproduct2bC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 8 2011
Temp. 22.0 C / 295.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
7232 repetitions
OBSERVE C13, 75.4536377 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 47 min
17b
ppm

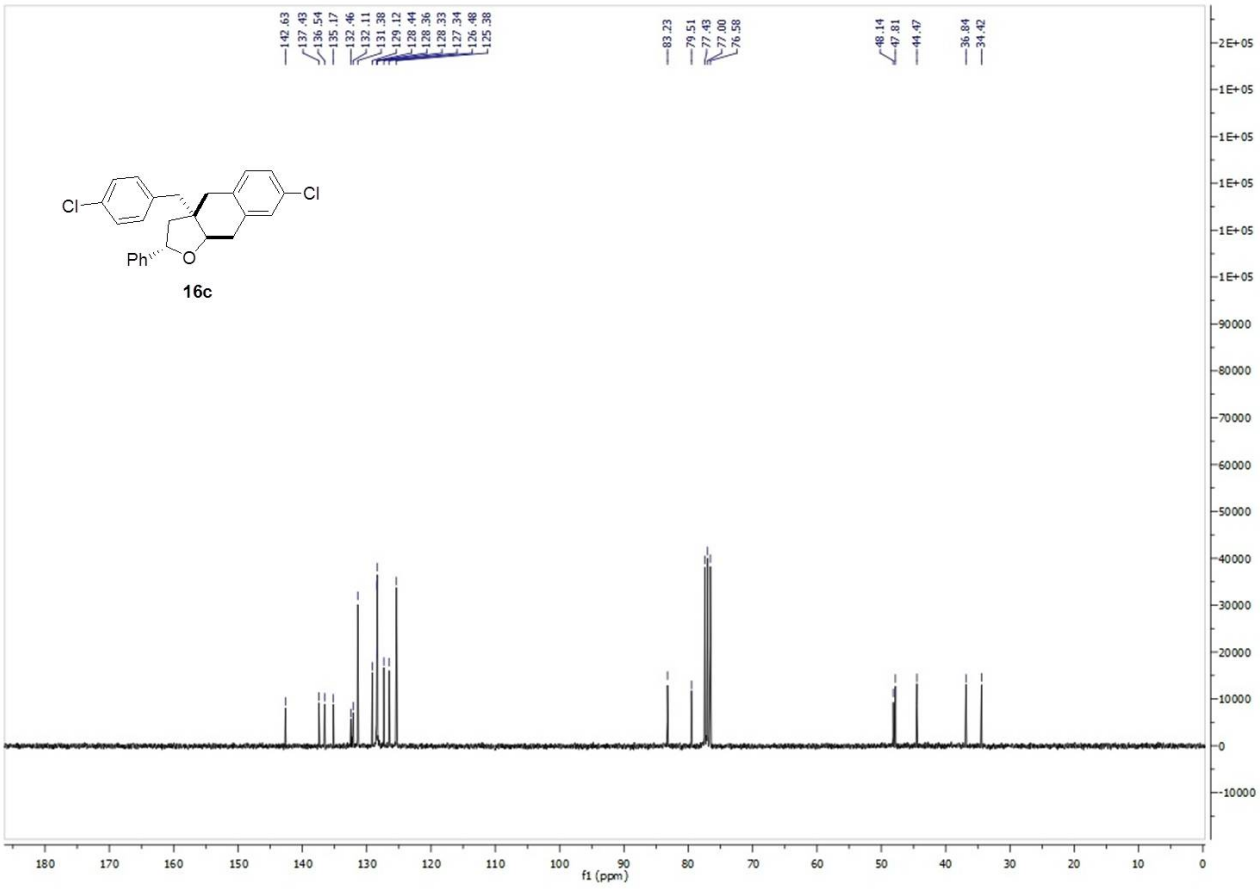


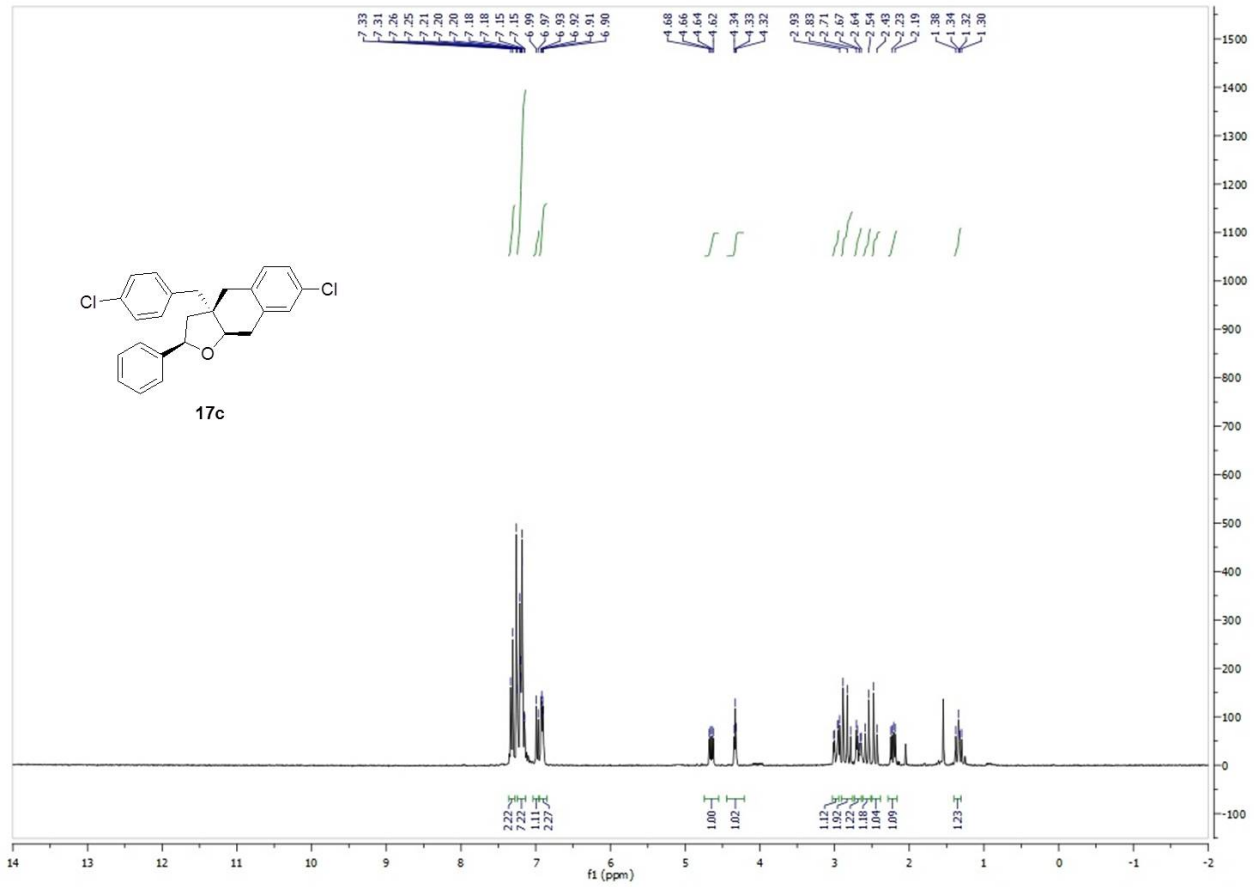
17b

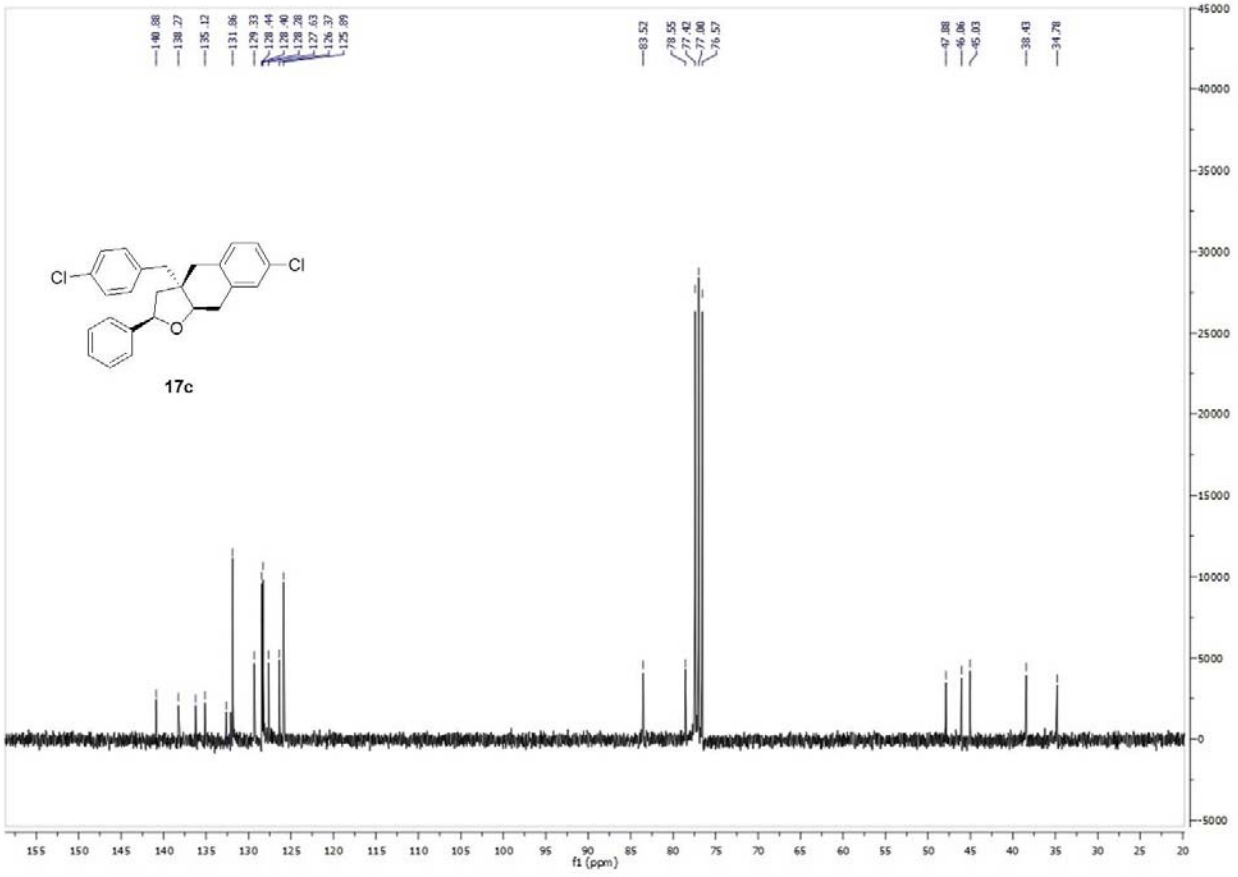
```
20110804dibenzylallylproduct2bNOE

 Sample Name:

 Data Collected on:
   chemmmr500.chem.buffalo.edu-inova500
 Archive directory:

 Sample directory:

 FidFile: NOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Aug  4 2011

Operator: Chemler

 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 2.284 sec
 Width 3586.8 Hz
 9088 repetitions
OBSERVE   H1, 499.8983908 MHz
DATA PROCESSING
FT size 16384
Total time 10 hr, 23 min
```

