Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Stereoselective Synthesis of (*E*)-3,3-diaryl and (*E*)-3-aryl-3-aryloxy Allylamines and Allylalcohols from *trans*-Cinnamyl chloride and alcohol

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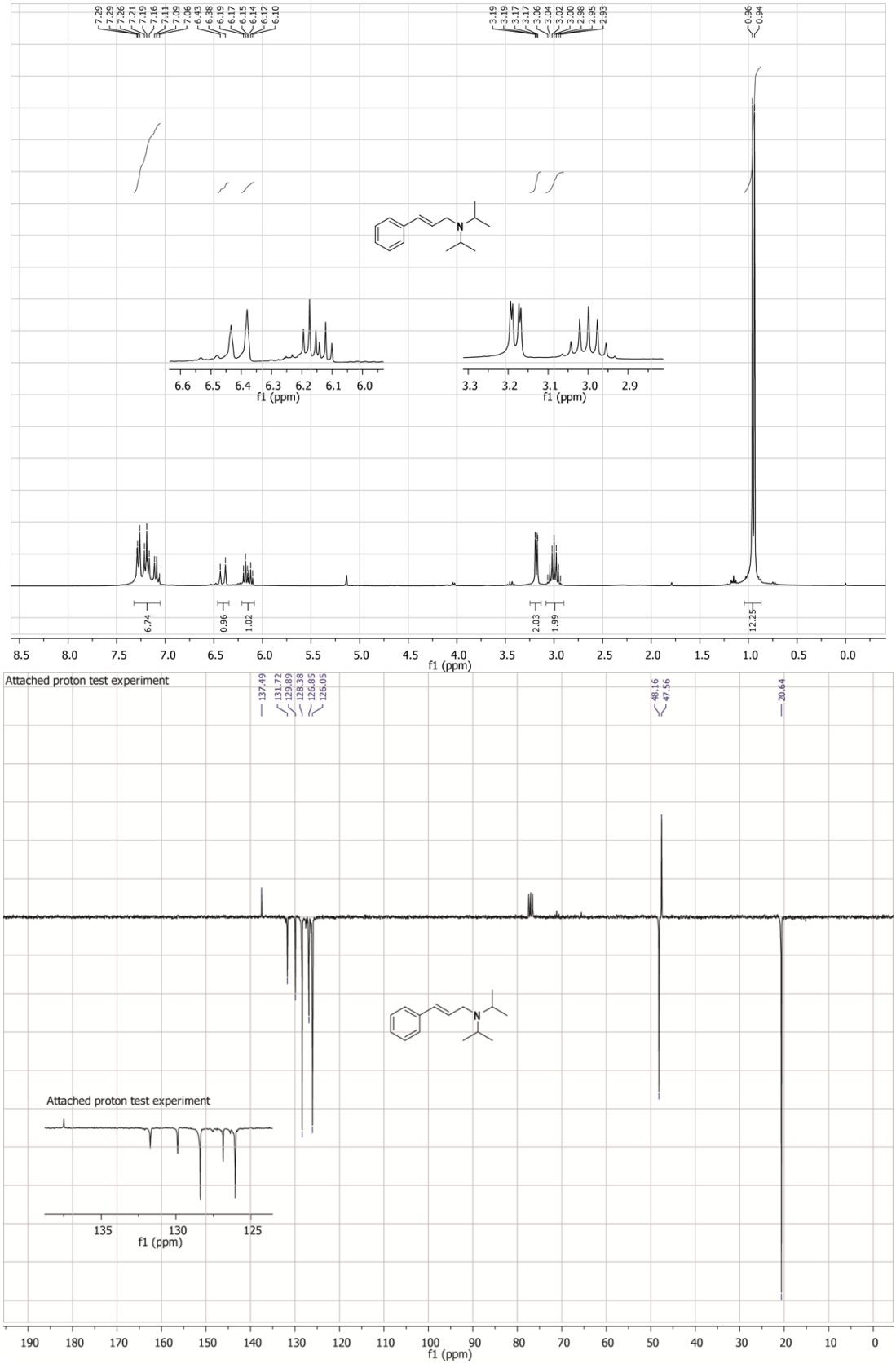
1. **Dehydrobromination optimization**

Table S1: Optimization of 4a dehydrobromintion conditions

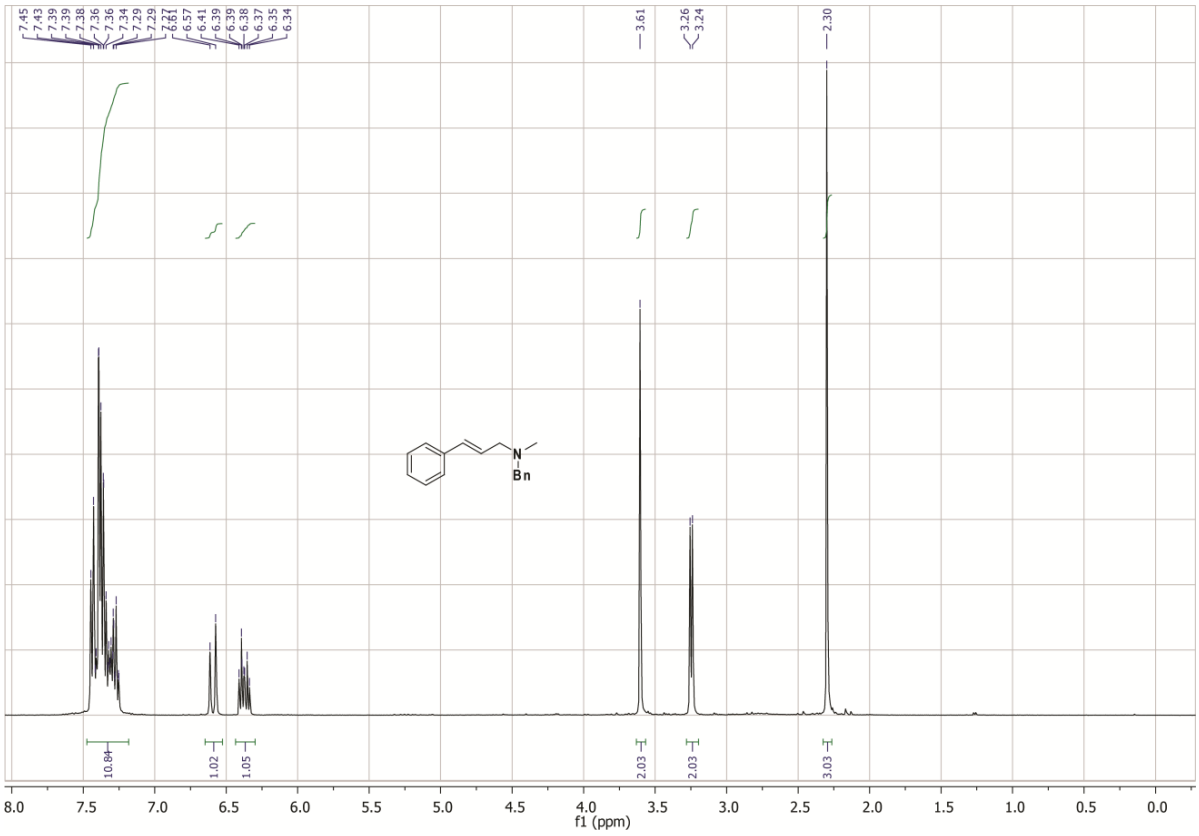
Entry	Temp. (°C)	Solvent	Base	Conversion (%)	Seletivity 5a (%)
1[a]	60	MeOH/THF	K_2CO_3	39	72
2[a]	60	THF/MeOH	KOH	33	76
3[a]	60	THF	K_2CO_3	38	51
4[a]	60	THF	KOH	37	53
5[a]	25	THF	KOH	40	98
6[b]	35	THF	KOH	100	97 (88)

Conditions: **4a** (1 mmol), base (2 mmol), solvent (8 ml). Internal standard: undecane. [a] 16 h, [b] 48 h. the value in brackets corresponds to isolated yield. Conversion determined by 1H-NMR and the isomer distribution (selectivity) determined by GC and GC-MS.

2. ^{1}H-NMR and ^{13}C-NMR Compounds Spectra



Compound **3a**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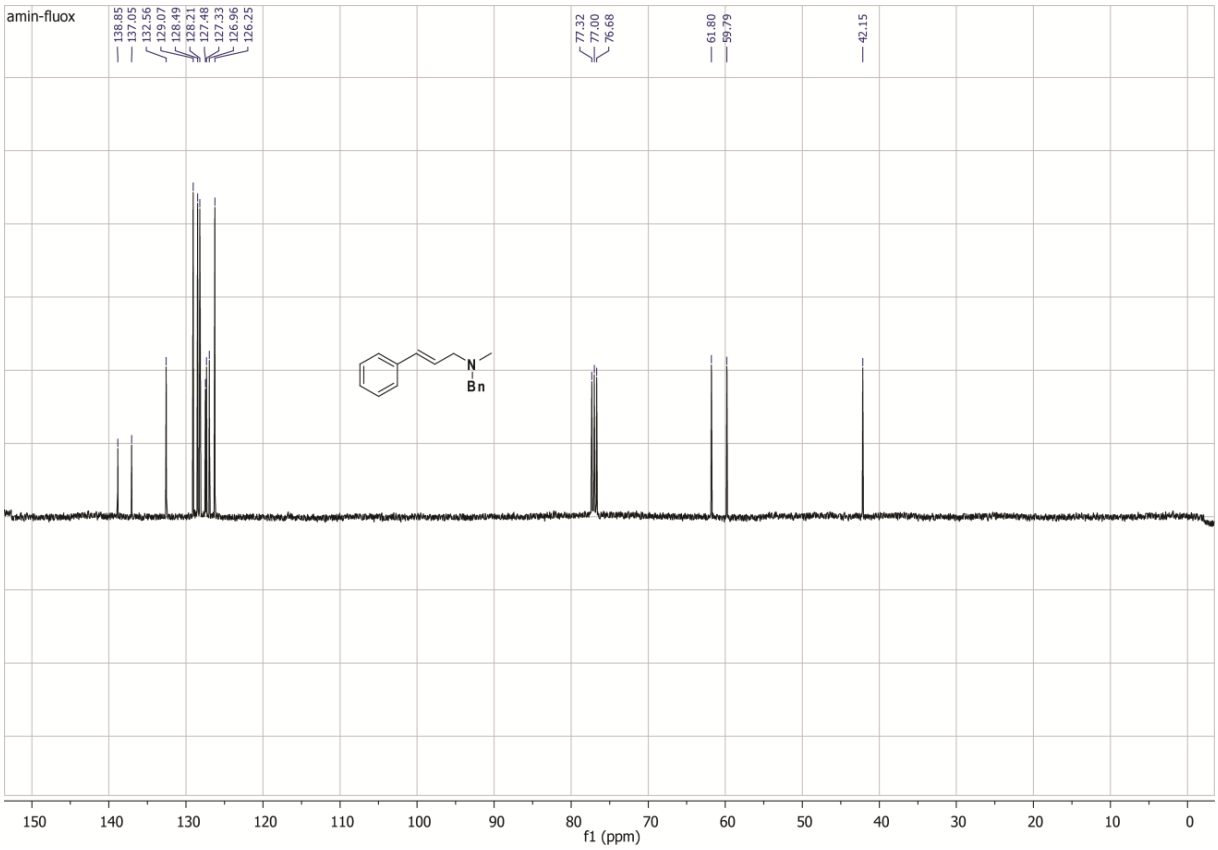
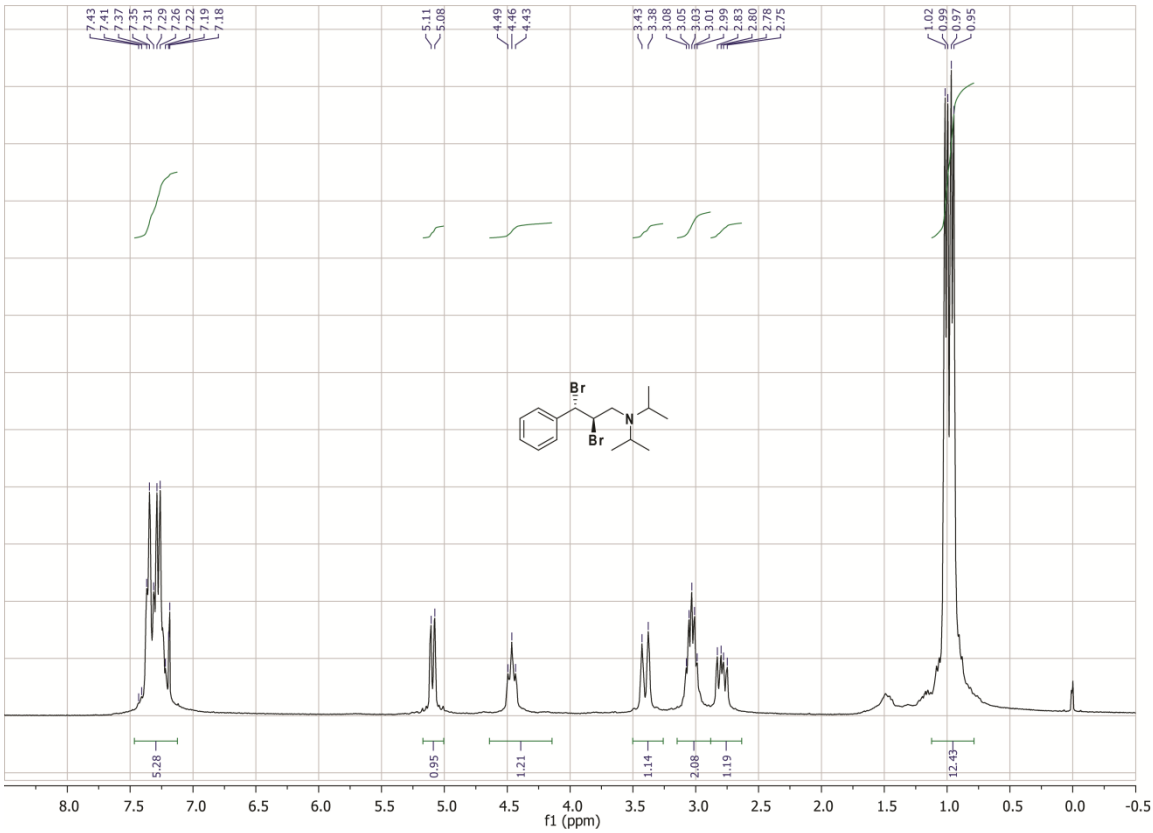
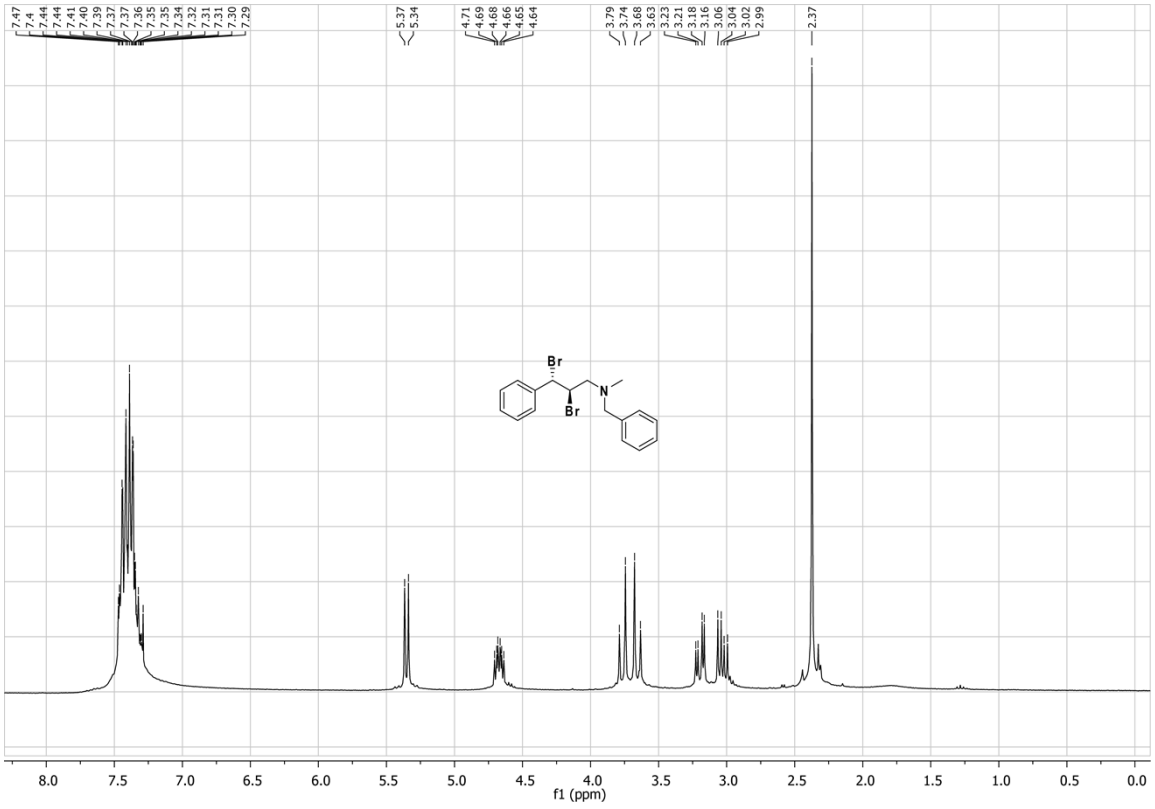
7.43
7.39
7.39
7.38
7.36
7.36
7.34
7.29
7.29
7.27
6.61
6.57
6.41
6.39
6.39
6.38
6.37
6.35
6.34
3.61
3.26
3.24
2.30
N
Bn
10.84
1.02
1.05
2.03
2.03
3.03
f1 (ppm)


amin-fluox
138.85
137.05
132.56
129.07
128.49
128.21
127.48
127.33
126.96
126.25
77.32
77.00
76.68
61.80
59.79
42.15
N
Bn
f1 (ppm)

