Supplementary Material

Preparation of cyclopropanone 2,2,2-trifluoroethoxy hemiacetals *via* oxyallyl cation

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Table of Contents

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General

NMR spectra were recorded on Varian/Agilent 400 (^{1}H NMR at 400 MHz, ^{13}C NMR at 100 MHz) and on Bruker Avance III 500 (^{1}H NMR at 500 MHz, ^{13}C NMR at 125 MHz), in deuterated chloroform, if not otherwise stated. Chemical shifts are expressed in ppm (δ) using tetramethylsilane as internal standard, coupling constants (*J*) are in Hz.

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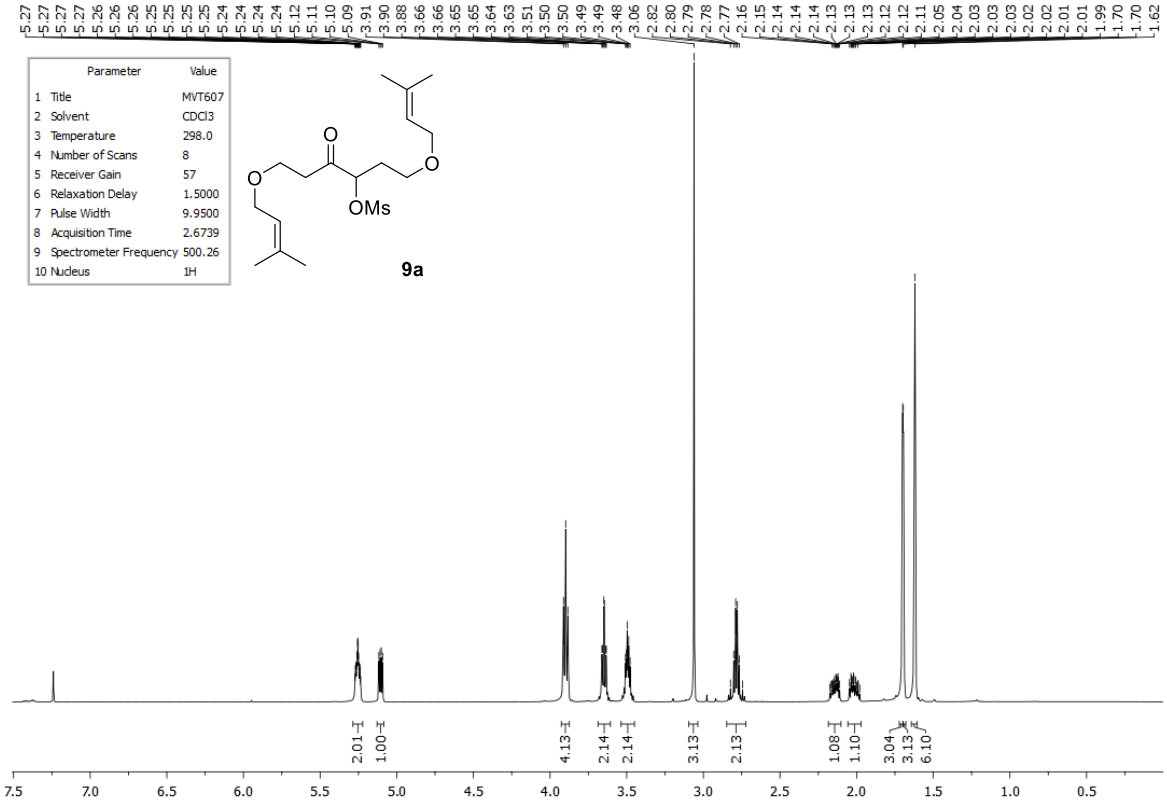
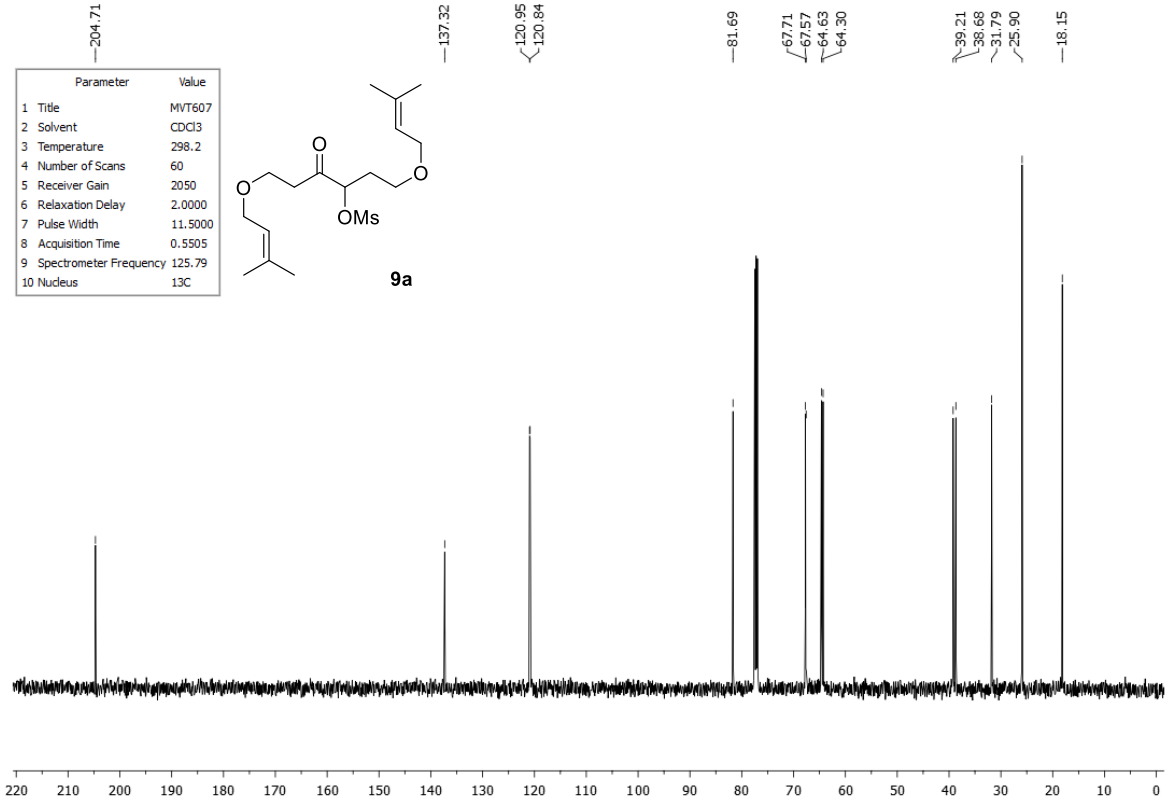
Copies of NMR spectra





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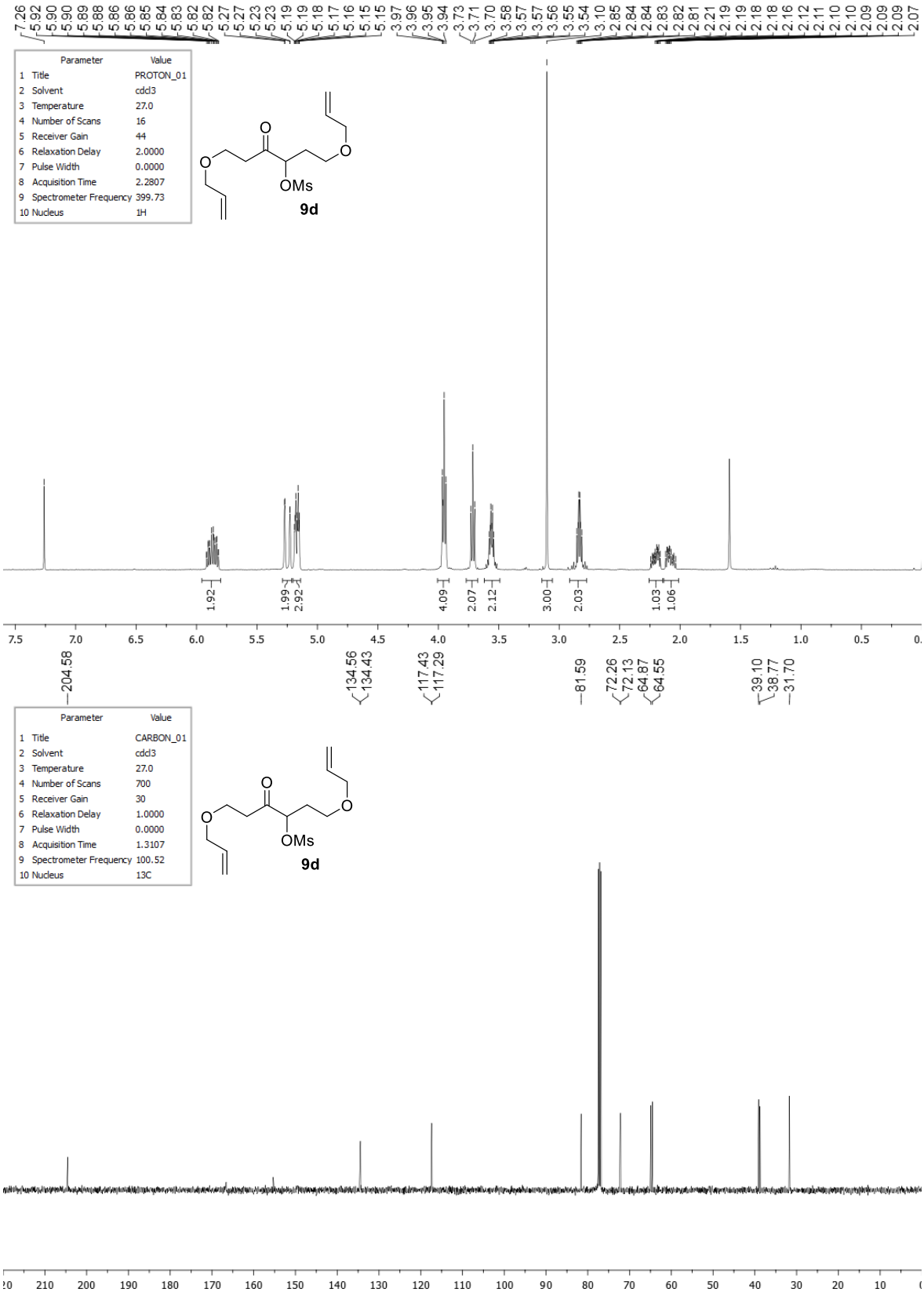
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9d
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OMs
9d