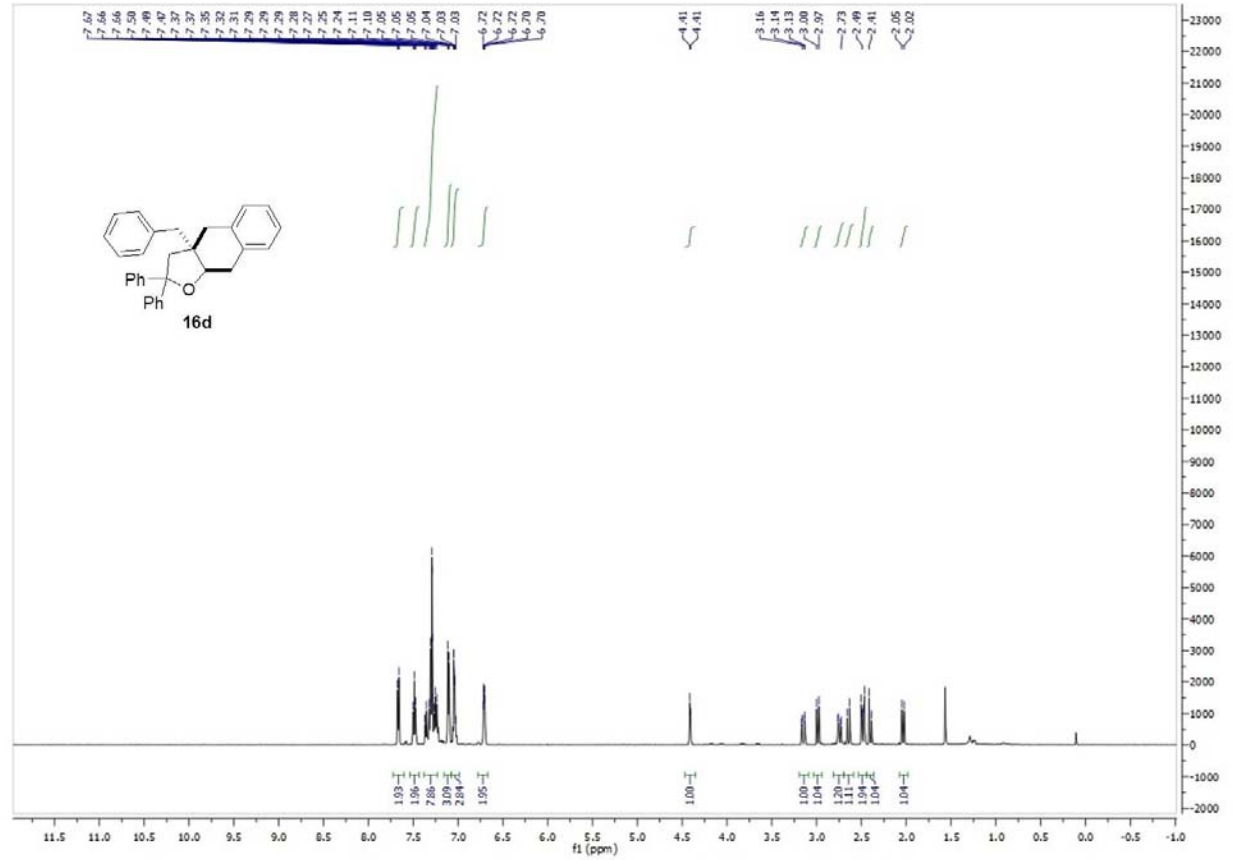


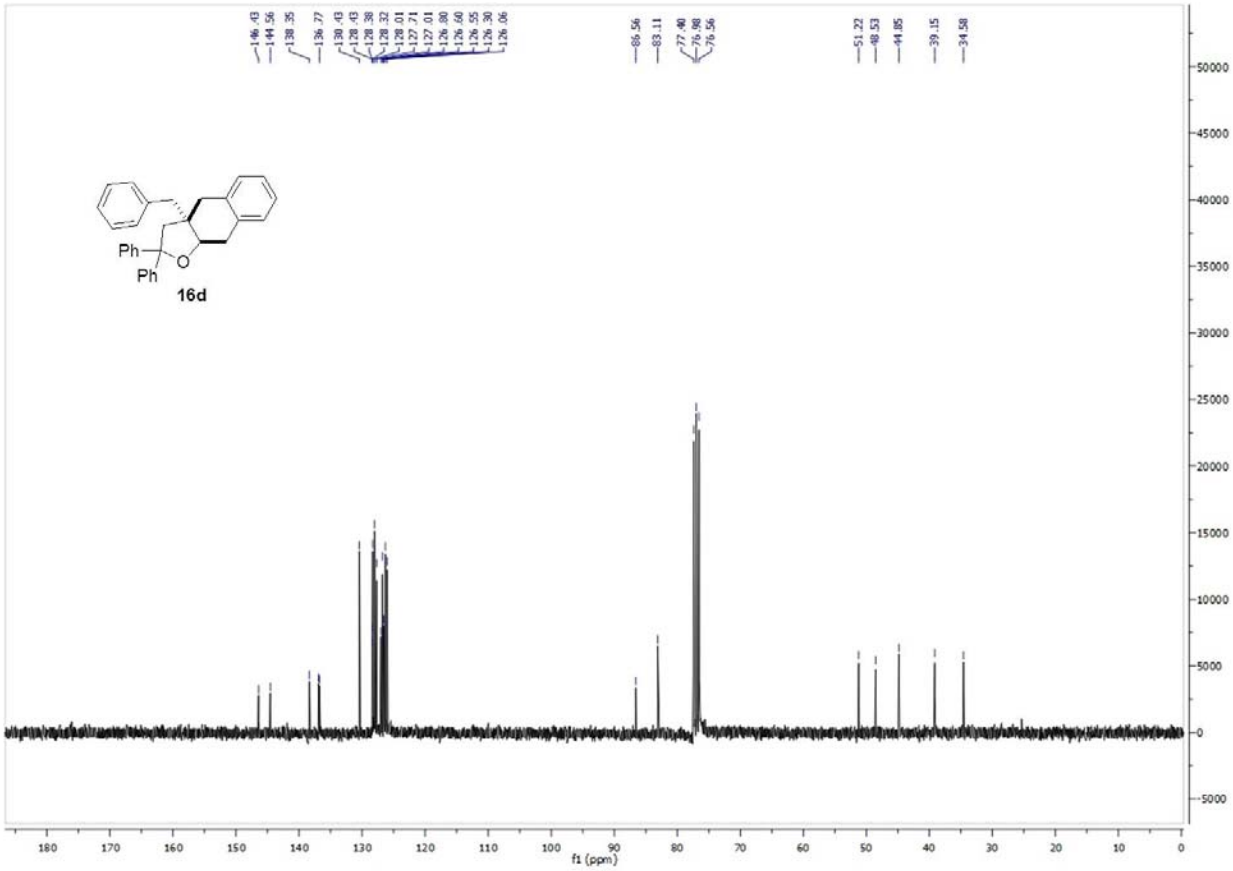

Cl
Cl
Ph
O
16c
f1 (ppm)

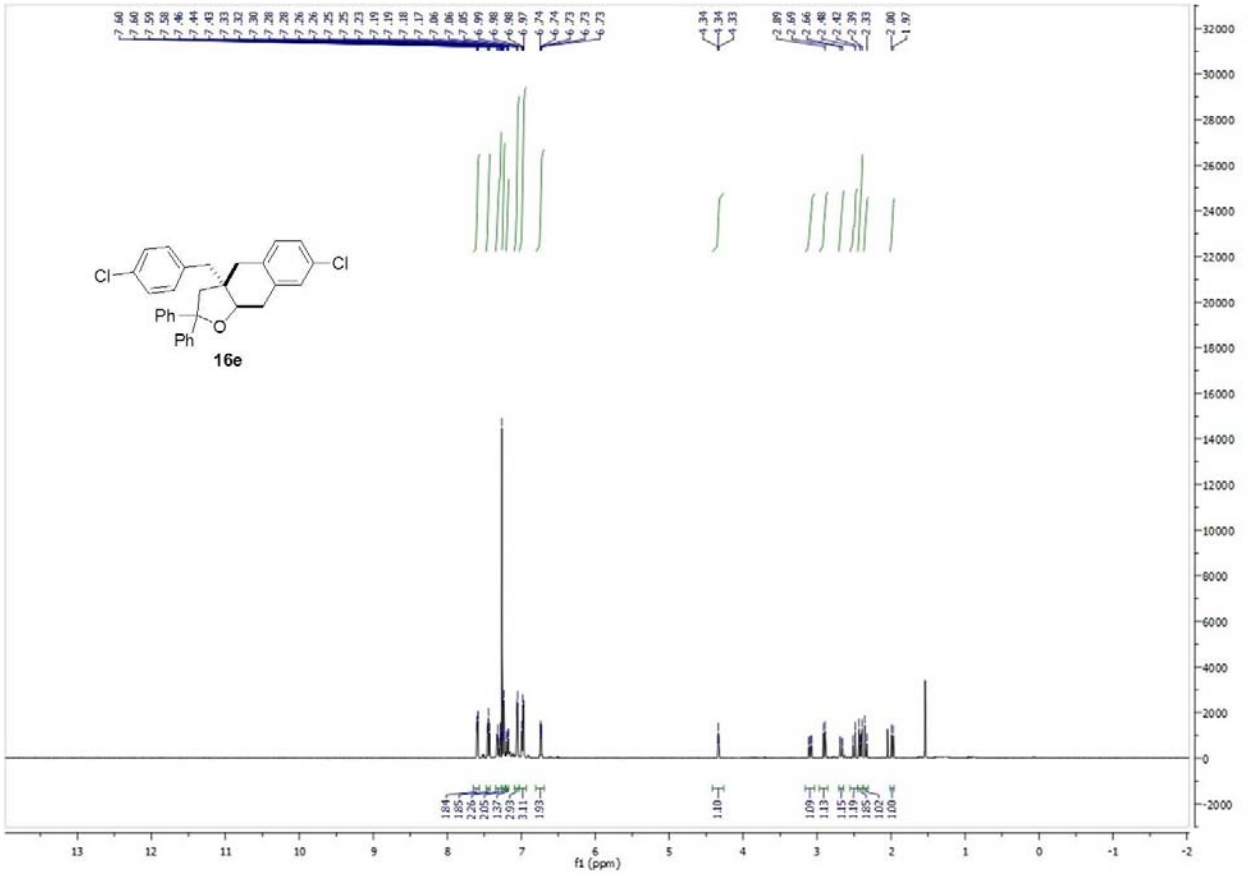

Cl
Cl
Ph
O
16c
f1 (ppm)

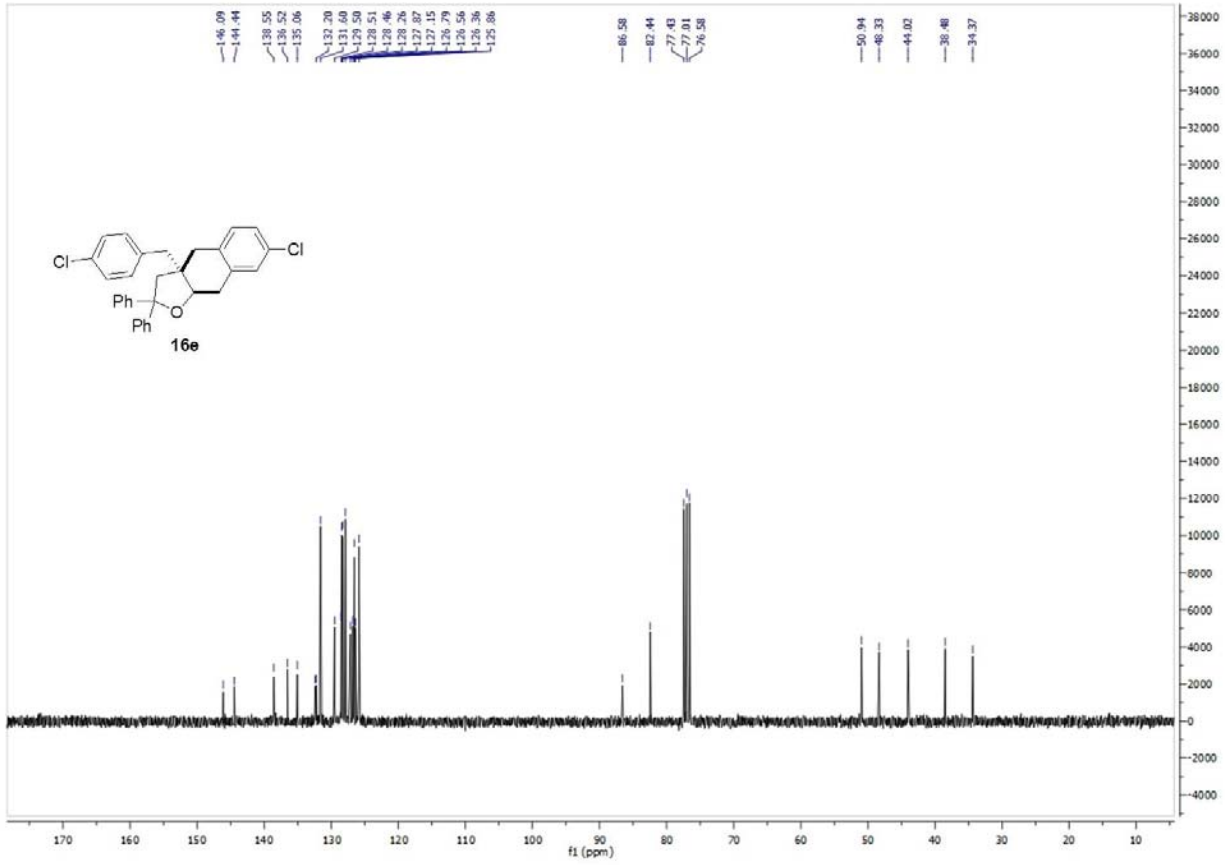

Cl
Cl
O
17c
f1 (ppm)

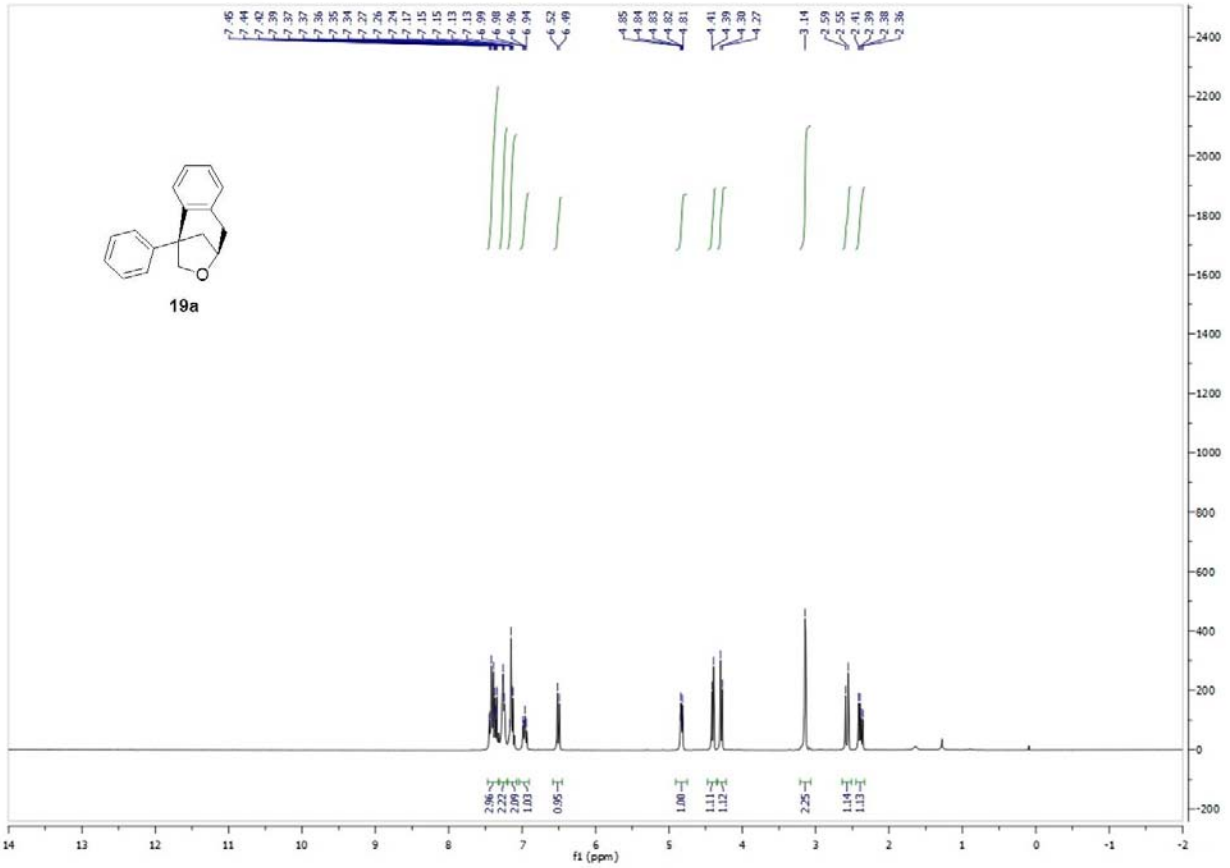

Cl
Cl
O
17c
f1 (ppm)