Compound **3b**


7.43
7.41
7.37
7.35
7.31
7.29
7.26
7.22
7.19
7.18
5.11
5.08
4.49
4.46
4.43
3.43
3.38
3.08
3.05
3.03
3.01
2.99
2.83
2.80
2.78
2.75
1.02
0.99
0.97
0.95
Br
N
Br
5.28
0.95
1.21
1.14
2.08
1.19
12.43
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
-0.5
f1 (ppm)

Compound **4a**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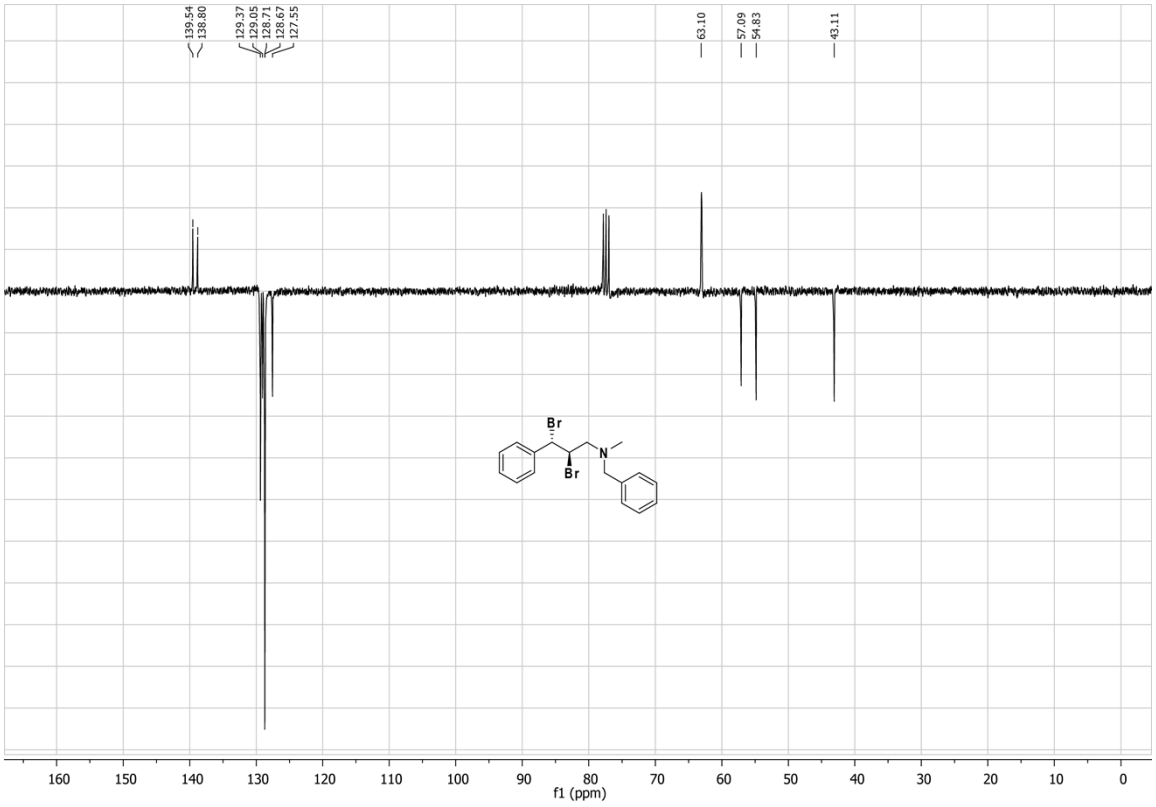
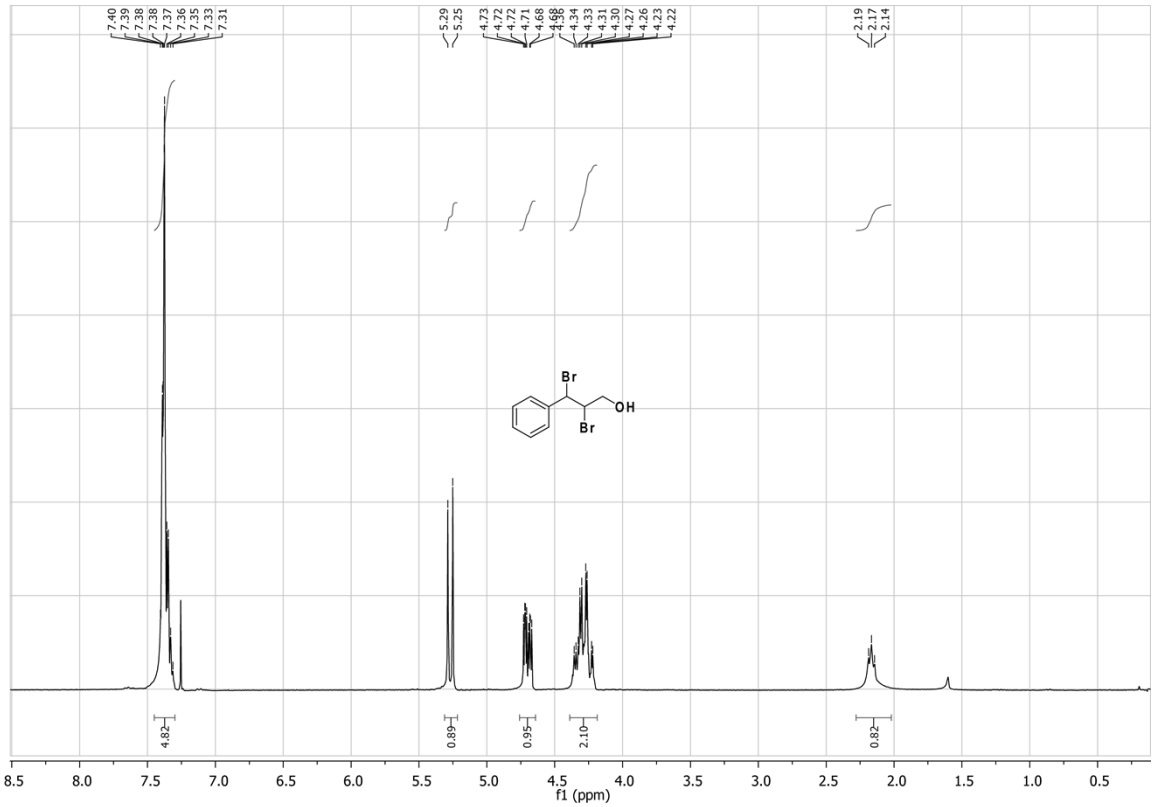
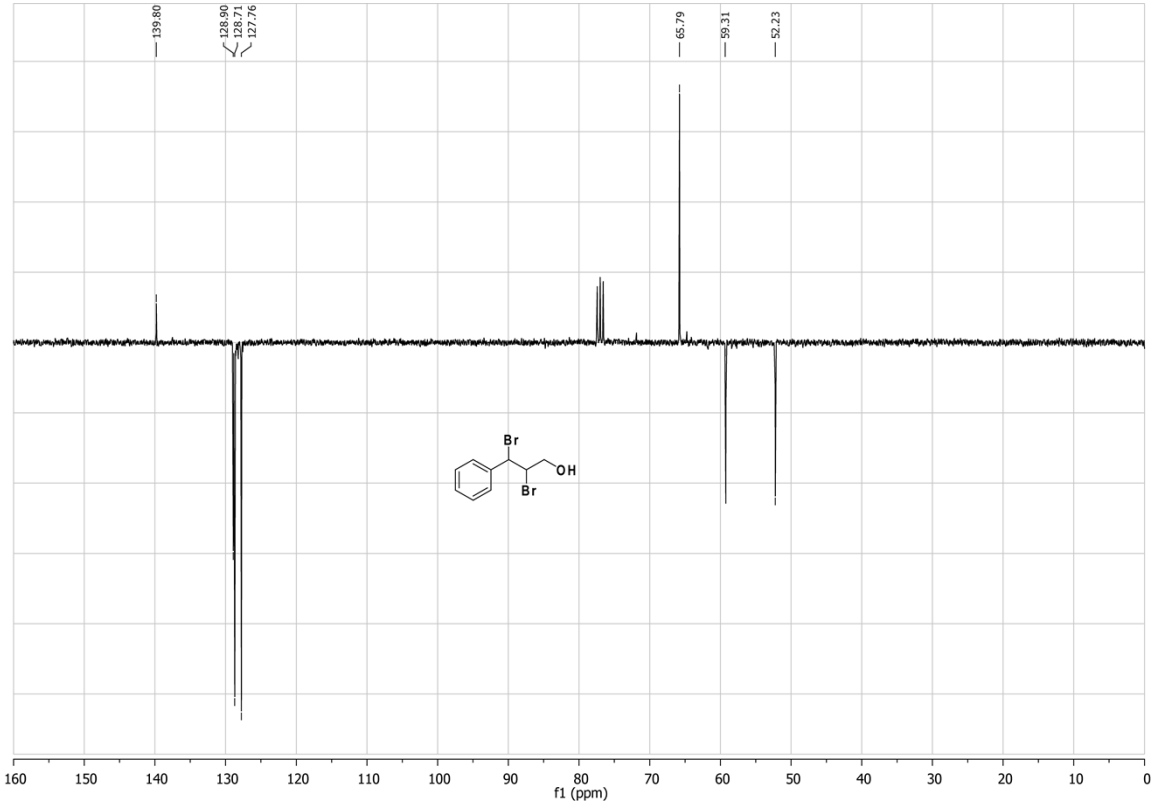
7.44
7.44
7.41
7.40
7.39
7.37
7.37
7.36
7.35
7.35
7.34
7.32
7.31
7.31
7.30
7.29
5.37
5.34
4.71
4.69
4.68
4.66
4.65
4.64
3.79
3.74
3.68
3.63
3.23
3.21
3.18
3.16
3.06
3.04
3.02
2.99
2.37
Br
Br
N
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

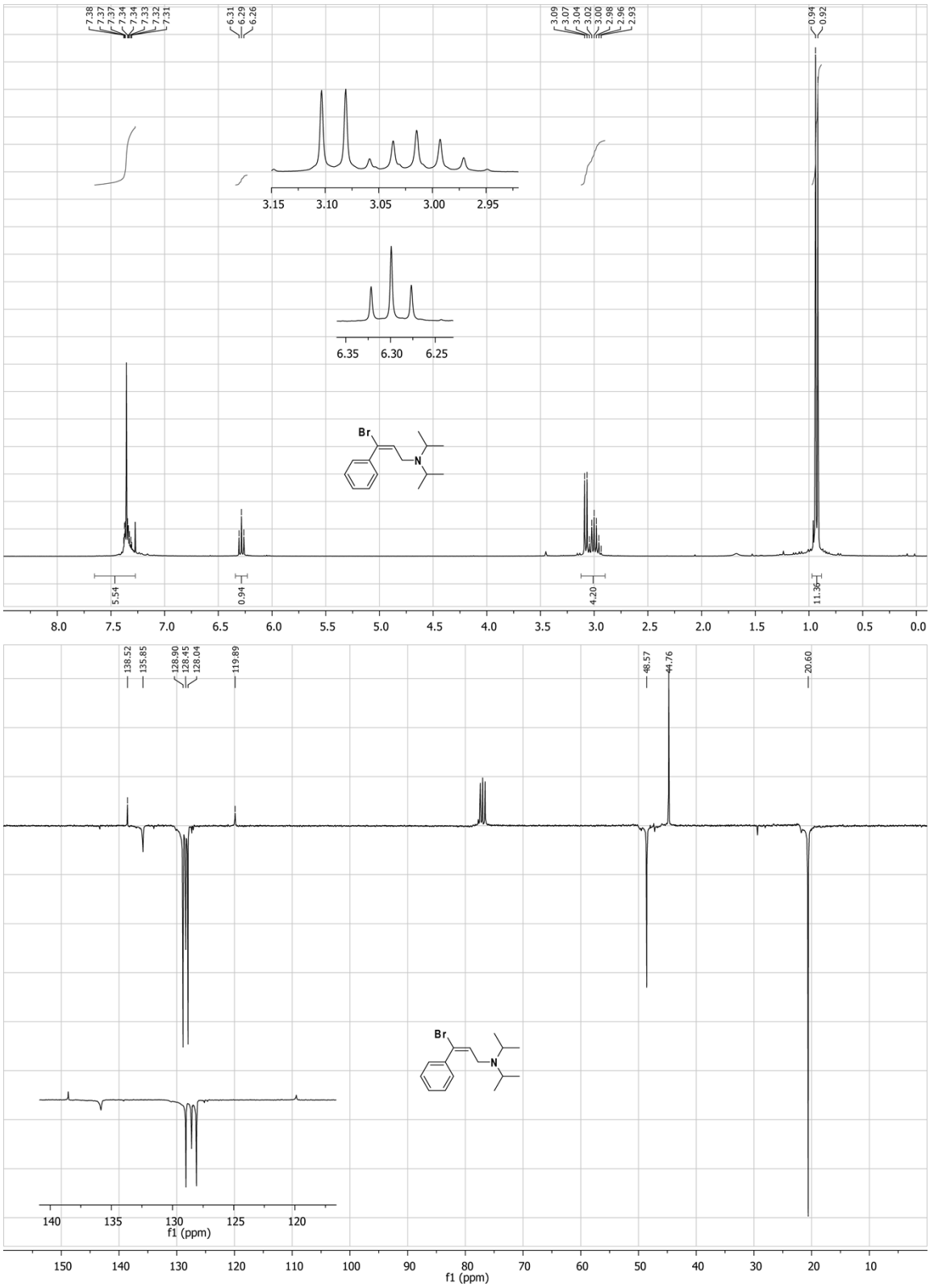

139.54
138.80
129.37
129.05
128.71
128.67
127.55
63.10
57.09
54.83
43.11
Br
Br
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Compound **4b**

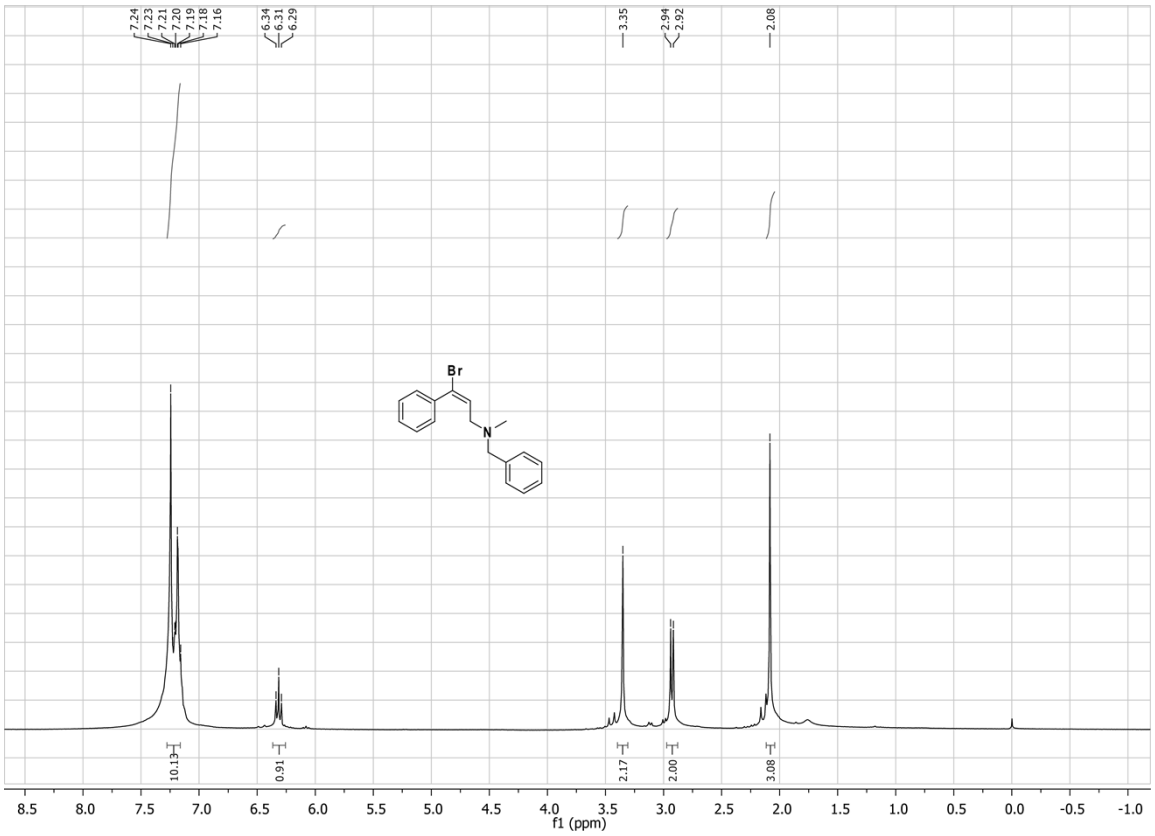

7.40
7.39
7.38
7.38
7.37
7.36
7.35
7.33
7.31
5.29
5.25
4.73
4.72
4.72
4.71
4.68
4.66
4.34
4.33
4.31
4.30
4.27
4.26
4.23
4.22
2.19
2.17
2.14
Br
OH
Br
4.82
0.89
0.95
2.10
0.82
f1 (ppm)