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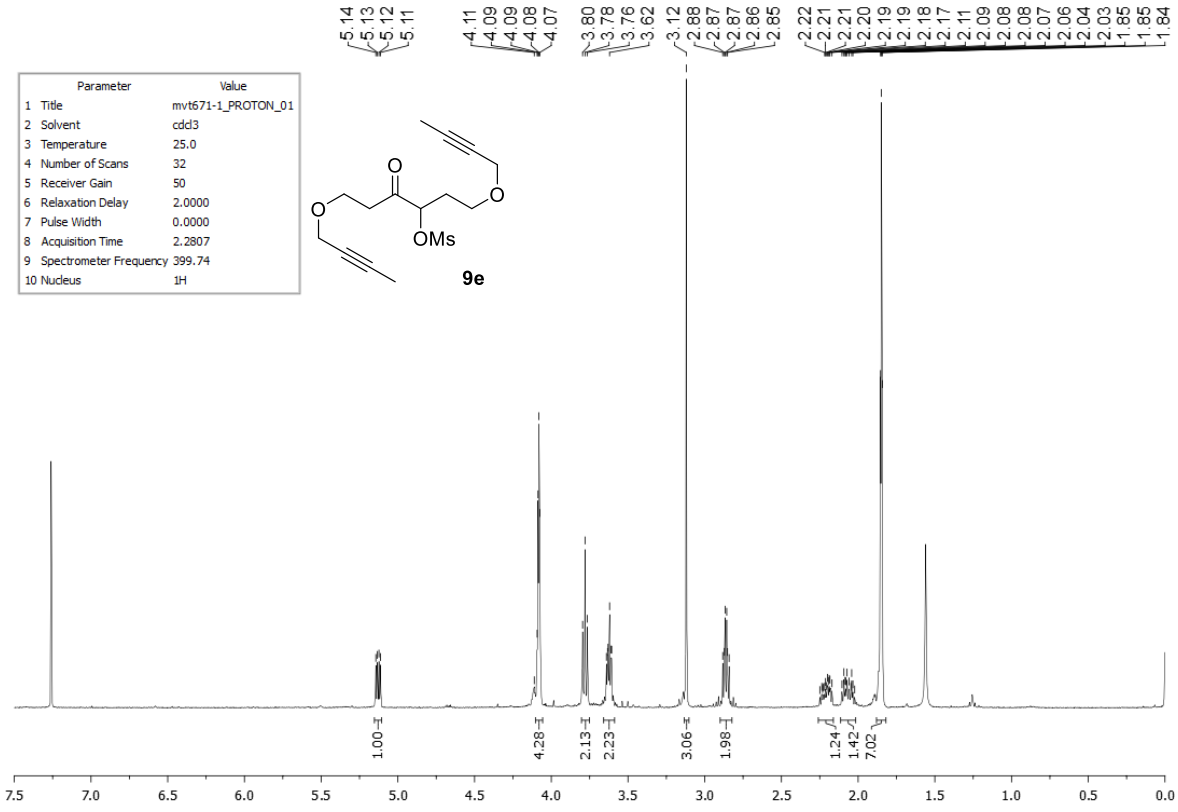
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2.85
2.22
2.21
2.21
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2.19
2.19
2.18
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2.04
2.03
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1.85
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OMs
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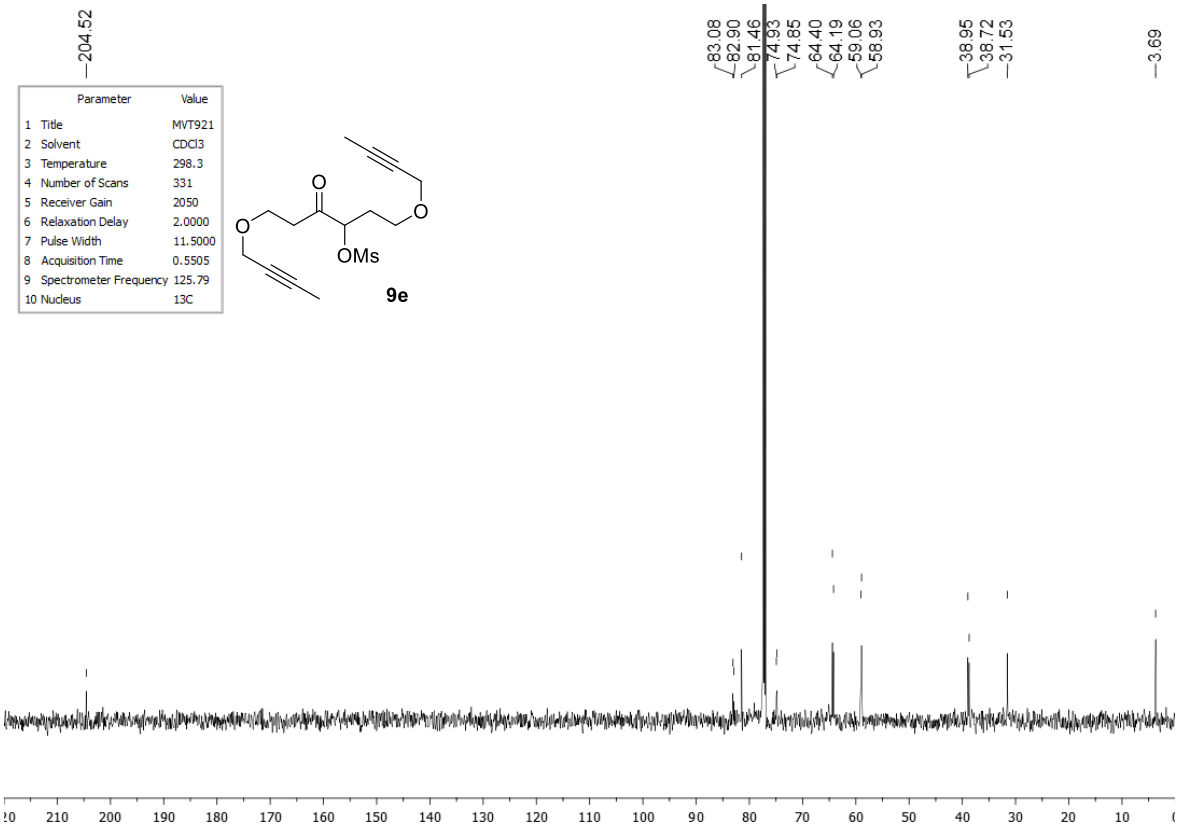
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OMs
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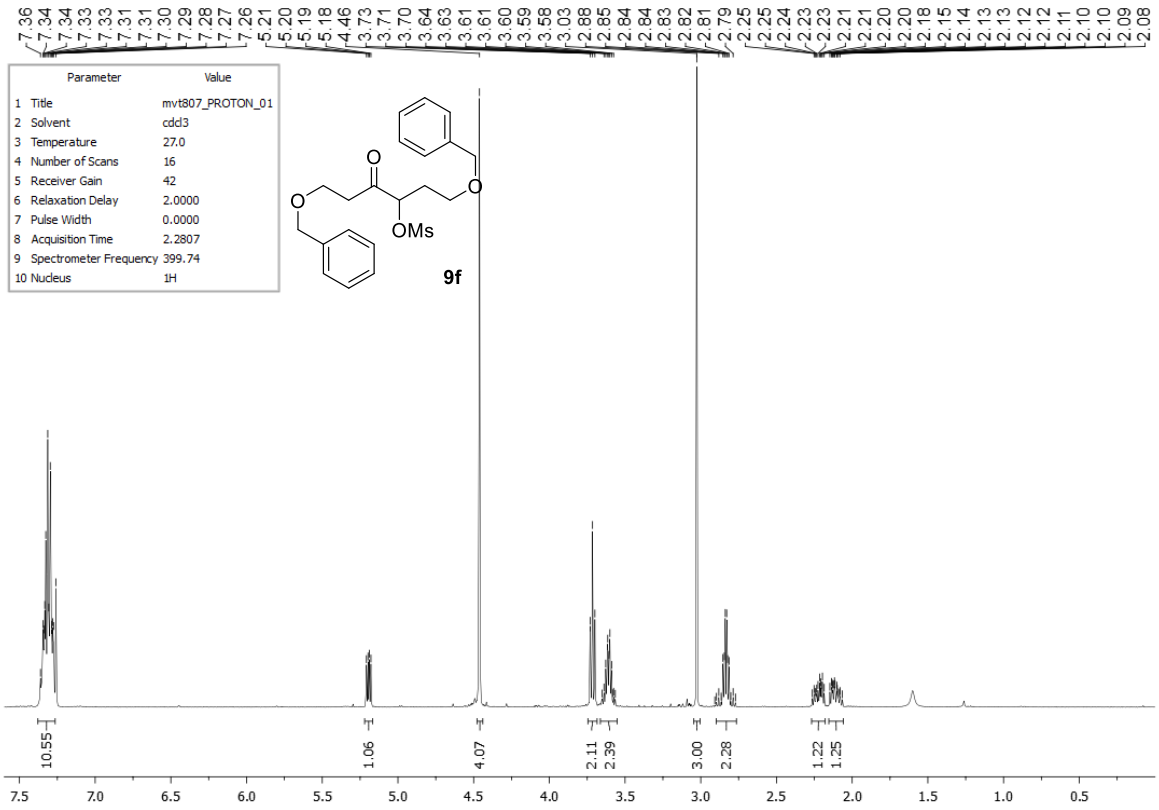
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O
O
OMs
9f
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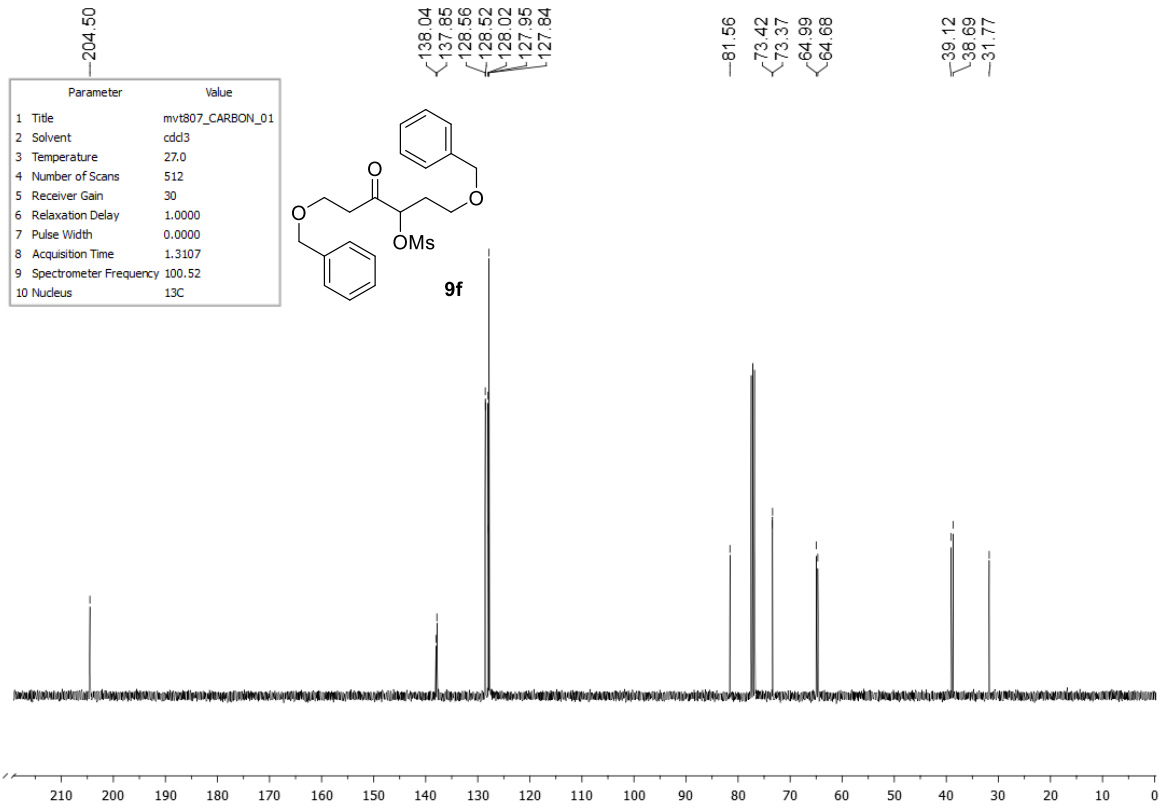
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O
O
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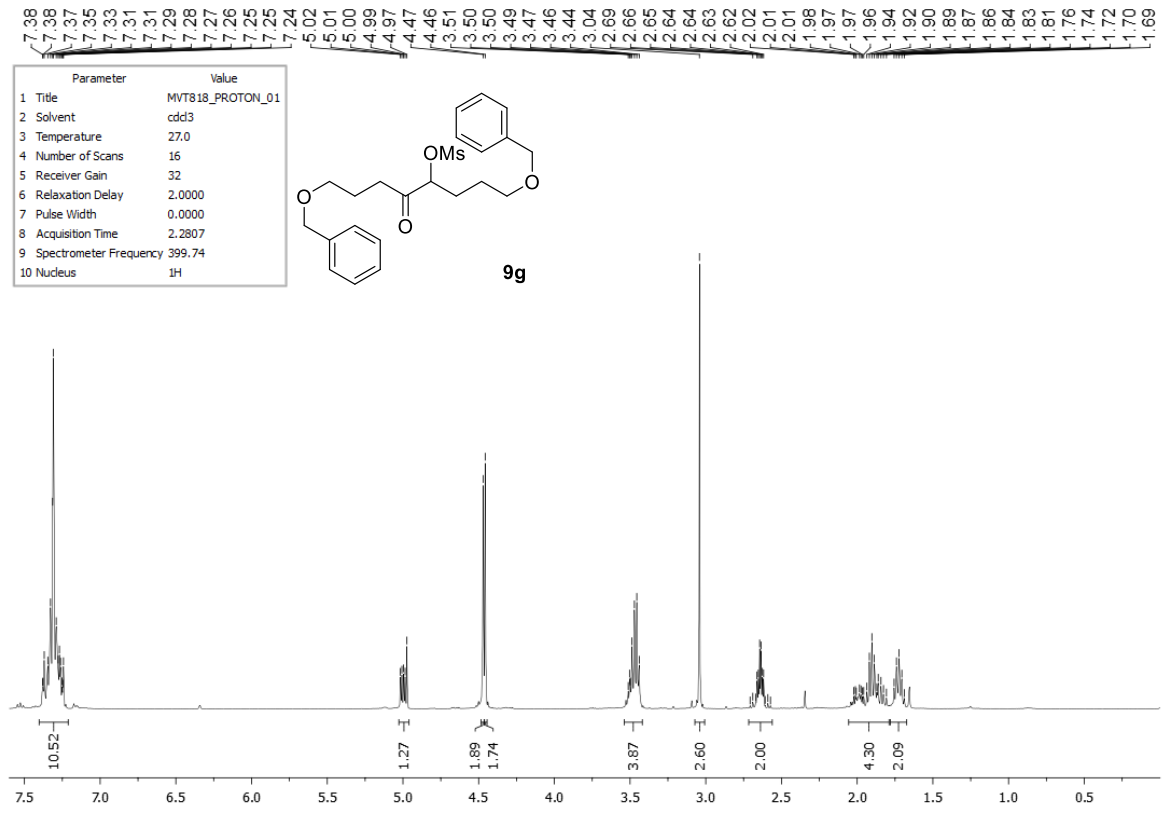
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10 Nucleus 1H
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O
O
9g
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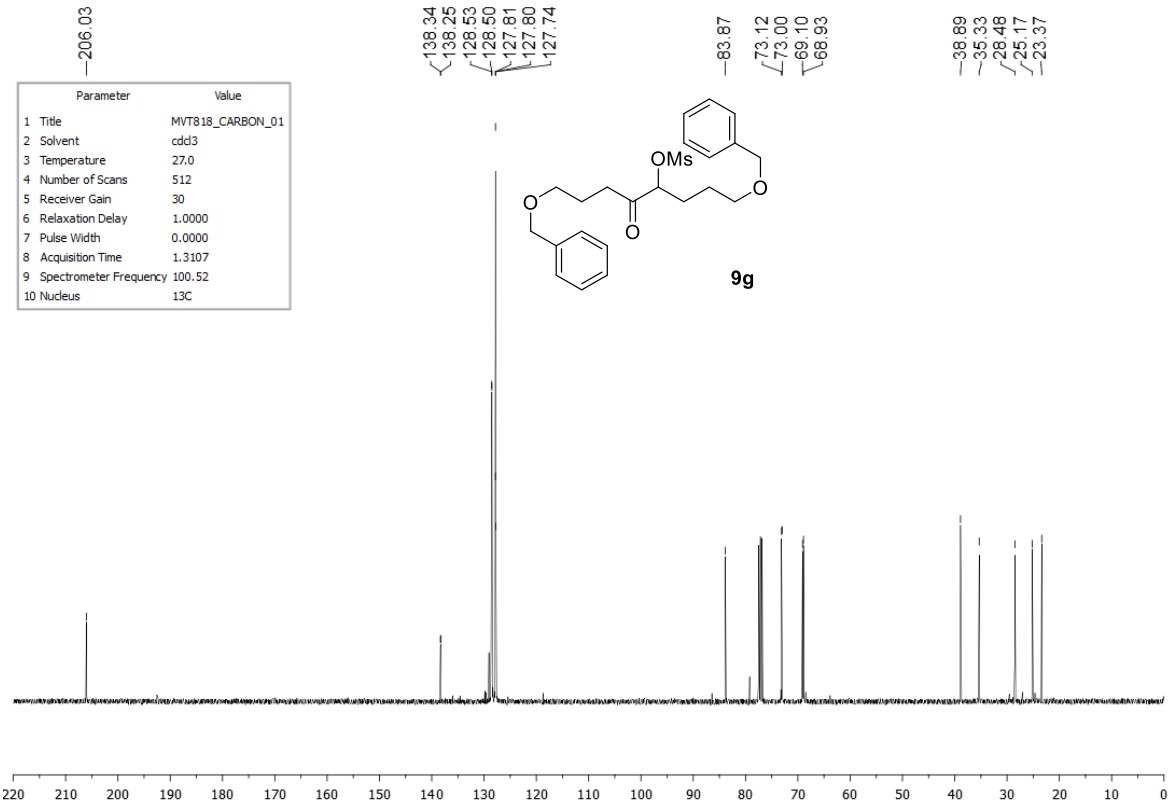
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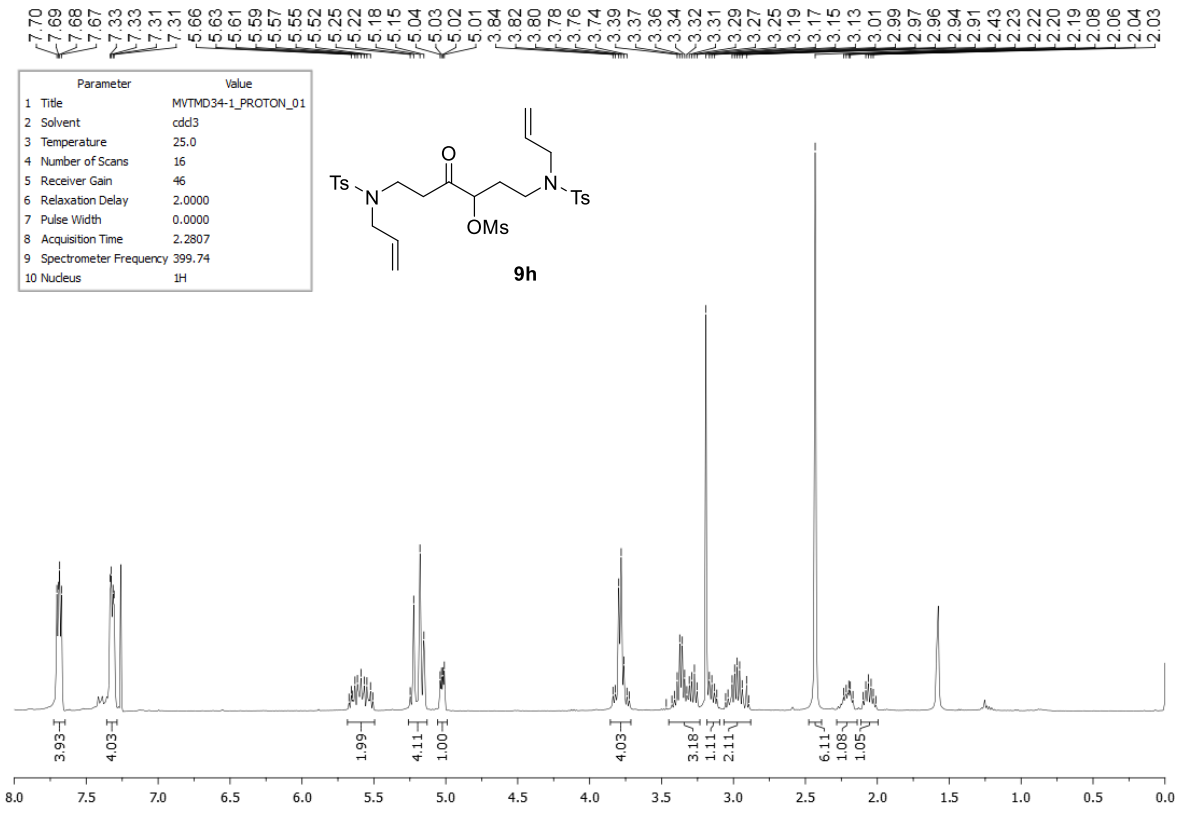
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OMs
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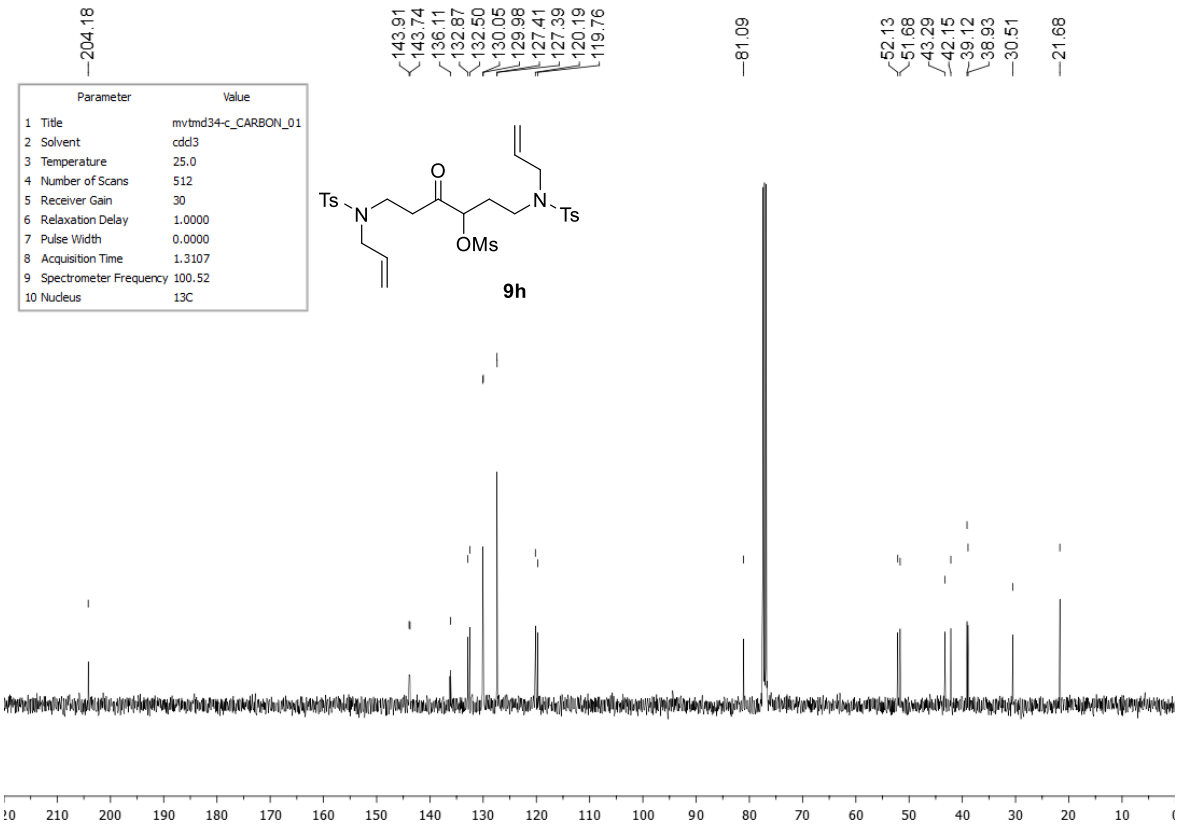
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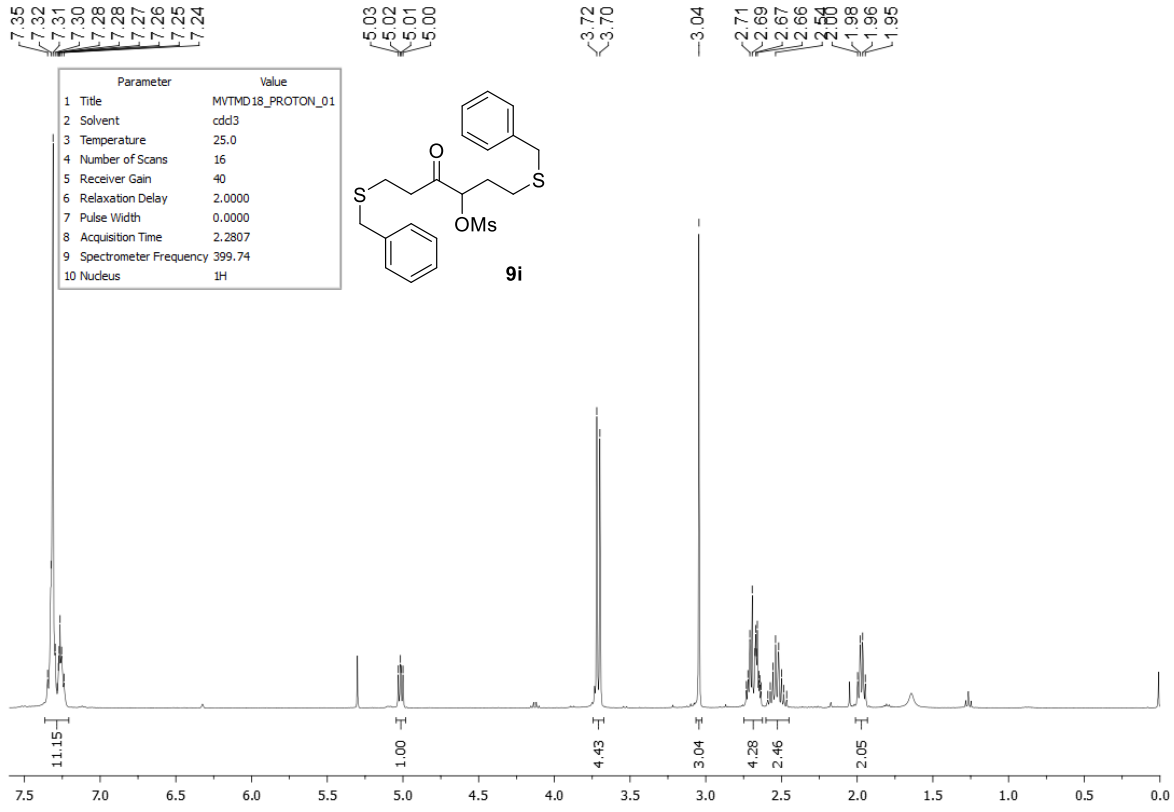
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S
S
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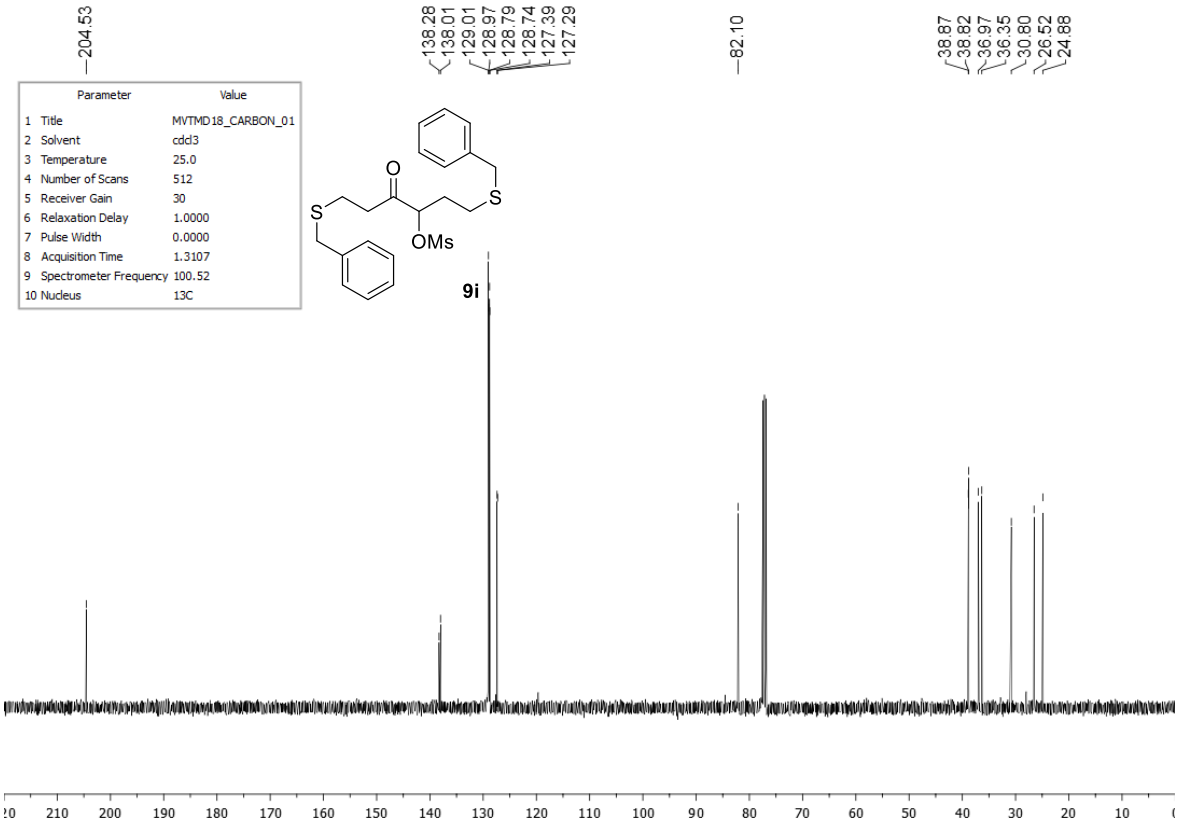
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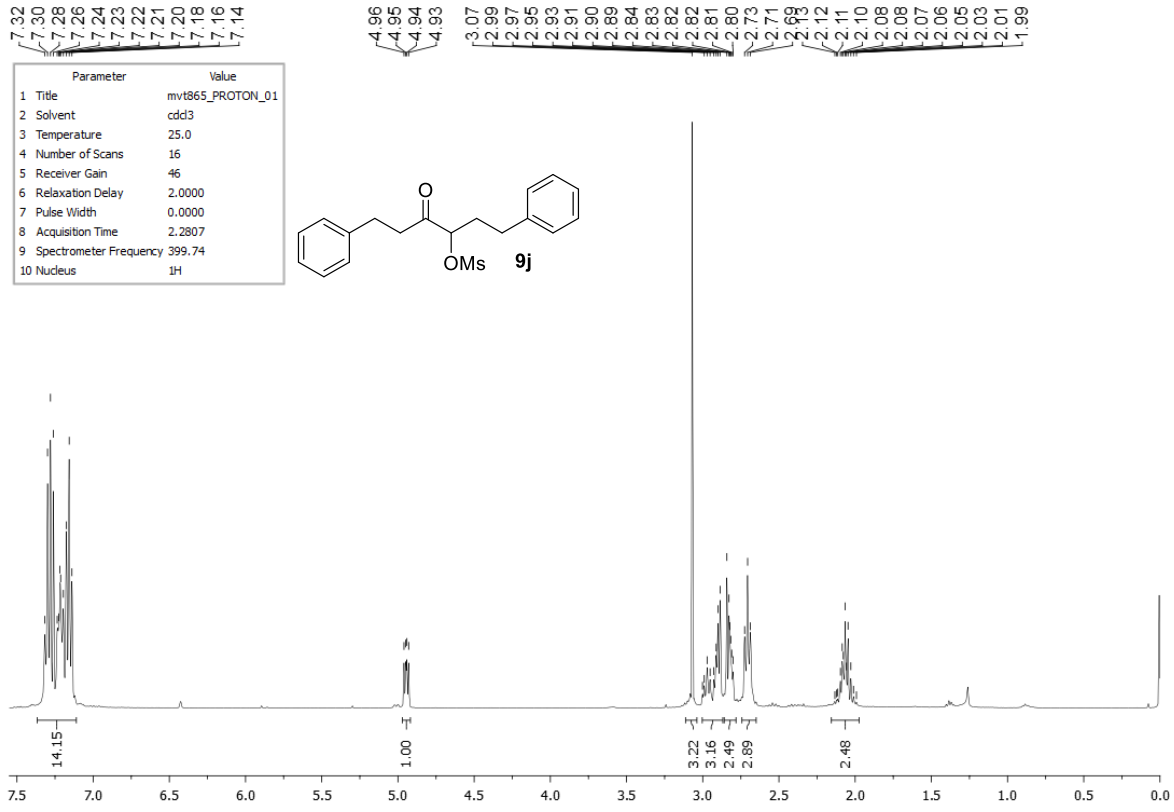
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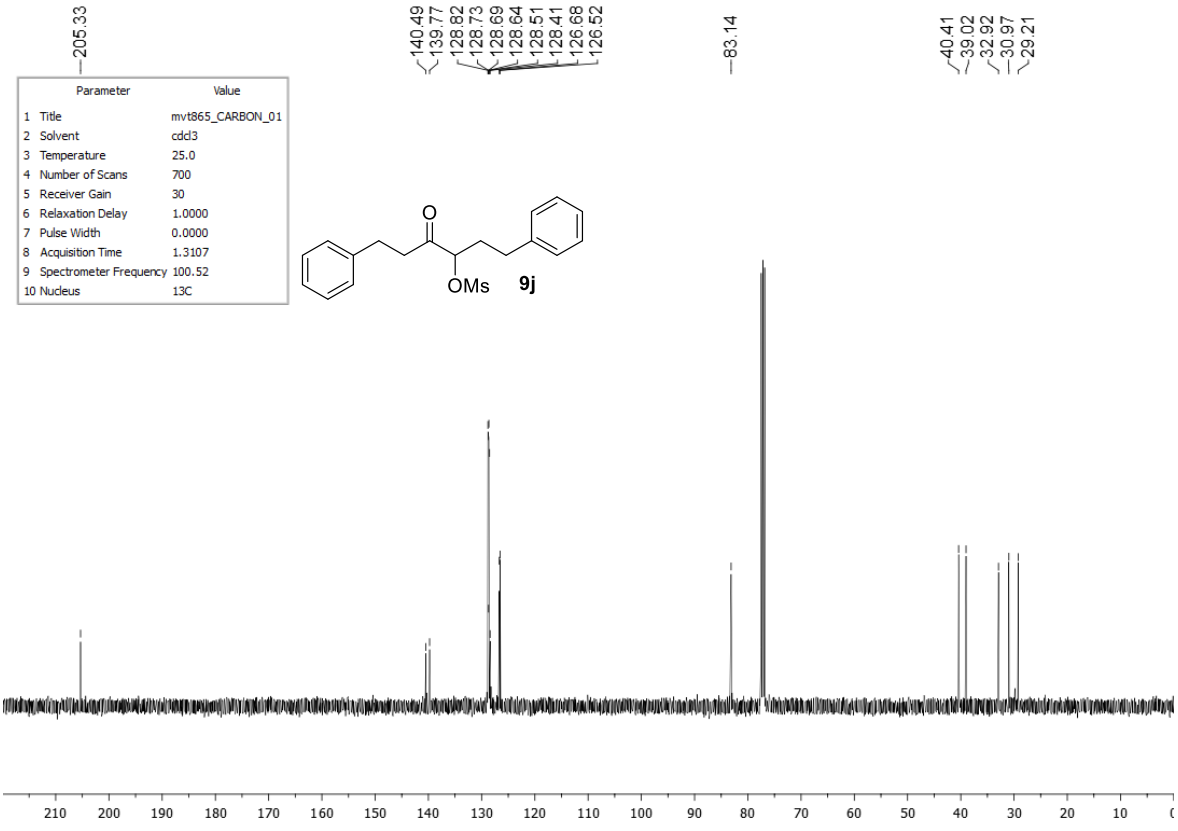
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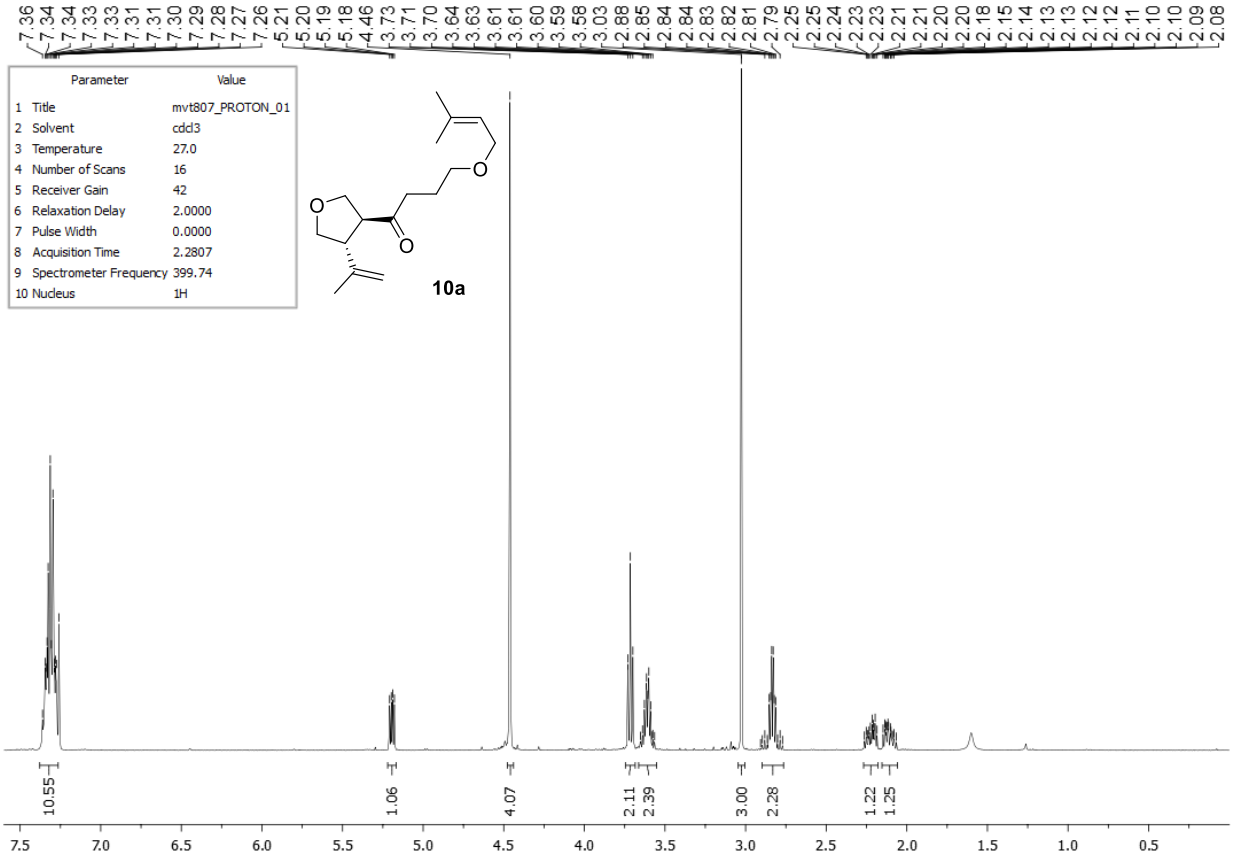
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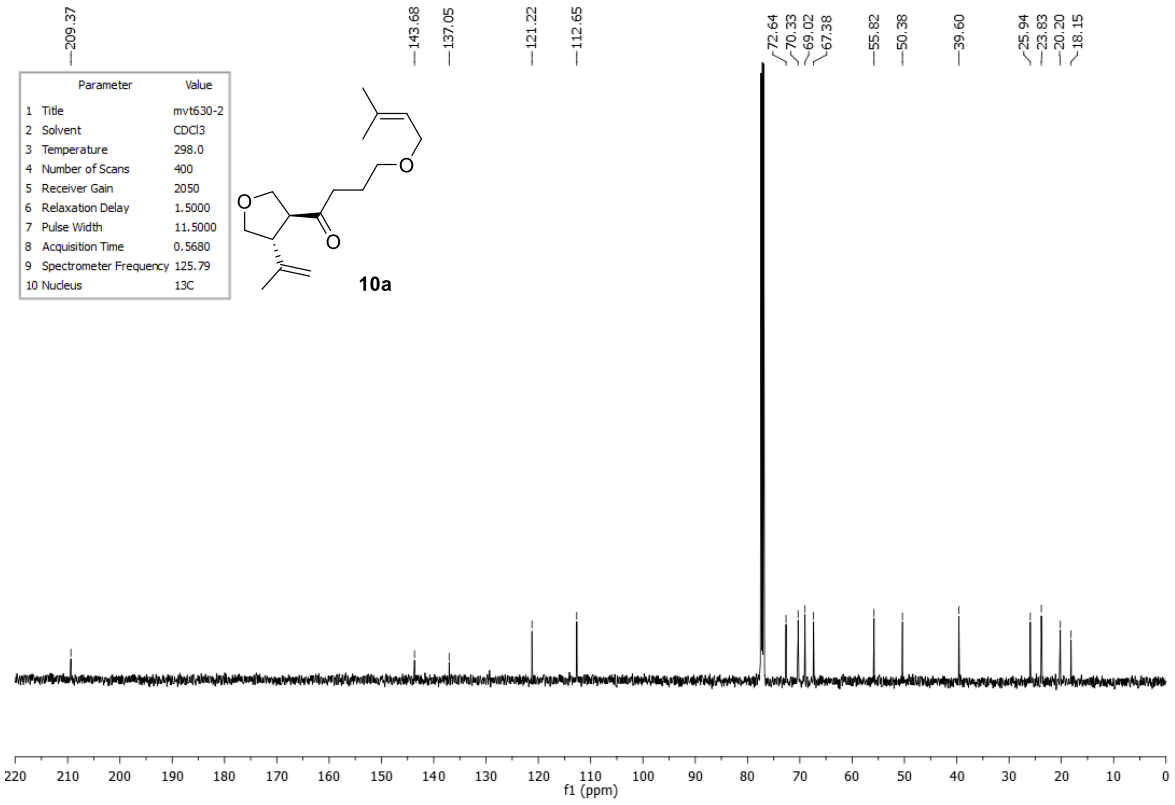
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f1 (ppm)