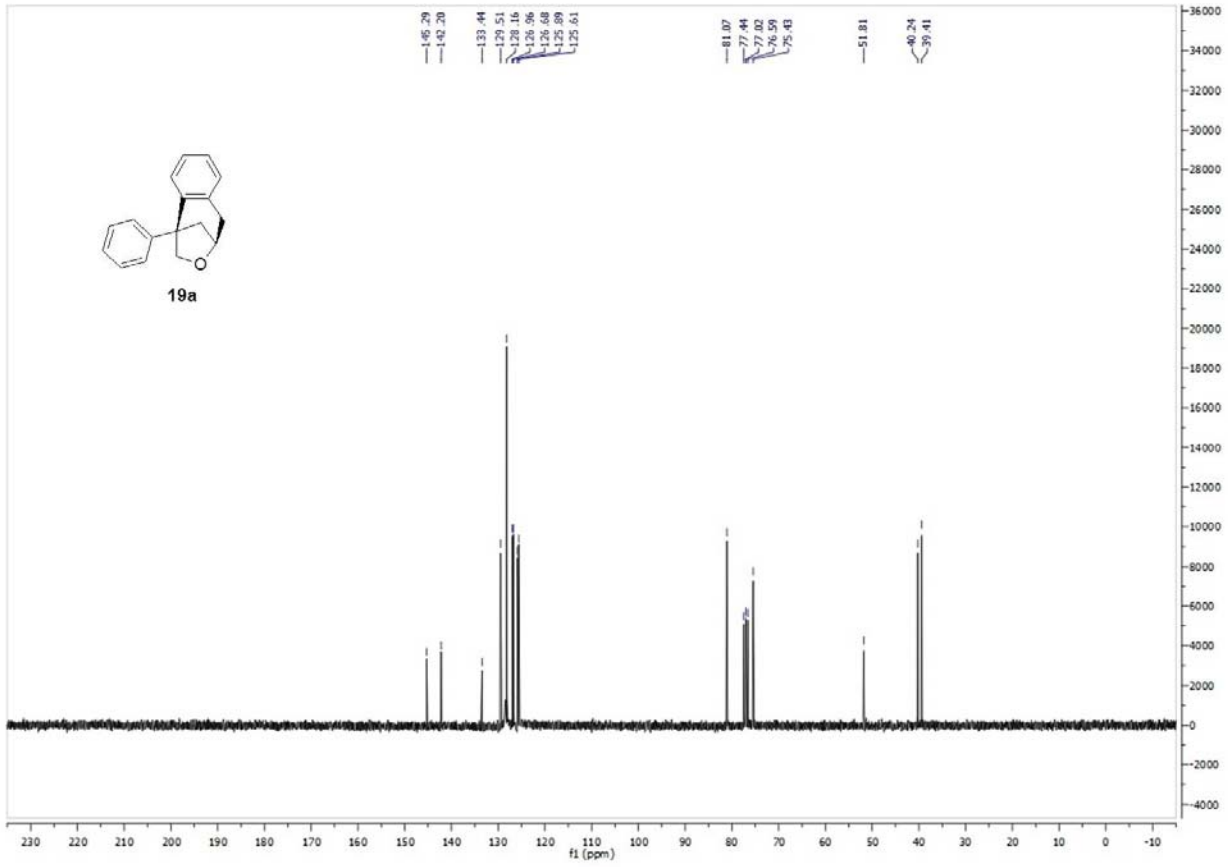

Ph
Ph
O
16d
f1 (ppm)

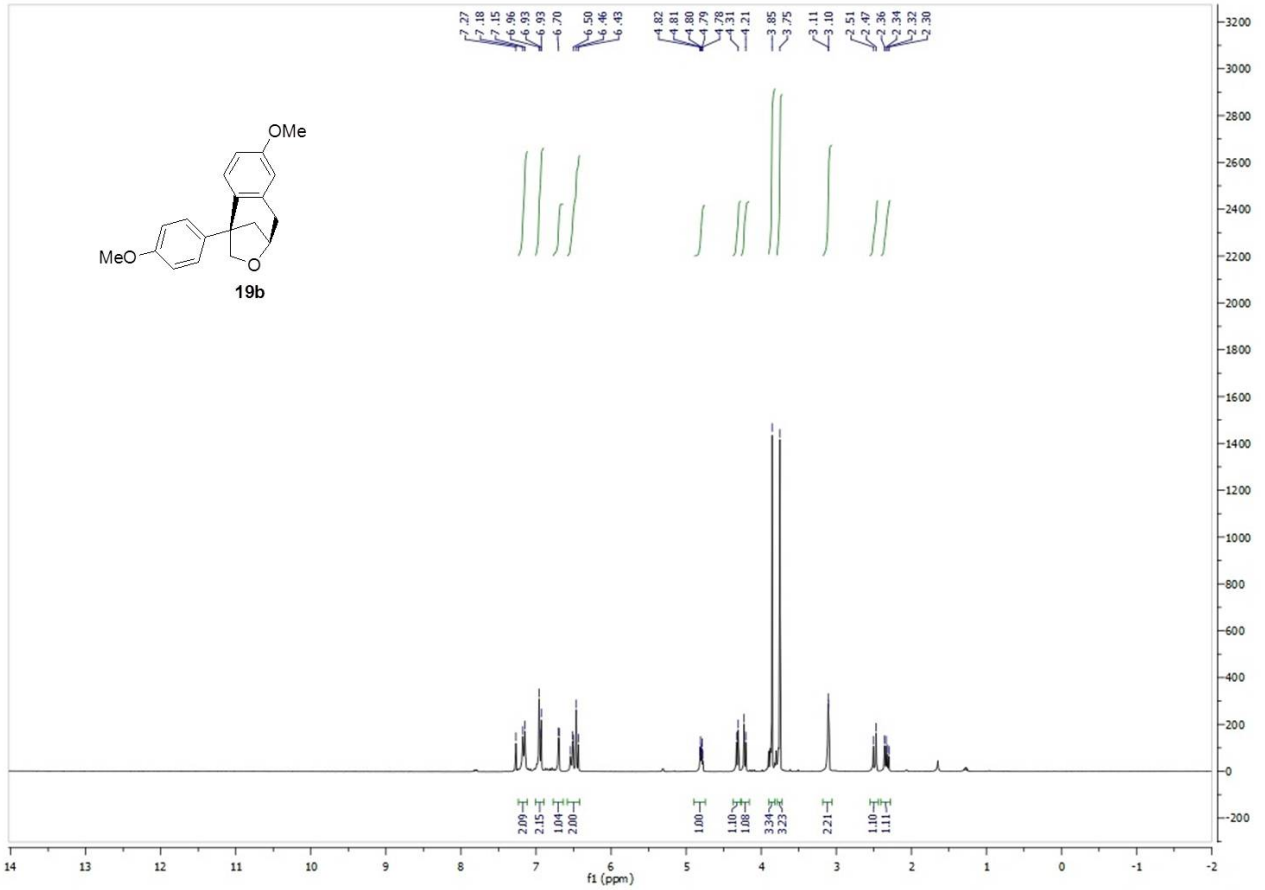

Ph
Ph
O
16d
f1 (ppm)

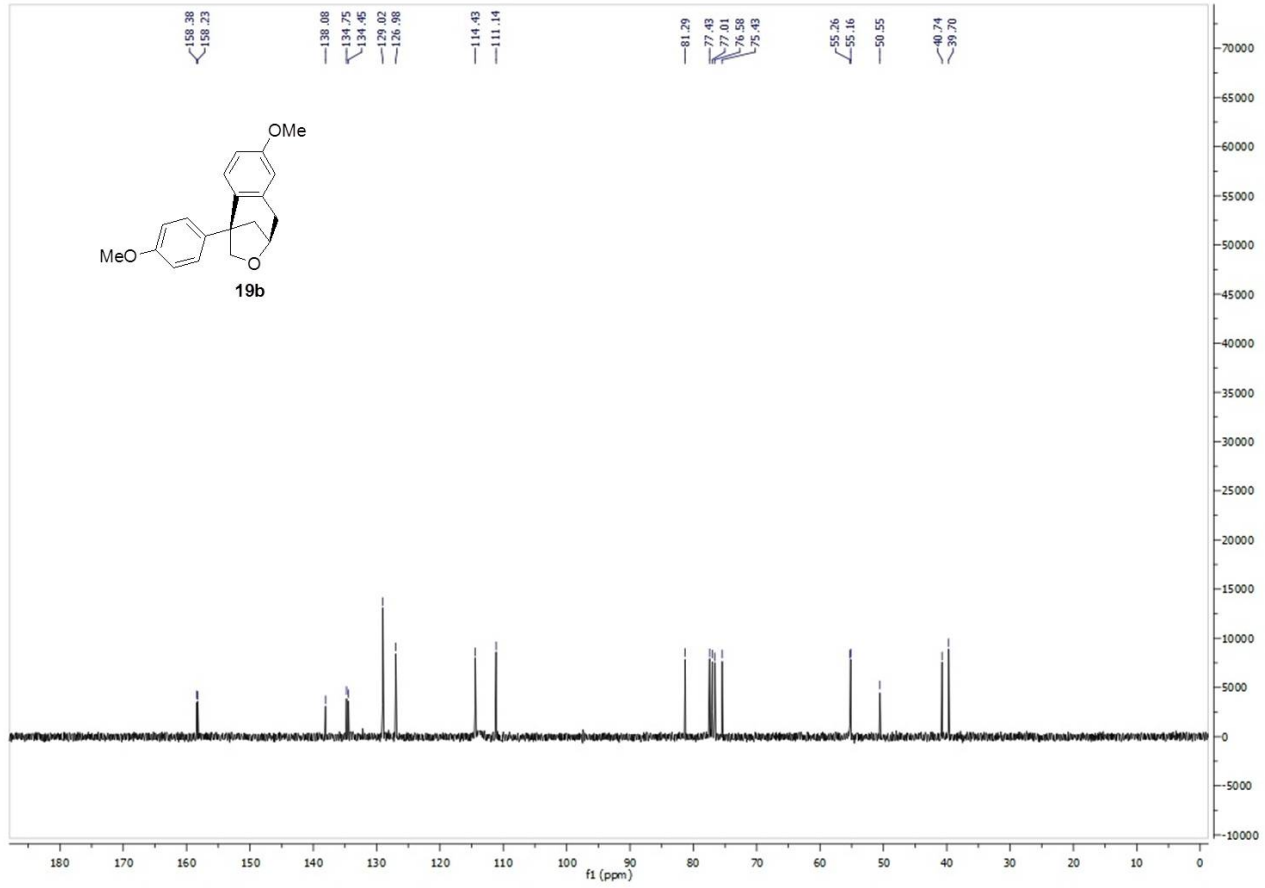

Cl
Cl
Ph
Ph
O
16e
f1 (ppm)

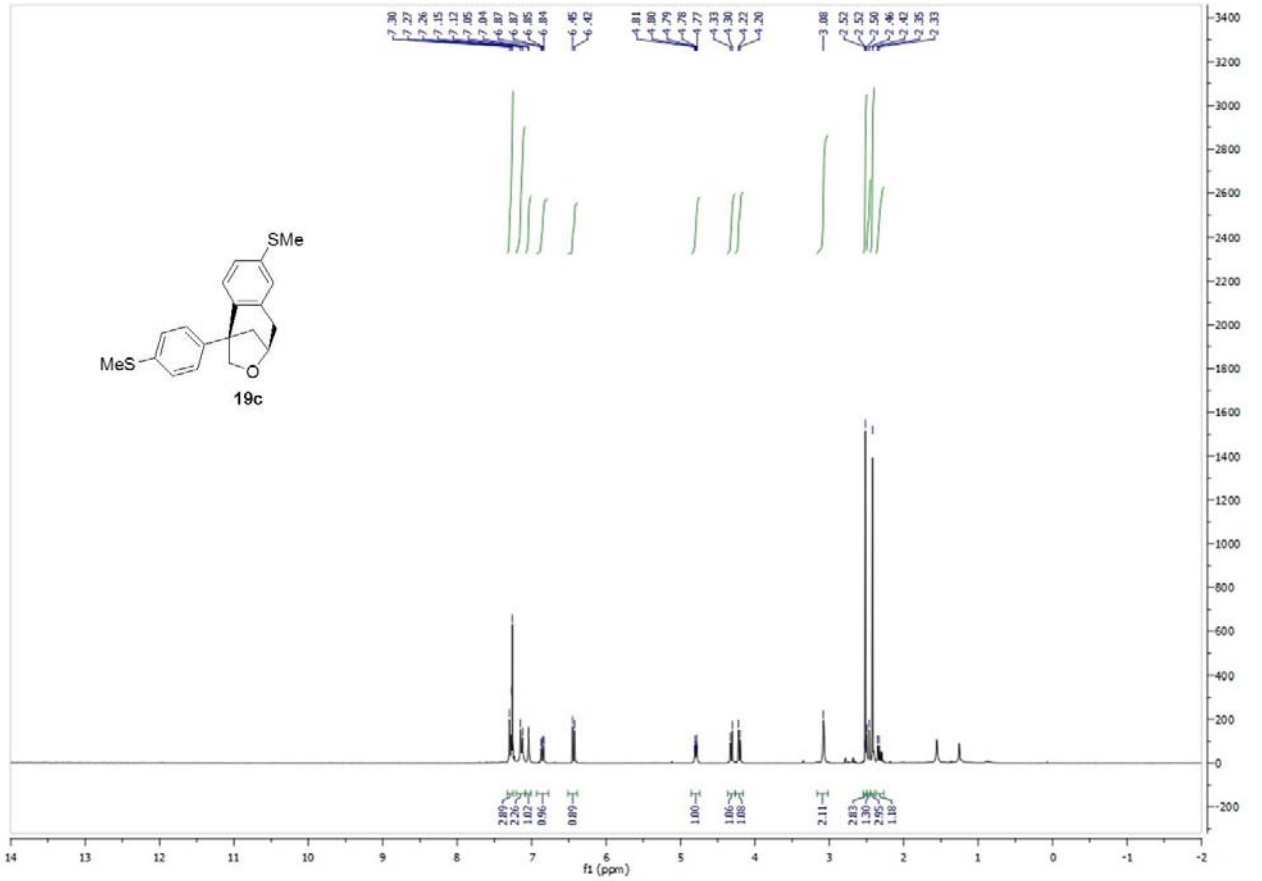

Cl
Cl
Ph
Ph
O
16e
f1 (ppm)