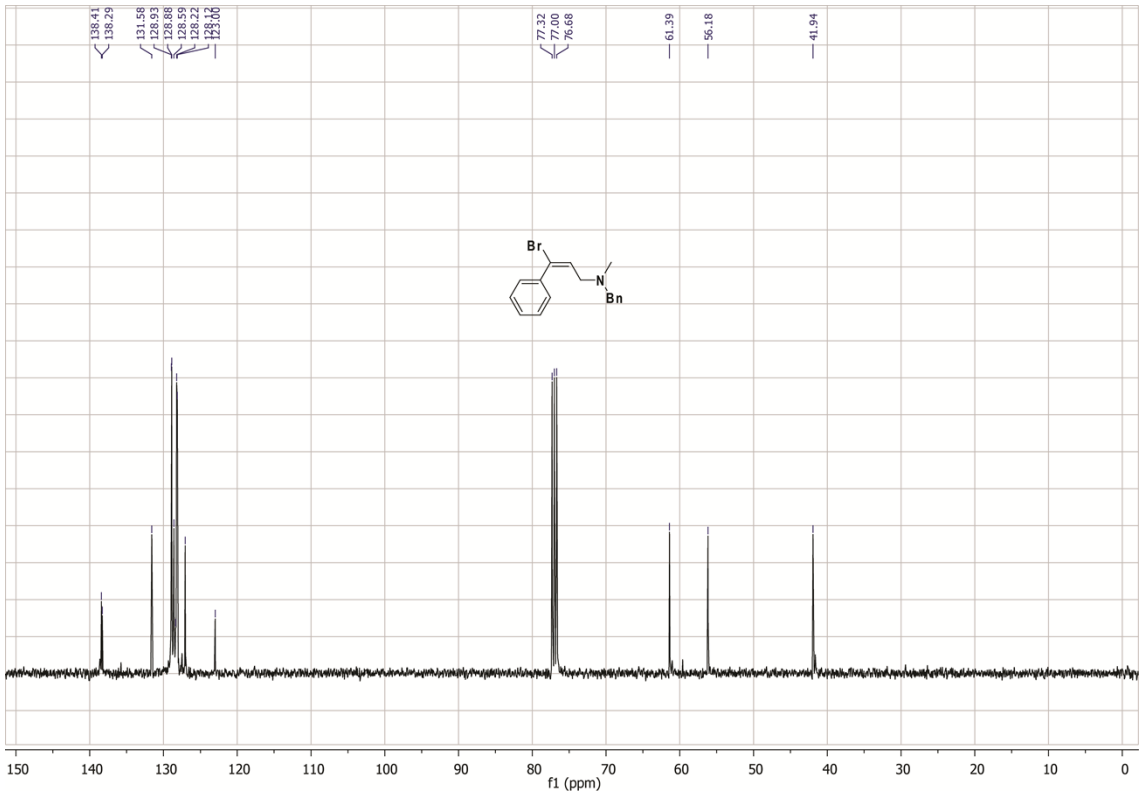

139.80
128.90
128.71
127.76
65.79
59.31
52.23
Br
OH
Br
f1 (ppm)

Compound **4c**

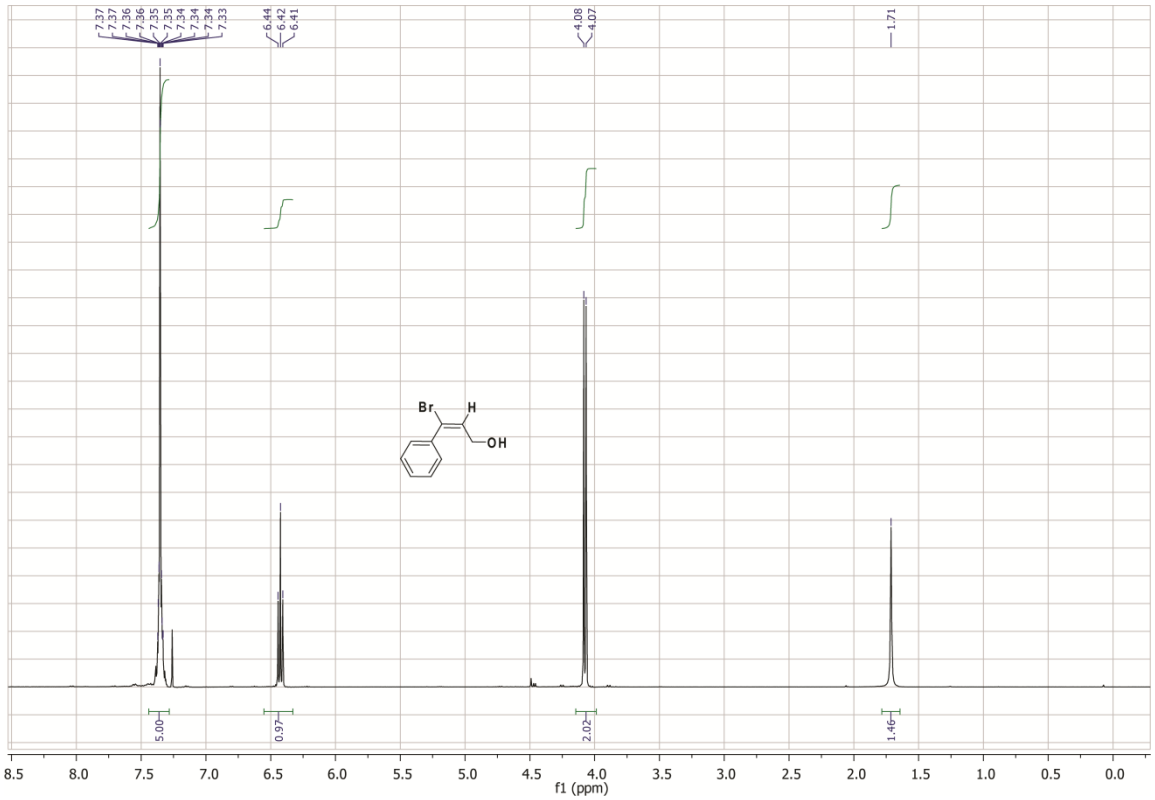

7.38
7.37
7.37
7.34
7.34
7.33
7.32
7.31
6.31
6.29
6.26
3.09
3.07
3.04
3.02
3.00
2.98
2.96
2.93
0.94
0.92
3.15
3.10
3.05
3.00
2.95
6.35
6.30
6.25
Br
N
5.54
0.94
4.20
11.36
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
138.52
135.85
128.90
128.45
128.04
119.89
48.57
44.76
20.60
Br
N
140
135
130
125
120
f1 (ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

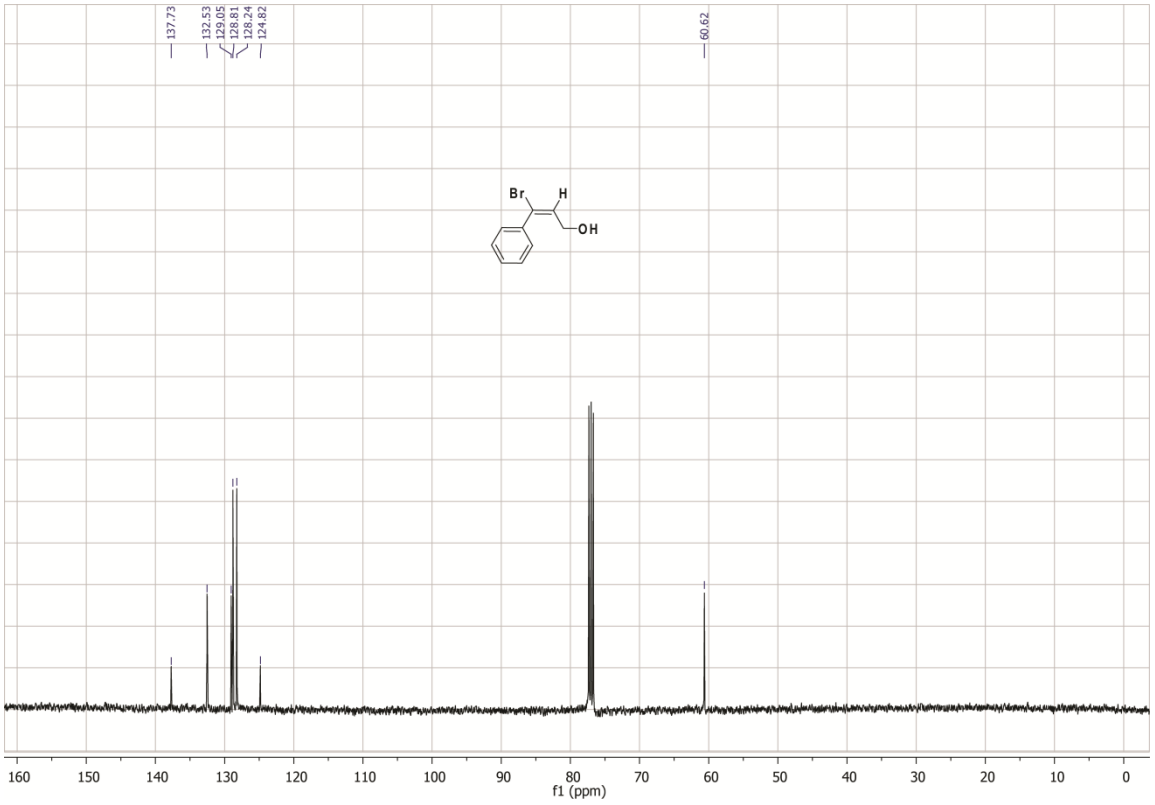
Compound **5a**


7.24
7.23
7.21
7.20
7.19
7.18
7.16
6.34
6.31
6.29
3.35
2.94
2.92
2.08
Br
N
10.13
0.91
2.17
2.00
3.08
8.5
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
-0.5
-1.0
f1 (ppm)

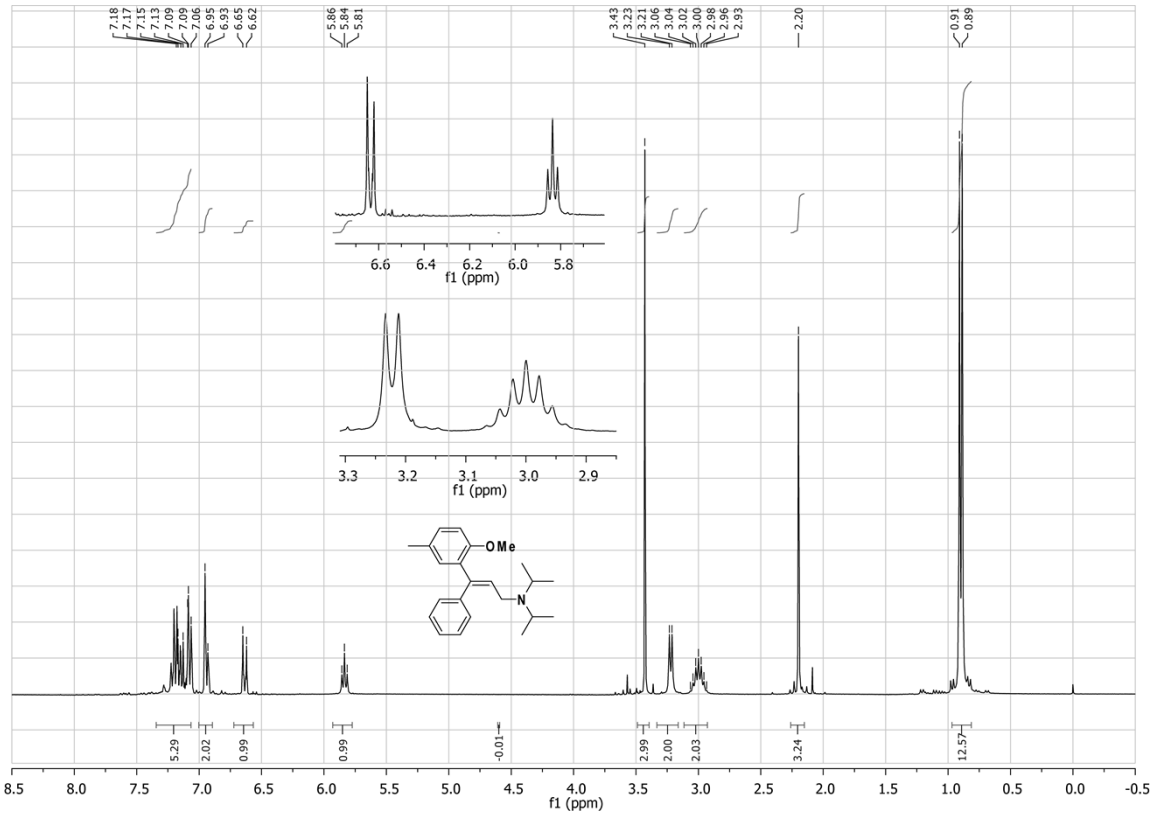

138.41
138.29
131.58
128.93
128.88
128.59
128.22
128.12
123.00
77.32
77.00
76.68
61.39
56.18
41.94
Br
N
Bn
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

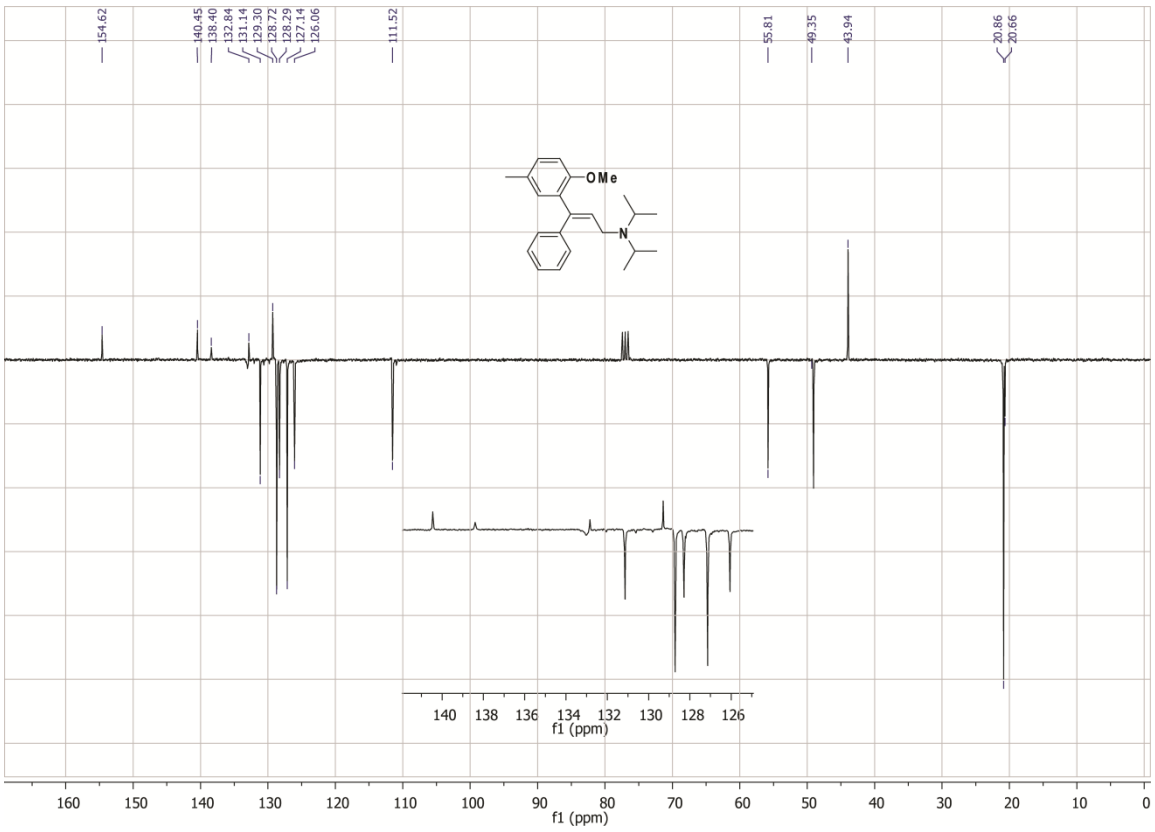
Compound **5b**


7.37
7.37
7.36
7.35
7.35
7.34
7.34
7.34
7.33
6.44
6.42
6.41
4.08
4.07
1.71
Br
H
OH
5.00
0.97
2.02
1.46
f1 (ppm)