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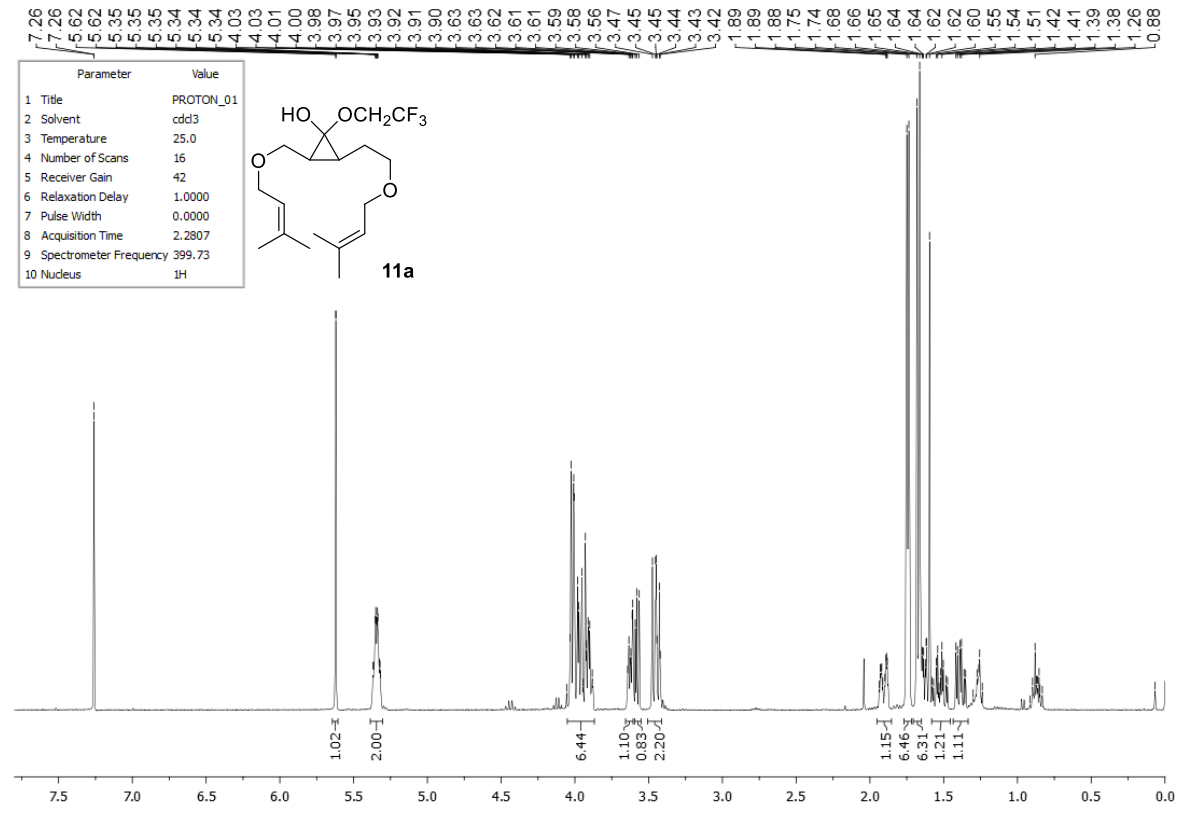
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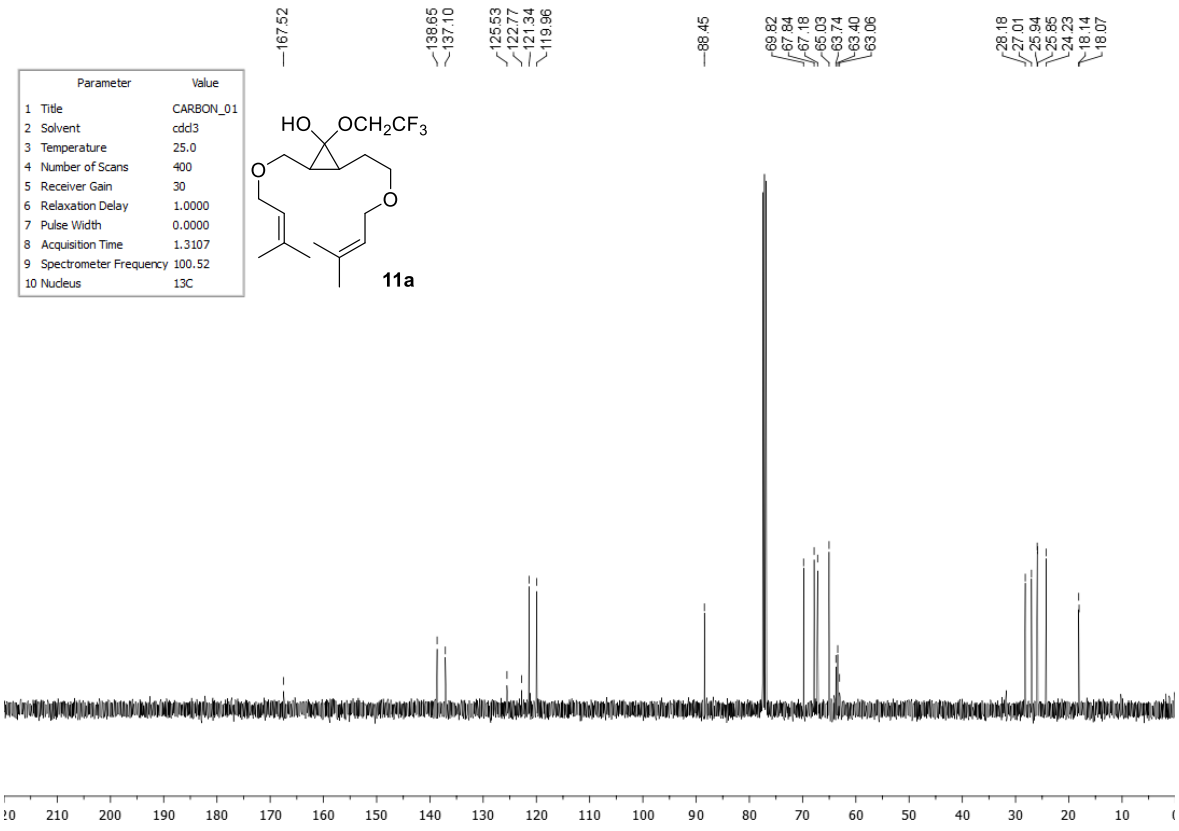
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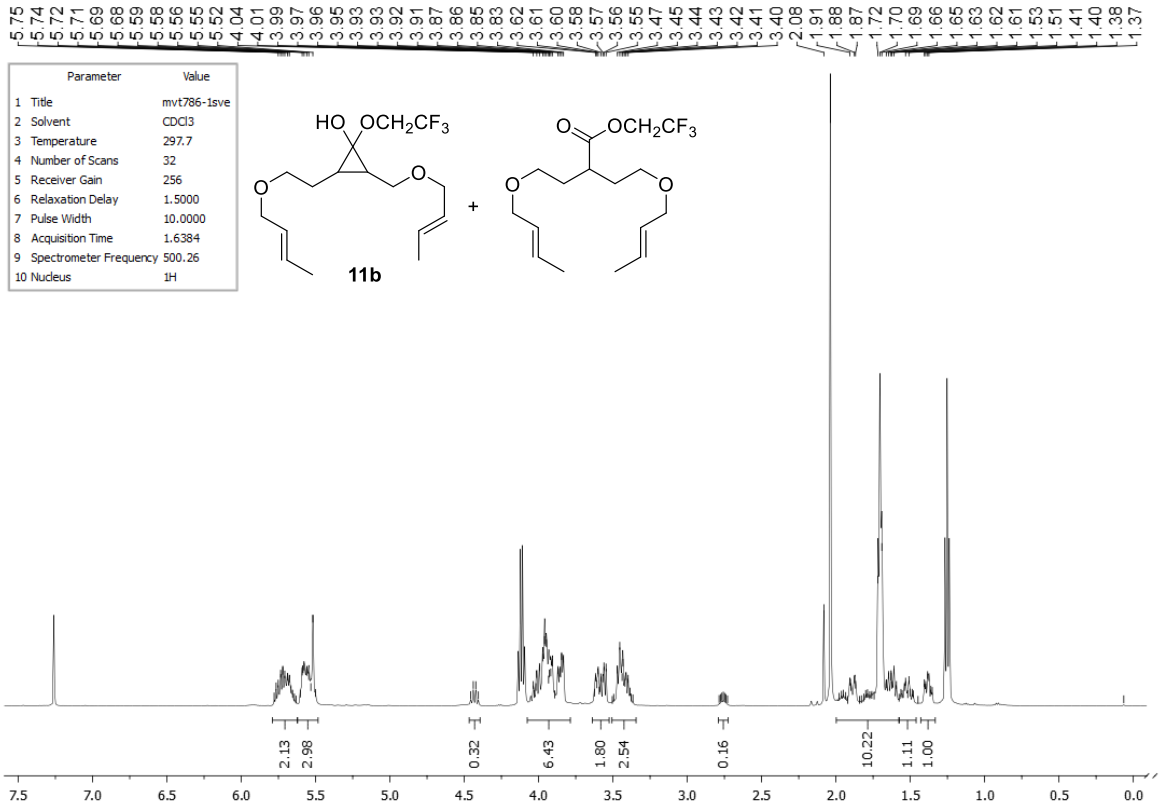
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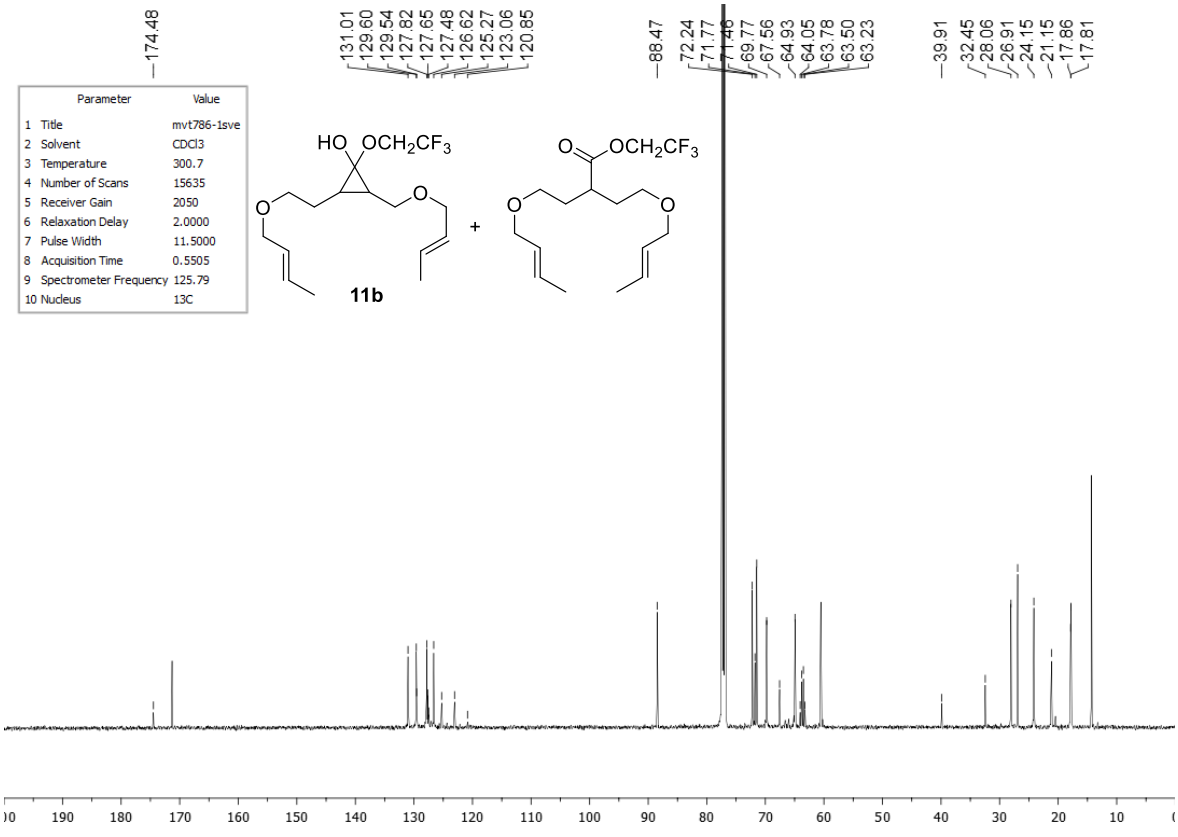
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11b

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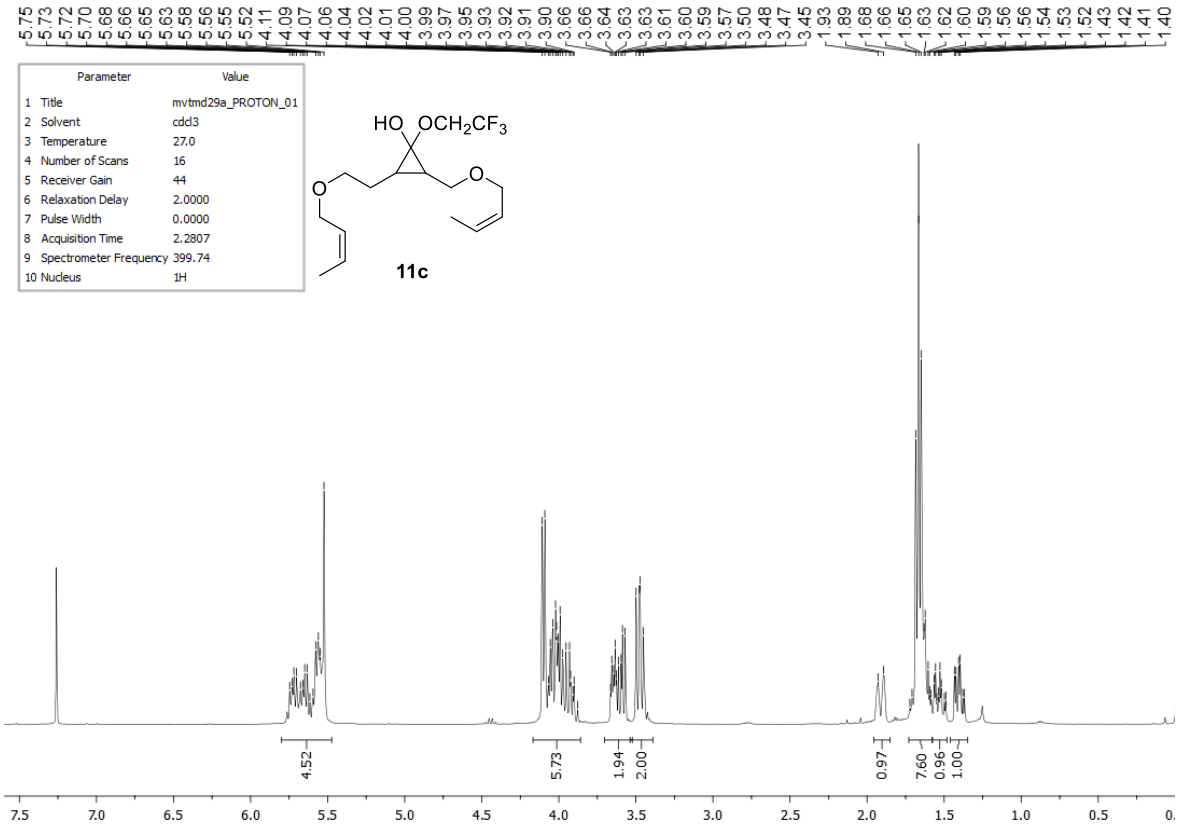
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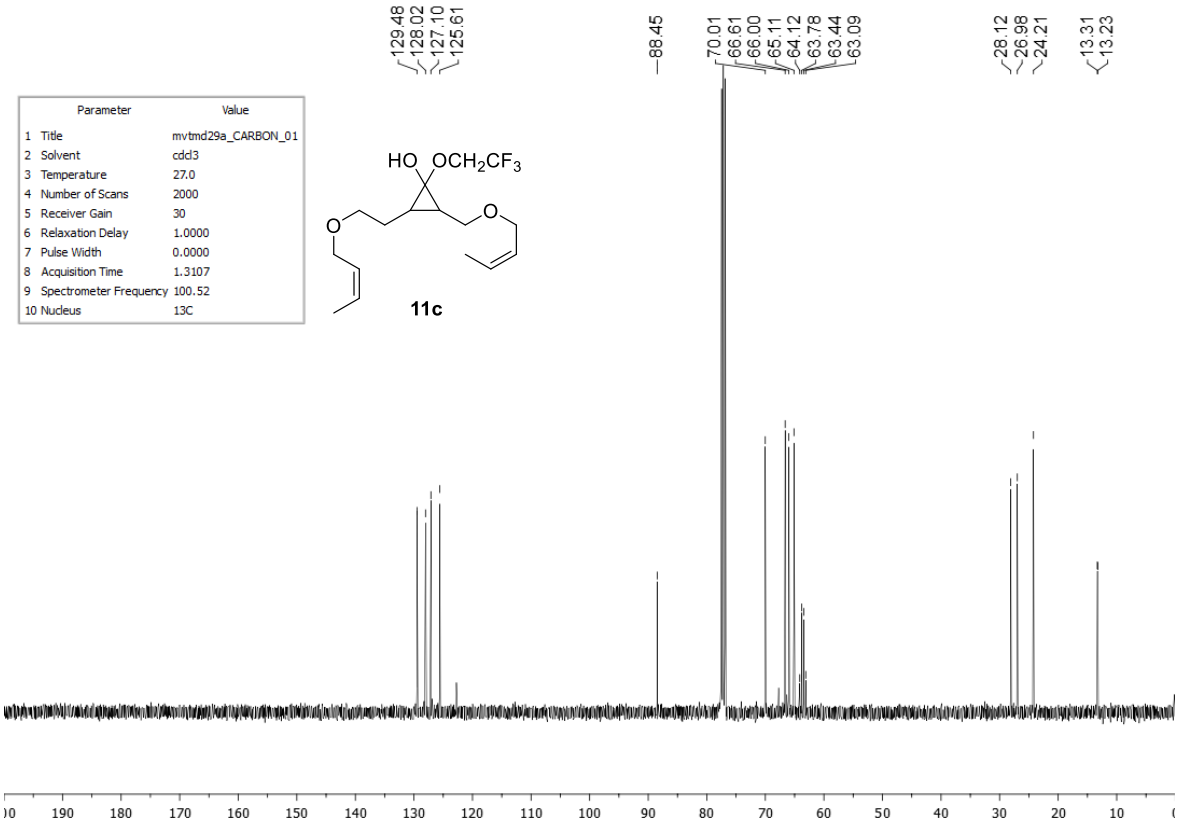
11c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10 Nucleus 13C
HO OCH2CF3
11c

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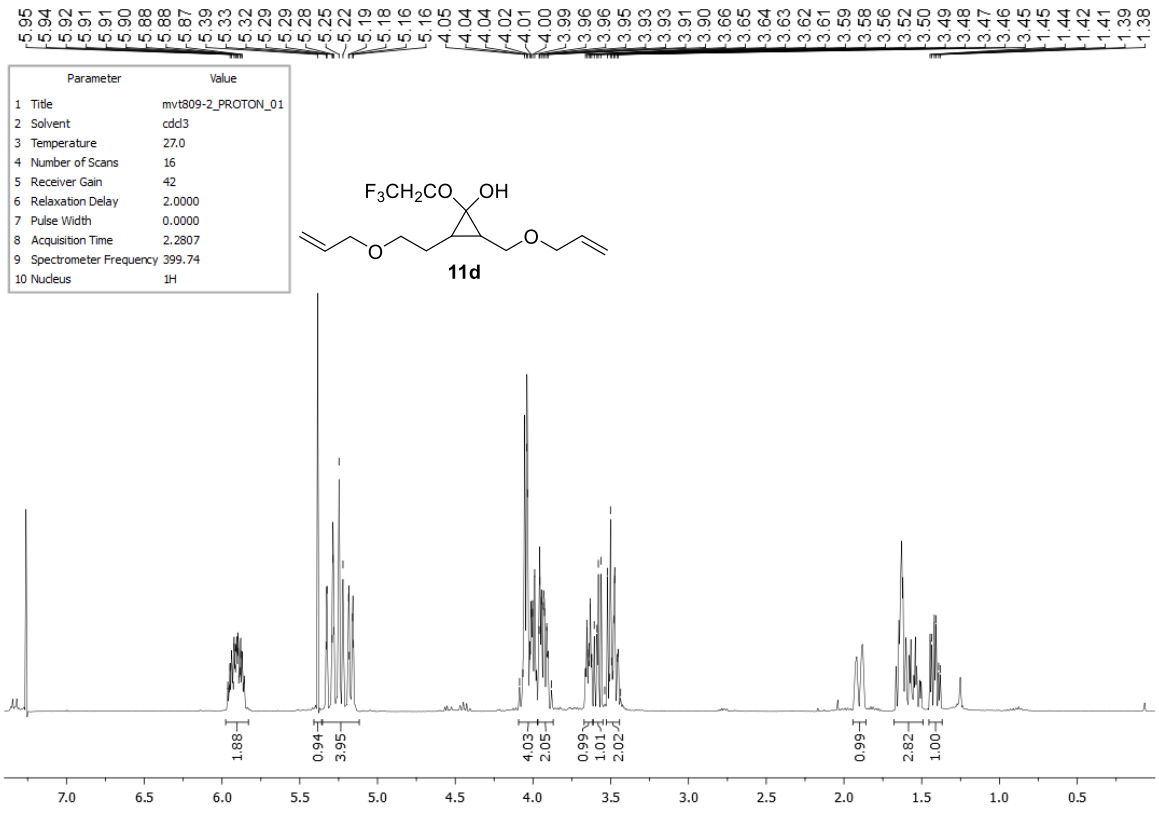
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1.88 0.94 3.95 4.03 2.05 0.99 1.01 2.02 0.99 2.82 1.00
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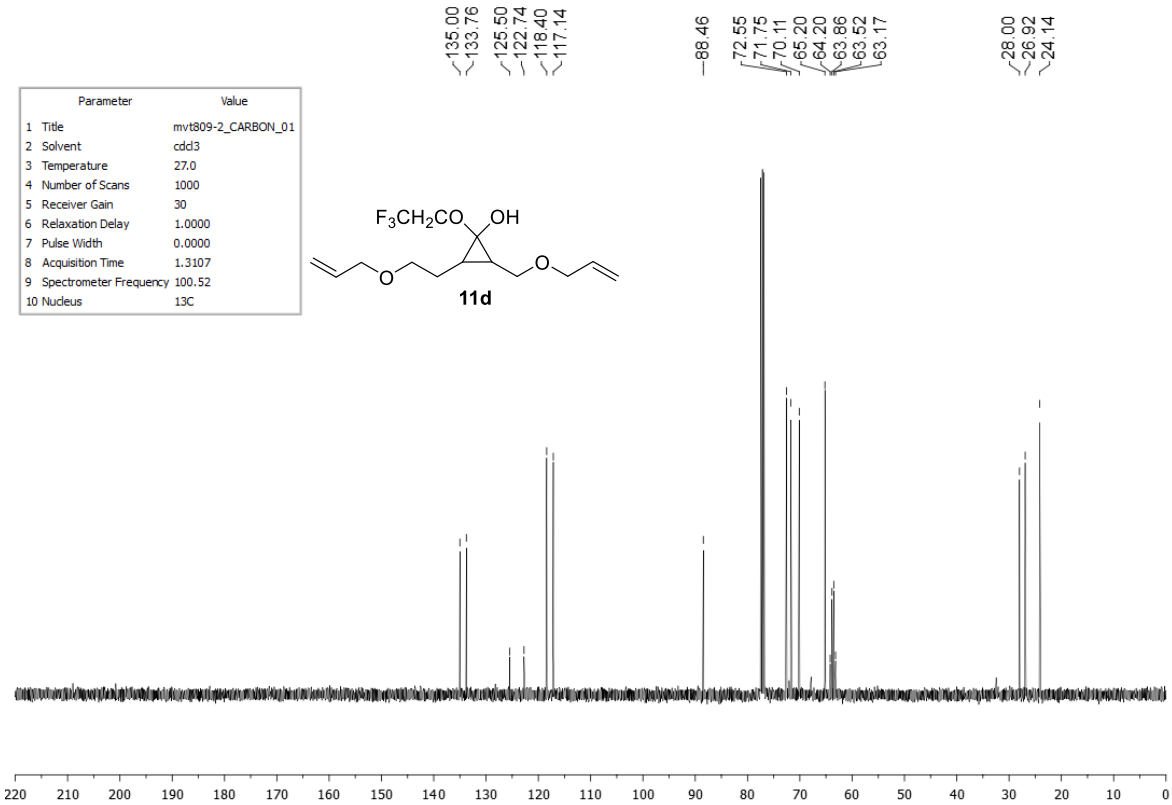
135.00 133.76 125.50 122.74 118.40 117.14 88.46 72.55 71.75 70.11 65.20 64.20 63.86 63.52 63.17 28.00 26.92 24.14
Parameter Value
1 Title mvt809-2_CARBON_01
2 Solvent cdcl3
3 Temperature 27.0
4 Number of Scans 1000
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
F3CH2CO OH
O
O
11d
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

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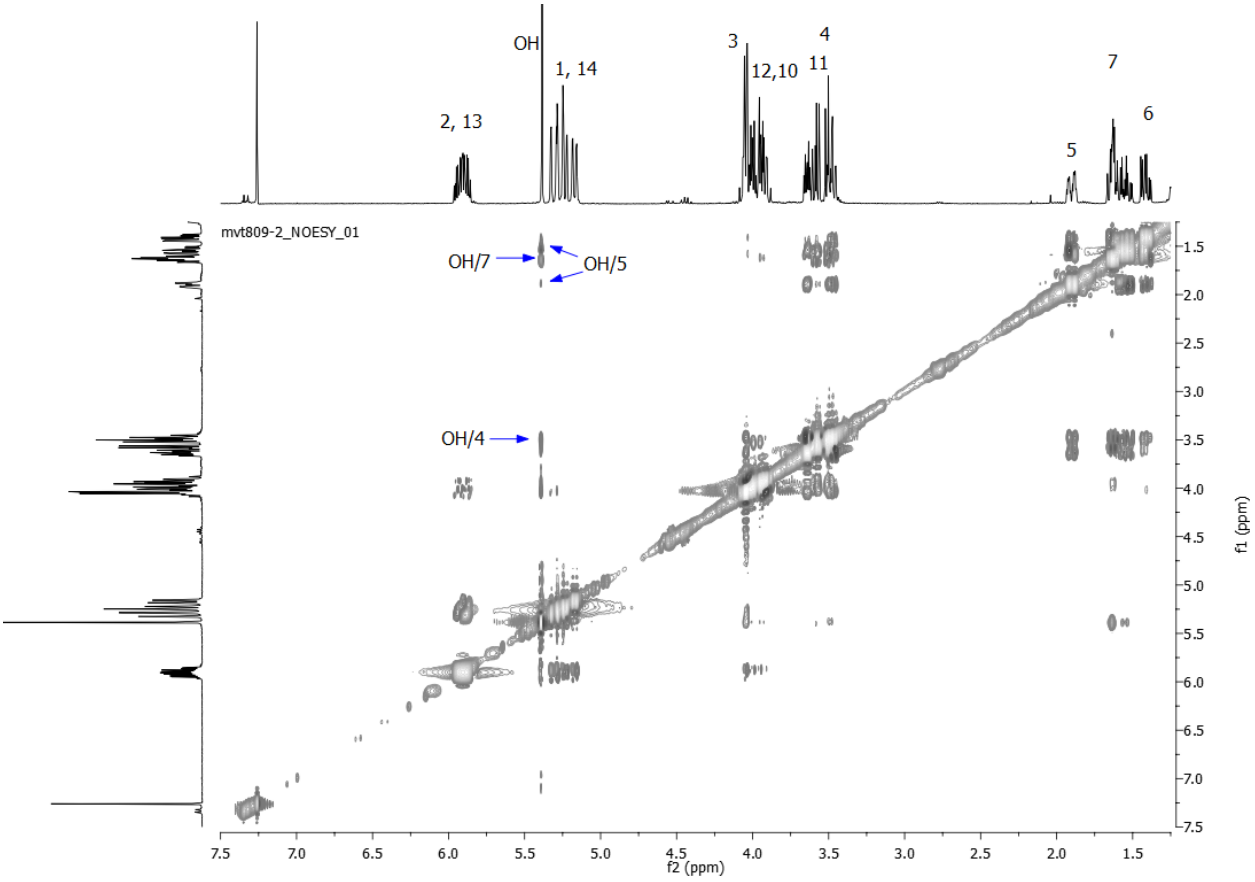