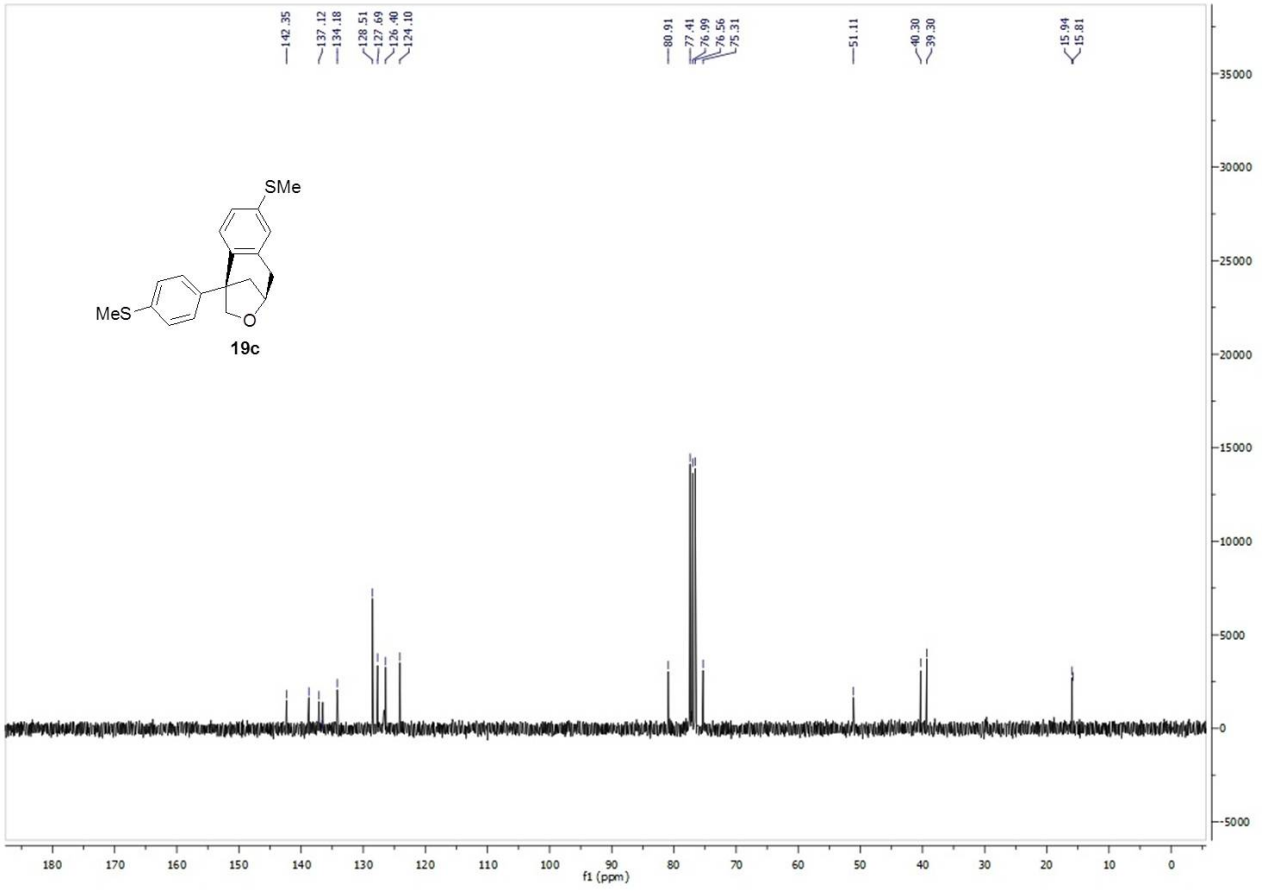

19a
f1 (ppm)

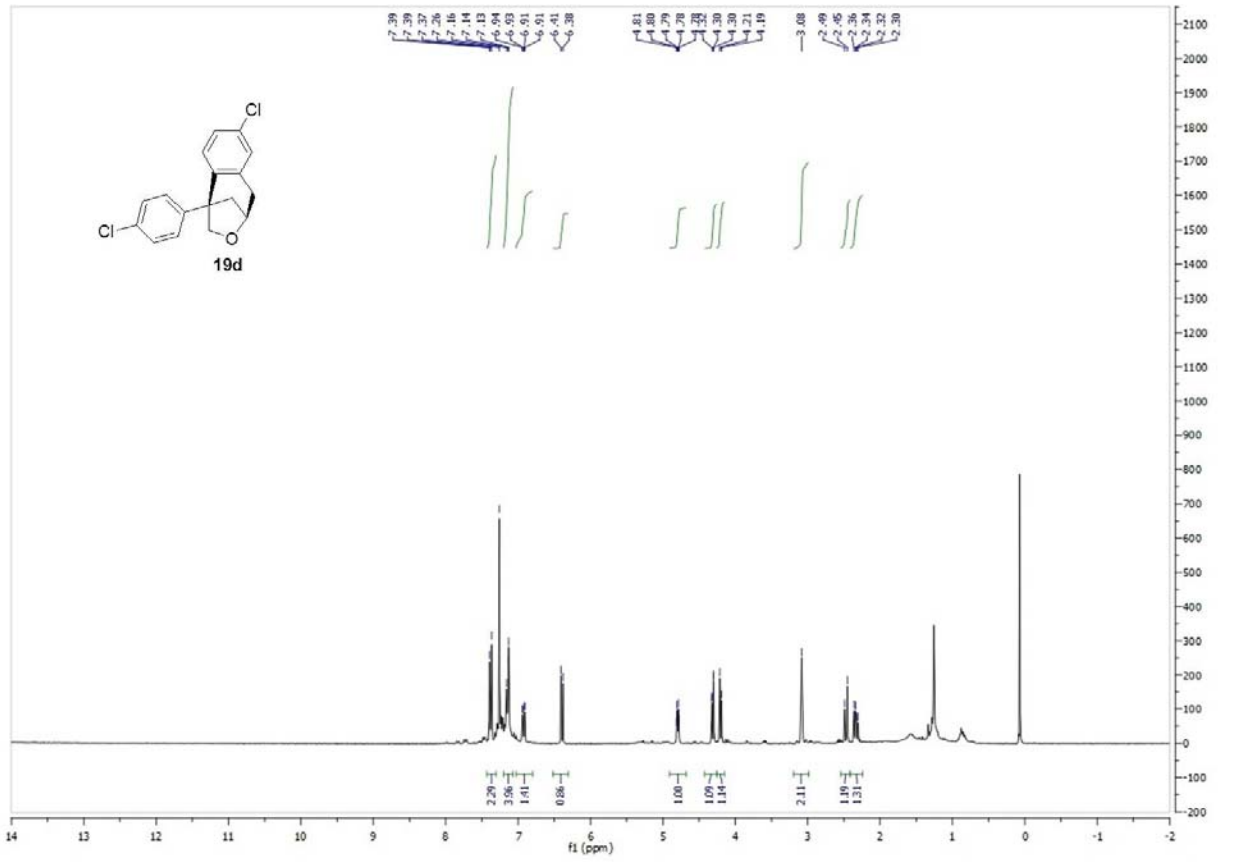

19a
f1 (ppm)

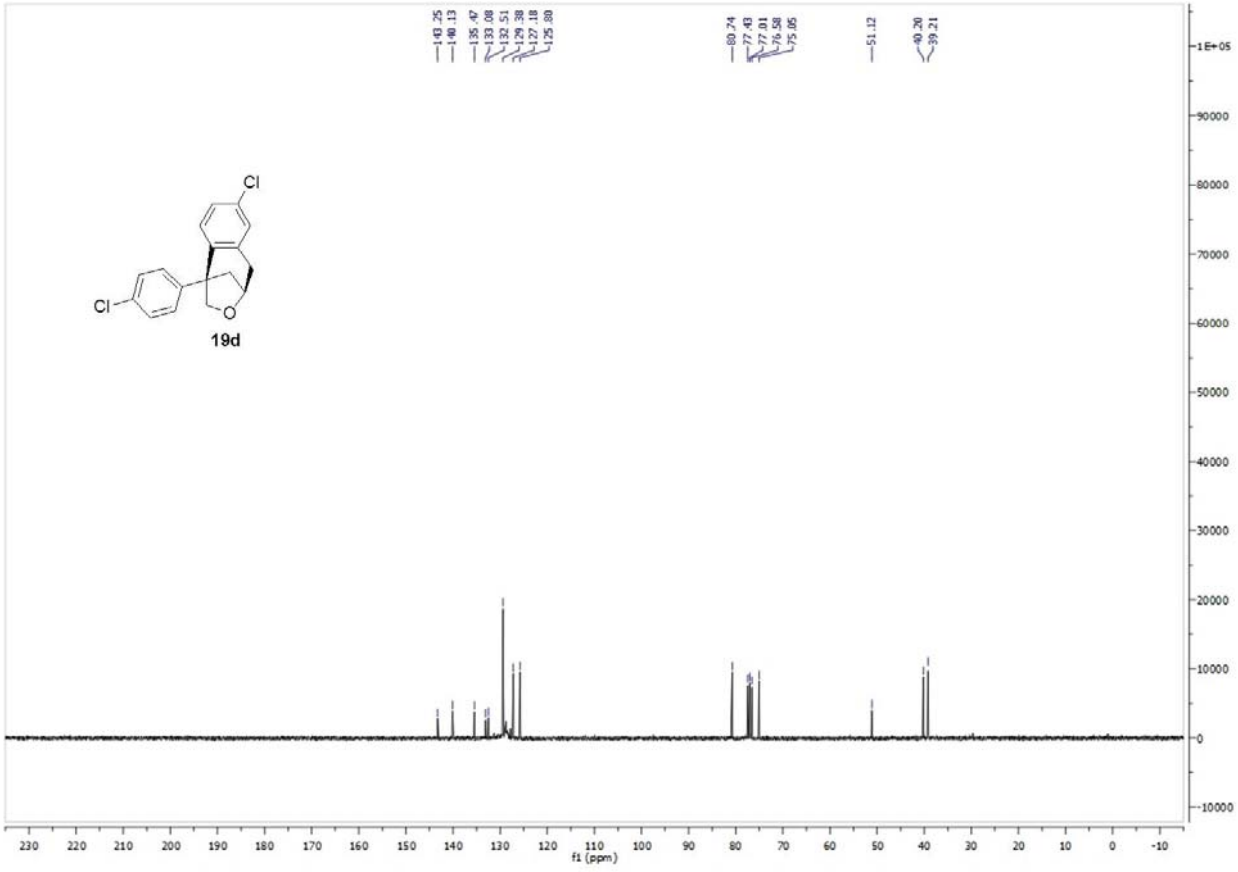

OMe
MeO
O
19b
f1 (ppm)

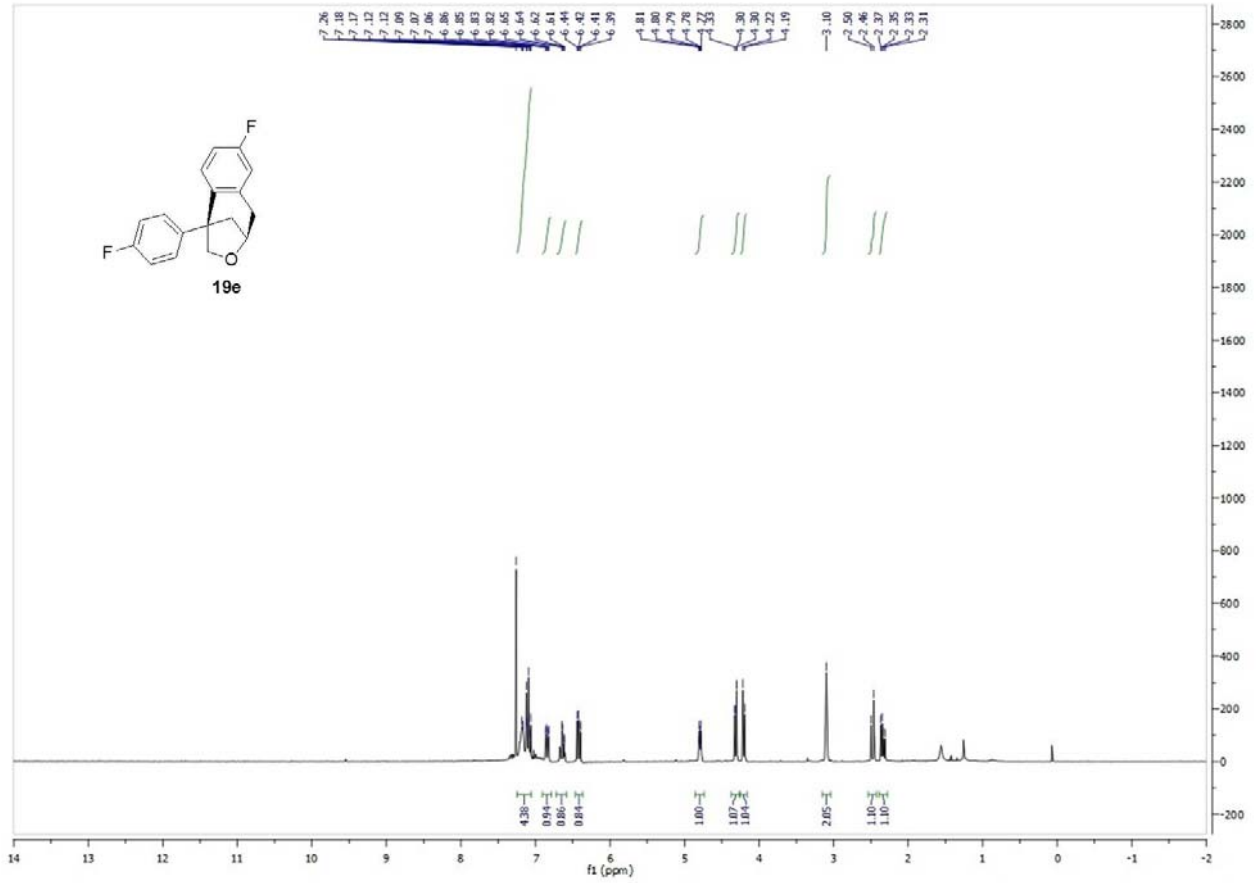

OMe
MeO
O
19b
f1 (ppm)