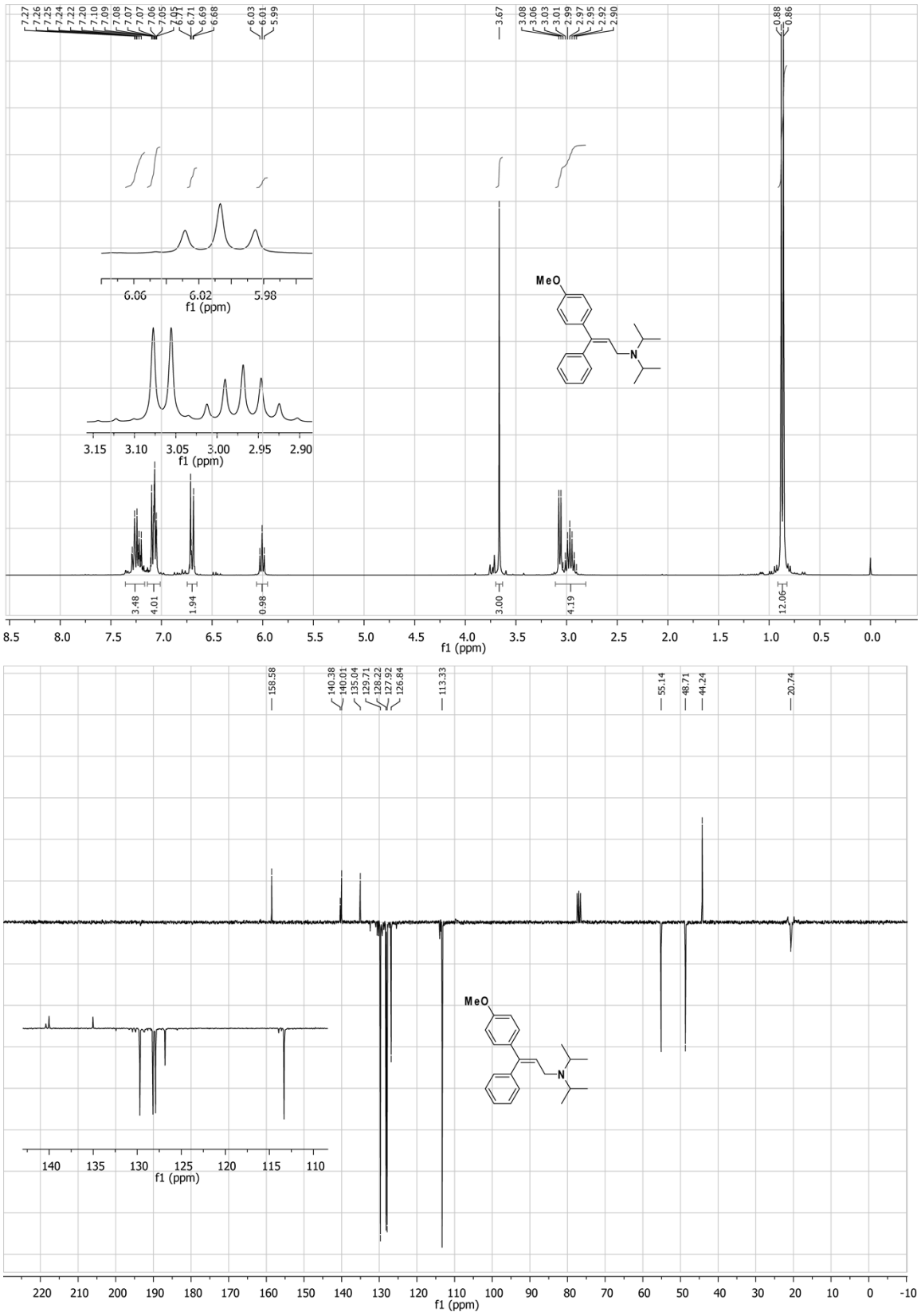

137.73
132.53
129.05
128.81
128.24
124.82
60.62
Br
H
OH
f1 (ppm)

Compound **5c**

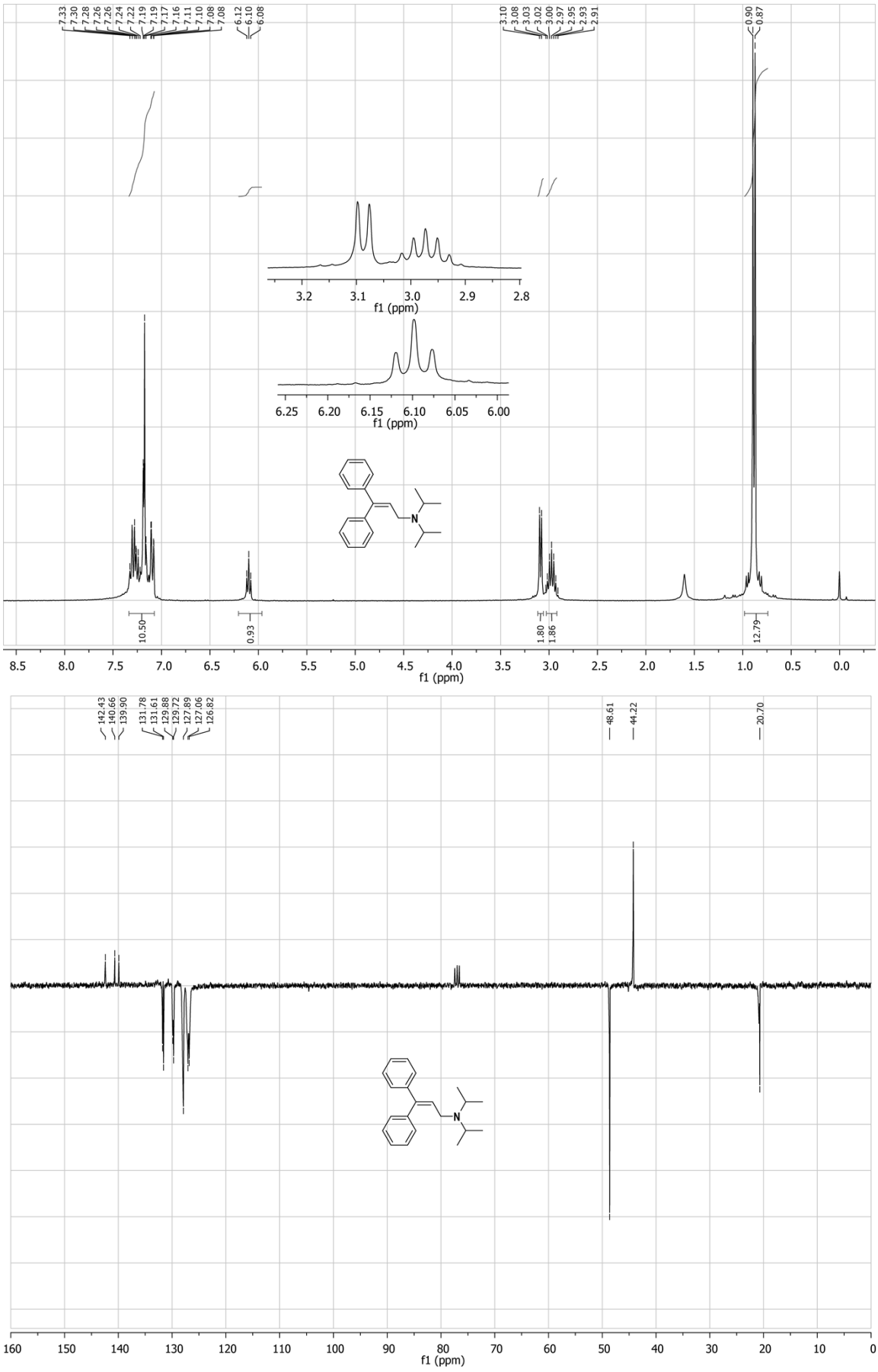

7.18
7.17
7.15
7.13
7.09
7.09
7.06
6.95
6.93
6.65
6.62
5.86
5.84
5.81
3.43
3.23
3.21
3.06
3.04
3.02
3.00
2.98
2.96
2.93
2.20
0.91
0.89
6.6 6.4 6.2 6.0 5.8
f1 (ppm)
3.3 3.2 3.1 3.0 2.9
f1 (ppm)
OMe
N
5.29
2.02
0.99
0.99
-0.01
2.99
2.00
2.03
3.24
12.57
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


154.62
140.45
138.40
132.84
131.14
129.30
128.72
128.29
127.14
126.06
111.52
55.81
49.35
43.94
20.86
20.66
OMe
N
140 138 136 134 132 130 128 126
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

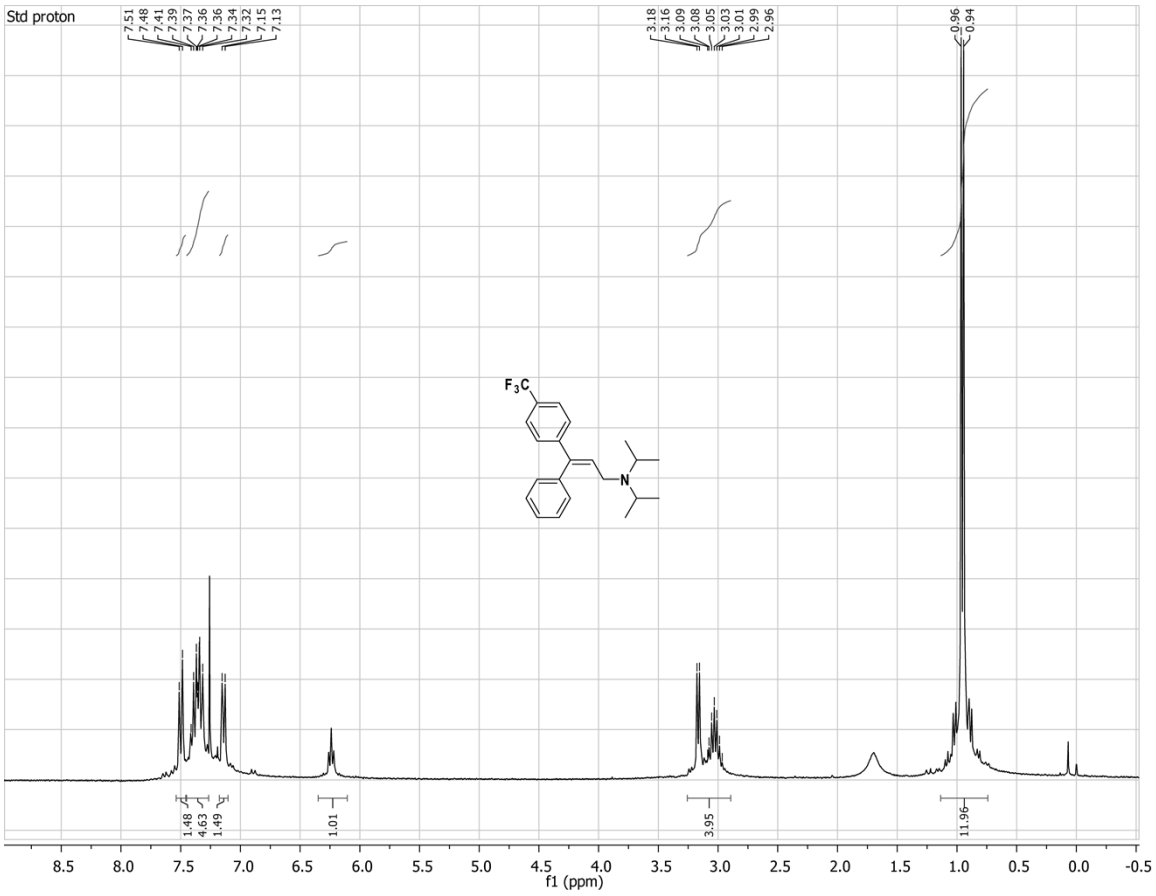
Compound **6a**

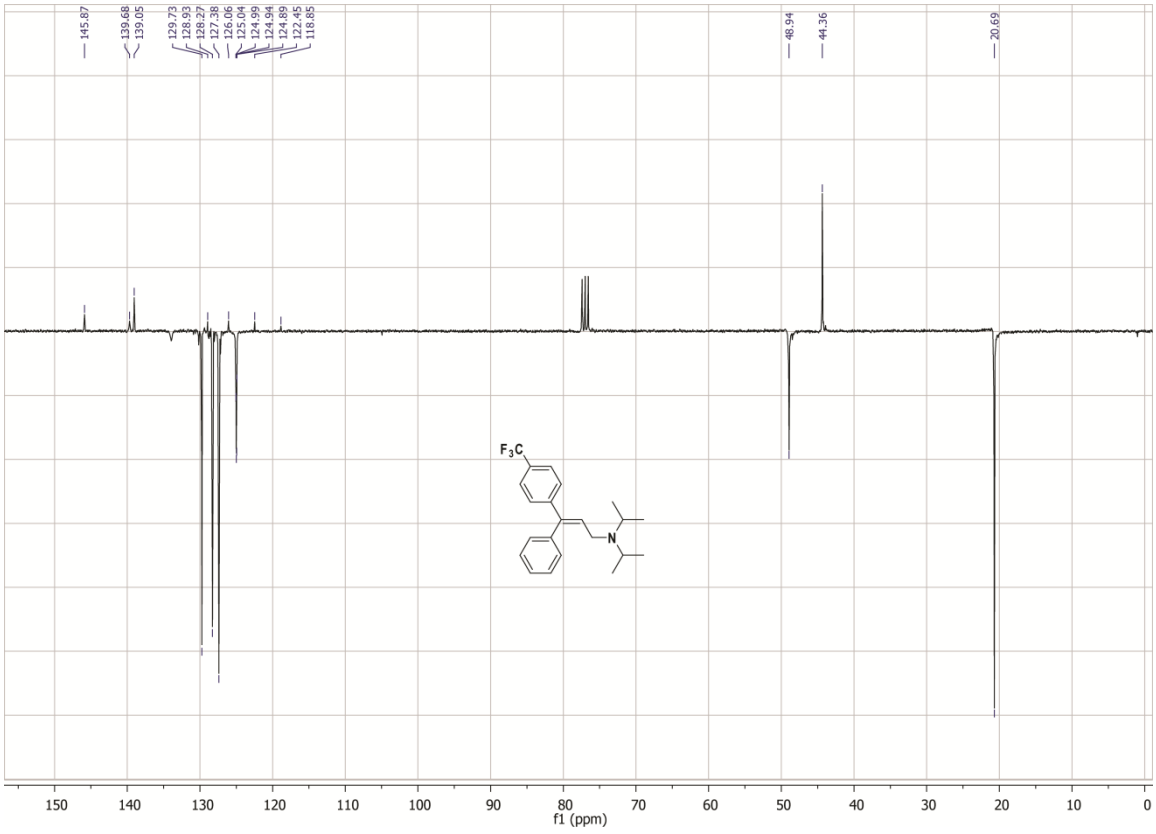

7.27
7.26
7.25
7.24
7.22
7.20
7.10
7.09
7.08
7.07
7.07
7.06
7.05
7.05
6.71
6.69
6.68
6.03
6.01
5.99
3.67
3.08
3.06
3.03
3.01
2.99
2.97
2.95
2.92
2.90
0.88
0.86
MeO
N
6.06
6.02
5.98
f1 (ppm)
3.15
3.10
3.05
3.00
2.95
2.90
f1 (ppm)
3.48
4.01
1.94
0.98
3.00
4.19
12.06
f1 (ppm)
158.58
140.38
140.01
135.04
129.71
128.22
127.92
126.84
113.33
55.14
48.71
44.24
20.74
MeO
N
140
135
130
125
120
115
110
f1 (ppm)
f1 (ppm)

Compound **7a**

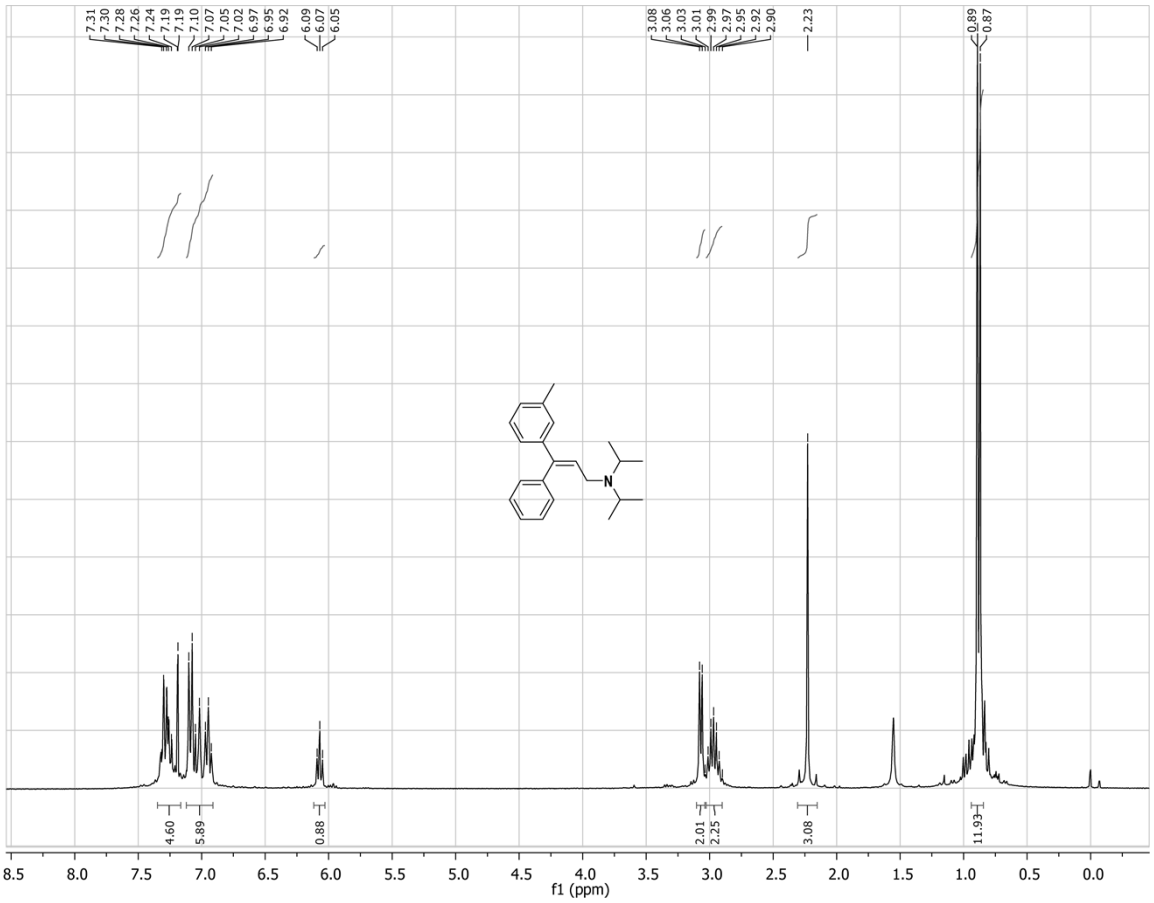

7.33
7.30
7.28
7.26
7.26
7.24
7.22
7.19
7.19
7.17
7.16
7.11
7.10
7.08
7.08
6.12
6.10
6.08
3.10
3.08
3.03
3.02
3.00
2.97
2.95
2.93
2.91
0.90
0.87
3.2
3.1
3.0
2.9
2.8
f1 (ppm)
6.25
6.20
6.15
6.10
6.05
6.00
f1 (ppm)
N
10.50
0.93
1.80
1.86
12.79
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
142.43
140.66
139.90
131.78
131.61
129.88
129.72
127.89
127.06
126.82
48.61
44.22
20.70
N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