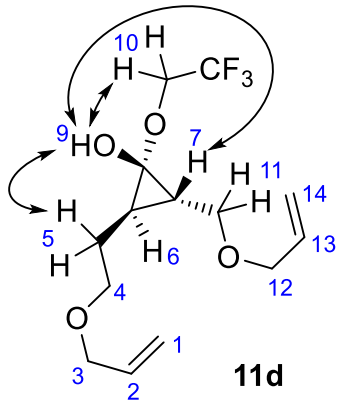

11d

NOESY correlations

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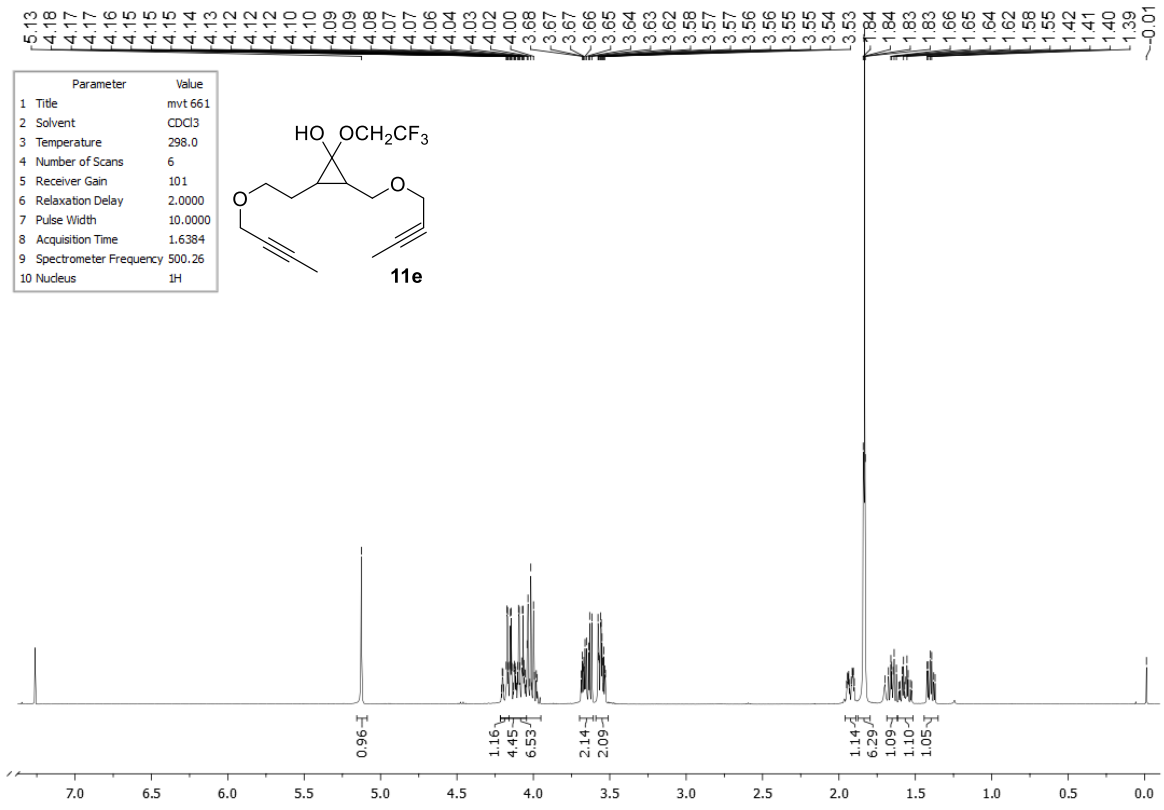
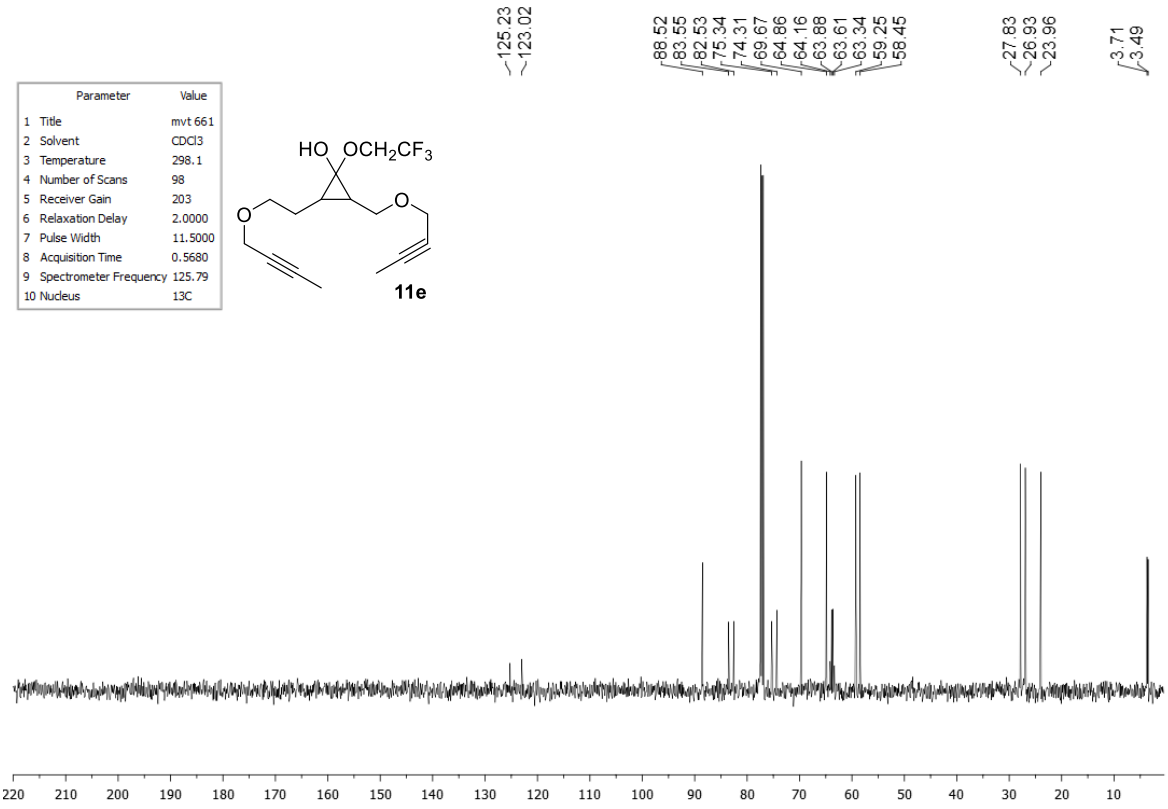

Parameter Value
1 Title mvt 661
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 6
5 Receiver Gain 101
6 Relaxation Delay 2.0000
7 Pulse Width 10.0000
8 Acquisition Time 1.6384
9 Spectrometer Frequency 500.26
10 Nucleus 1H
HO OCH2CF3
O
O
11e


Parameter Value
1 Title mvt 661
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 98
5 Receiver Gain 203
6 Relaxation Delay 2.0000
7 Pulse Width 11.5000
8 Acquisition Time 0.5680
9 Spectrometer Frequency 125.79
10 Nucleus 13C
HO OCH2CF3
O
O
11e

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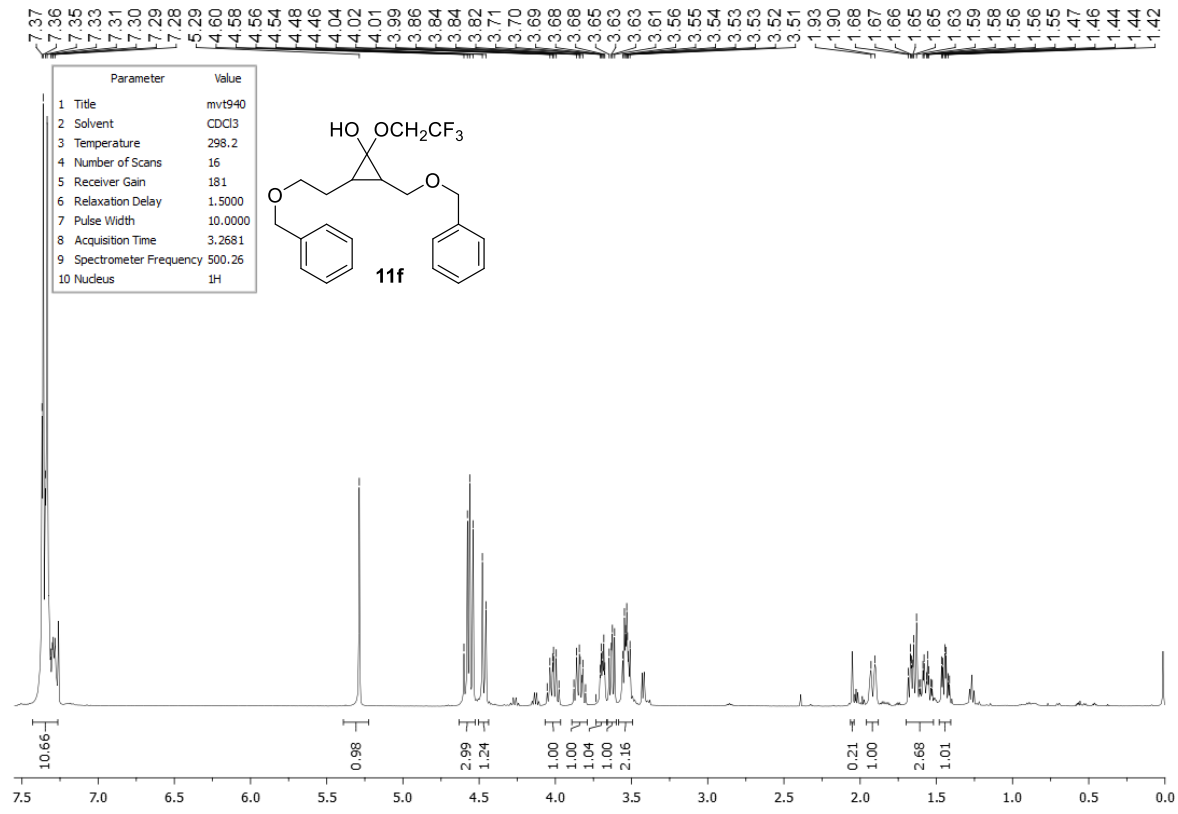
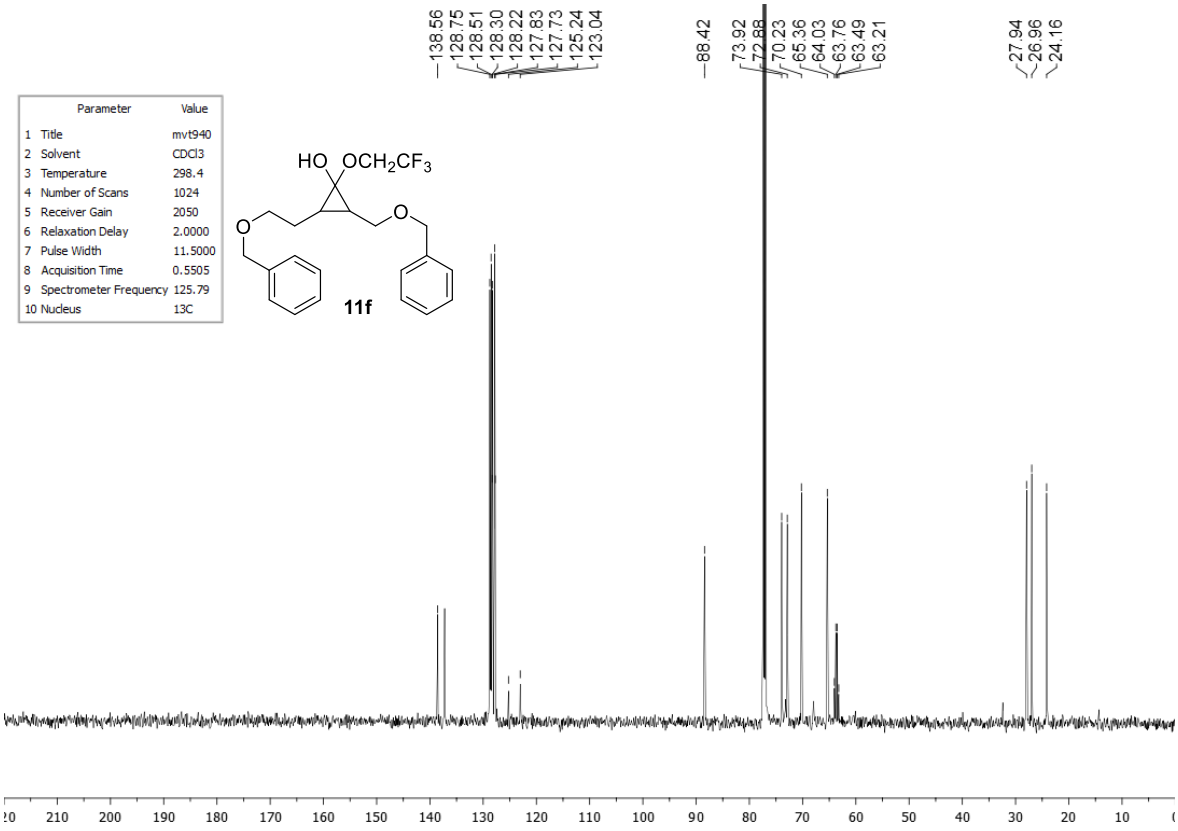
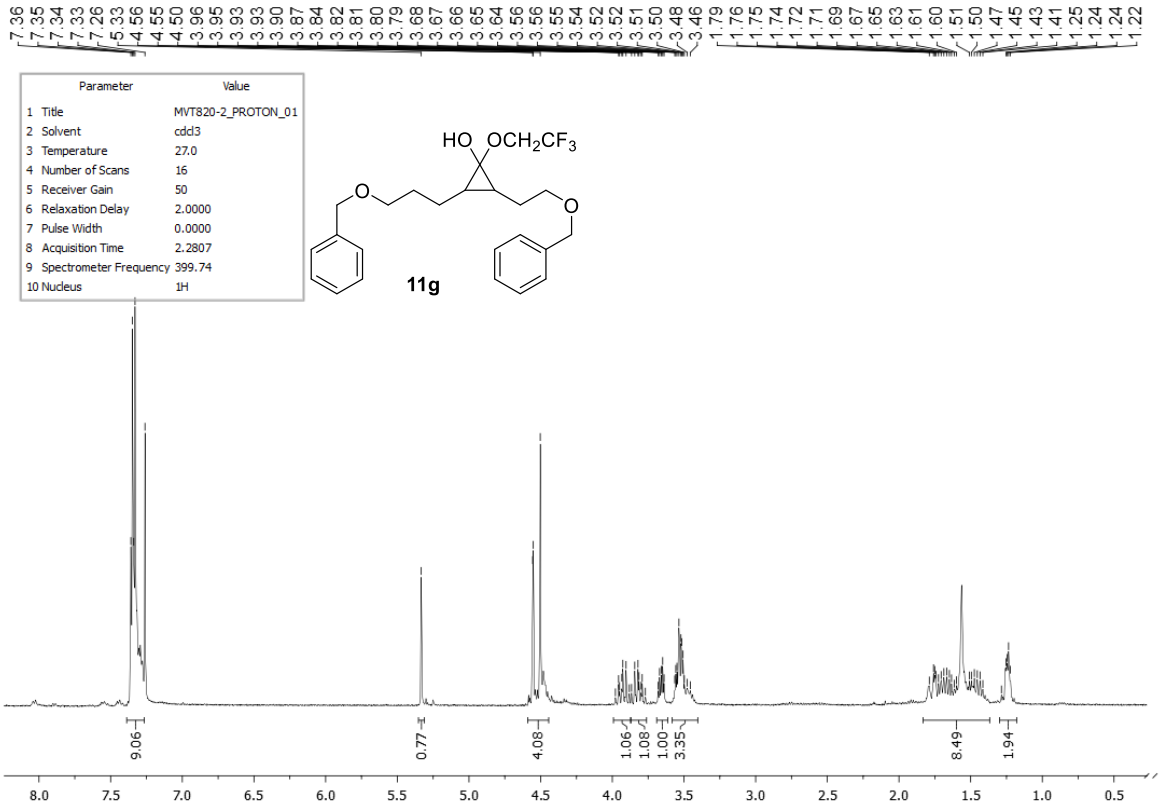
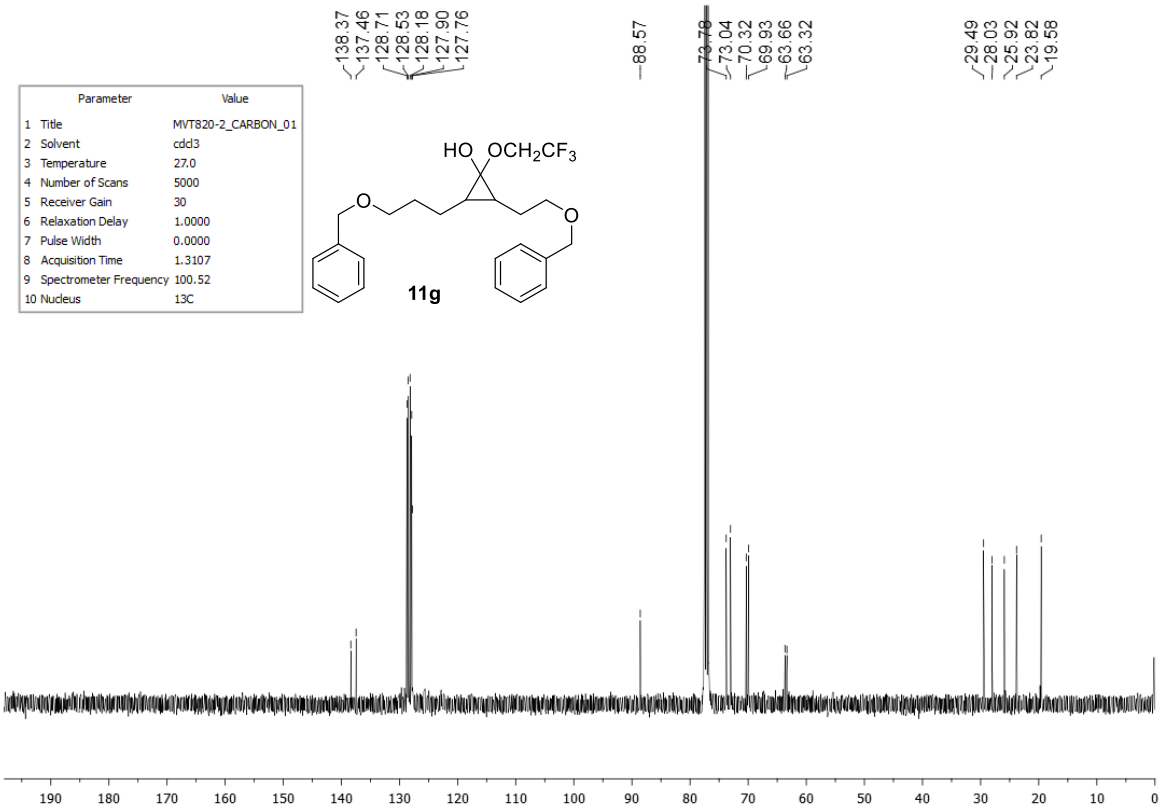

Parameter Value
1 Title mvt940
2 Solvent CDCl3
3 Temperature 298.2
4 Number of Scans 16
5 Receiver Gain 181
6 Relaxation Delay 1.5000
7 Pulse Width 10.0000
8 Acquisition Time 3.2681
9 Spectrometer Frequency 500.26
10 Nucleus 1H
HO OCH2CF3
O
O
11f


Parameter Value
1 Title mvt940
2 Solvent CDCl3
3 Temperature 298.4
4 Number of Scans 1024
5 Receiver Gain 2050
6 Relaxation Delay 2.0000
7 Pulse Width 11.5000
8 Acquisition Time 0.5505
9 Spectrometer Frequency 125.79
10 Nucleus 13C
HO OCH2CF3
O
O
11f


7.36 7.35 7.34 7.33 7.26 5.33 4.56 4.55 4.50 3.96 3.95 3.93 3.93 3.90 3.87 3.84 3.82 3.81 3.80 3.79 3.68 3.67 3.66 3.65 3.64 3.56 3.56 3.55 3.54 3.52 3.52 3.51 3.50 3.48 3.46 1.79 1.76 1.75 1.74 1.72 1.71 1.69 1.67 1.65 1.63 1.61 1.60 1.51 1.50 1.47 1.45 1.43 1.41 1.25 1.24 1.24 1.22
Parameter Value
1 Title MVT820-2_PROTON_01
2 Solvent cdcl3
3 Temperature 27.0
4 Number of Scans 16
5 Receiver Gain 50
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.74
10 Nucleus 1H
HO OCH2CF3
O
O
11g
9.06
0.77
4.08
1.06
1.08
1.00
3.35
8.49
1.94
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5


138.37 137.46 128.71 128.53 128.18 127.90 127.76 88.57 73.78 73.04 70.32 69.93 63.66 63.32 29.49 28.03 25.92 23.82 19.58
Parameter Value
1 Title MVT820-2_CARBON_01
2 Solvent cdcl3
3 Temperature 27.0
4 Number of Scans 5000
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
HO OCH2CF3
O
O
11g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

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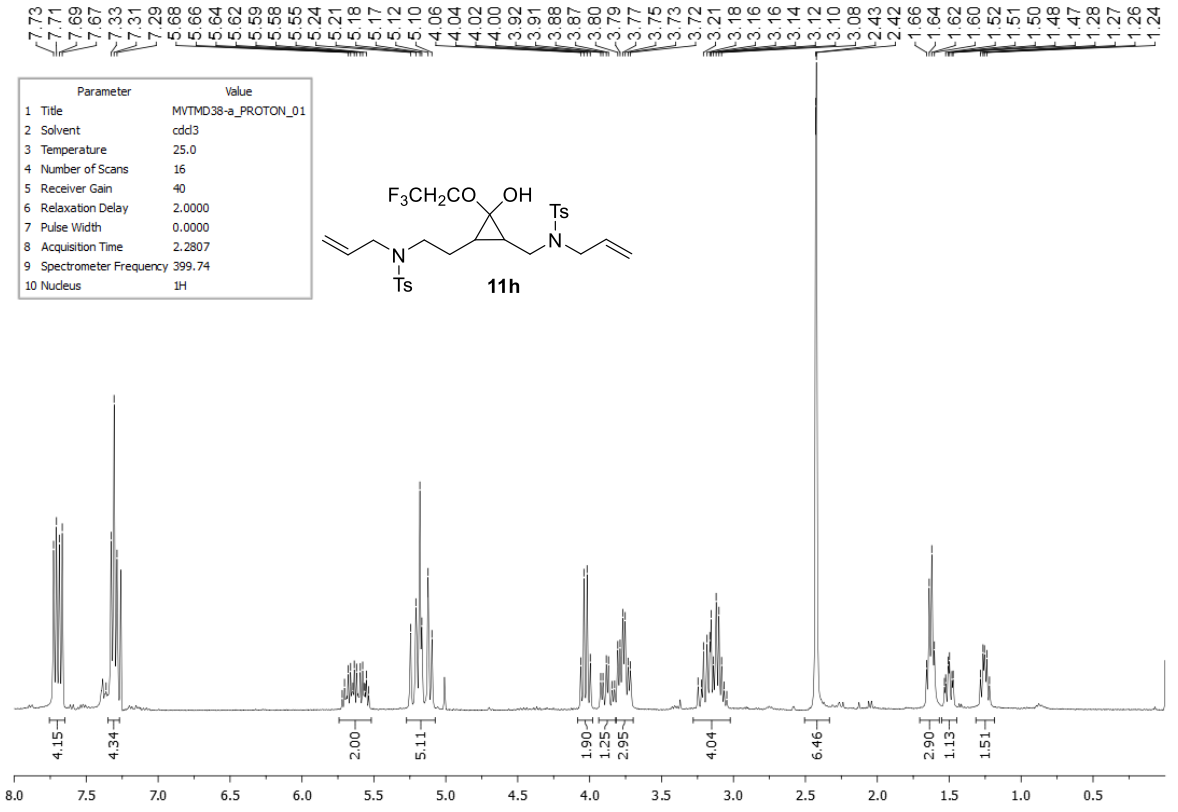
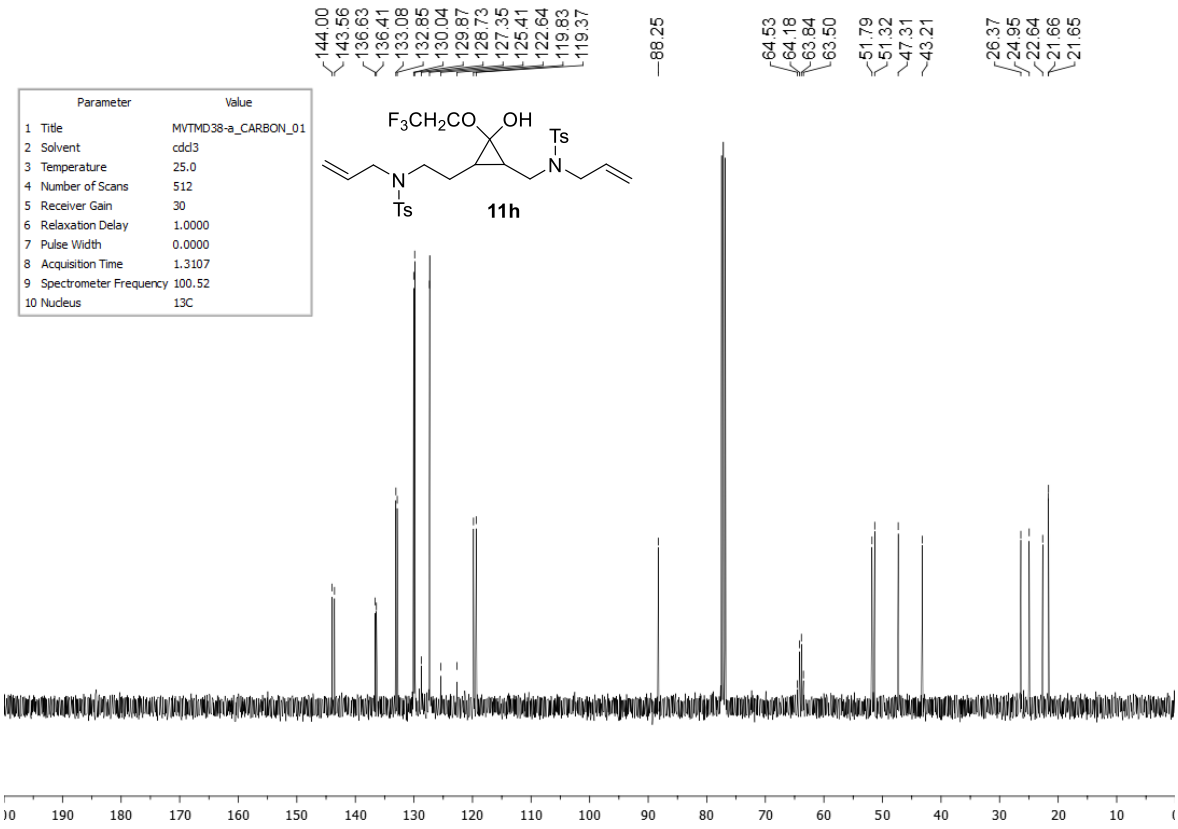

Parameter Value
1 Title MVTMD38-a_PROTON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 16
5 Receiver Gain 40
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.74
10 Nucleus 1H
F3CH2CO
OH
Ts
N
Ts
11h


Parameter Value
1 Title MVTMD38-a_CARBON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 512
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
F3CH2CO
OH
Ts
N
Ts
11h