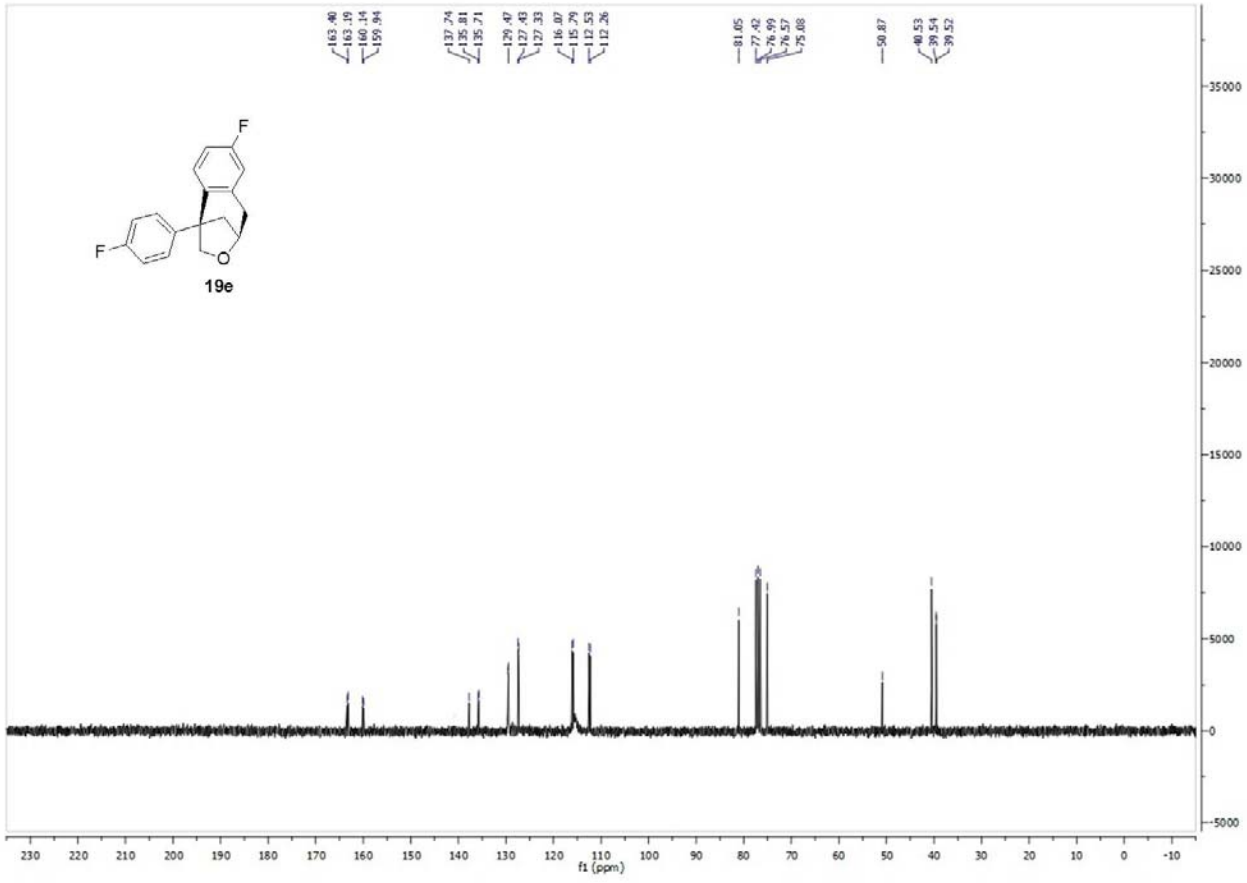

SMe
MeS
O
19c
f1 (ppm)

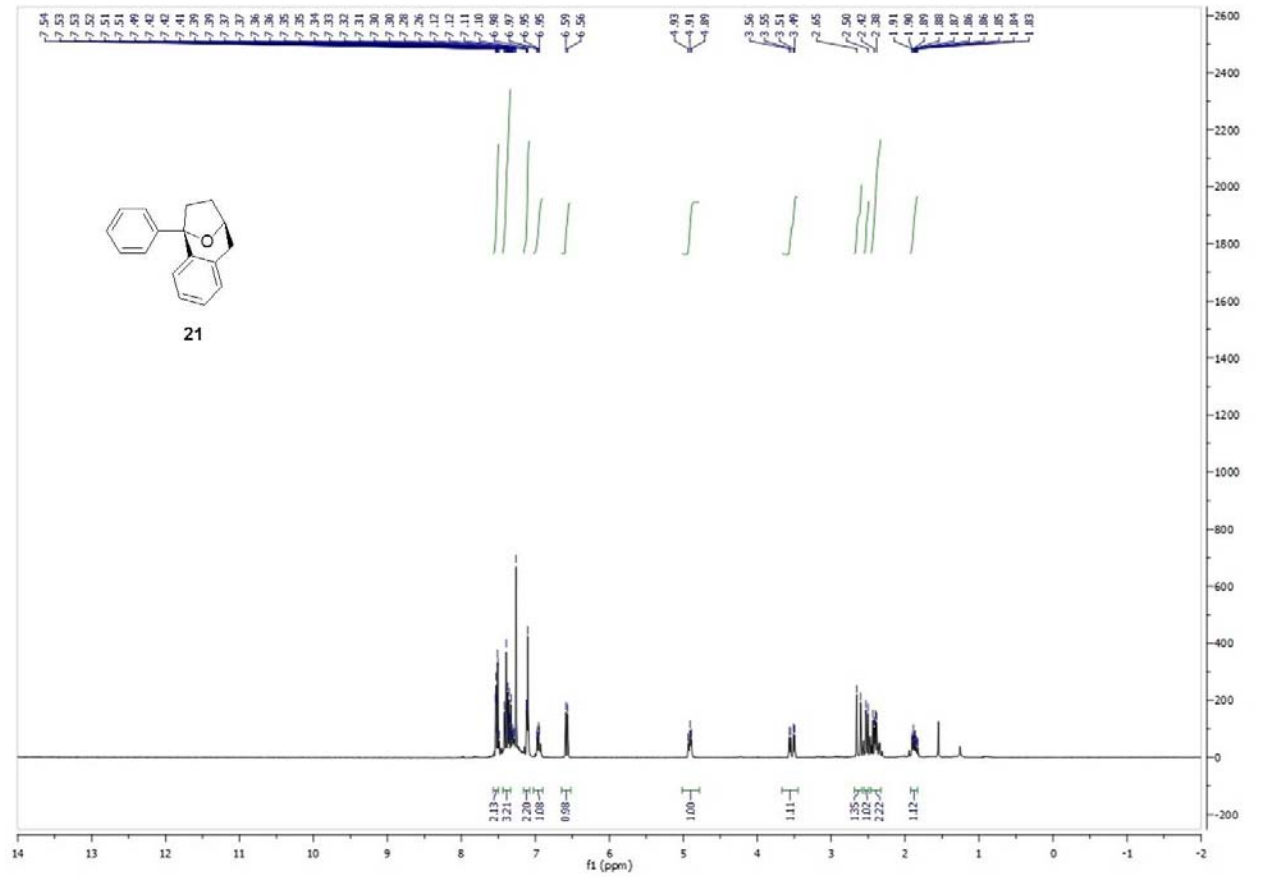

SMe
MeS
O
19c
f1 (ppm)

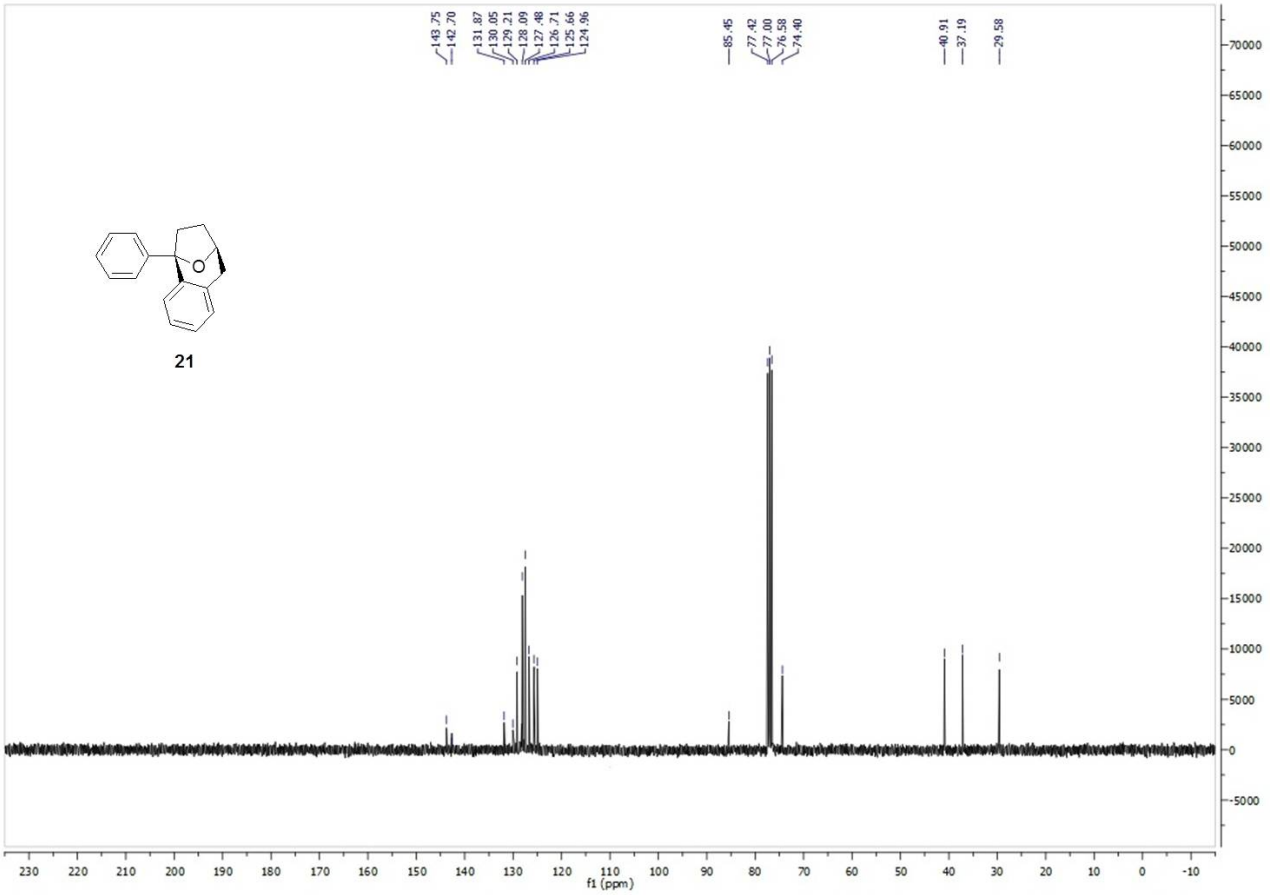

Cl
Cl
O
19d
f1 (ppm)

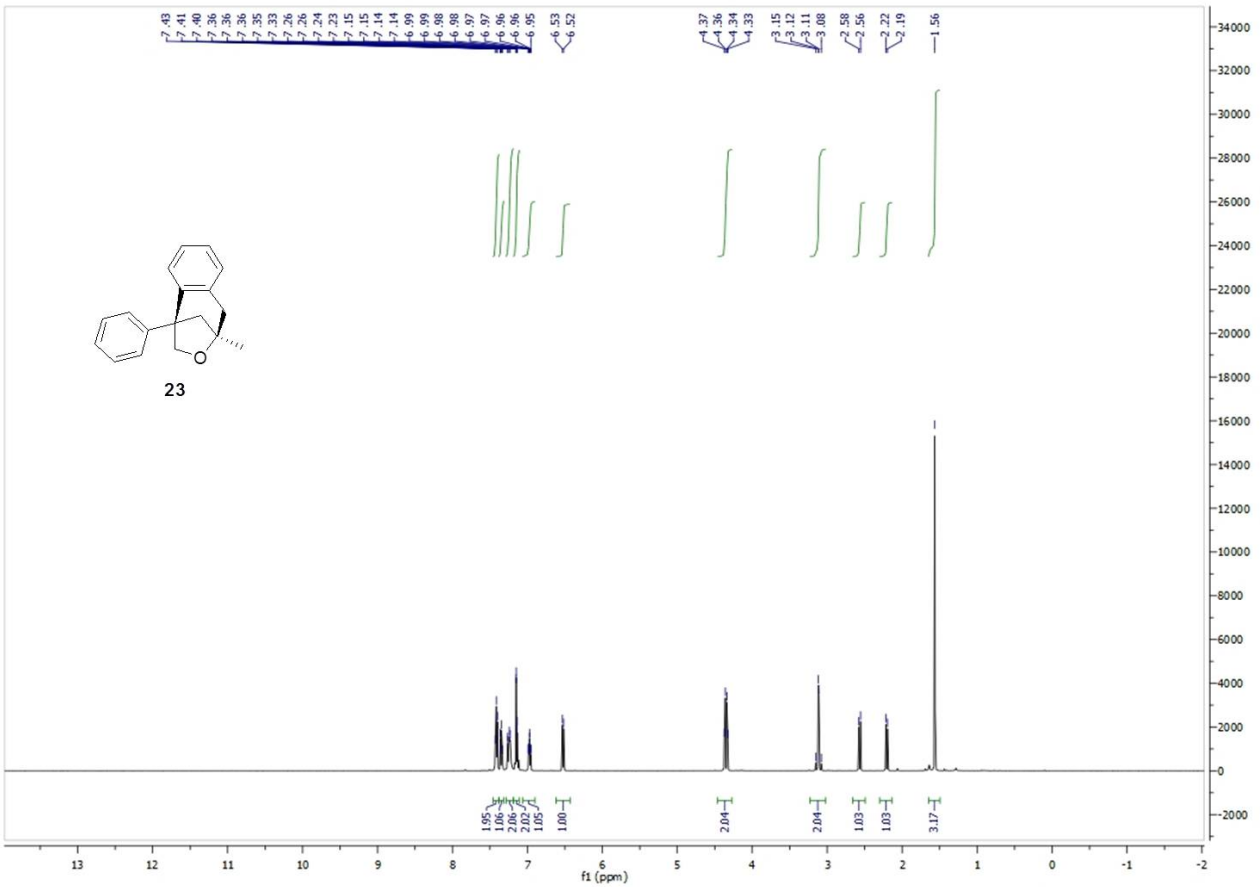

Cl
Cl
O
19d
f1 (ppm)