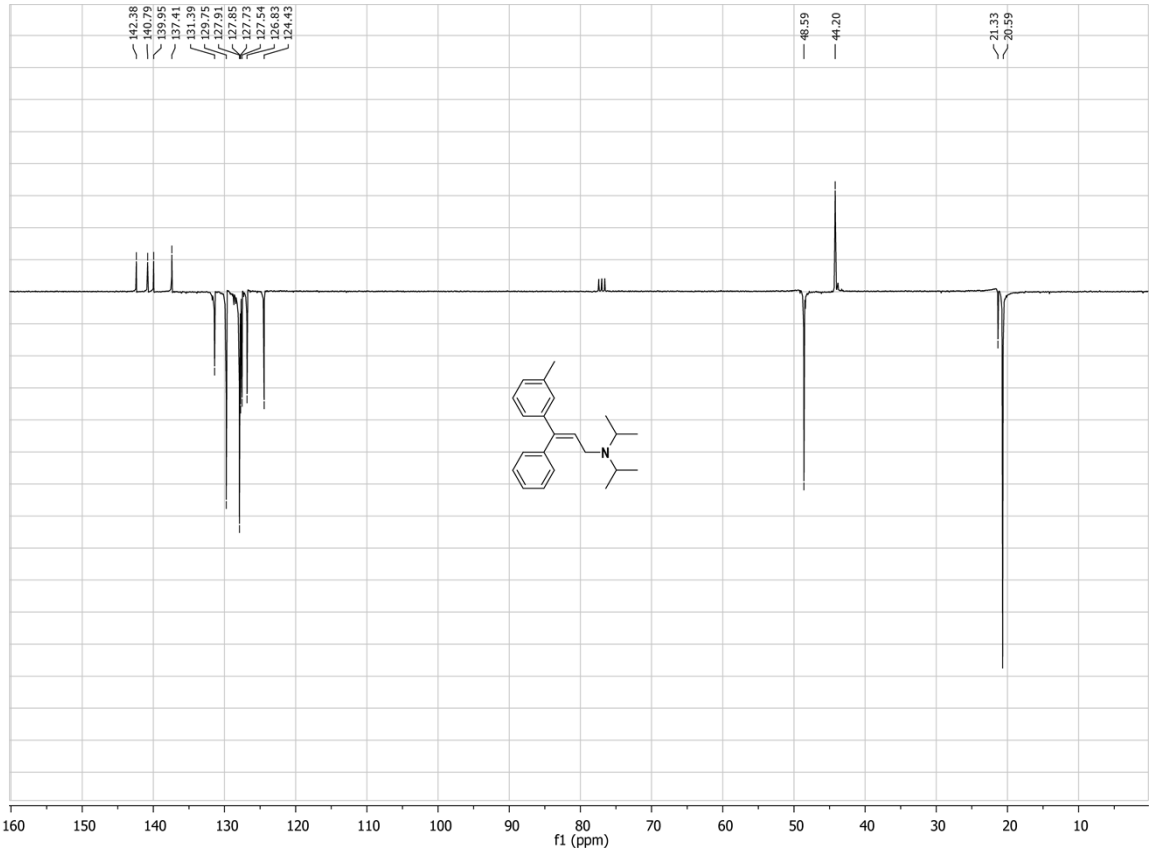
Compound **8a**


Std proton
7.51
7.48
7.41
7.39
7.37
7.36
7.36
7.34
7.32
7.15
7.13
3.18
3.16
3.09
3.08
3.05
3.03
3.01
2.99
2.96
0.96
0.94
F3C
N
1.48
4.63
1.49
1.01
3.95
11.96
f1 (ppm)

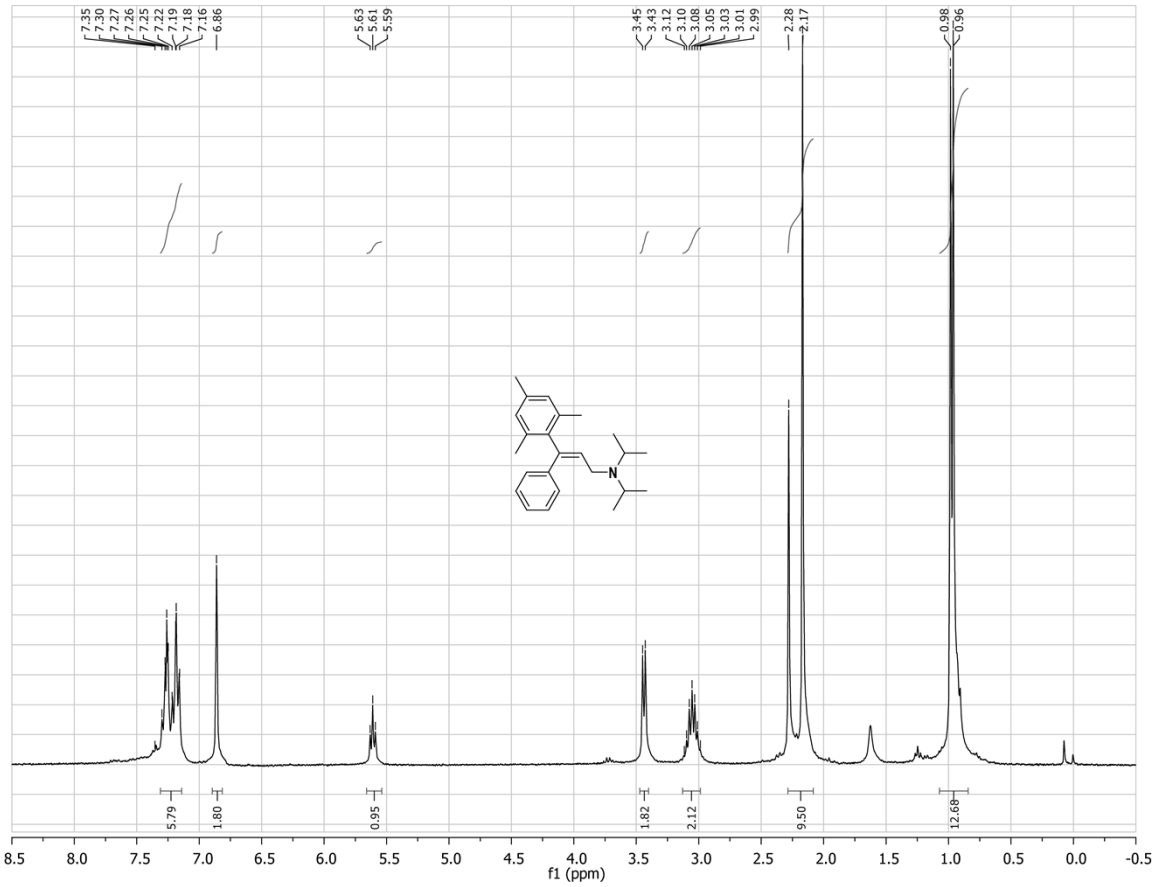

145.87
139.68
139.05
129.73
128.93
128.27
127.38
126.06
125.04
124.99
124.94
124.89
122.45
118.65
48.94
44.36
20.69
F3C
N
f1 (ppm)