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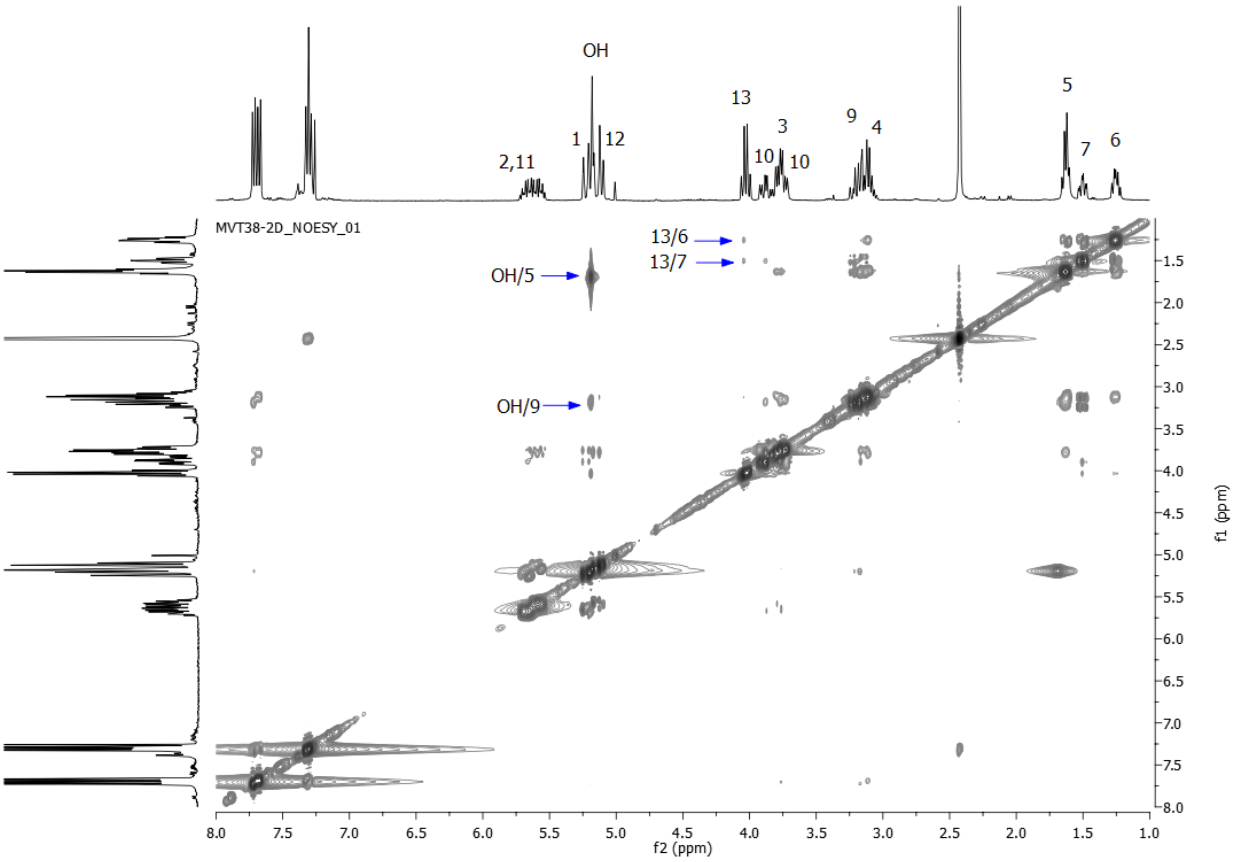

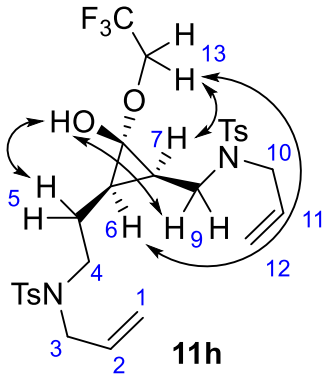

11h

NOESY correlations

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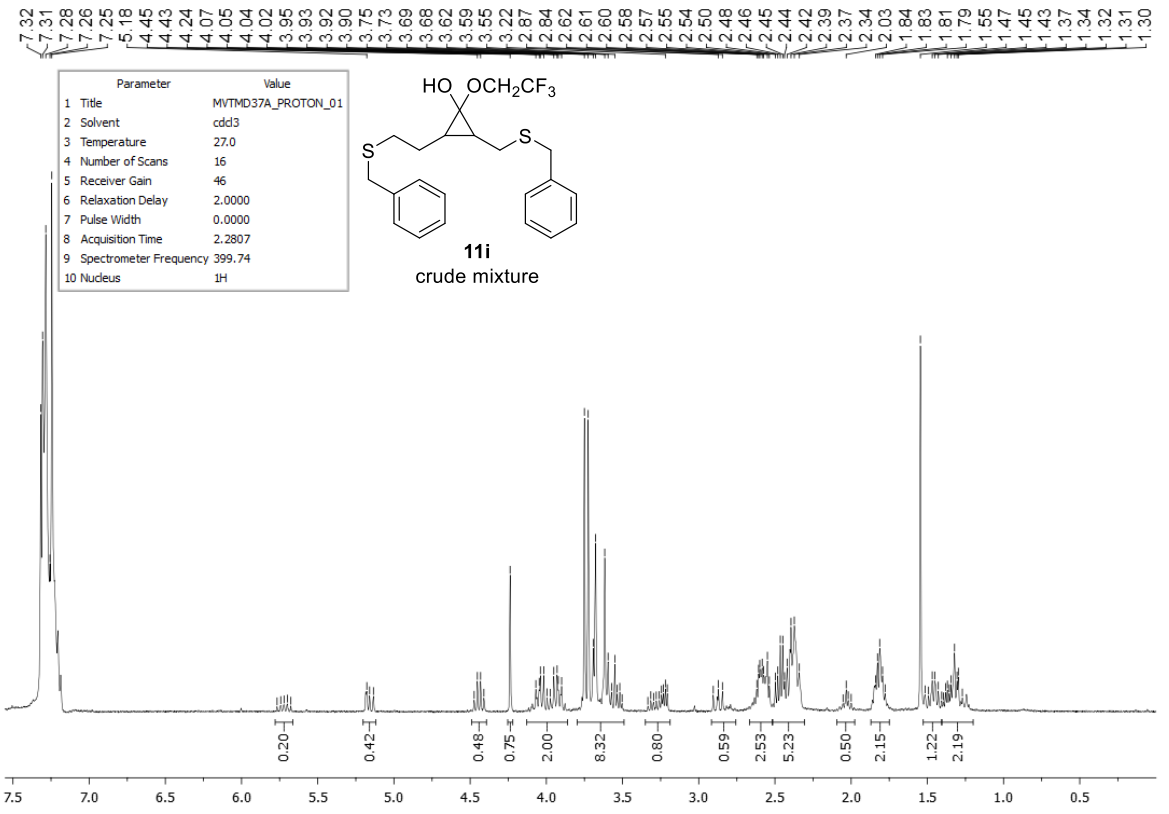
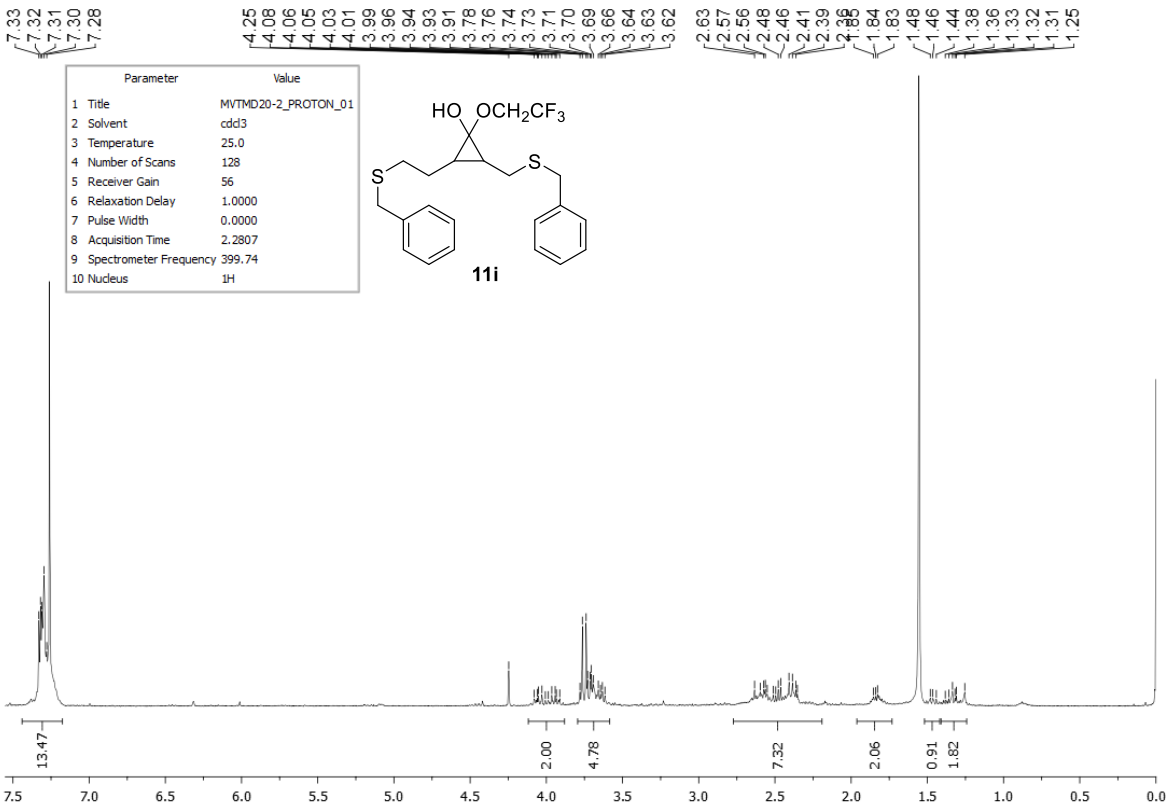

Parameter Value
1 Title MVTMD37A_PROTON_01
2 Solvent cdcl3
3 Temperature 27.0
4 Number of Scans 16
5 Receiver Gain 46
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.74
10 Nucleus 1H
HO OCH2CF3
S
S
11i
crude mixture


Parameter Value
1 Title MVTMD20-2_PROTON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 128
5 Receiver Gain 56
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.74
10 Nucleus 1H
HO OCH2CF3
S
S
11i

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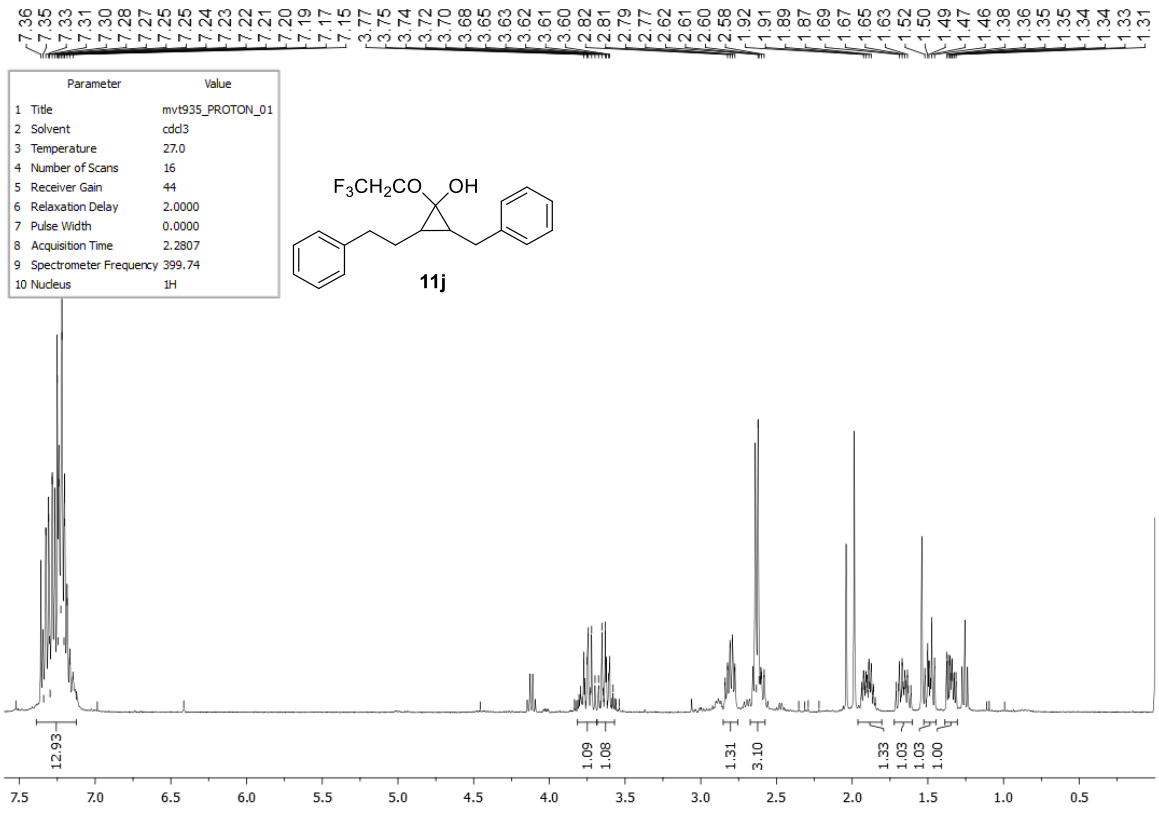
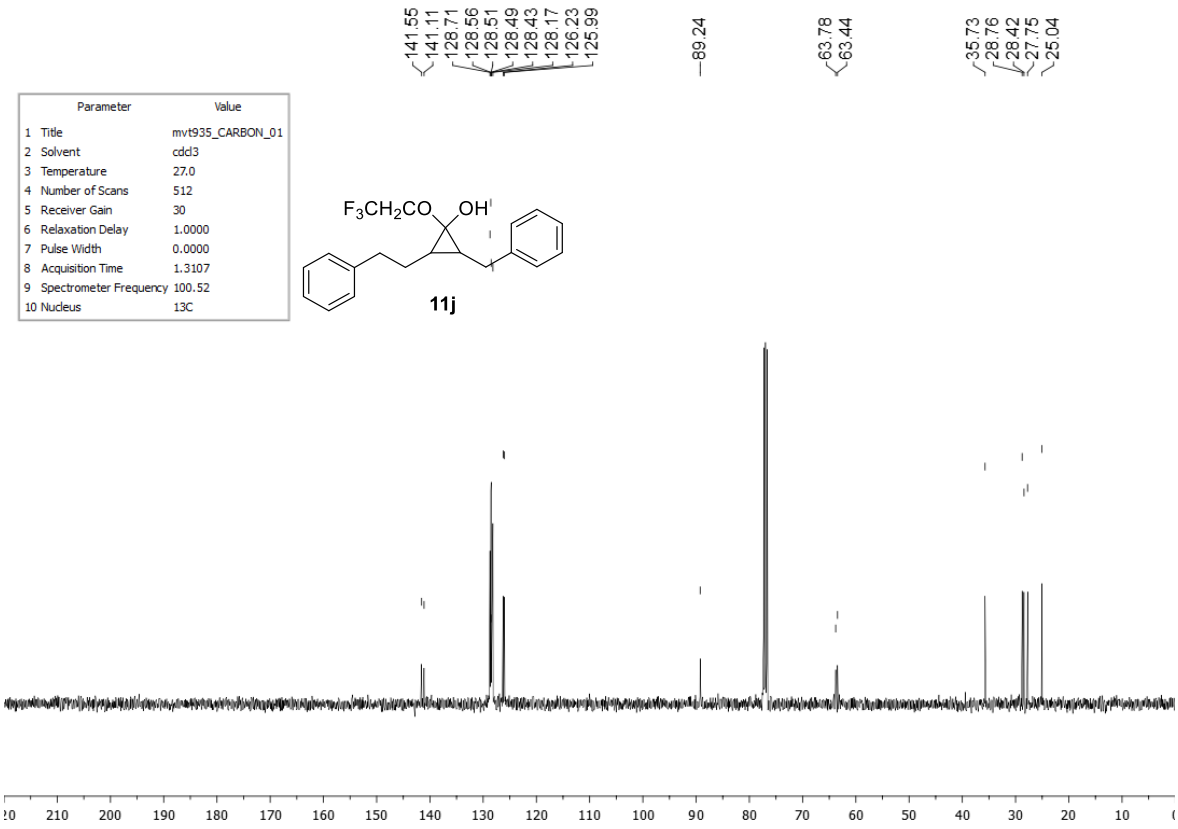
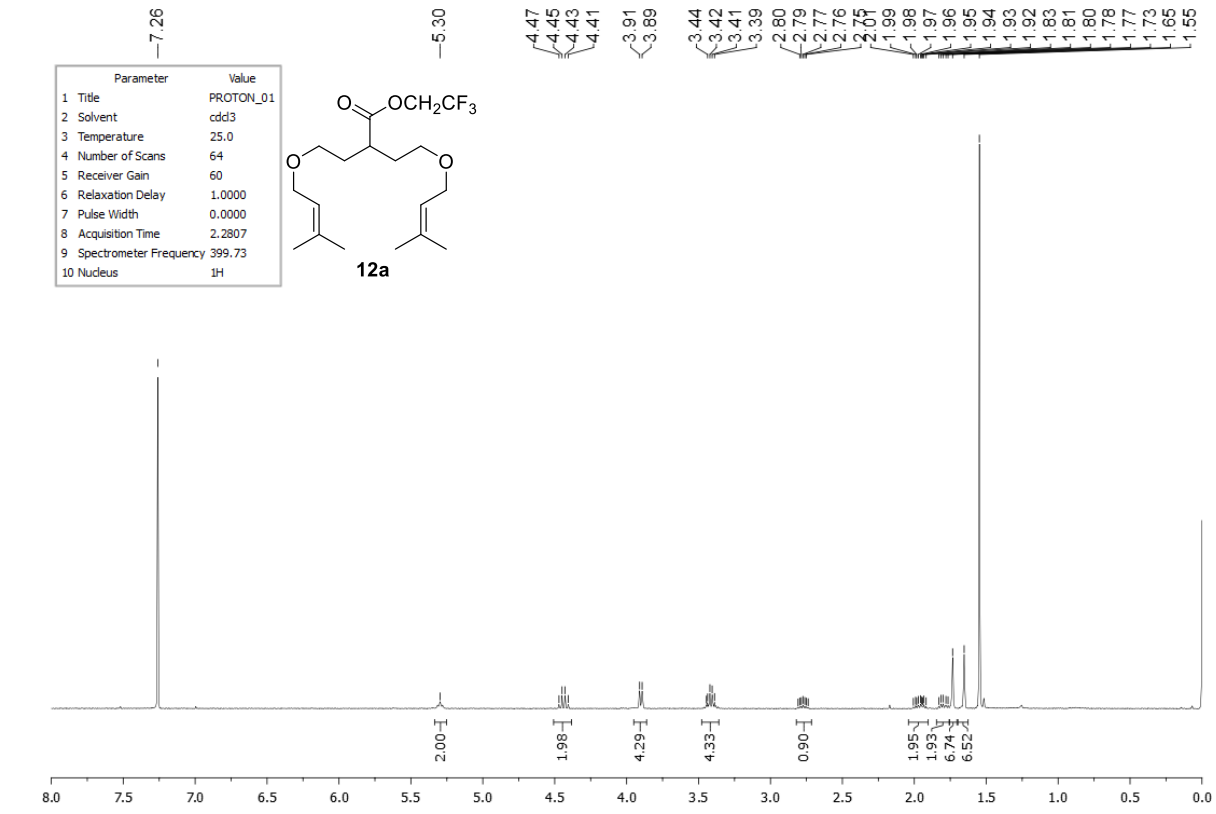
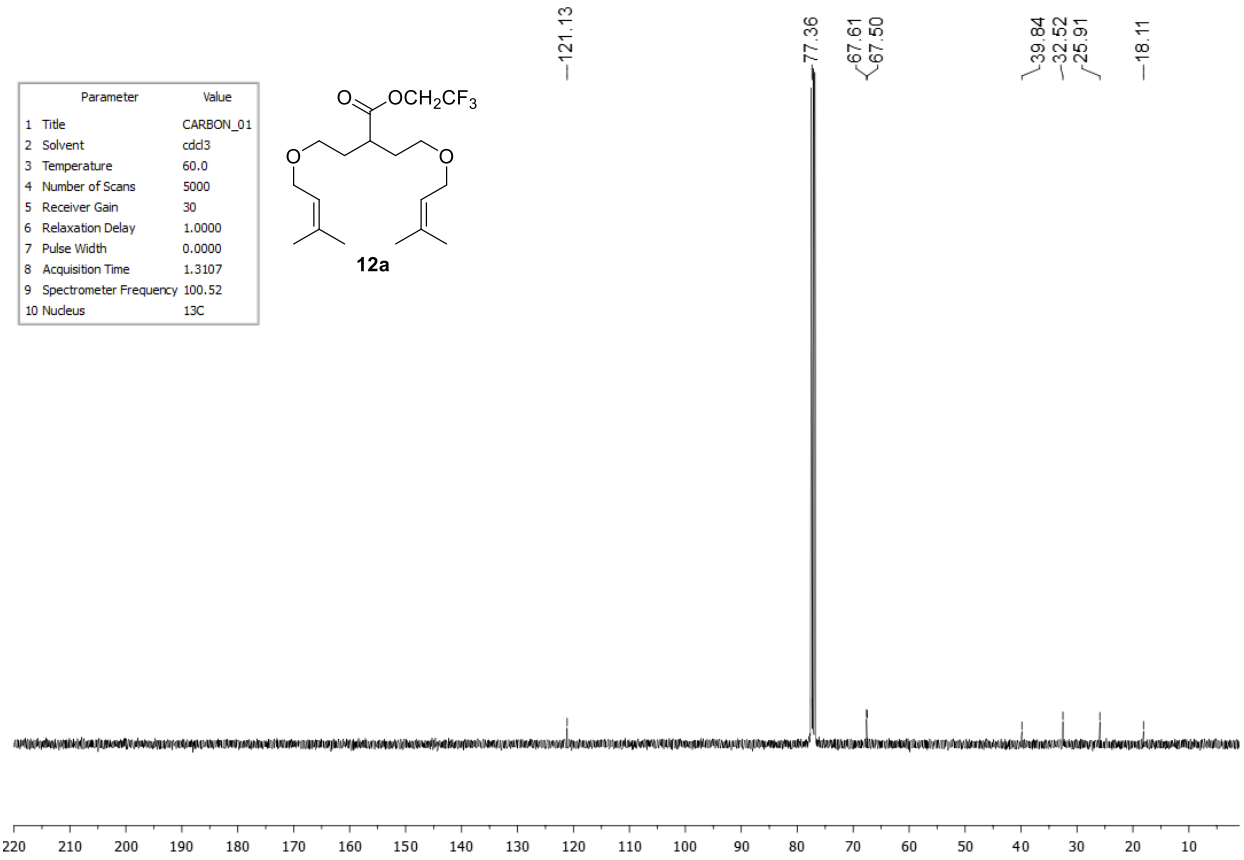
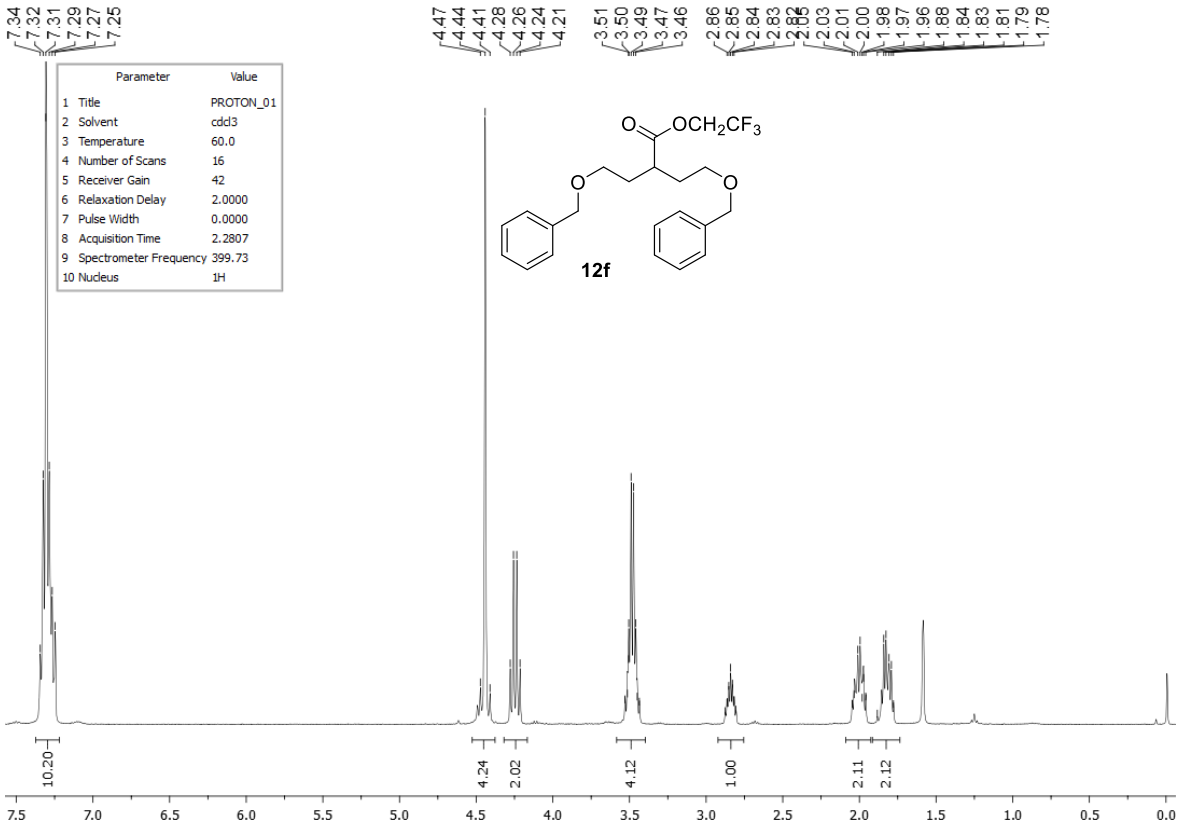
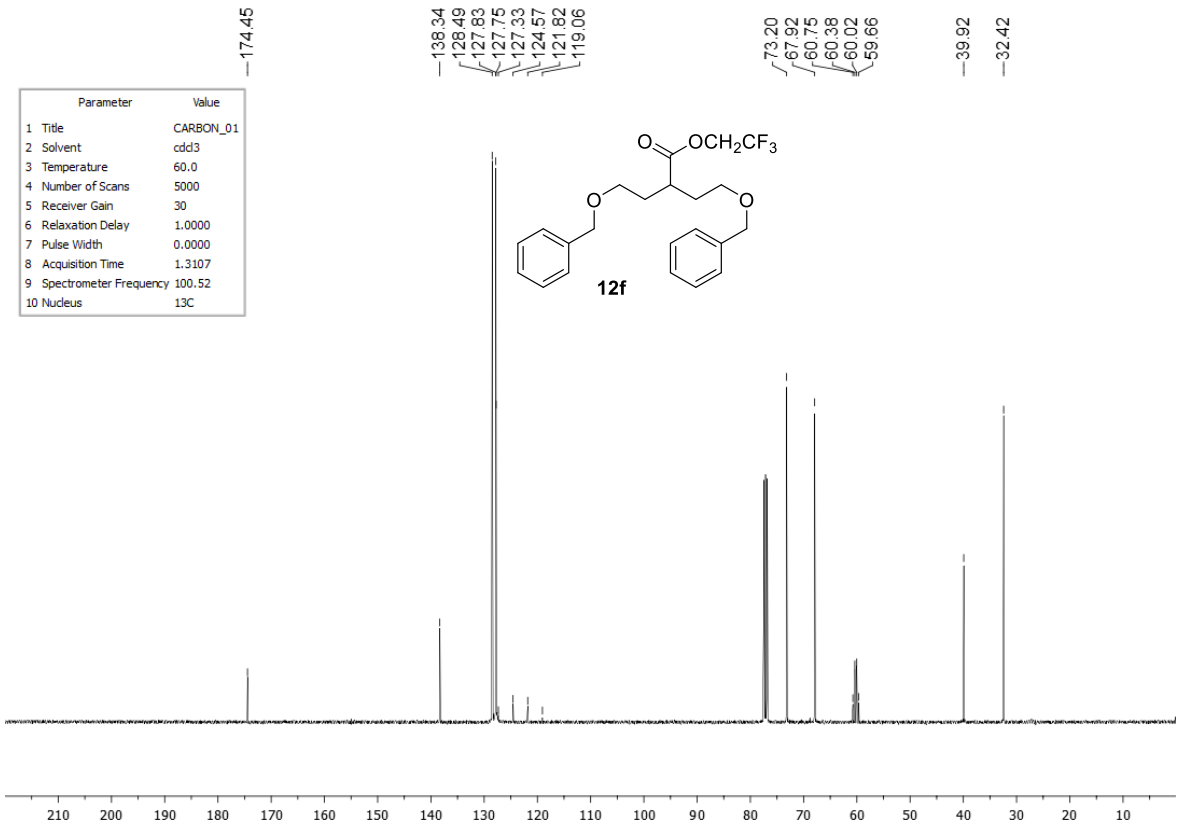