19e
f1 (ppm)

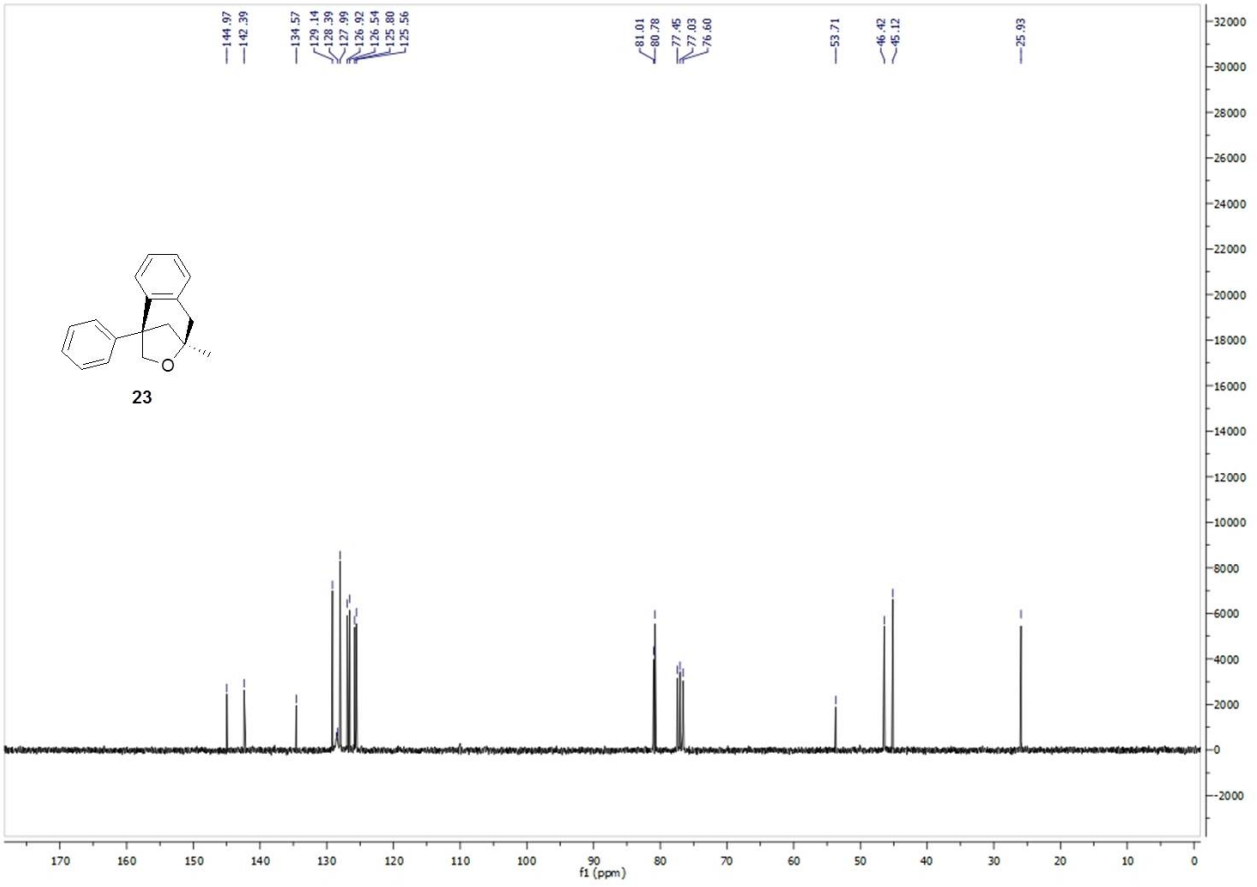

19e
f1 (ppm)


21
f1 (ppm)

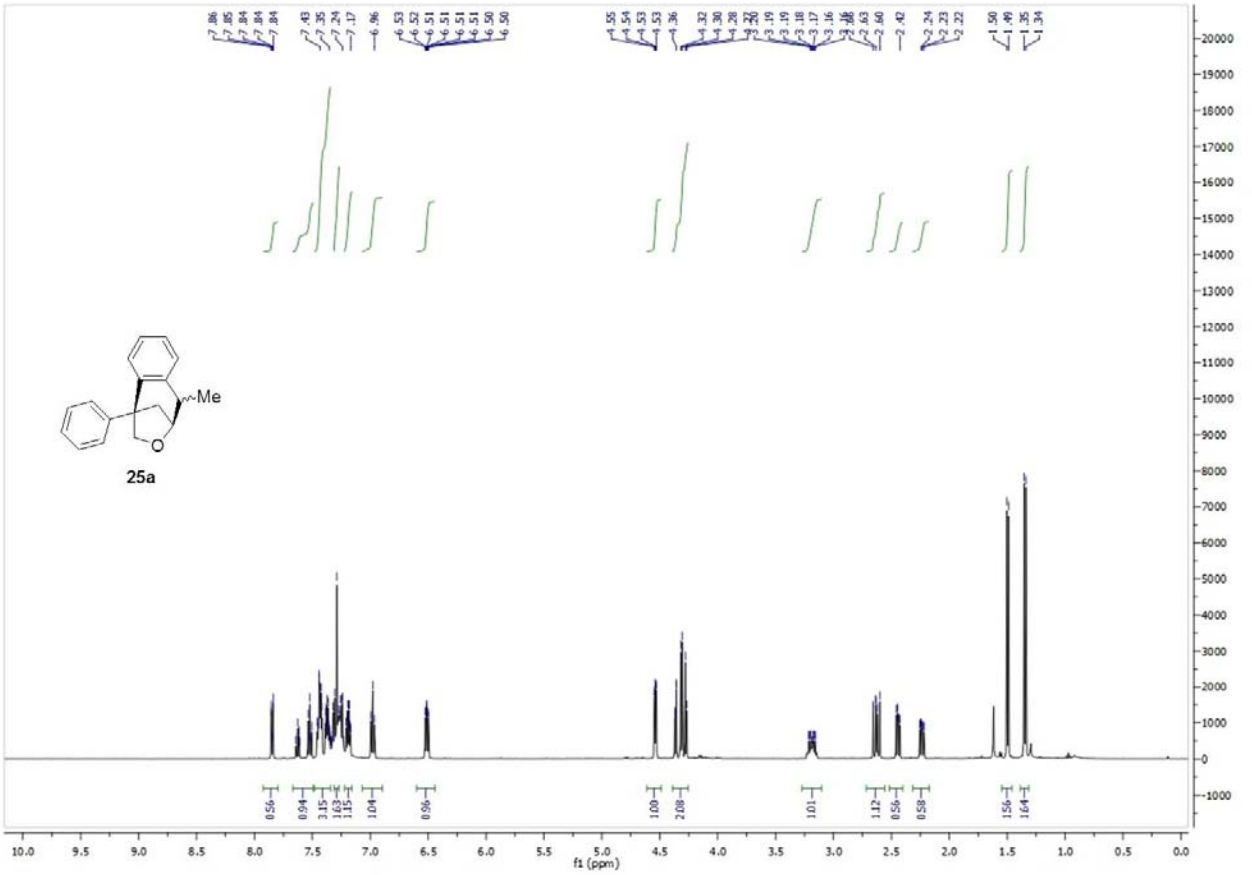

21
f1 (ppm)

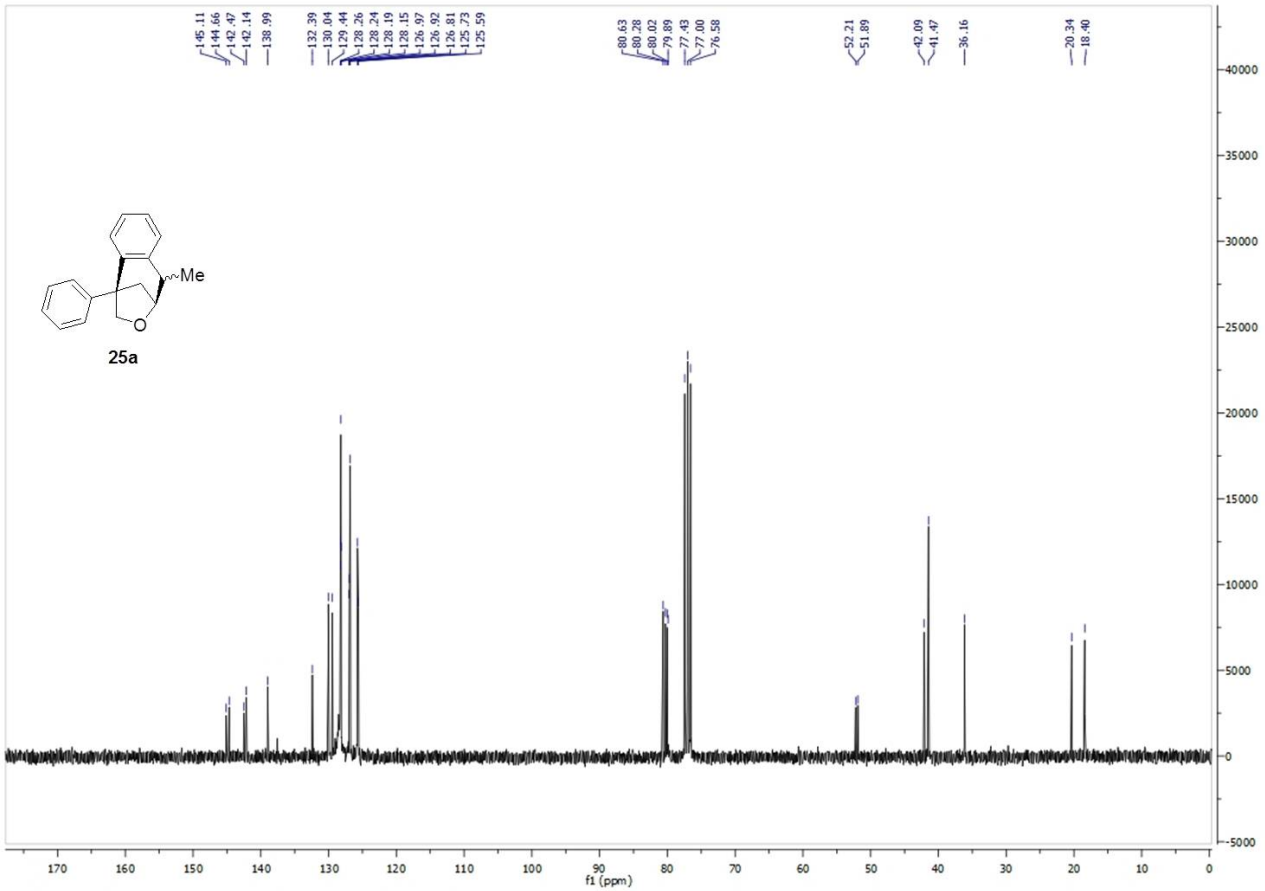

7.43
7.41
7.40
7.36
7.36
7.36
7.35
7.33
7.26
7.26
7.24
7.23
7.15
7.15
7.14
7.14
6.99
6.99
6.98
6.98
6.97
6.97
6.96
6.96
6.96
6.95
6.53
6.52
4.37
4.36
4.34
4.33
3.15
3.12
3.11
3.08
2.58
2.56
2.22
2.19
1.56
1.95
1.06
2.06
2.02
1.05
1.00
2.04
2.04
1.03
1.03
3.17
f1 (ppm)