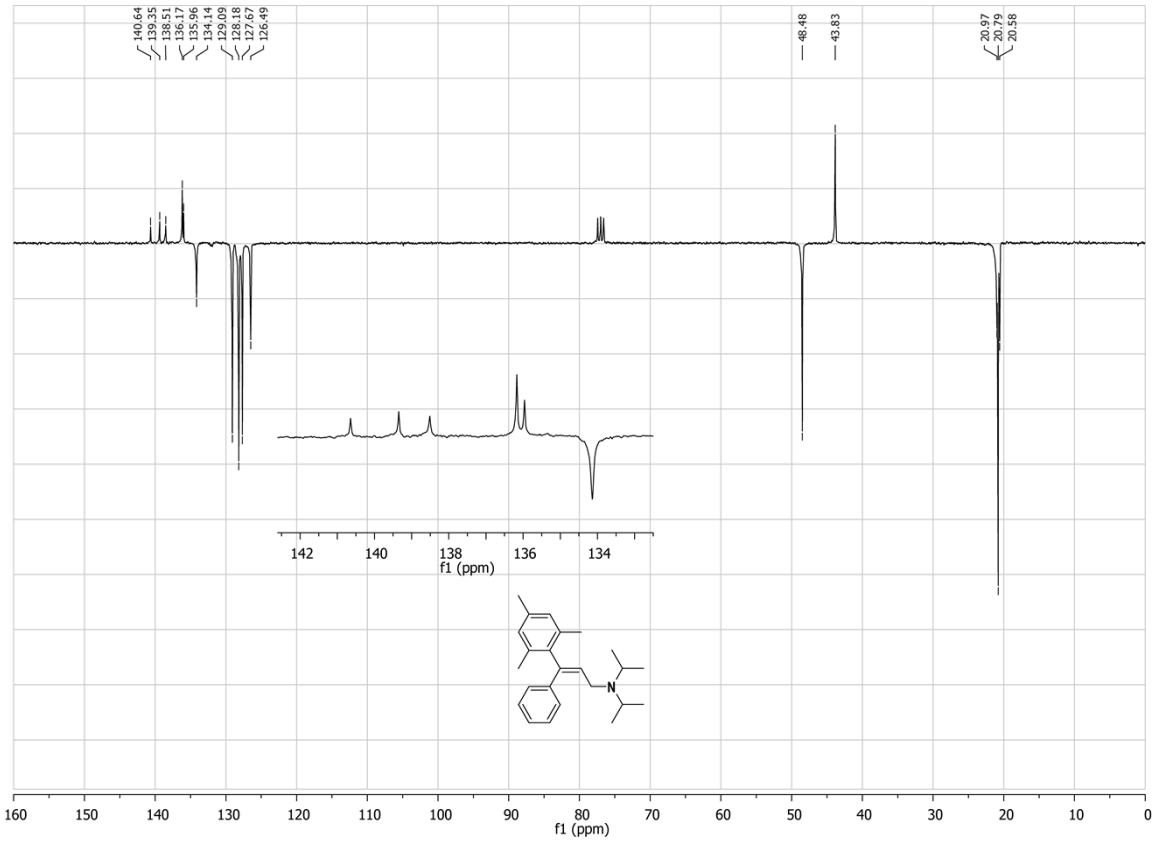
Compound **9a**



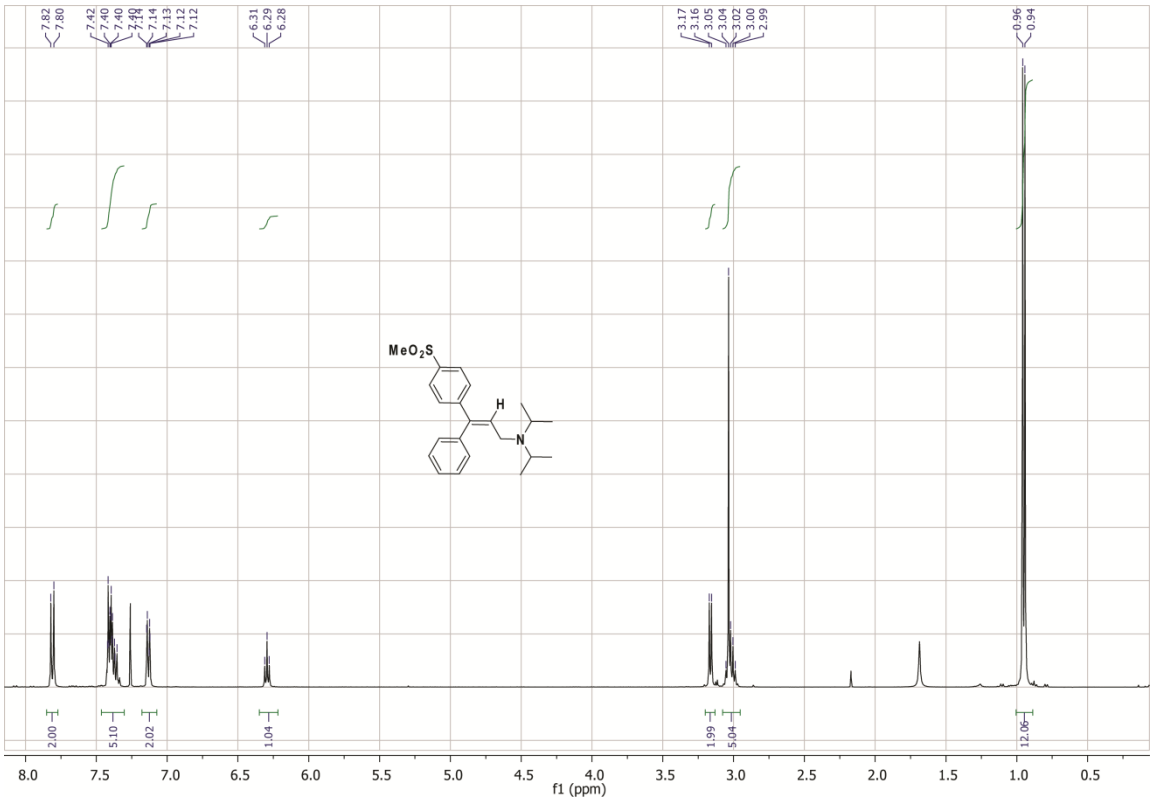


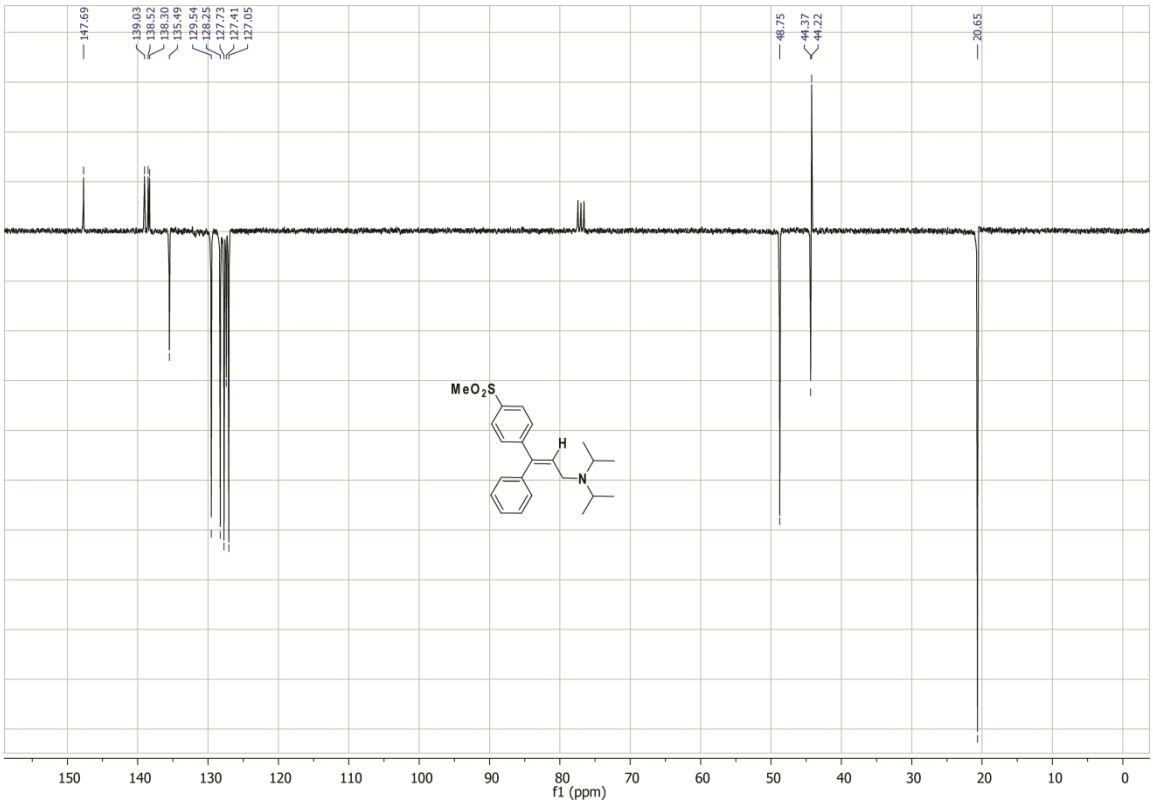
Compound **10a**



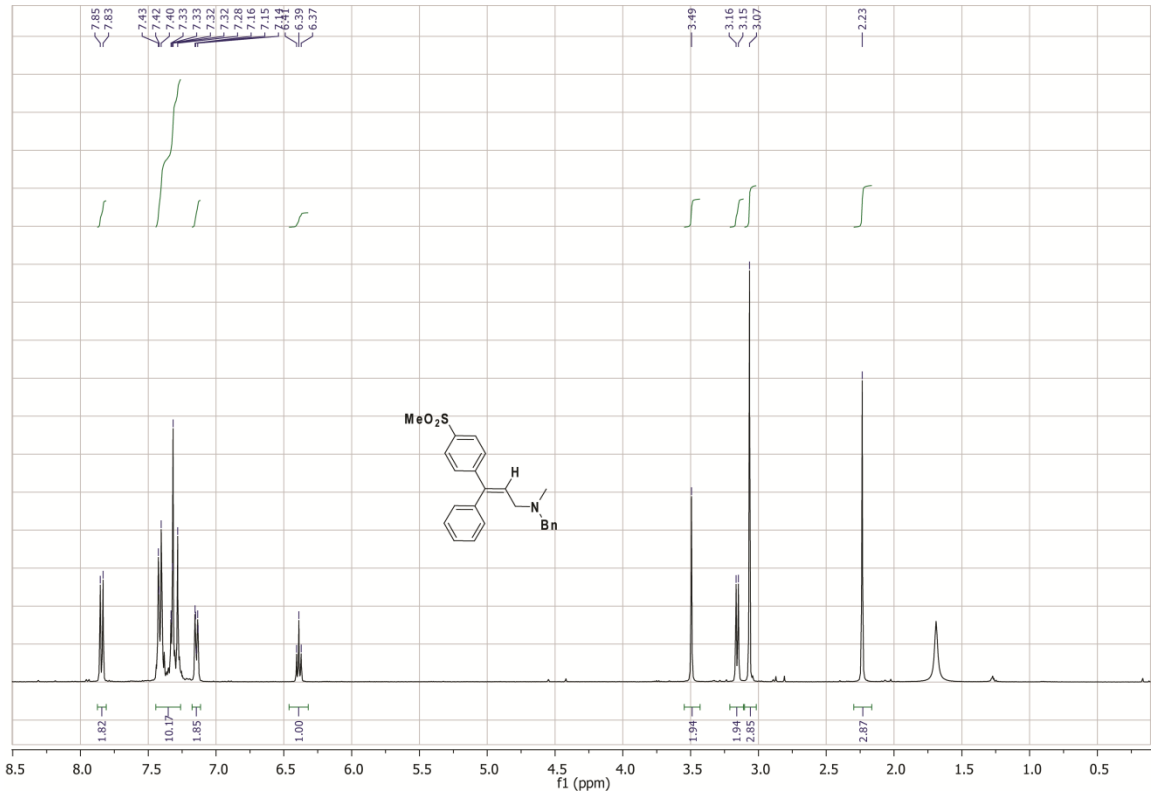


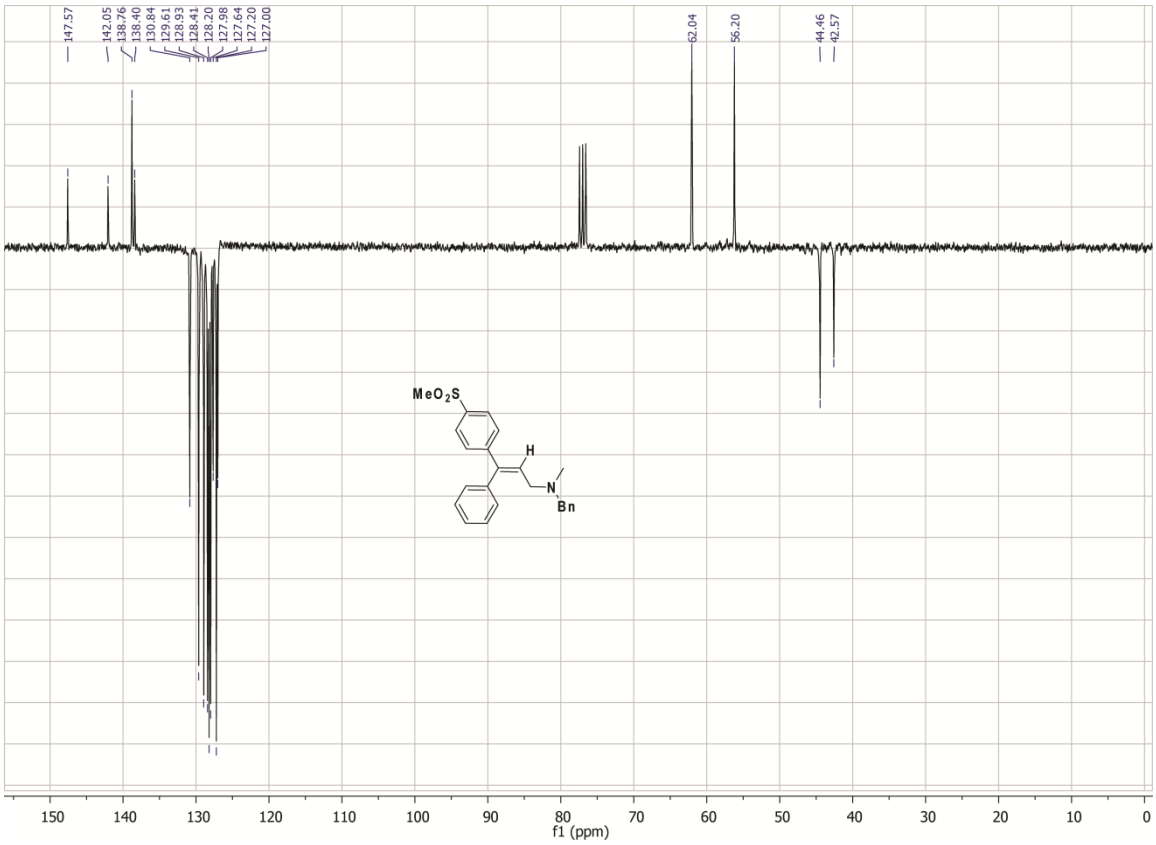
Compound **11a**



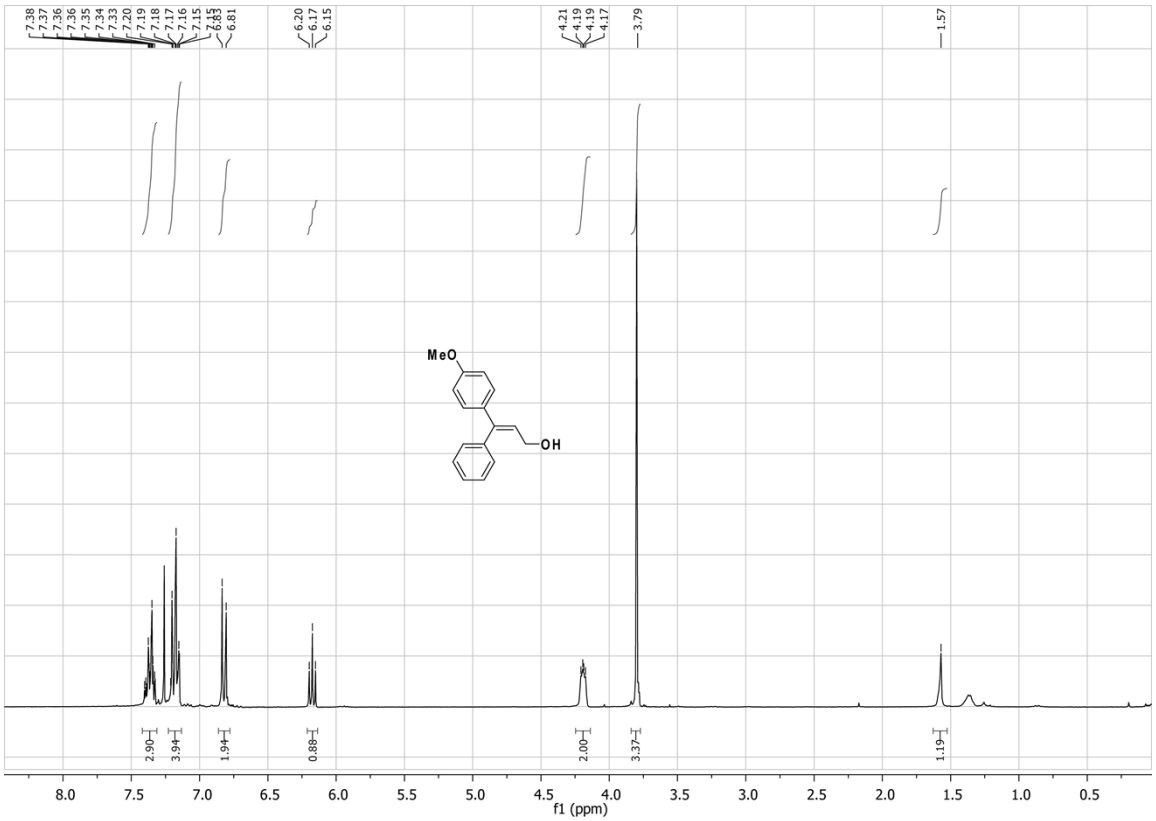


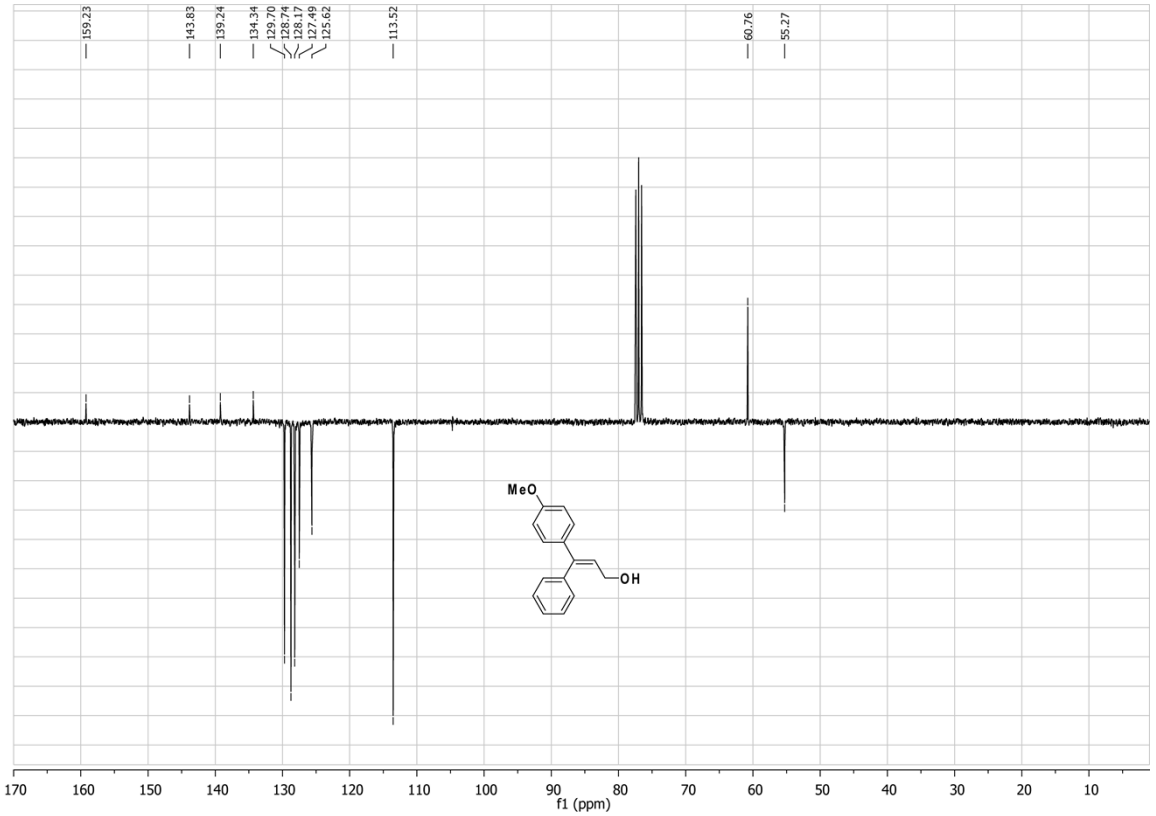
Compound **12a**


7.85
7.83
7.43
7.42
7.40
7.33
7.32
7.28
7.16
7.15
7.14
6.41
6.39
6.37
3.49
3.16
3.15
3.07
2.23
MeO2S
H
N
Bn
1.82
10.17
1.85
1.00
1.94
1.94
2.85
2.87
f1 (ppm)

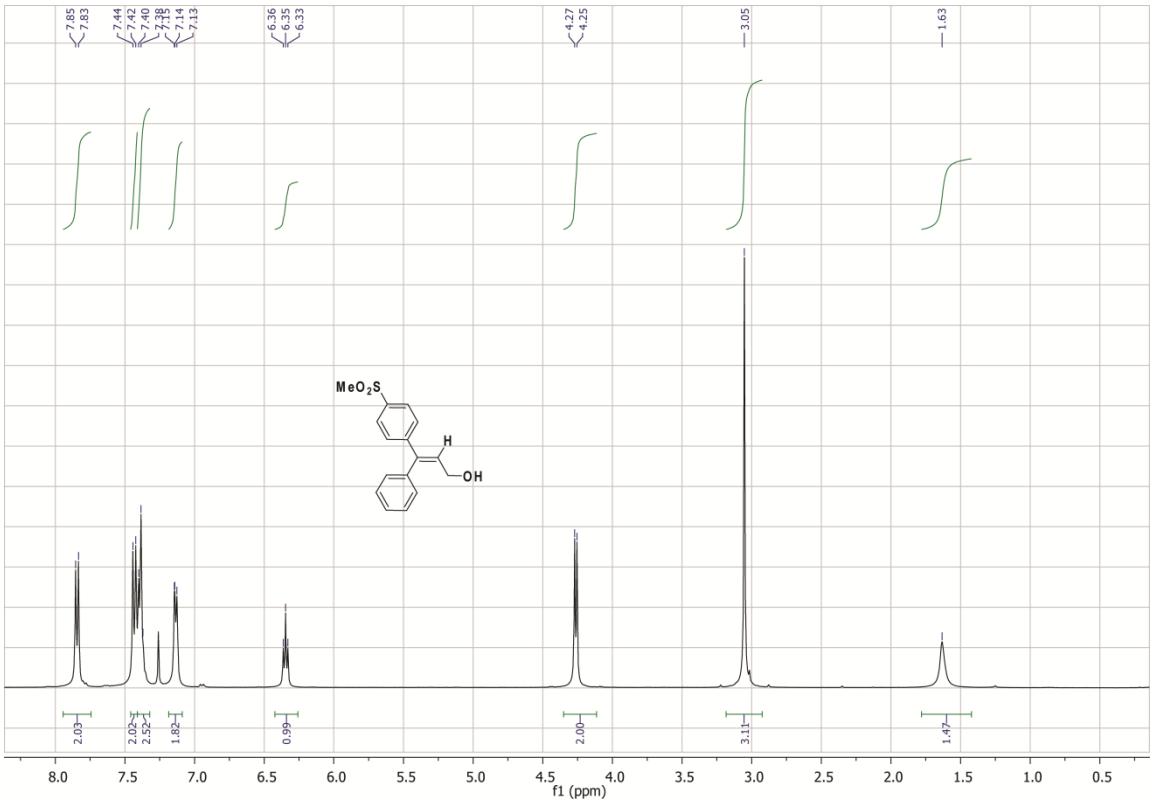

147.57
142.05
138.76
138.40
130.84
129.61
128.93
128.41
128.20
127.98
127.64
127.20
127.00
62.04
56.20
44.46
42.57
MeO2S
H
N
Bn
f1 (ppm)

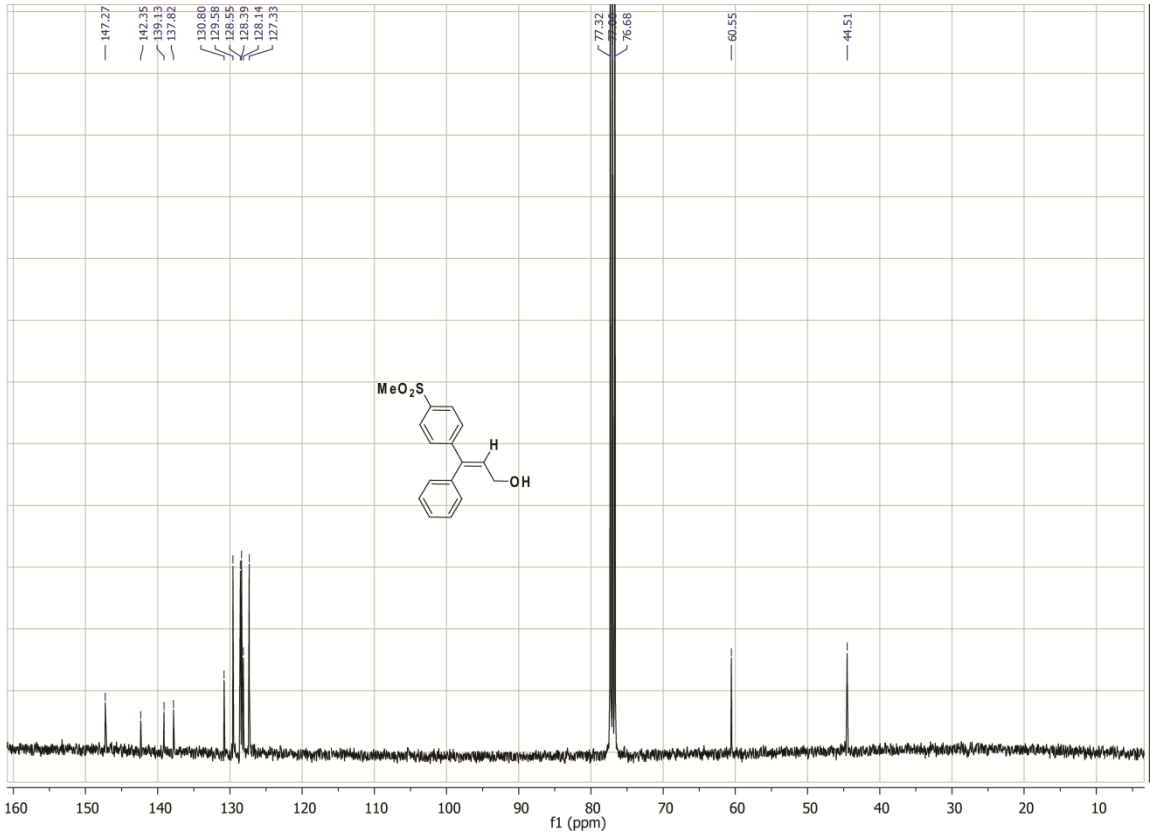
Compound **6b**


7.38
7.37
7.36
7.36
7.35
7.34
7.33
7.20
7.19
7.18
7.17
7.16
7.15
6.83
6.81
6.20
6.17
6.15
4.21
4.19
4.19
4.19
4.17
3.79
1.57
MeO
OH
2.90
3.94
1.94
0.88
2.00
3.37
1.19
f1 (ppm)