7.36 7.35 7.33 7.31 7.30 7.28 7.27 7.25 7.25 7.24 7.23 7.22 7.21 7.20 7.19 7.17 7.15 3.77 3.75 3.74 3.72 3.70 3.68 3.65 3.63 3.62 3.61 3.60 2.82 2.81 2.79 2.77 2.62 2.61 2.60 2.58 1.92 1.91 1.89 1.87 1.69 1.67 1.65 1.63 1.52 1.50 1.49 1.47 1.46 1.38 1.36 1.35 1.35 1.34 1.34 1.33 1.31
Parameter Value
1 Title mvt935_PROTON_01
2 Solvent cdcl3
3 Temperature 27.0
4 Number of Scans 16
5 Receiver Gain 44
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.74
10 Nucleus 1H
F3CH2CO OH
11j
12.93 1.09 1.08 1.31 3.10 1.33 1.03 1.03 1.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5


141.55 141.11 128.71 128.56 128.51 128.49 128.43 128.17 126.23 125.99 89.24 63.78 63.44 35.73 28.76 28.42 27.75 25.04
Parameter Value
1 Title mvt935_CARBON_01
2 Solvent cdcl3
3 Temperature 27.0
4 Number of Scans 512
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
F3CH2CO OH
11j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


7.26
5.30
4.47
4.45
4.43
4.41
3.91
3.89
3.44
3.42
3.41
3.39
2.80
2.79
2.77
2.76
2.75
2.01
1.99
1.98
1.97
1.96
1.95
1.94
1.93
1.92
1.83
1.81
1.80
1.78
1.77
1.73
1.65
1.55
Parameter Value
1 Title PROTON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 64
5 Receiver Gain 60
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.73
10 Nucleus 1H
O
OCH2CF3
O
O
12a
2.00
1.98
4.29
4.33
0.90
1.95
1.93
6.74
6.52
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


121.13
77.36
67.61
67.50
39.84
32.52
25.91
18.11
Parameter Value
1 Title CARBON_01
2 Solvent cdcl3
3 Temperature 60.0
4 Number of Scans 5000
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
O
OCH2CF3
O
O
12a
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


7.34
7.32
7.31
7.29
7.27
7.25
4.47
4.44
4.41
4.28
4.26
4.24
4.21
3.51
3.50
3.49
3.47
3.46
2.86
2.85
2.84
2.83
2.03
2.01
2.00
1.98
1.97
1.96
1.88
1.84
1.83
1.81
1.79
1.78
Parameter Value
1 Title PROTON_01
2 Solvent cdcl3
3 Temperature 60.0
4 Number of Scans 16
5 Receiver Gain 42
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.73
10 Nucleus 1H
O
OCH2CF3
O
O
12f
10.20
4.24
2.02
4.12
1.00
2.11
2.12
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


174.45
138.34
128.49
127.83
127.75
127.33
124.57
121.82
119.06
73.20
67.92
60.75
60.38
60.02
59.66
39.92
32.42
Parameter Value
1 Title CARBON_01
2 Solvent cdcl3
3 Temperature 60.0
4 Number of Scans 5000
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
O
OCH2CF3
O
O
12f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

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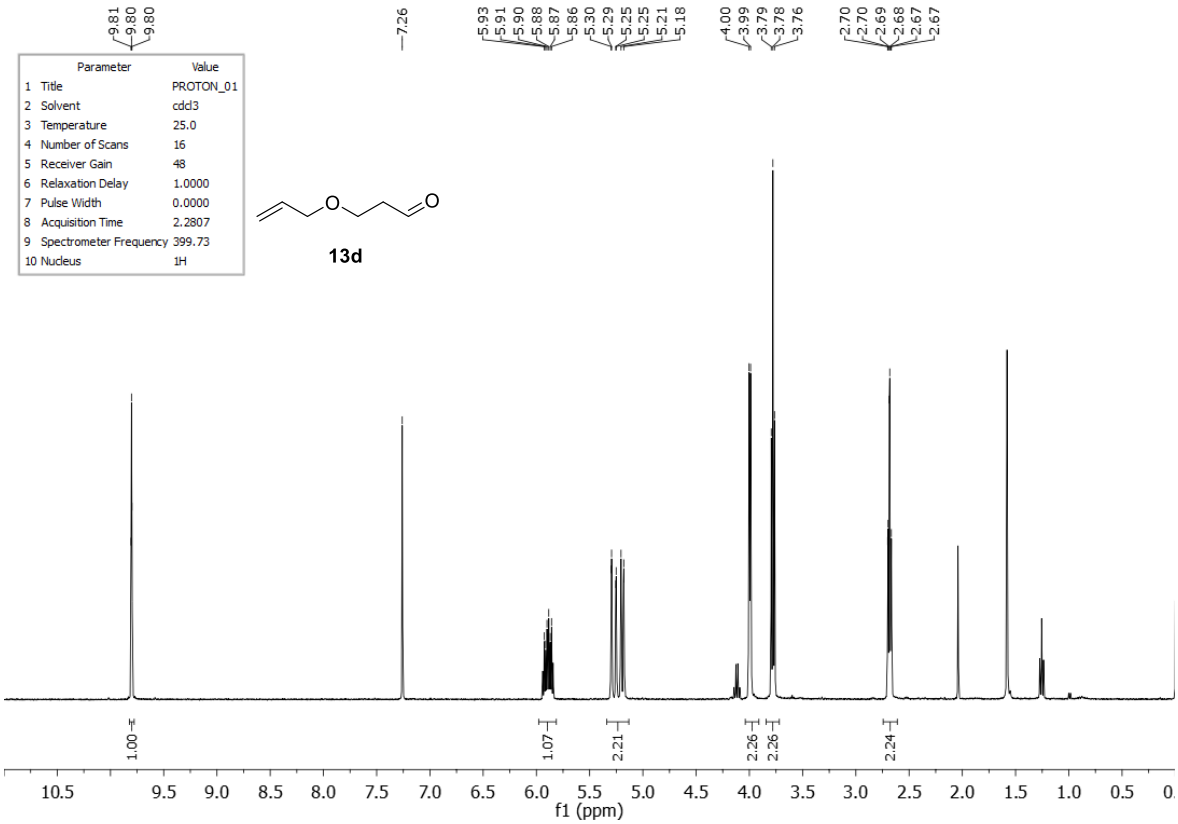
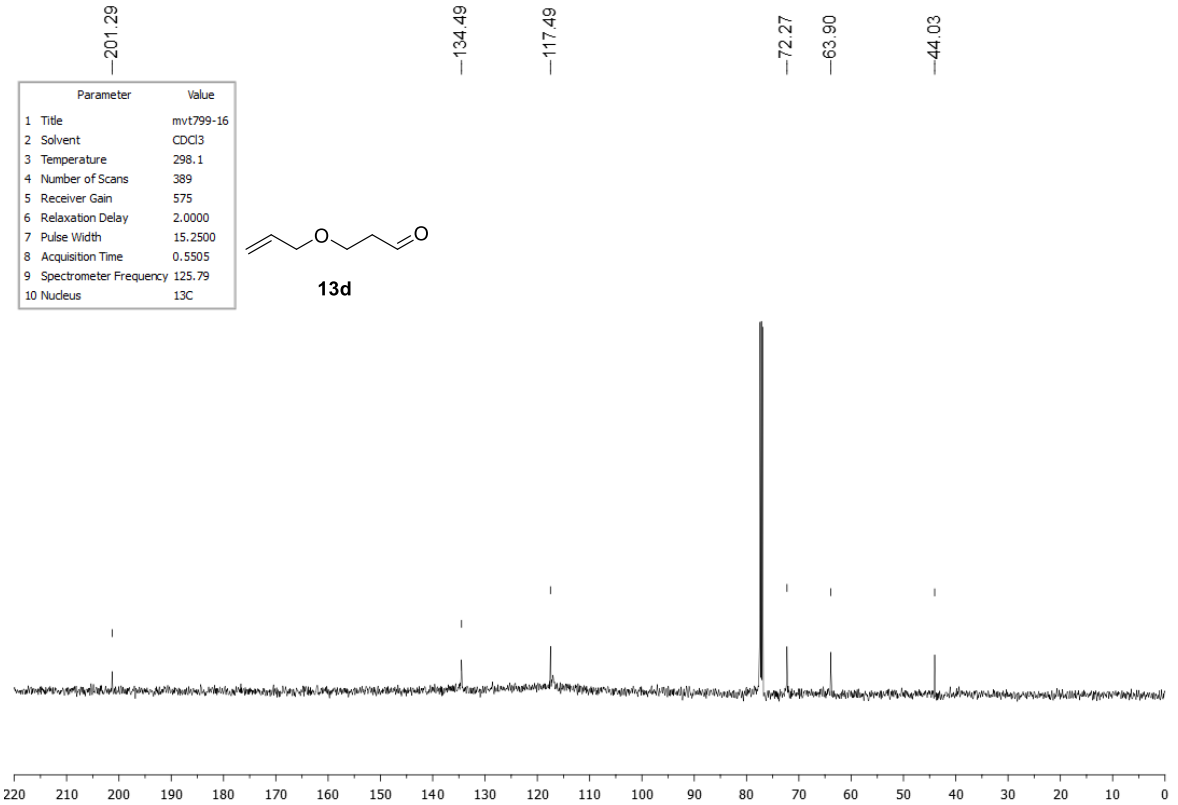

9.81
9.80
9.80
7.26
5.93
5.91
5.90
5.88
5.87
5.86
5.30
5.29
5.25
5.25
5.21
5.18
4.00
3.99
3.79
3.78
3.76
2.70
2.70
2.69
2.68
2.67
2.67
Parameter Value
1 Title PROTON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 16
5 Receiver Gain 48
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.73
10 Nucleus 1H
13d
1.00
1.07
2.21
2.26
2.26
2.24
f1 (ppm)


201.29
134.49
117.49
72.27
63.90
44.03
Parameter Value
1 Title mvt799-16
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 389
5 Receiver Gain 575
6 Relaxation Delay 2.0000
7 Pulse Width 15.2500
8 Acquisition Time 0.5505
9 Spectrometer Frequency 125.79
10 Nucleus 13C
13d

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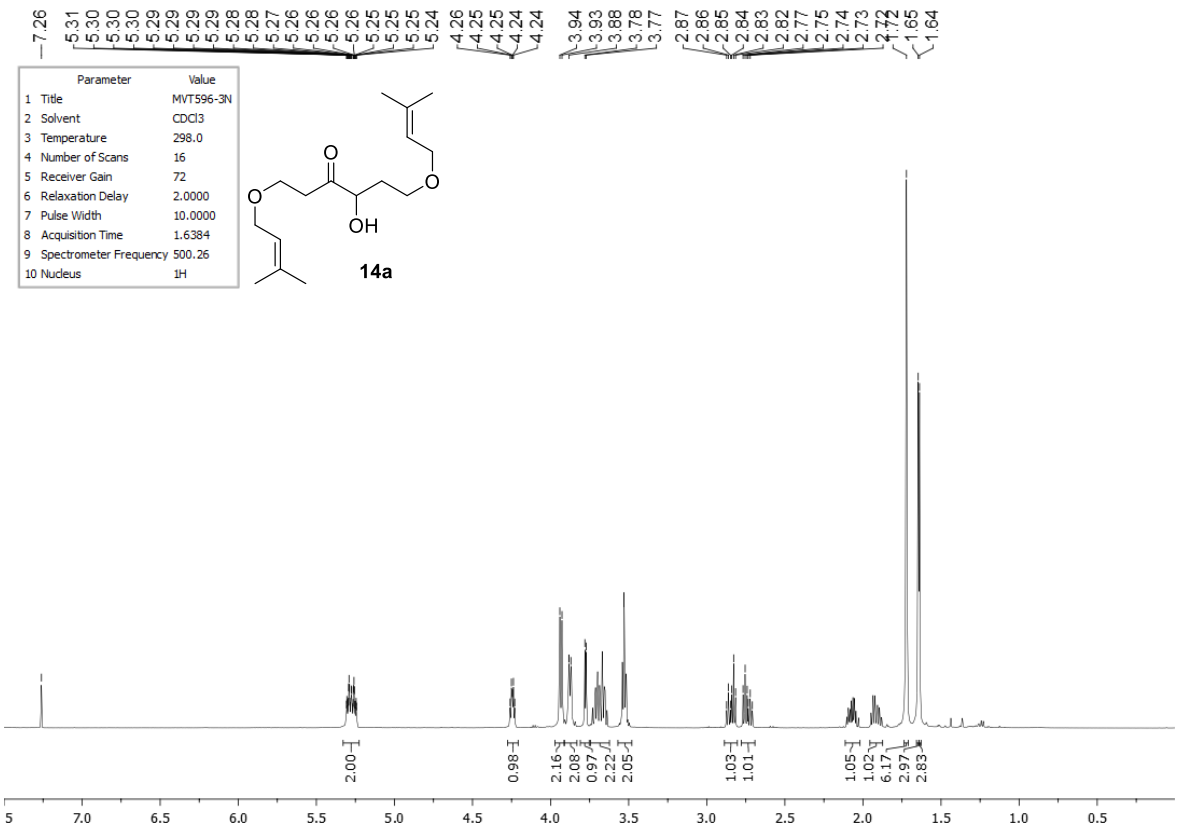
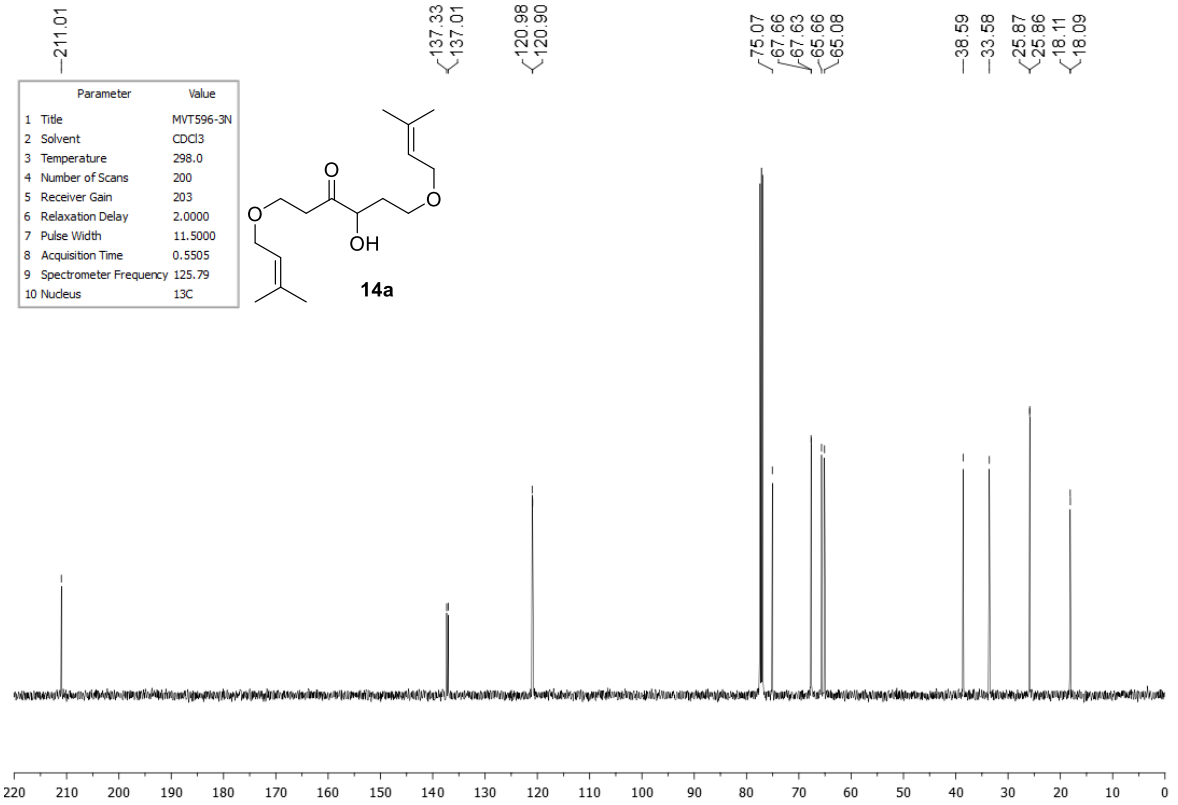

7.26
5.31
5.30
5.30
5.30
5.29
5.29
5.29
5.29
5.28
5.28
5.27
5.26
5.26
5.26
5.26
5.25
5.25
5.25
5.24
4.26
4.25
4.25
4.24
4.24
3.94
3.93
3.88
3.78
3.77
2.87
2.86
2.85
2.84
2.83
2.82
2.77
2.75
2.74
2.73
1.72
1.65
1.64
Parameter Value
1 Title MVT596-3N
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 16
5 Receiver Gain 72
6 Relaxation Delay 2.0000
7 Pulse Width 10.0000
8 Acquisition Time 1.6384
9 Spectrometer Frequency 500.26
10 Nucleus 1H
O
O
O
OH
14a
2.00
0.98
2.16
2.08
0.97
2.22
2.05
1.03
1.01
1.05
1.02
6.17
2.97
2.83
5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5


211.01
137.33
137.01
120.98
120.90
75.07
67.66
67.63
65.66
65.08
38.59
33.58
25.87
25.86
18.11
18.09
Parameter Value
1 Title MVT596-3N
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 200
5 Receiver Gain 203
6 Relaxation Delay 2.0000
7 Pulse Width 11.5000
8 Acquisition Time 0.5505
9 Spectrometer Frequency 125.79
10 Nucleus 13C
O
O
O
OH
14a
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

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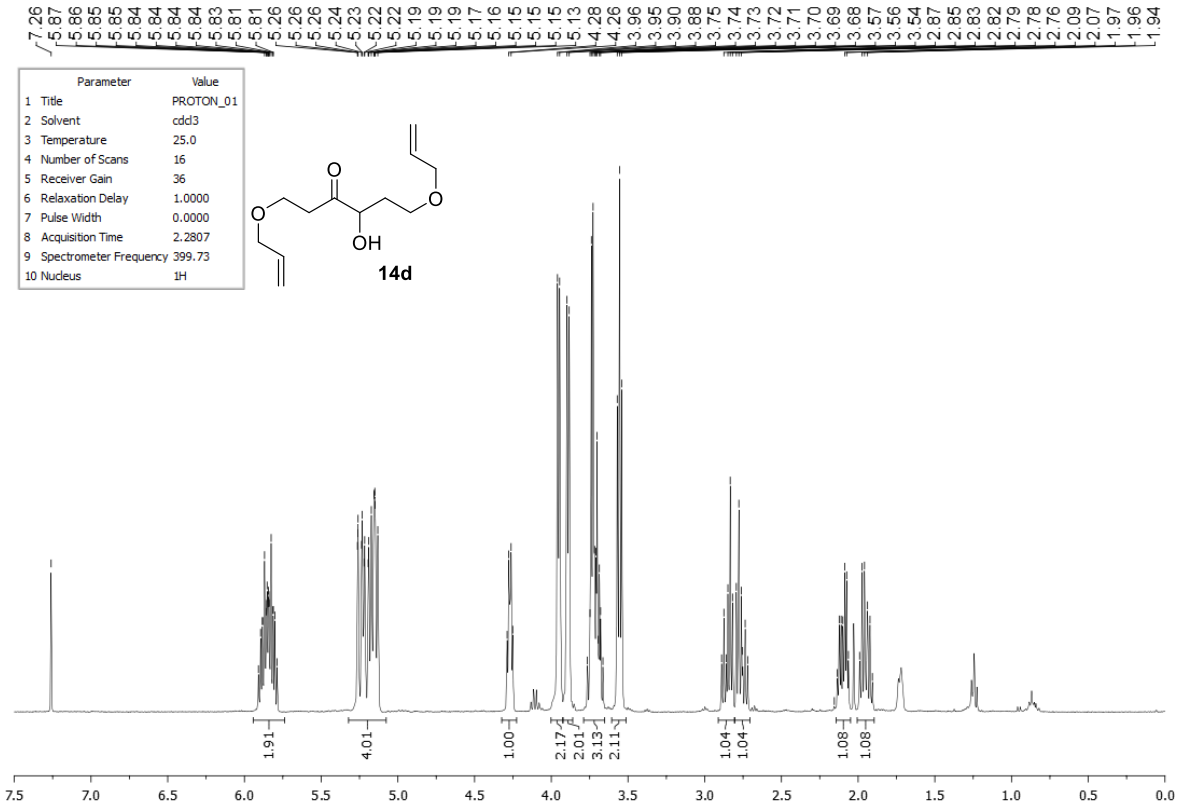
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Parameter Value
1 Title PROTON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 16
5 Receiver Gain 36
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.73
10 Nucleus 1H
O
O
O
OH
14d
1.91 4.01 1.00 2.17 2.01 3.13 2.11 1.04 1.04 1.08 1.08
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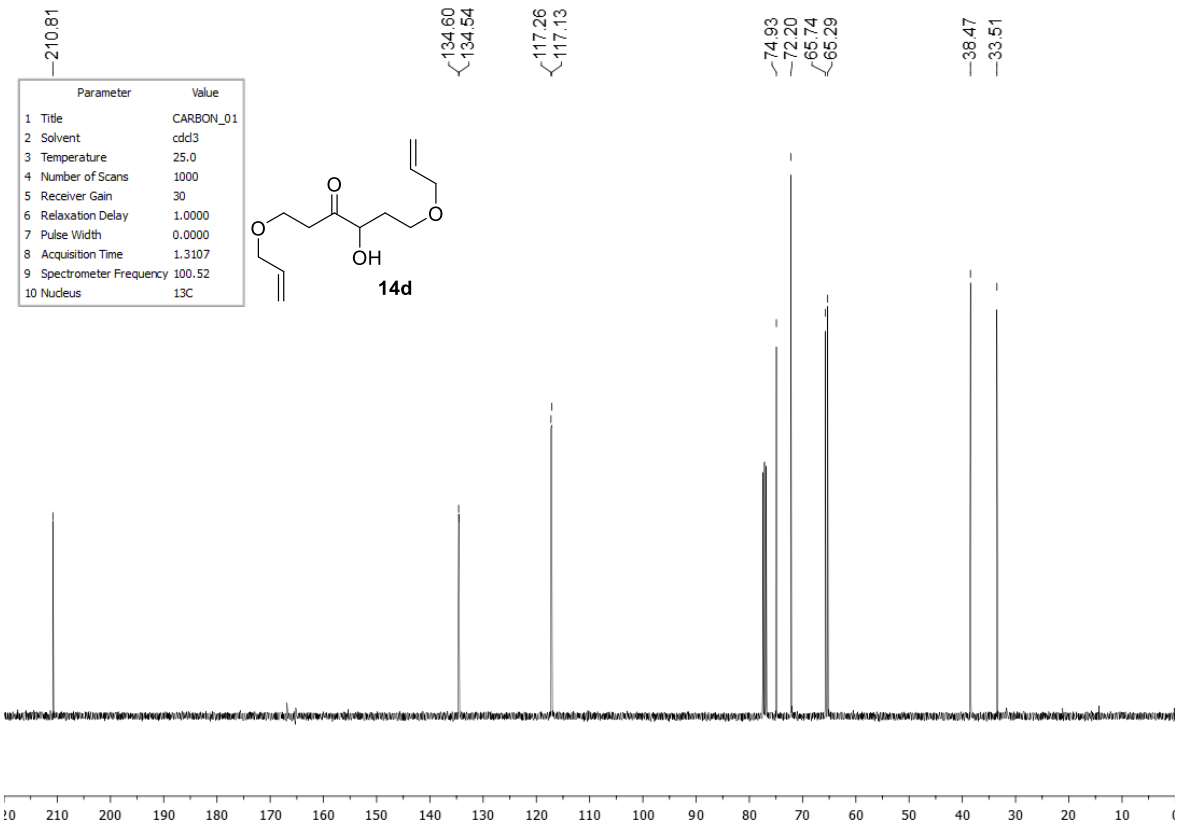
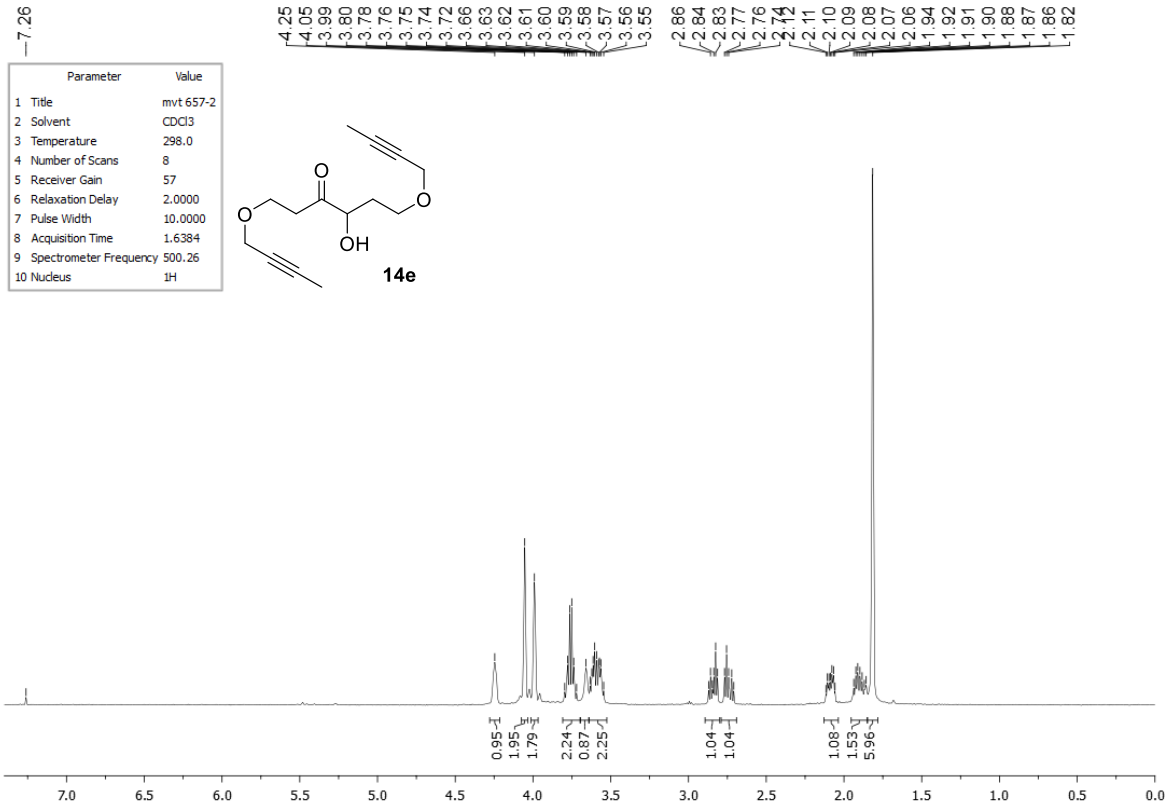