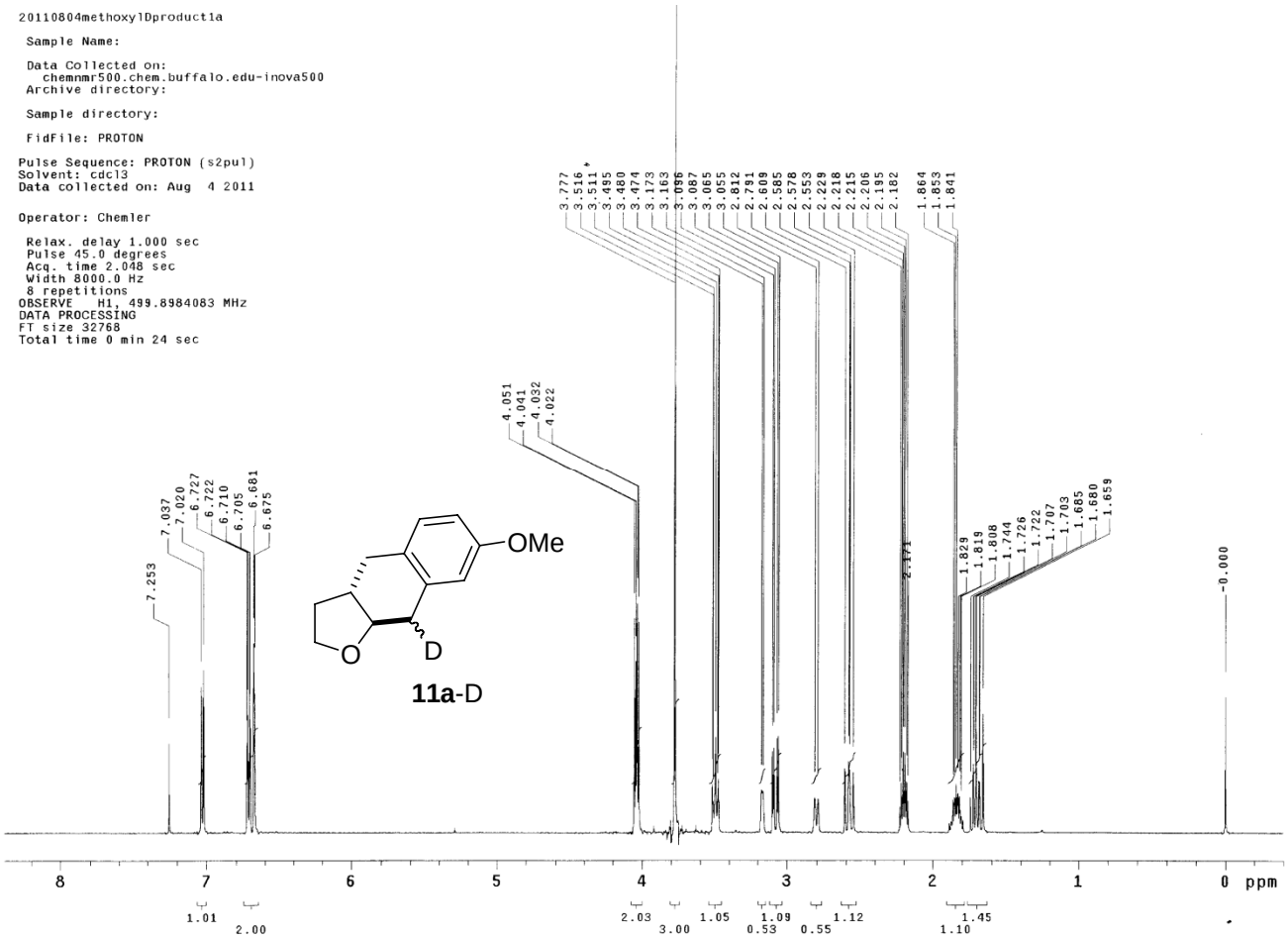
23

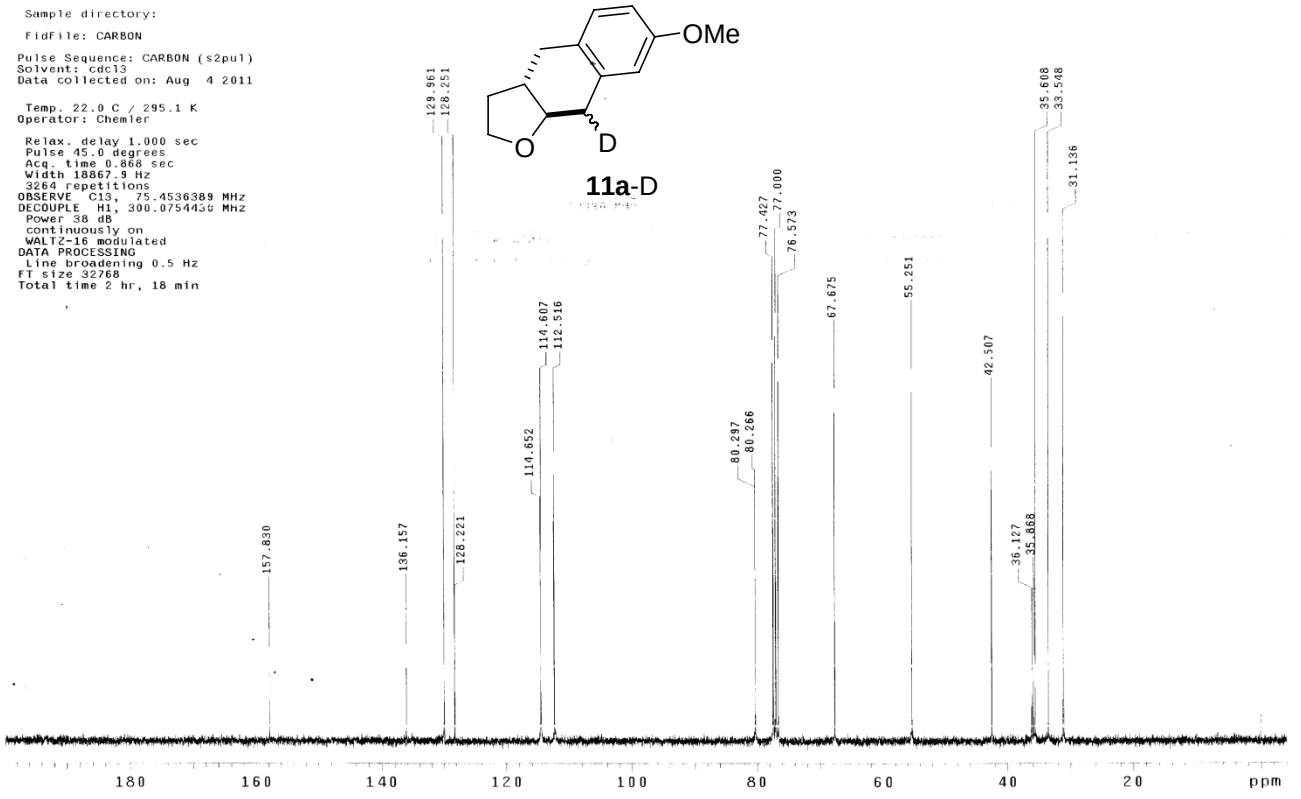

144.97
142.39
134.57
129.14
128.39
127.99
126.92
126.54
125.80
125.56
81.01
80.78
77.45
77.03
76.60
53.71
46.42
45.12
25.93
f1 (ppm)

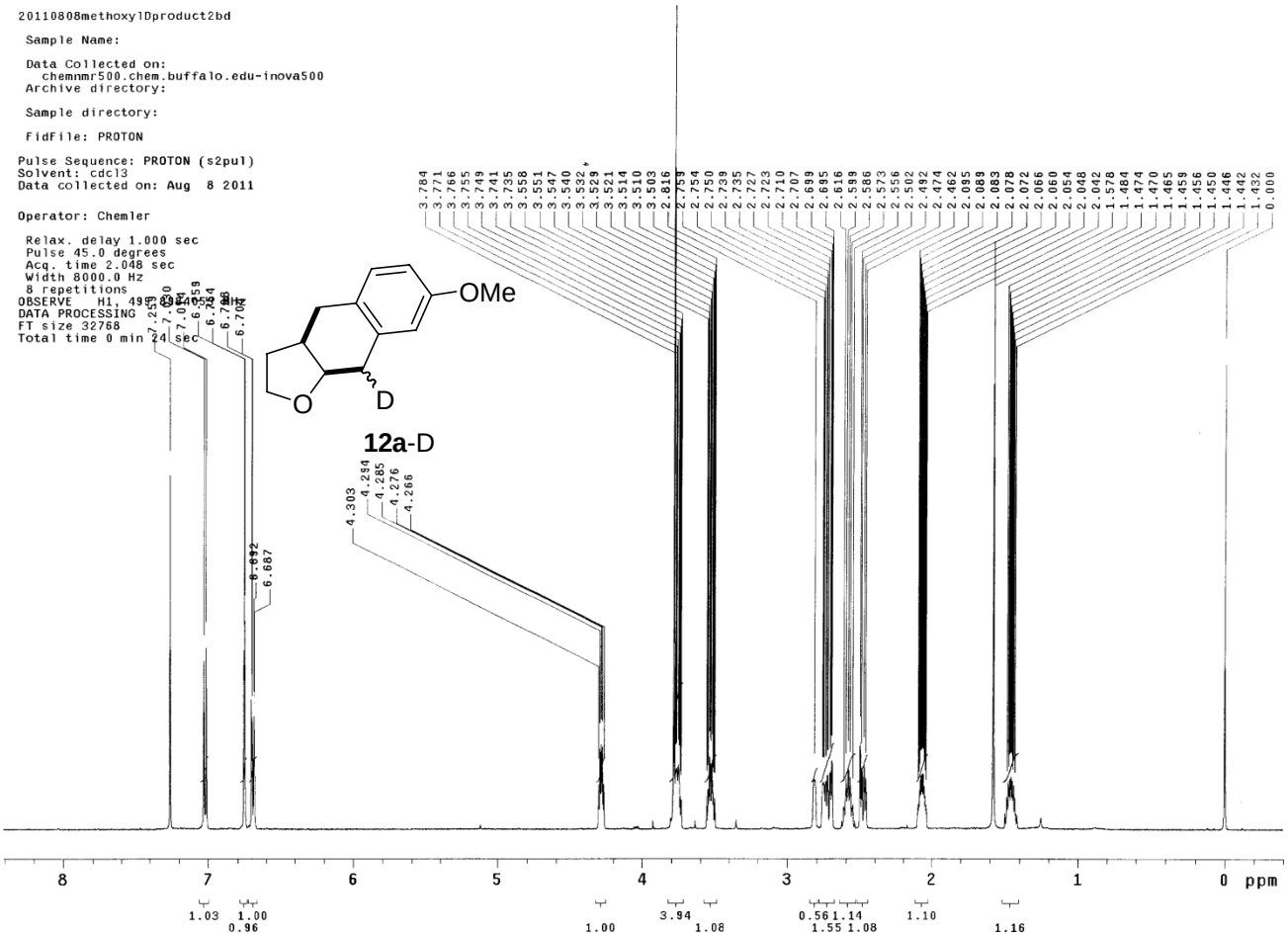
23

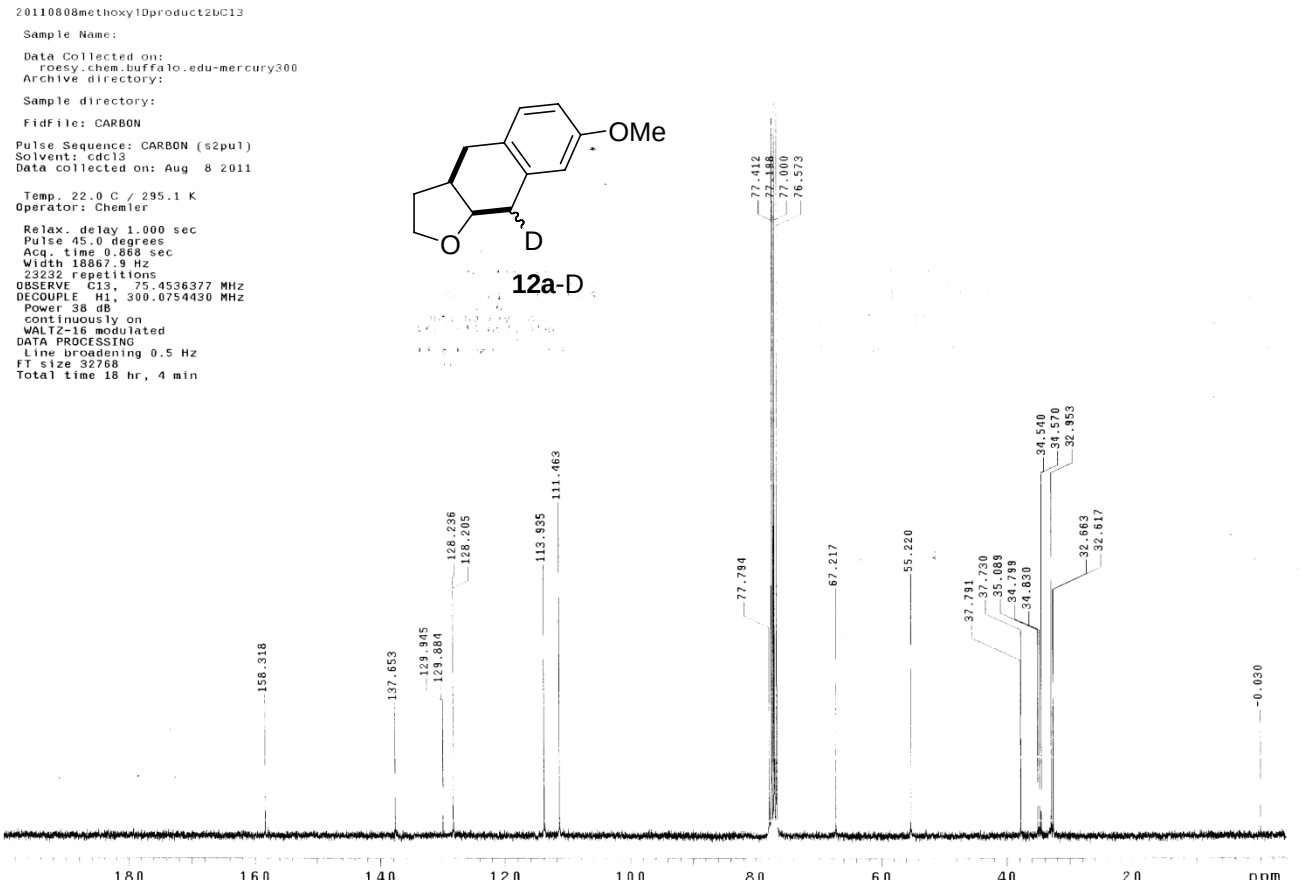

Me
O
25a
f1 (ppm)