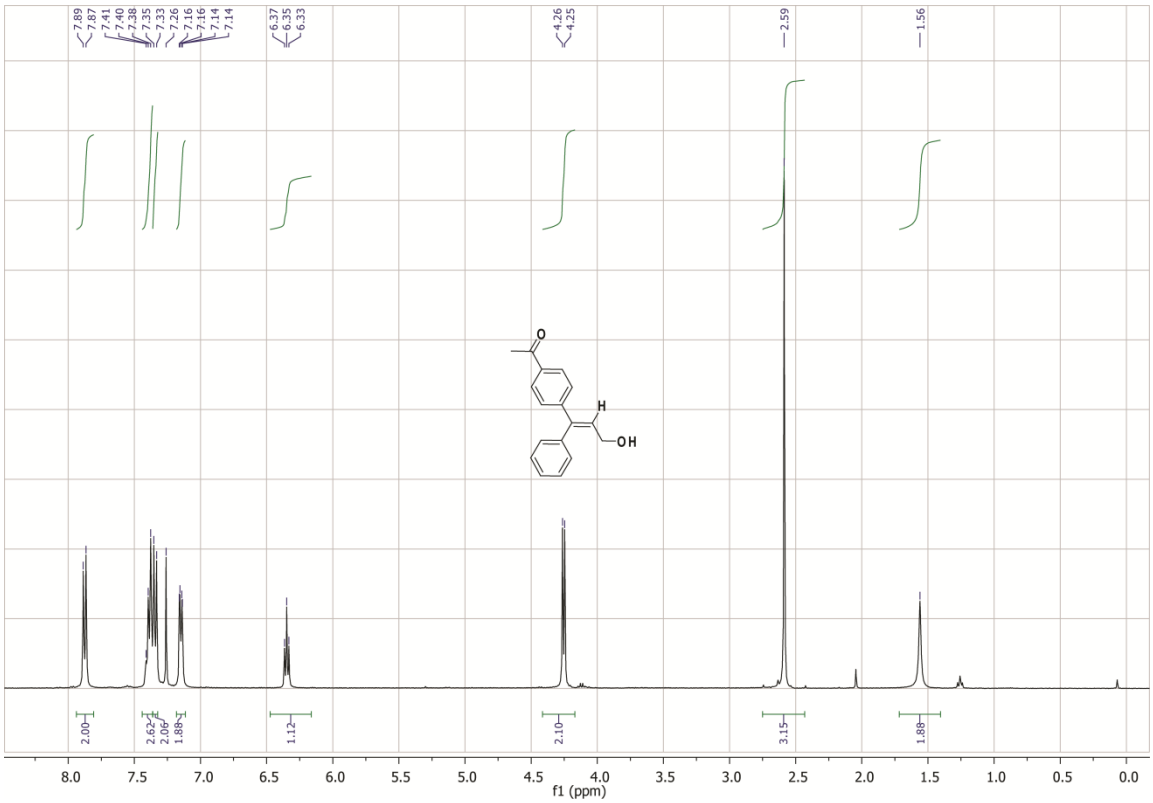

159.23
143.83
139.24
134.34
129.70
128.74
128.17
127.49
125.62
113.52
60.76
55.27
MeO
OH
f1 (ppm)

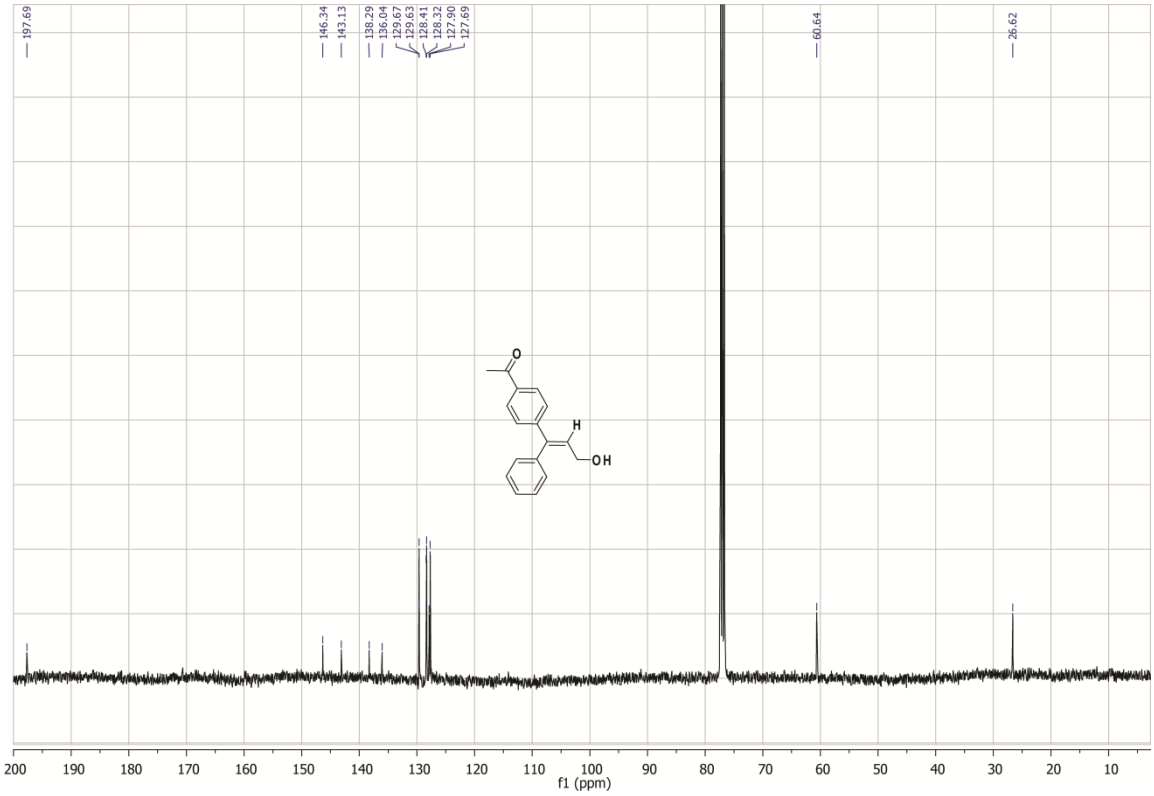
Compound **6c**


7.85
7.83
7.44
7.42
7.40
7.18
7.14
7.13
6.36
6.35
6.33
4.27
4.25
3.05
1.63
MeO2S
H
OH
2.03
2.02
2.52
1.82
0.99
2.00
3.11
1.47
f1 (ppm)

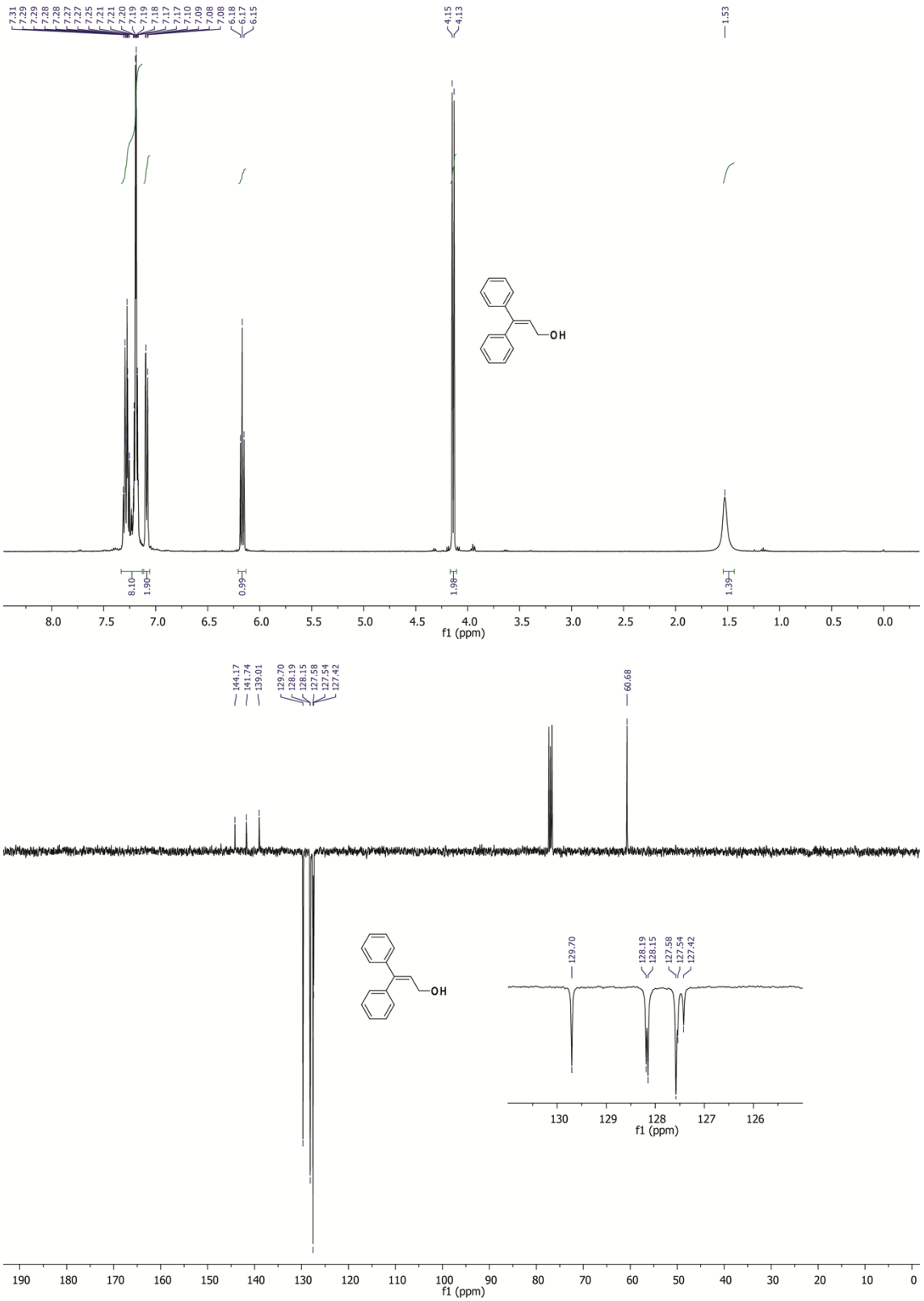

147.27
142.35
139.13
137.82
130.80
129.58
128.55
128.39
128.14
127.33
77.32
76.68
60.55
44.51
MeO2S
H
OH
f1 (ppm)

Compound **7c**

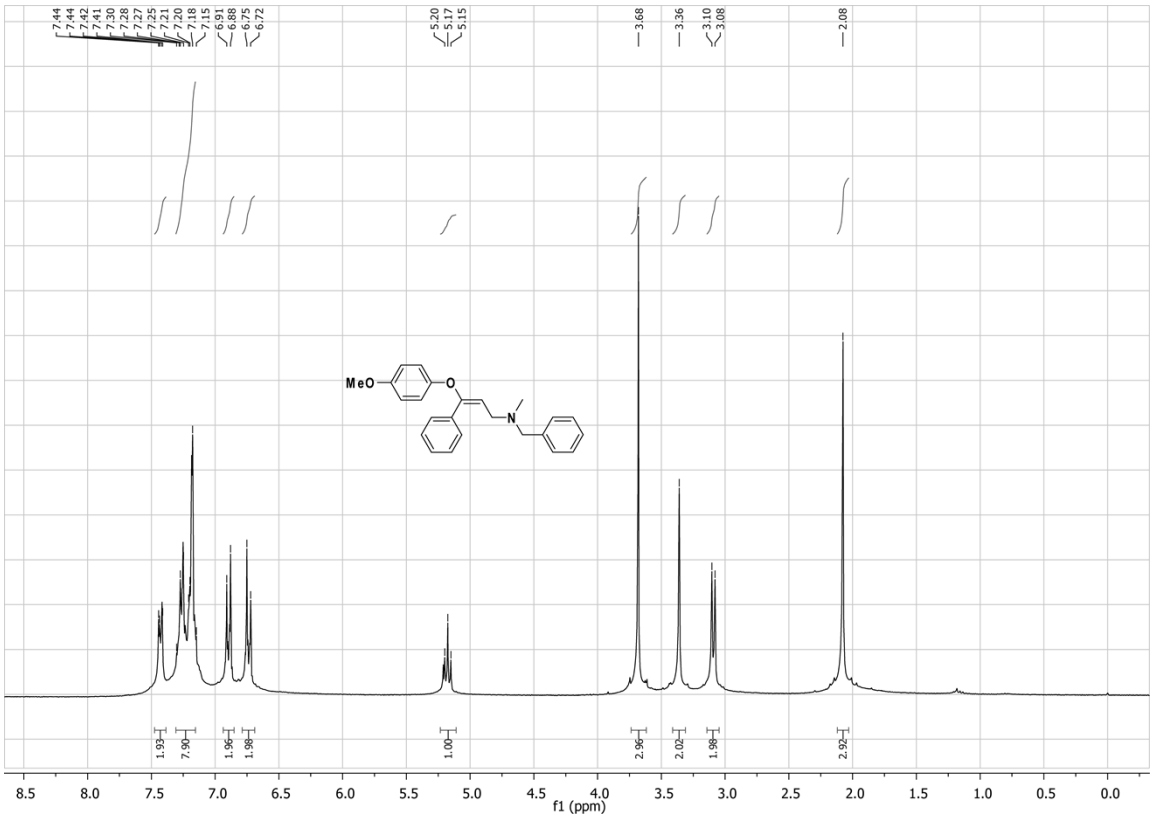

7.89
7.87
7.41
7.40
7.38
7.35
7.33
7.26
7.16
7.16
7.14
7.14
6.37
6.35
6.33
4.26
4.25
2.59
1.56
O
H
OH
2.00
2.62
2.06
1.89
1.12
2.10
3.15
1.88
f1 (ppm)

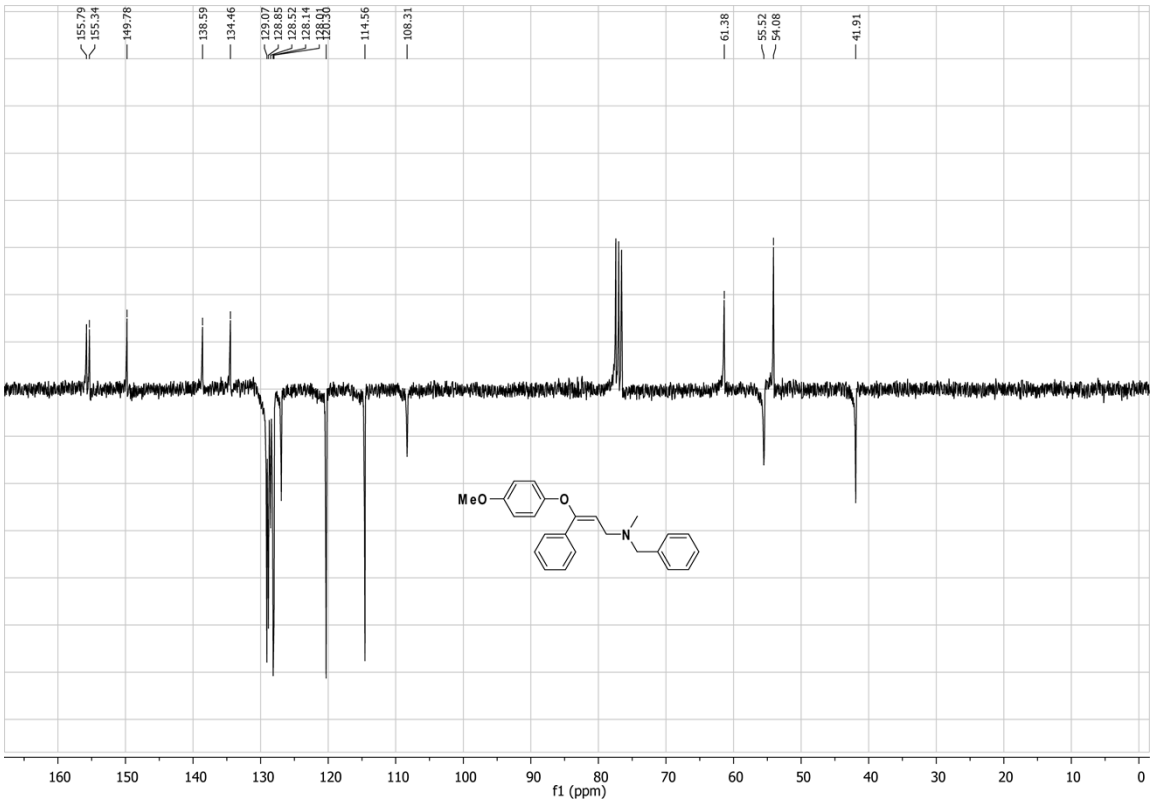

197.69
146.34
143.13
138.29
136.04
129.67
129.63
128.41
128.32
127.90
127.69
60.64
26.62
O
H
OH
f1 (ppm)