210.81 134.60 134.54 117.26 117.13 74.93 72.20 65.74 65.29 38.47 33.51
Parameter Value
1 Title CARBON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 1000
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
O
O
O
OH
14d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10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4.25
4.05
3.99
3.80
3.78
3.76
3.75
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3.72
3.66
3.63
3.62
3.61
3.60
3.59
3.58
3.57
3.56
3.55
2.86
2.84
2.83
2.77
2.76
2.74
2.12
2.11
2.10
2.09
2.08
2.07
2.06
1.94
1.92
1.91
1.90
1.88
1.87
1.86
1.82
Parameter Value
1 Title mvt 657-2
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 8
5 Receiver Gain 57
6 Relaxation Delay 2.0000
7 Pulse Width 10.0000
8 Acquisition Time 1.6384
9 Spectrometer Frequency 500.26
10 Nucleus 1H
O
O
O
OH
14e
0.95
1.95
1.79
2.24
0.87
2.25
1.04
1.04
1.08
1.53
5.96
7.0
6.5
6.0
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2.0
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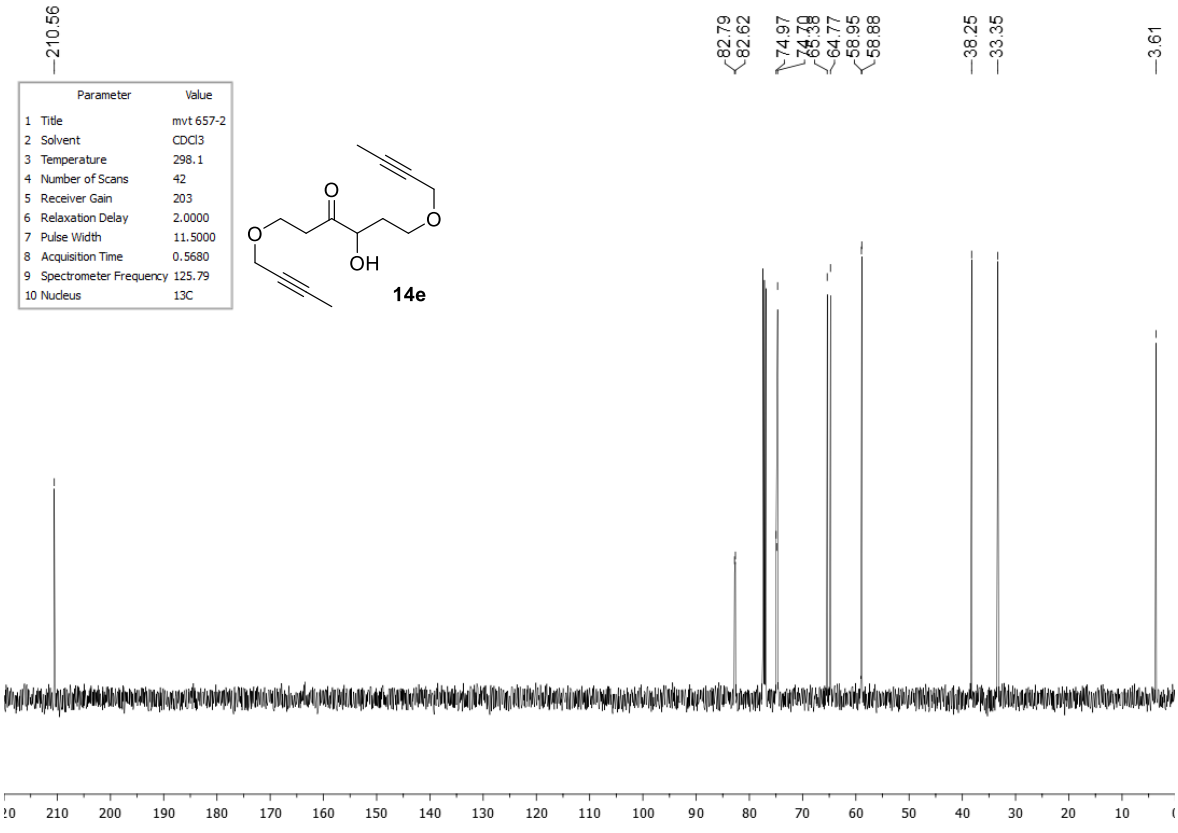
210.56
82.79
82.62
74.97
74.70
65.38
64.77
58.95
58.88
38.25
33.35
3.61
Parameter Value
1 Title mvt 657-2
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 42
5 Receiver Gain 203
6 Relaxation Delay 2.0000
7 Pulse Width 11.5000
8 Acquisition Time 0.5680
9 Spectrometer Frequency 125.79
10 Nucleus 13C
O
O
O
OH
14e
210
200
190
180
170
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130
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100
90
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70
60
50
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20
10

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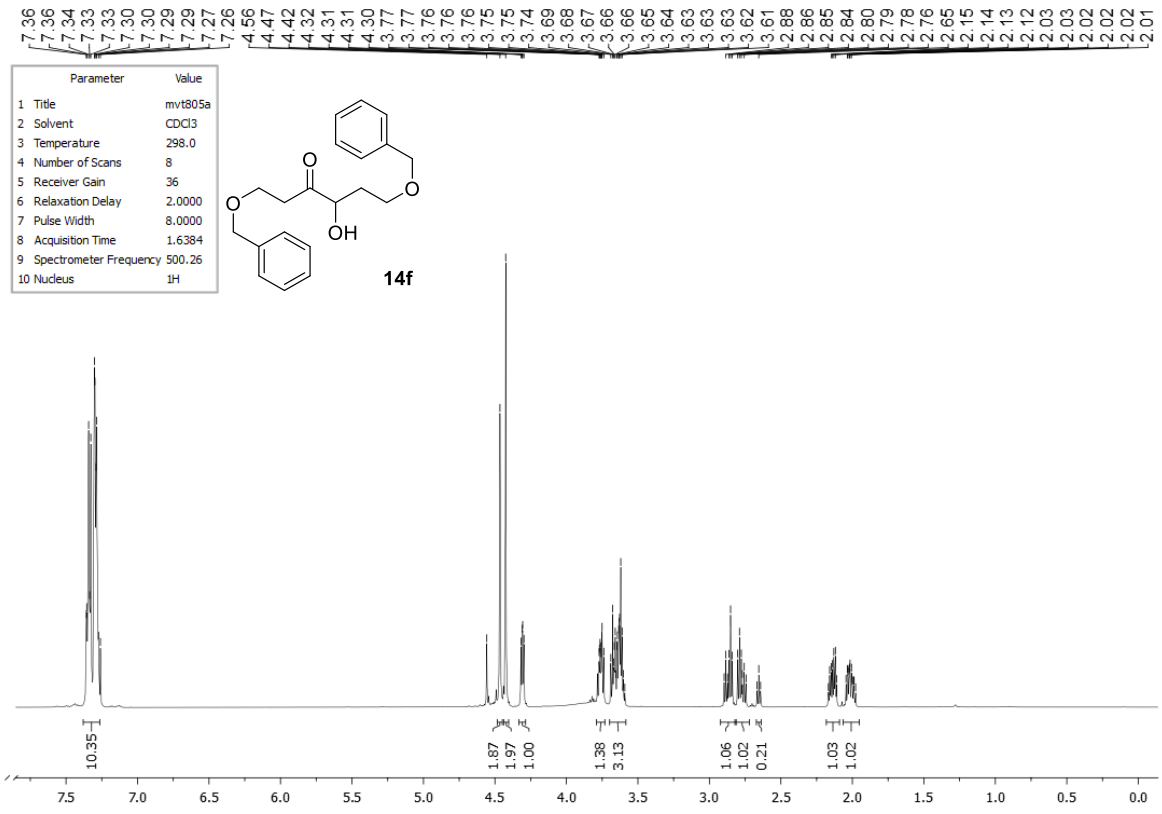
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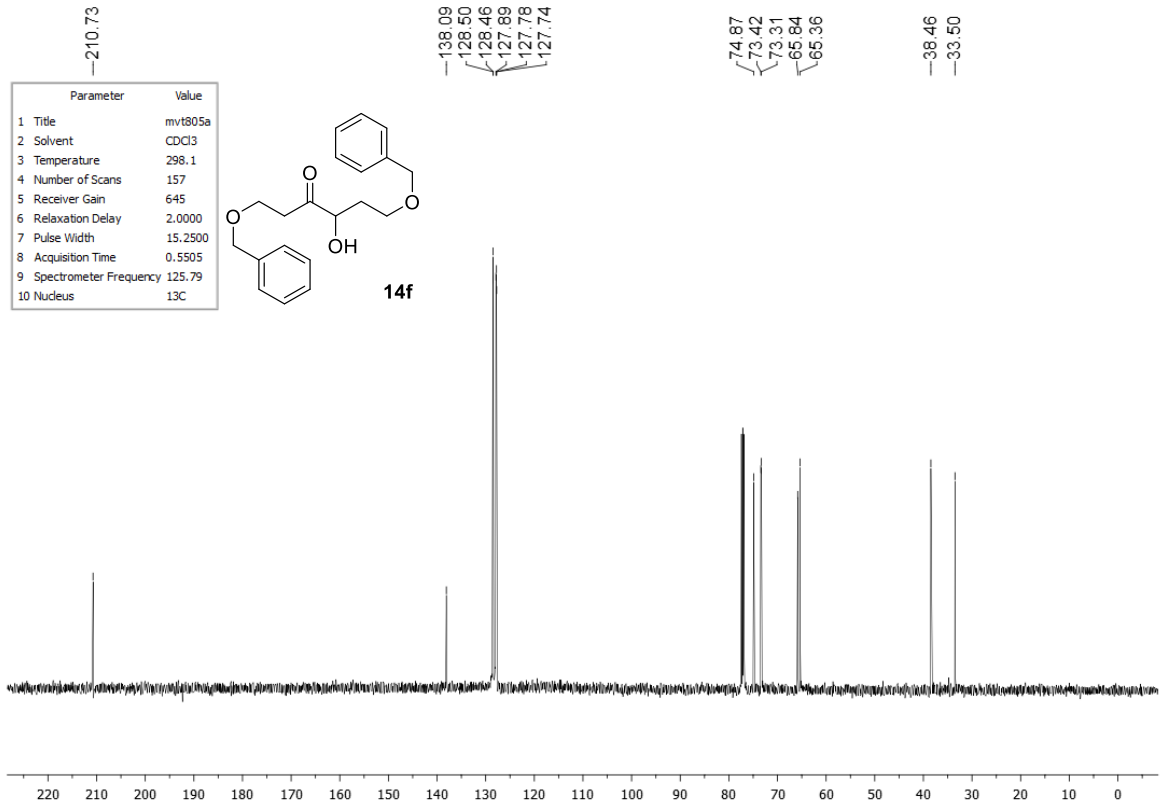
4.56 4.47 4.42 4.32 4.31 4.31 4.30 3.77 3.77 3.76 3.76 3.76 3.75 3.75 3.74 3.69 3.68 3.67 3.66 3.66 3.65 3.64 3.63 3.63 3.63 3.62 3.61 2.88 2.86 2.85 2.84 2.80 2.79 2.78 2.76 2.65 2.15 2.14 2.13 2.12 2.03 2.03 2.02 2.02 2.02 2.02 2.01
Parameter Value
1 Title mvt805a
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 8
5 Receiver Gain 36
6 Relaxation Delay 2.0000
7 Pulse Width 8.0000
8 Acquisition Time 1.6384
9 Spectrometer Frequency 500.26
10 Nucleus 1H
O
O
O
OH
14f
10.35
1.87 1.97 1.00
1.38 3.13
1.06 1.02 0.21
1.03 1.02
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


210.73
138.09 128.50 128.46 127.89 127.78 127.74
74.87 73.42 73.31 65.84 65.36
38.46 33.50
Parameter Value
1 Title mvt805a
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 157
5 Receiver Gain 645
6 Relaxation Delay 2.0000
7 Pulse Width 15.2500
8 Acquisition Time 0.5505
9 Spectrometer Frequency 125.79
10 Nucleus 13C
O
O
O
OH
14f
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

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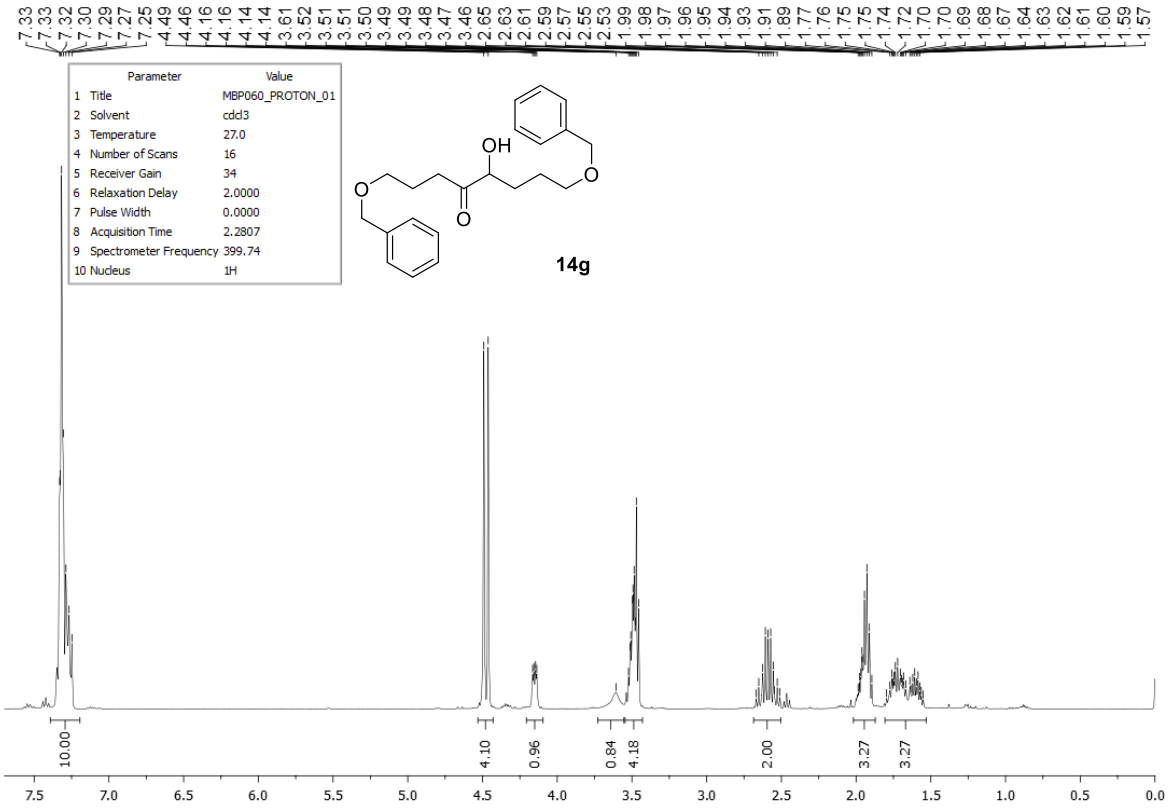
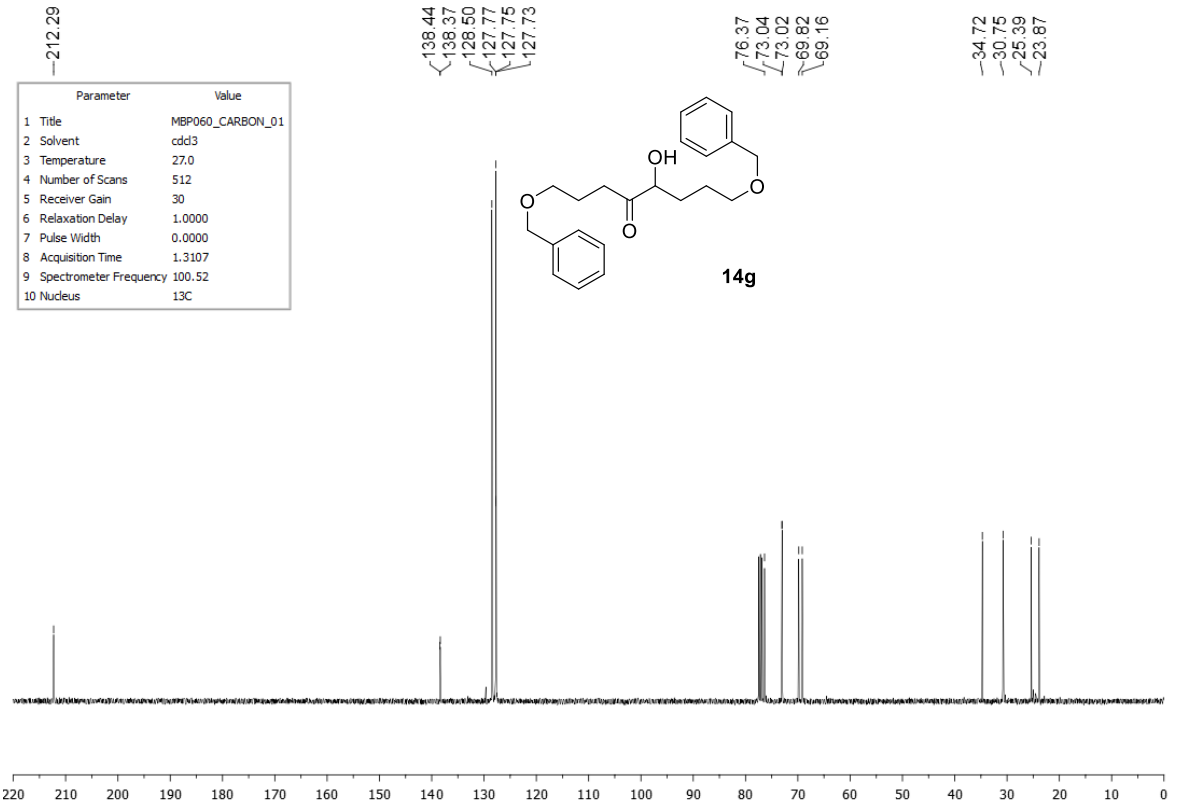

7.33 7.33 7.32 7.30 7.29 7.27 7.25 4.49 4.46 4.16 4.16 4.14 4.14 3.61 3.52 3.51 3.51 3.50 3.49 3.49 3.48 3.47 3.46 2.65 2.63 2.61 2.59 2.57 2.55 2.53 1.99 1.98 1.97 1.96 1.95 1.94 1.93 1.91 1.89 1.77 1.76 1.75 1.75 1.74 1.72 1.70 1.70 1.69 1.68 1.67 1.64 1.63 1.62 1.61 1.60 1.59 1.57
Parameter Value
1 Title MBP060_PROTON_01
2 Solvent cdcl3
3 Temperature 27.0
4 Number of Scans 16
5 Receiver Gain 34
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.74
10 Nucleus 1H
OH
O
O
O
14g
10.00 4.10 0.96 0.84 4.18 2.00 3.27 3.27
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


212.29
138.44 138.37 128.50 127.77 127.75 127.73
76.37 73.04 73.02 69.82 69.16
34.72 30.75 25.39 23.87
Parameter Value
1 Title MBP060_CARBON_01
2 Solvent cdcl3
3 Temperature 27.0
4 Number of Scans 512
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
OH
O
O
O
14g
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

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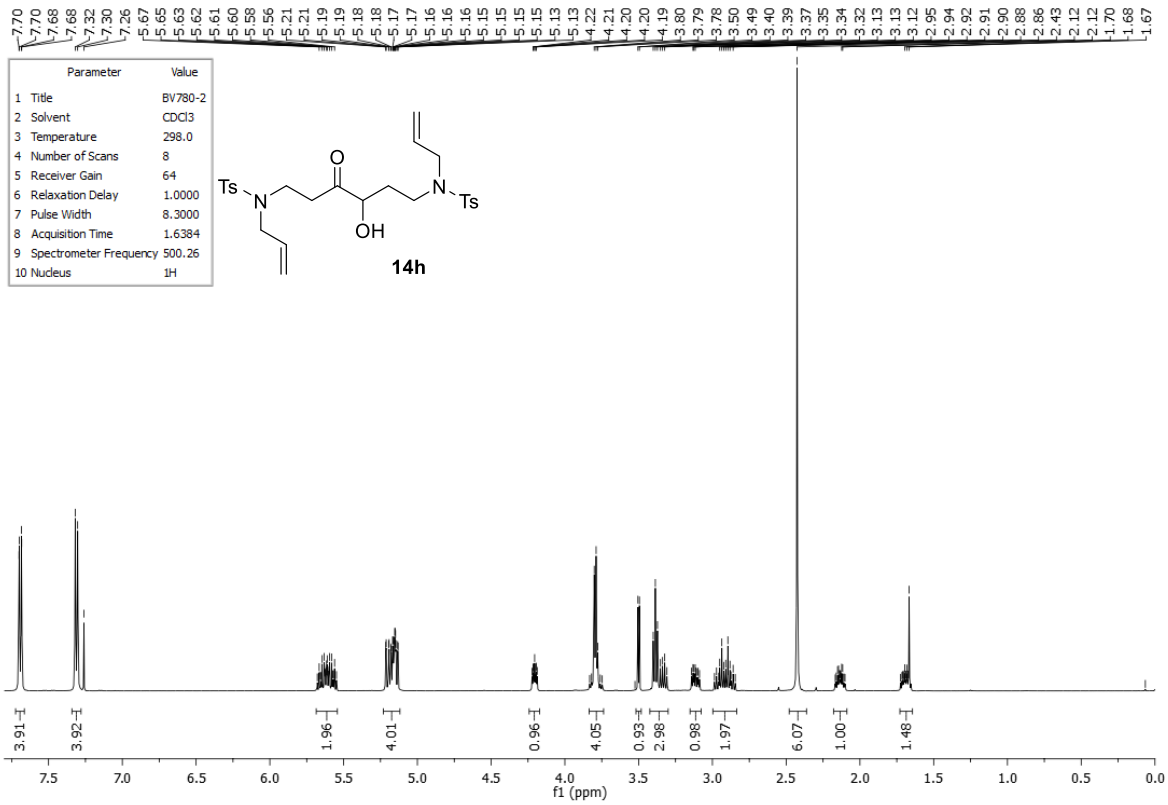
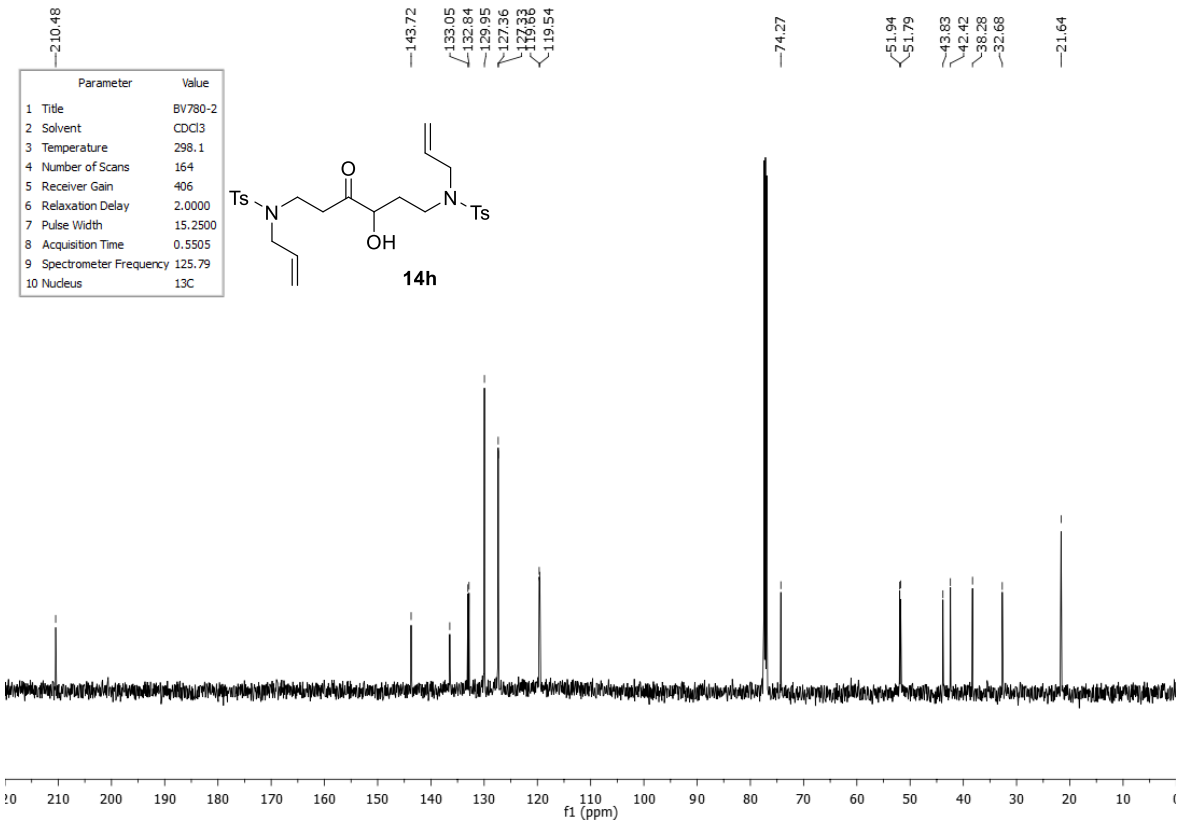

Parameter Value
1 Title BV780-2
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 8
5 Receiver Gain 64
6 Relaxation Delay 1.0000
7 Pulse Width 8.3000
8 Acquisition Time 1.6384
9 Spectrometer Frequency 500.26
10 Nucleus 1H
Ts
N
O
OH
14h
f1 (ppm)


Parameter Value
1 Title BV780-2
2 Solvent CDCl3
3 Temperature 298.1
4 Number of Scans 164
5 Receiver Gain 406
6 Relaxation Delay 2.0000
7 Pulse Width 15.2500
8 Acquisition Time 0.5505
9 Spectrometer Frequency 125.79
10 Nucleus 13C
Ts
N
O
OH
14h
f1 (ppm)