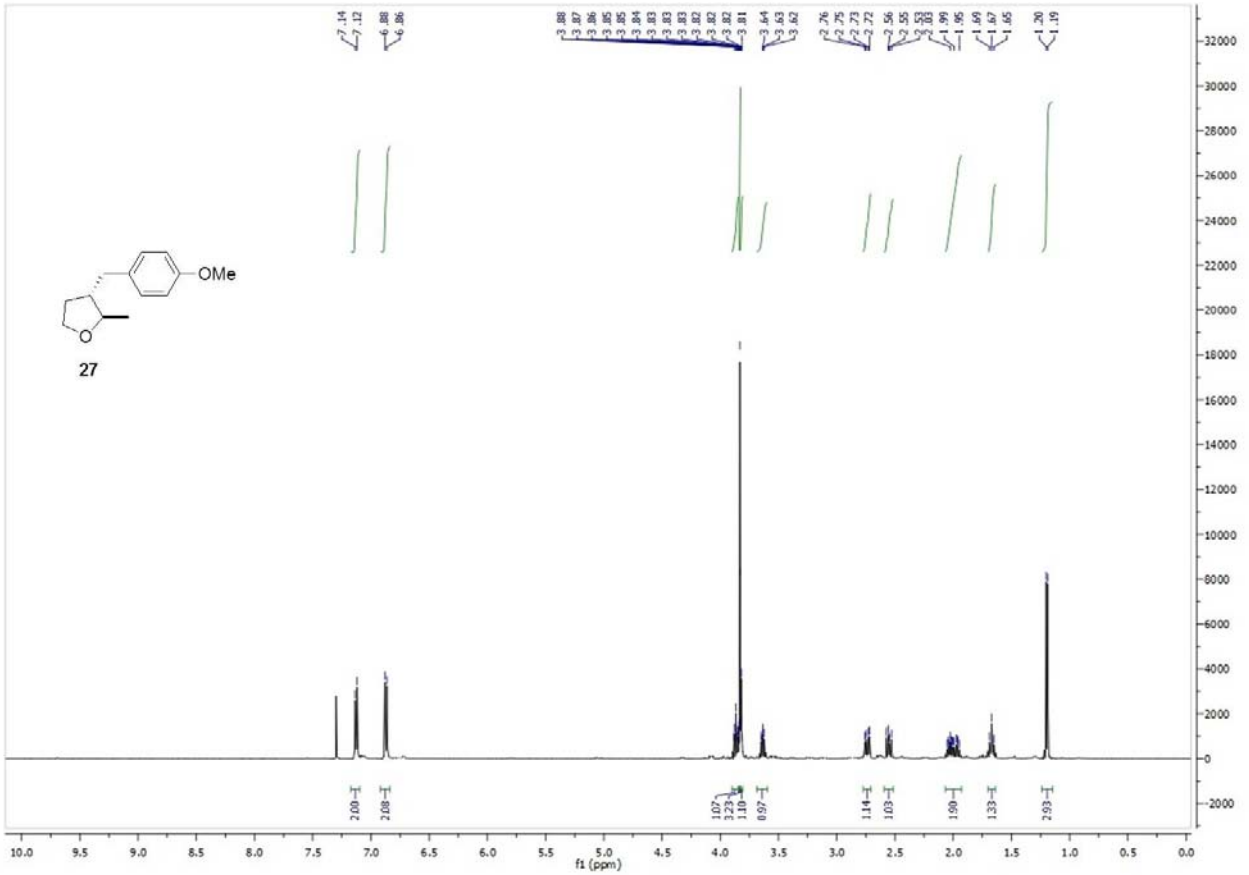

Me
O
25a
f1 (ppm)

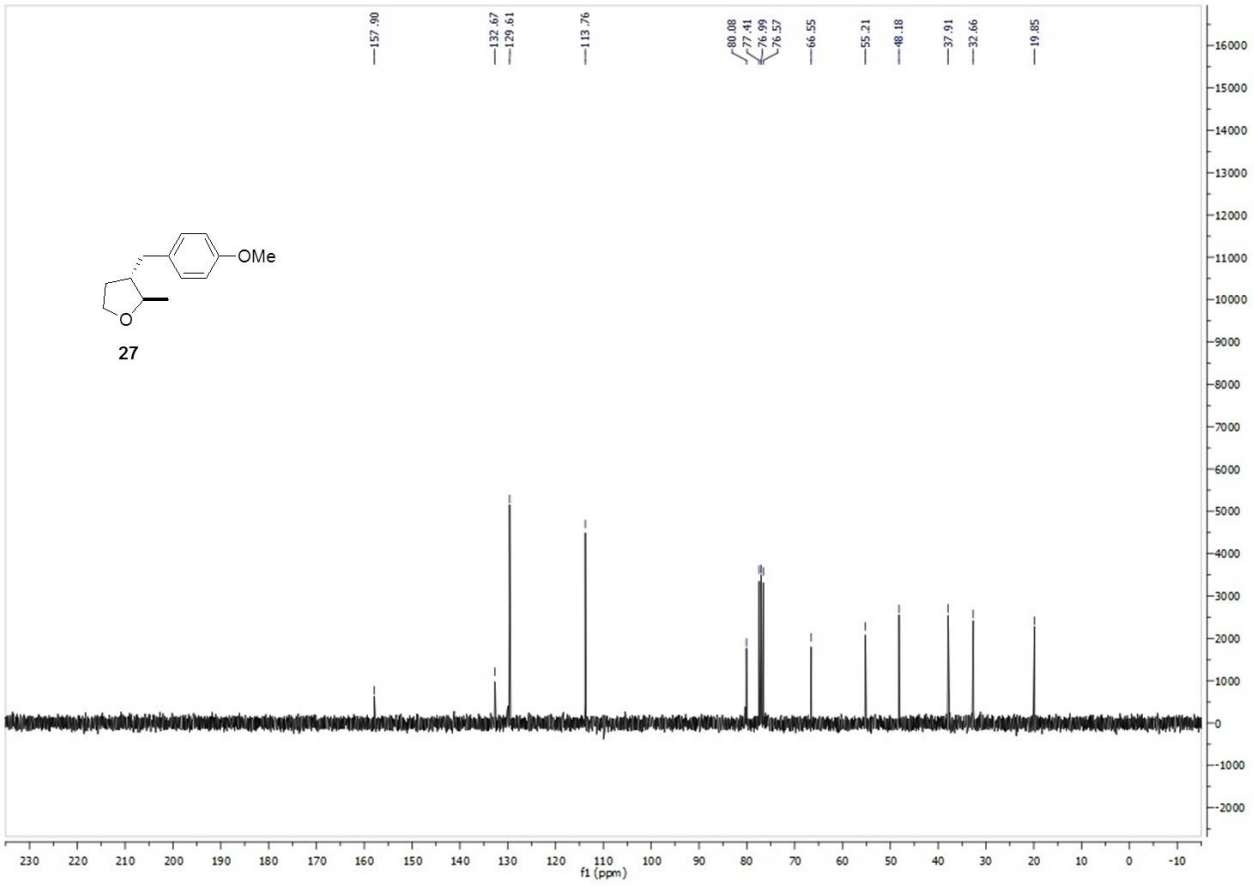

20110804methoxy1Dproduct1a
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 4 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984083 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
D
11a-D
ppm

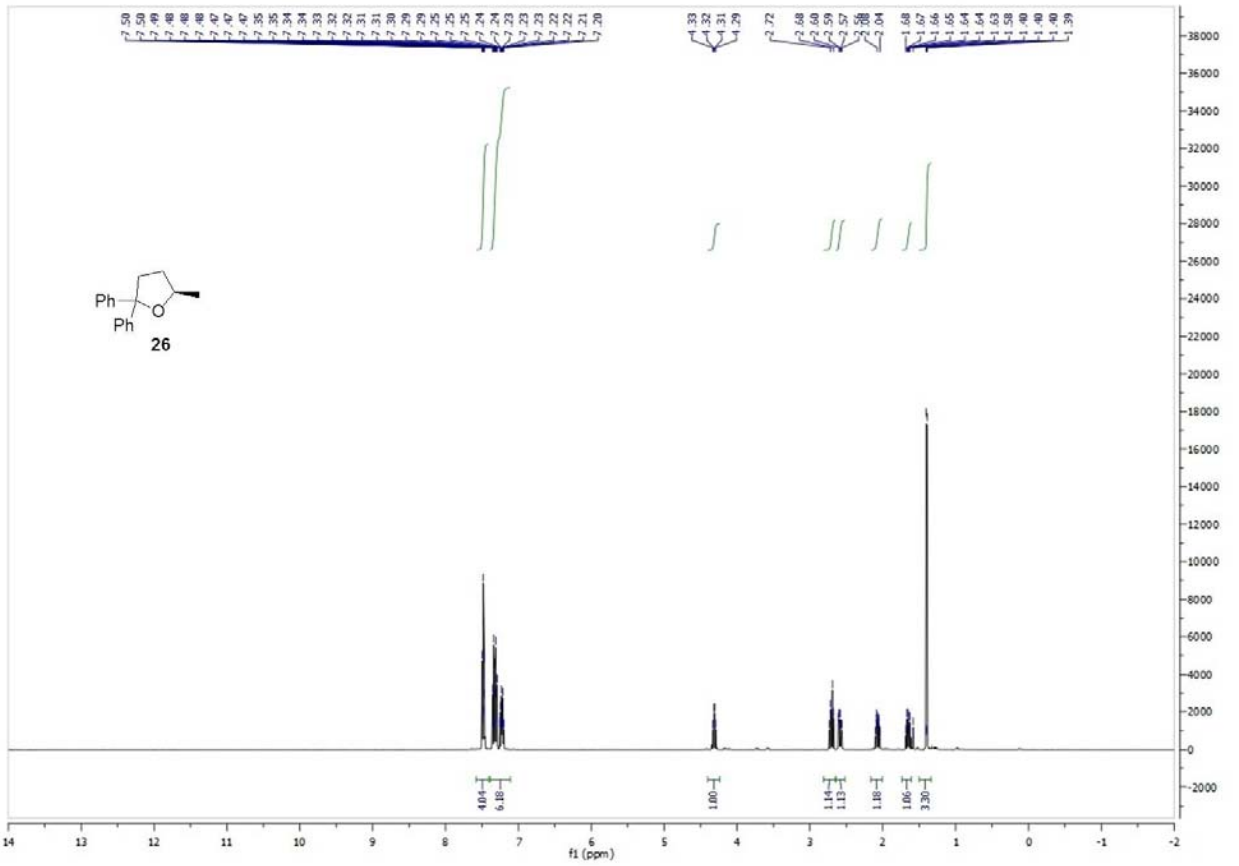

20110804methoxy1Dproduct1aC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 4 2011
Temp. 22.0 C / 295.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3264 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754435 Mhz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 2 hr, 18 min
OMe
D
11a-D
ppm

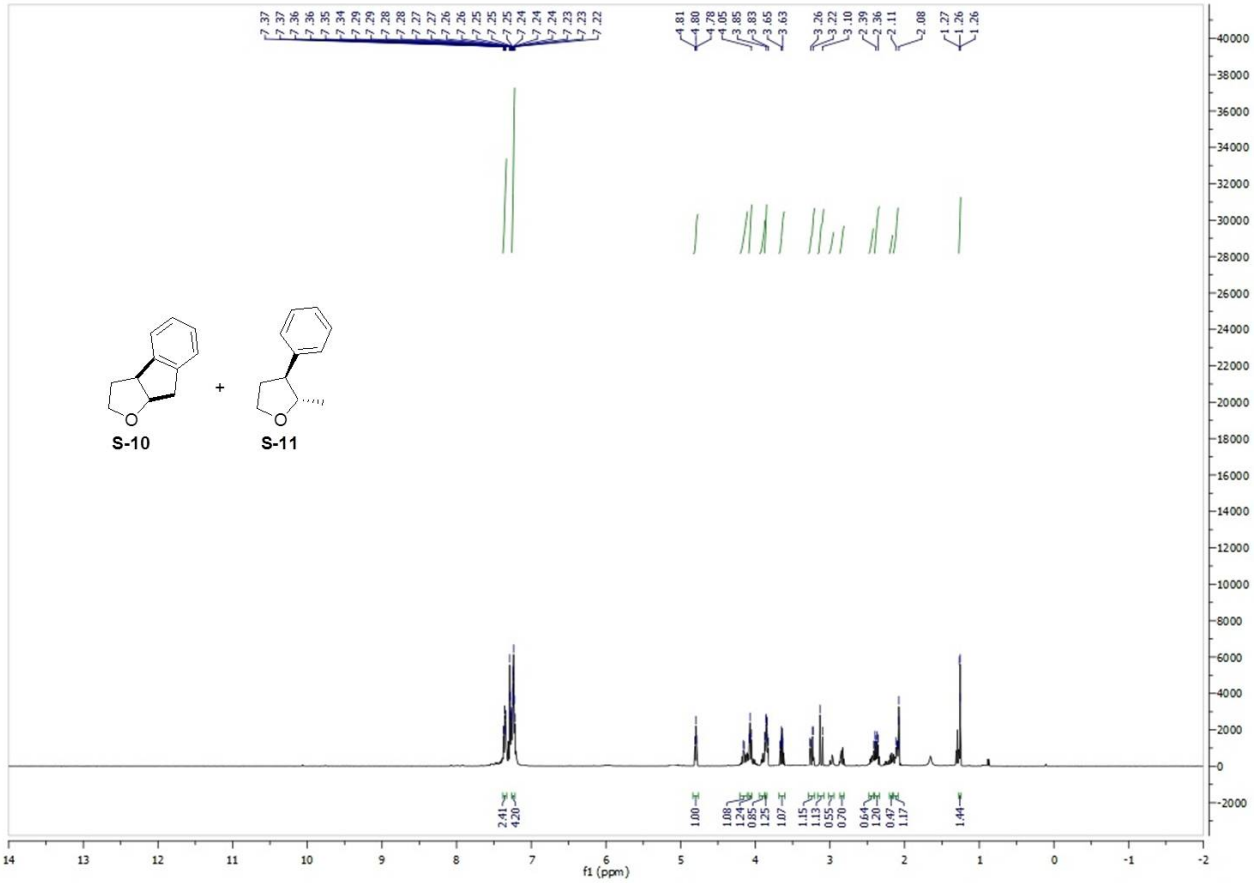

20110808methoxy1Dproduct2bd
Sample Name:
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 8 2011
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8840559 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec
OMe
D
12a-D
8
7
6
5
4
3
2
1
0 ppm
1.03
1.00
0.96
1.00
3.94
1.08
0.56
1.14
1.55
1.08
1.10
1.16


20110808methoxy1Dproduct2bC13
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 8 2011
Temp. 22.0 C / 295.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
23232 repetitions
OBSERVE C13, 75.4536377 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 18 hr, 4 min
OMe
D
12a-D
180
160
140
120
100
80
60
40
20
ppm


OMe
27
f1 (ppm)


OMe
27
f1 (ppm)


Ph
Ph
O
26
f1 (ppm)


S-10
+
S-11
f1 (ppm)