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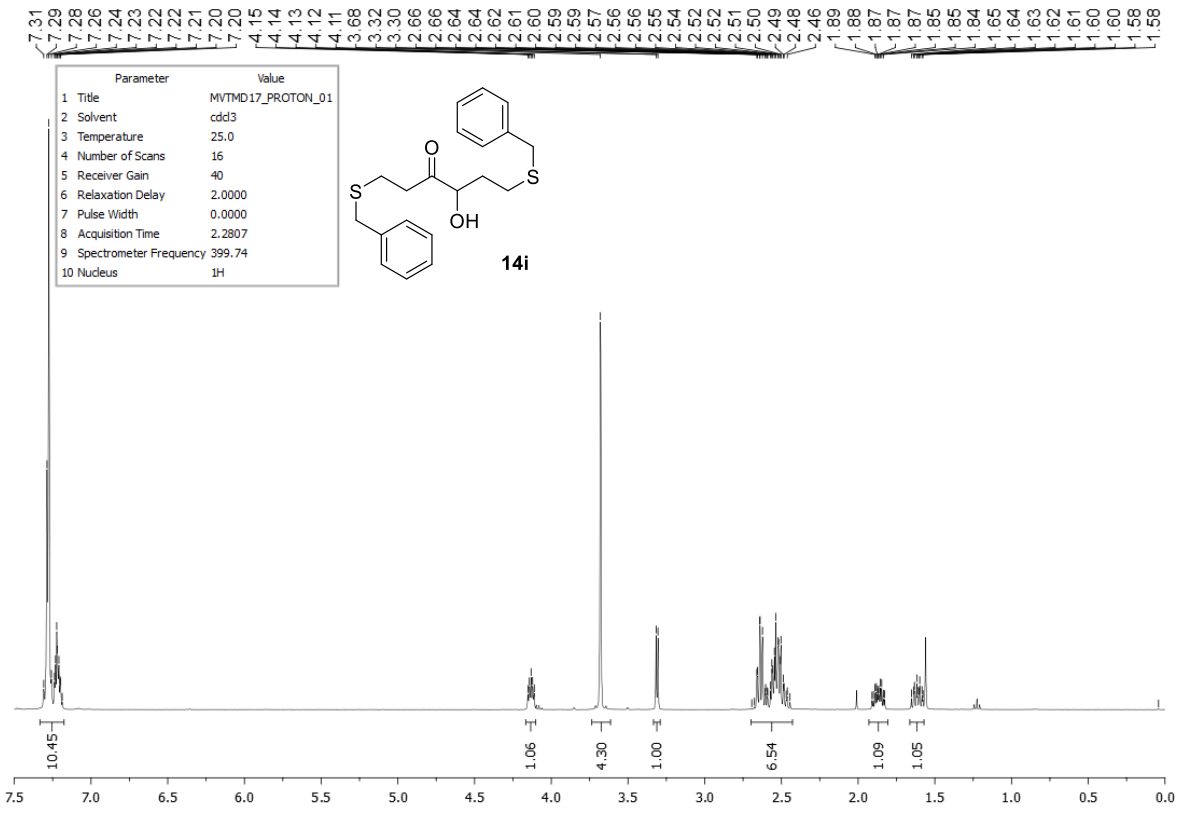
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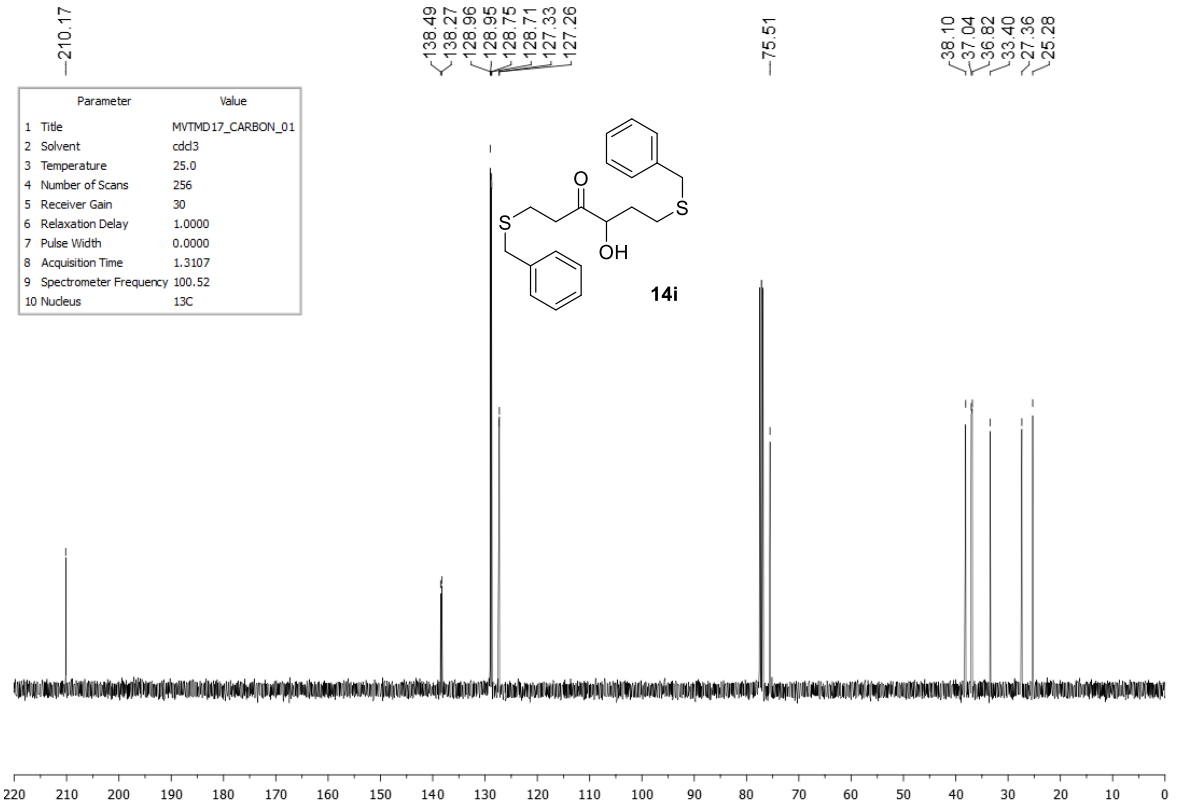
Parameter Value
1 Title MVTMD17_PROTON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 16
5 Receiver Gain 40
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.74
10 Nucleus 1H
O
S
S
OH
14i
10.45 1.06 4.30 1.00 6.54 1.09 1.05
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


210.17
138.49 138.27 128.96 128.95 128.75 128.71 127.33 127.26
75.51
38.10 37.04 36.82 33.40 27.36 25.28
Parameter Value
1 Title MVTMD17_CARBON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 256
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
10 Nucleus 13C
O
S
S
OH
14i
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

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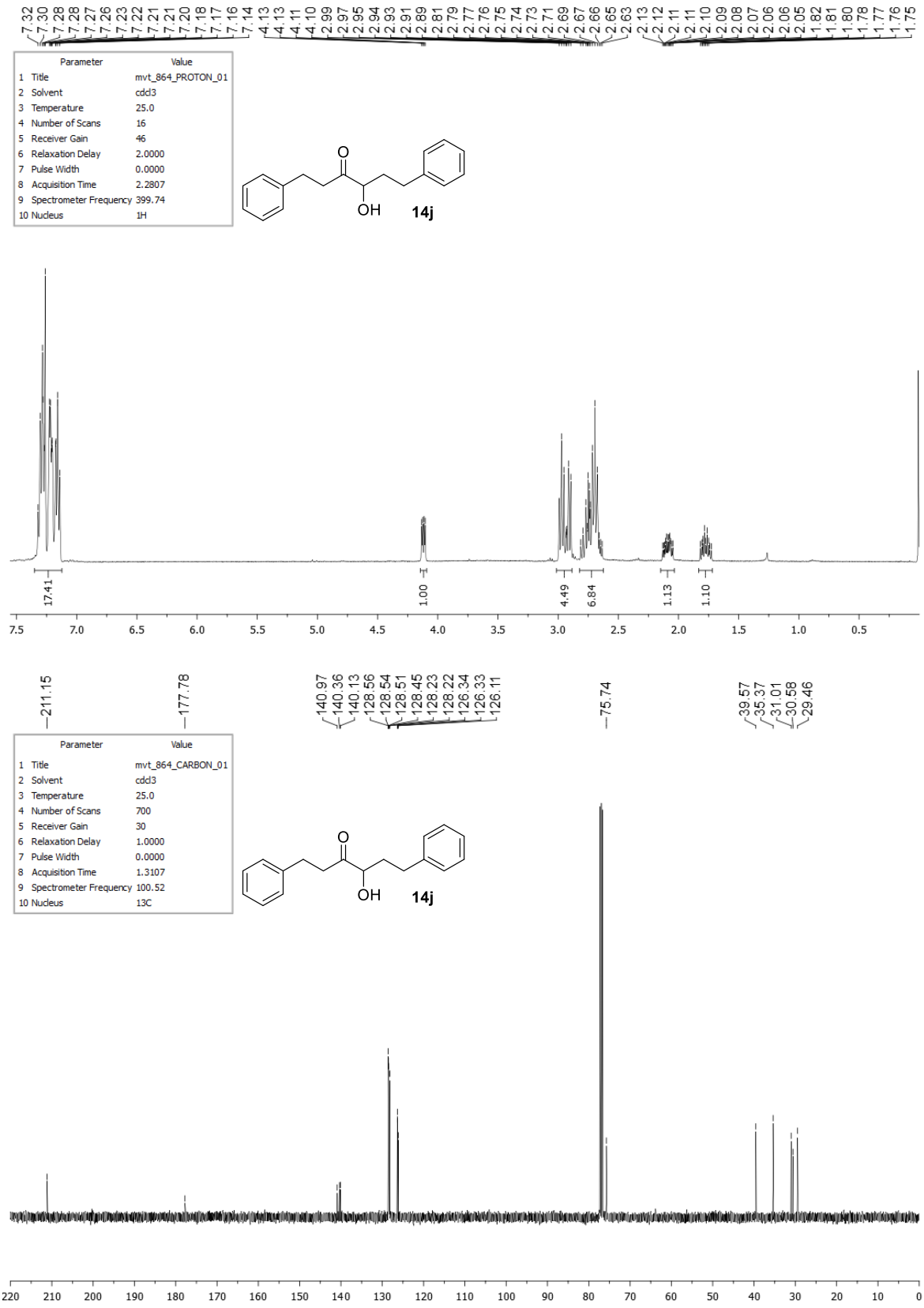
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Parameter Value
1 Title mvt_864_PROTON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 16
5 Receiver Gain 46
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.74
10 Nucleus 1H
O
OH
14j
17.41
1.00
4.49
6.84
1.13
1.10
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
211.15
177.78
140.97 140.36 140.13 128.56 128.54 128.51 128.45 128.23 128.22 126.34 126.33 126.11
75.74
39.57 35.37 31.01 30.58 29.46
Parameter Value
1 Title mvt_864_CARBON_01
2 Solvent cdcl3
3 Temperature 25.0
4 Number of Scans 700
5 Receiver Gain 30
6 Relaxation Delay 1.0000
7 Pulse Width 0.0000
8 Acquisition Time 1.3107
9 Spectrometer Frequency 100.52
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O
OH
14j
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

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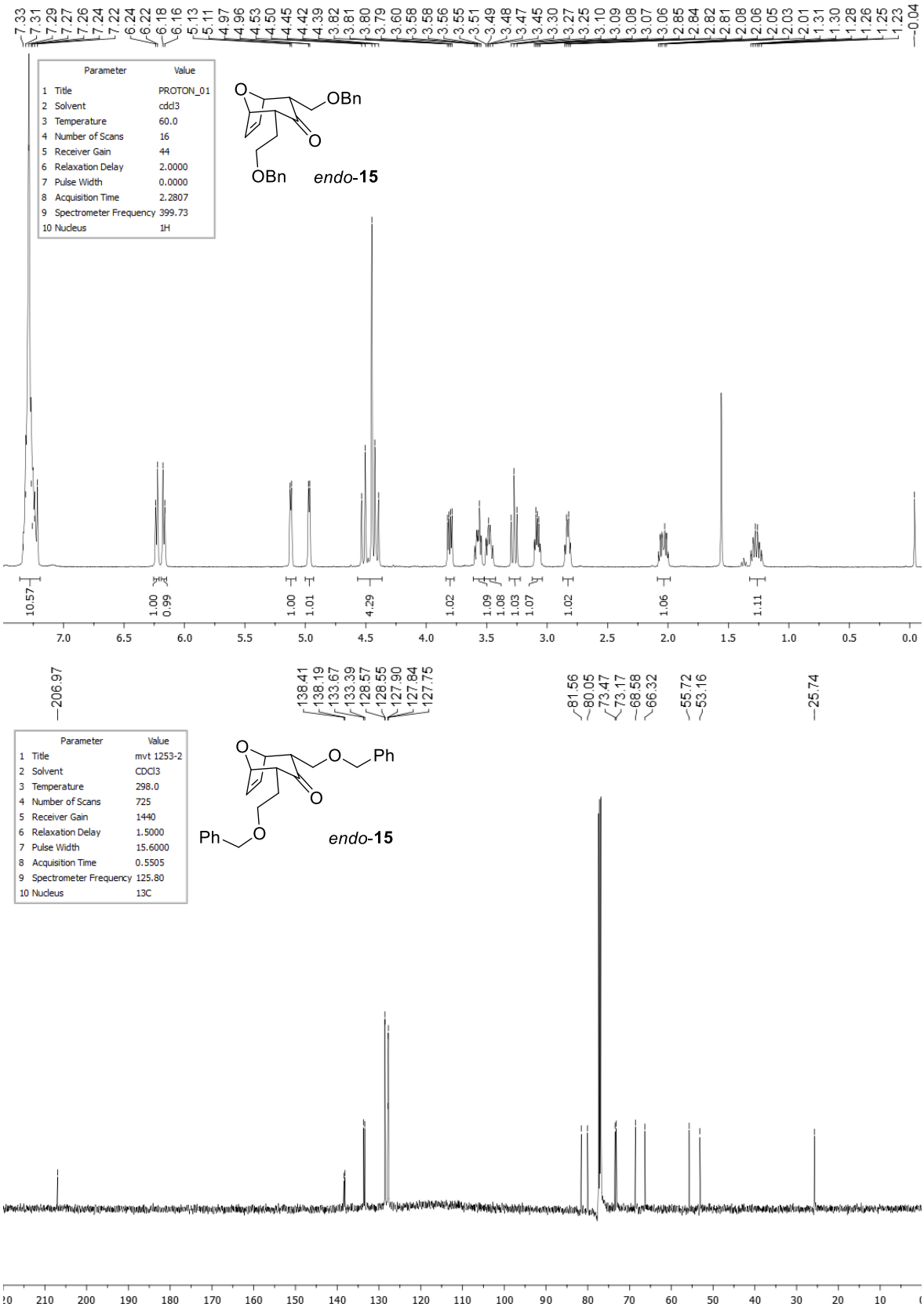
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1 Title PROTON_01
2 Solvent cdcl3
3 Temperature 60.0
4 Number of Scans 16
5 Receiver Gain 44
6 Relaxation Delay 2.0000
7 Pulse Width 0.0000
8 Acquisition Time 2.2807
9 Spectrometer Frequency 399.73
10 Nucleus 1H
OBn
OBn
endo-15
Parameter Value
1 Title mvt 1253-2
2 Solvent CDCl3
3 Temperature 298.0
4 Number of Scans 725
5 Receiver Gain 1440
6 Relaxation Delay 1.5000
7 Pulse Width 15.6000
8 Acquisition Time 0.5505
9 Spectrometer Frequency 125.80
10 Nucleus 13C
Ph
Ph
endo-15

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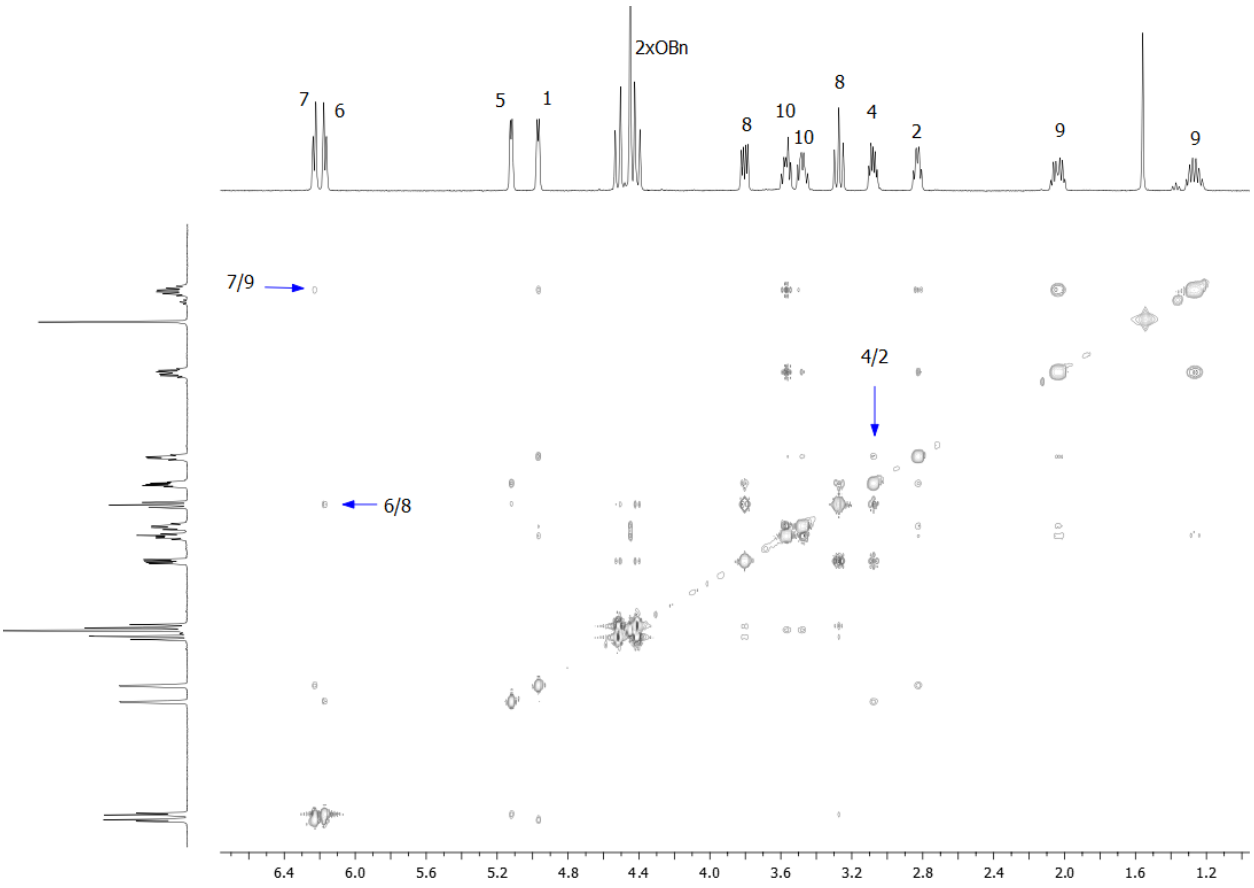

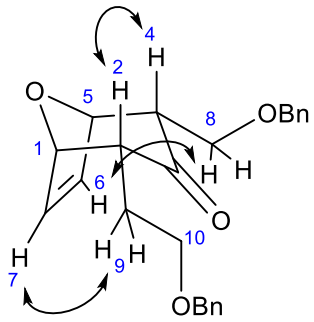

endo-**15**

NOESY correlations

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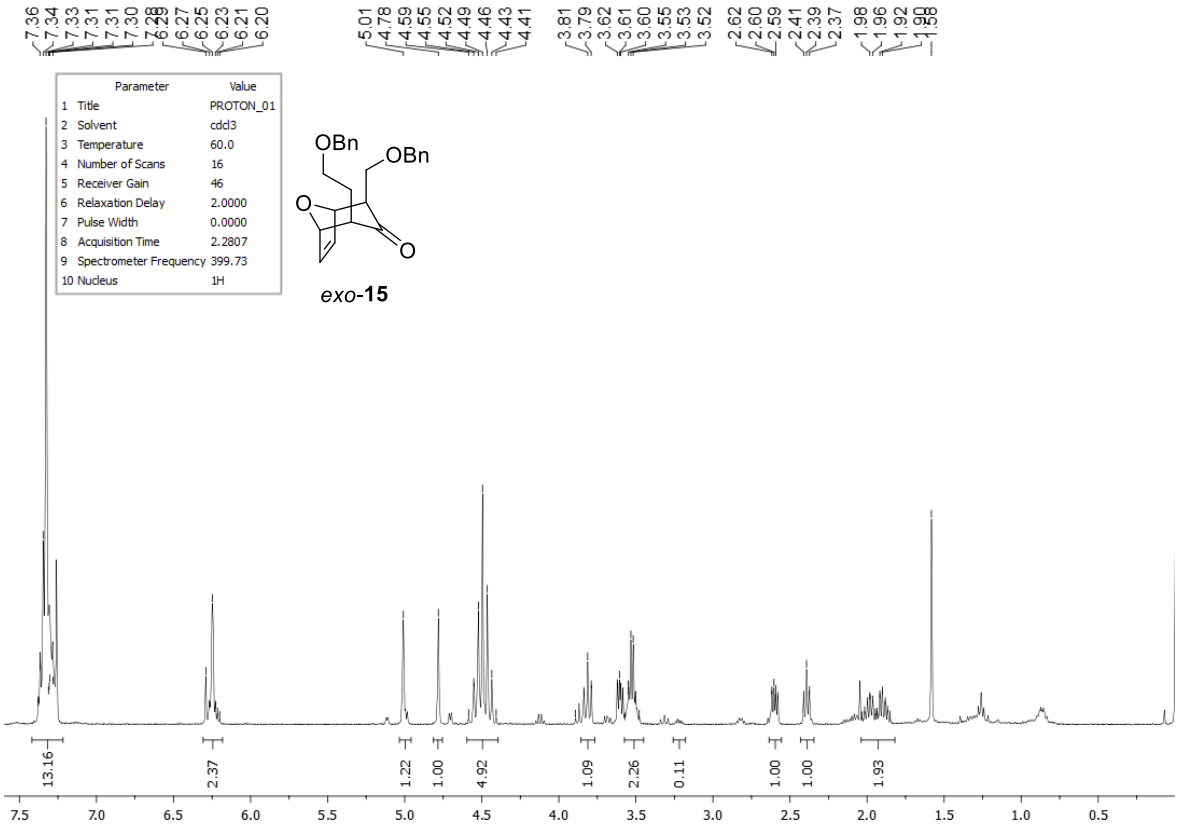
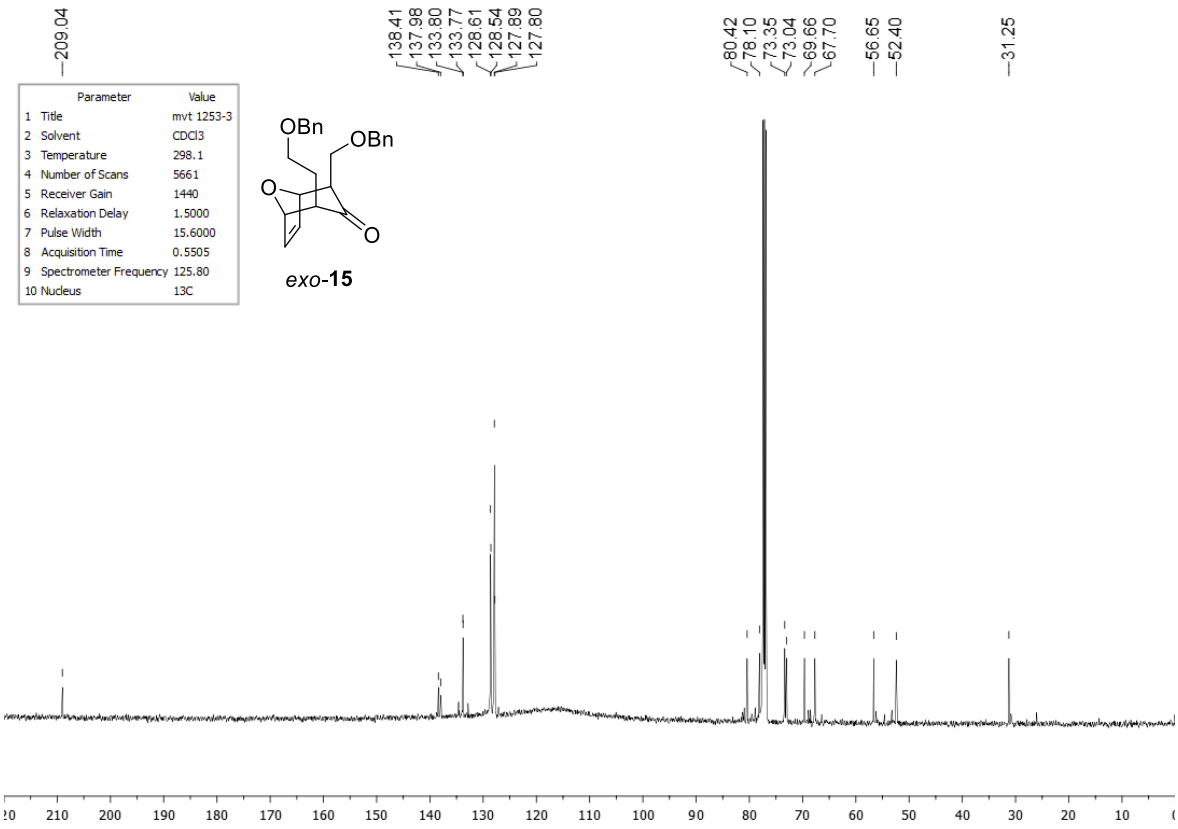


exo-**15**



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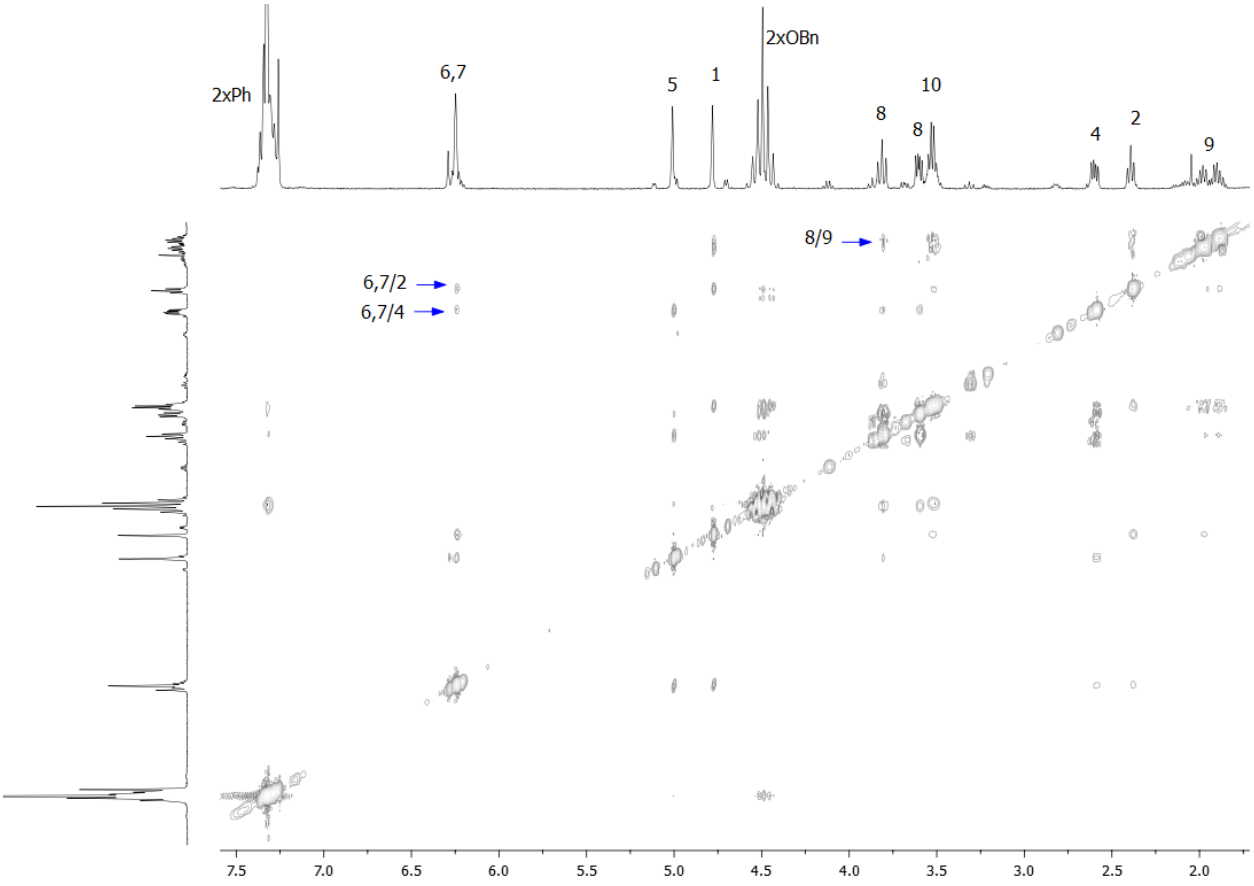

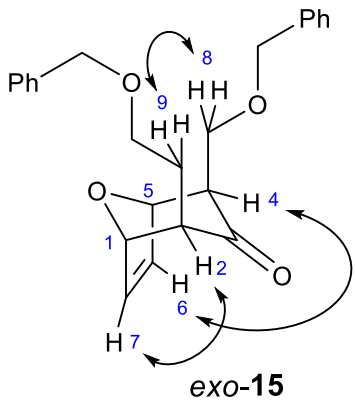

exo-**15**

NOESY correlations

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