Compound **8c**

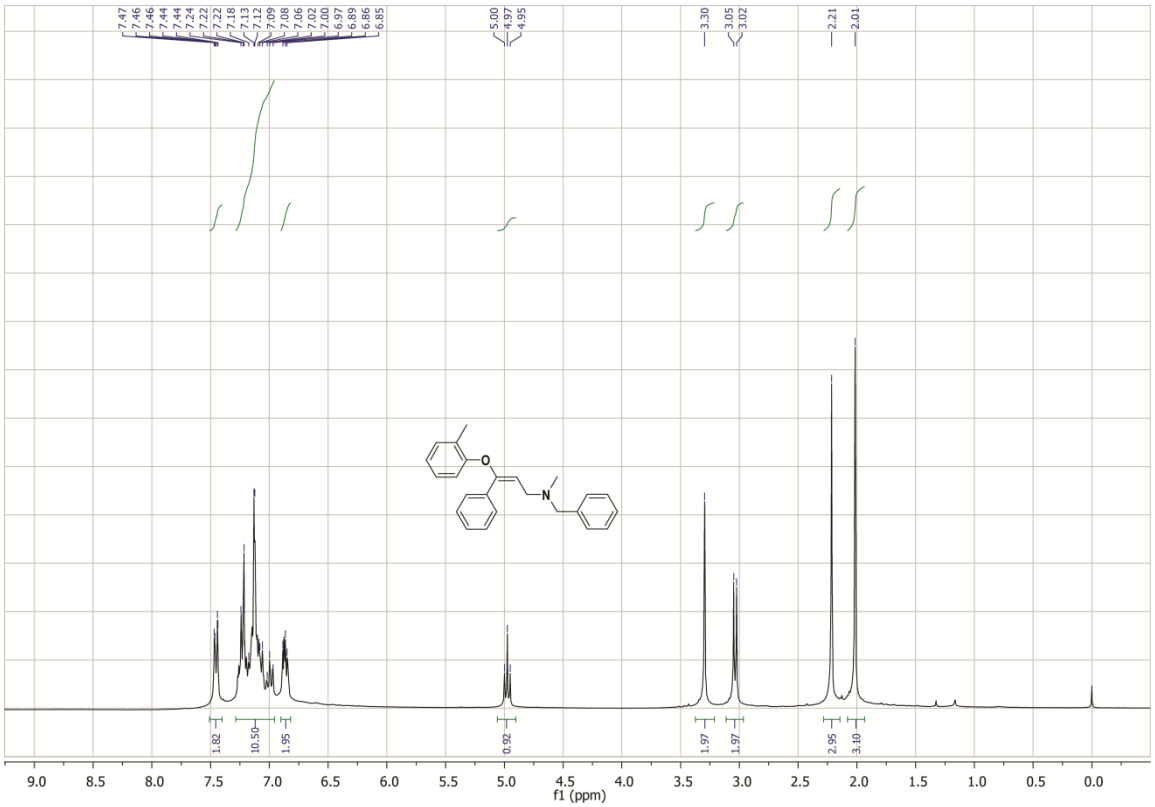

7.31
7.29
7.29
7.28
7.28
7.28
7.27
7.27
7.25
7.21
7.21
7.20
7.19
7.19
7.18
7.17
7.17
7.10
7.09
7.08
7.08
6.18
6.17
6.15
4.15
4.13
1.53
OH
8.10
1.90
0.99
1.98
1.39
f1 (ppm)
144.17
141.74
139.01
129.70
128.19
128.15
127.58
127.54
127.42
60.68
OH
129.70
128.19
128.15
127.58
127.54
127.42
f1 (ppm)

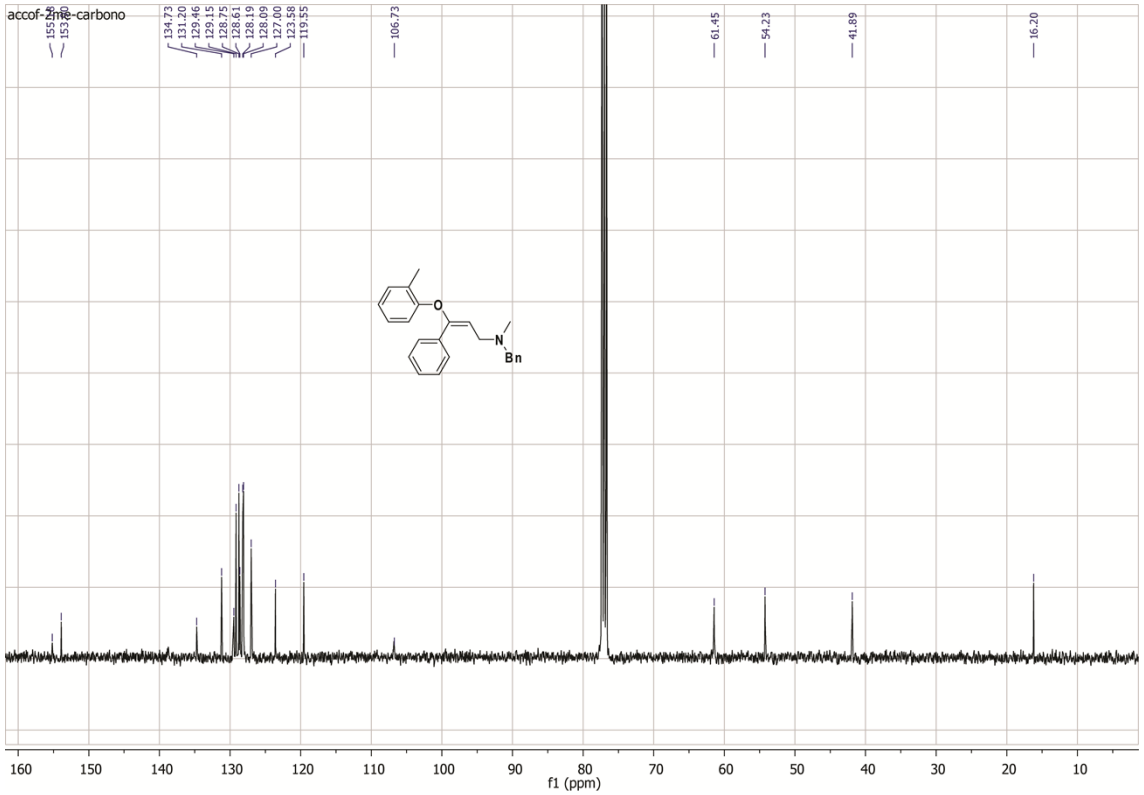
Compound 9c


7.44
7.44
7.42
7.41
7.30
7.28
7.27
7.25
7.21
7.20
7.18
7.15
6.91
6.88
6.75
6.72
5.20
5.17
5.15
3.68
3.36
3.10
3.08
2.08
MeO
O
N
1.93
7.90
1.96
1.98
1.00
2.96
2.02
1.98
2.92
f1 (ppm)

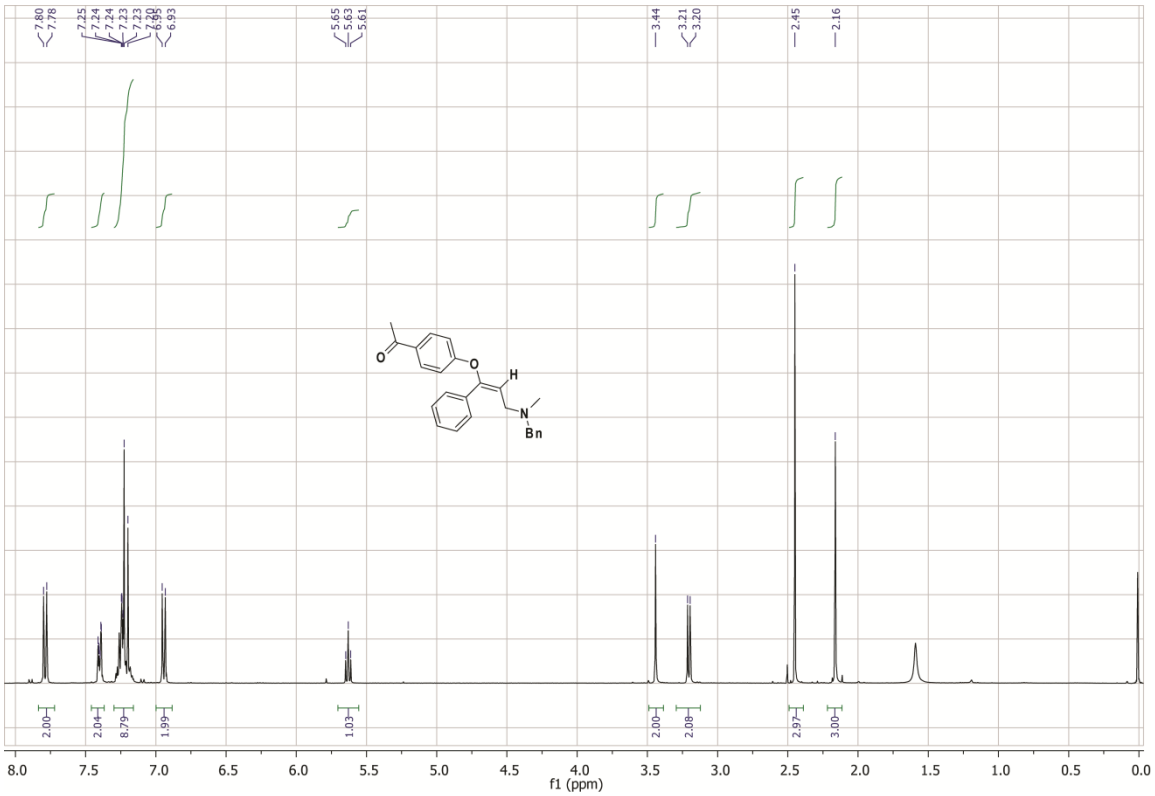

155.79
155.34
149.78
138.59
134.46
129.07
128.85
128.52
128.14
128.01
120.30
114.56
108.31
61.38
55.52
54.08
41.91
MeO
O
N
f1 (ppm)

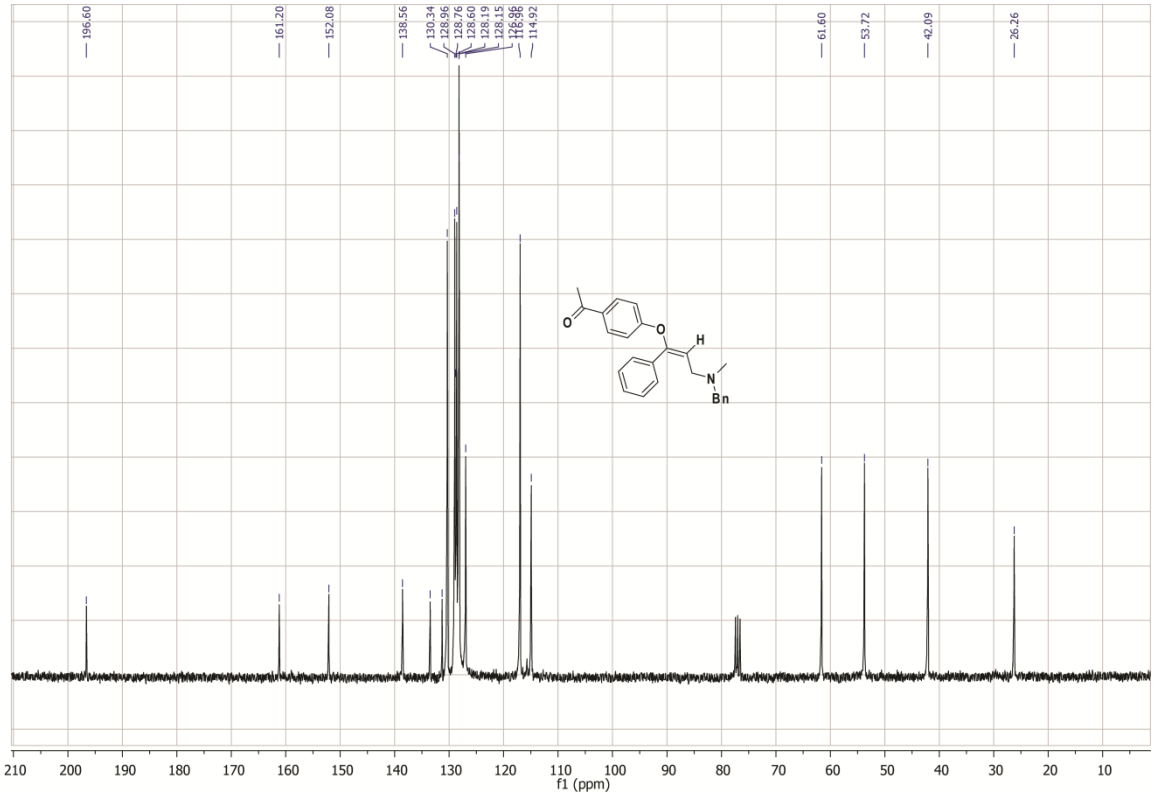
Compound **8b**


7.47
7.46
7.46
7.44
7.44
7.24
7.22
7.22
7.18
7.13
7.12
7.09
7.08
7.06
7.02
7.00
6.97
6.89
6.86
6.85
5.00
4.97
4.95
3.30
3.05
3.02
2.21
2.01
1.82
10.50
1.95
0.92
1.97
1.97
2.95
3.10
O
N
9.0 8.5 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
f1 (ppm)

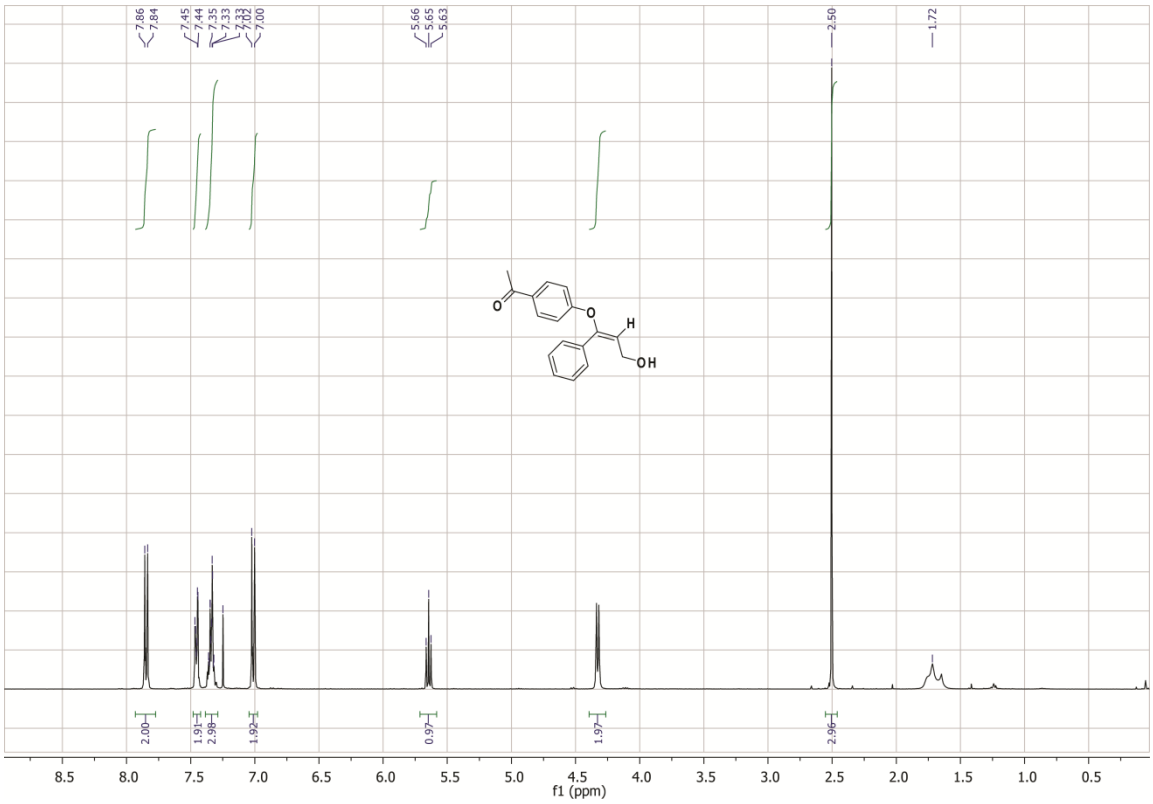

accof-2me-carbono
159.48
153.20
134.73
131.20
129.46
129.15
128.75
128.61
128.19
128.09
127.00
123.58
119.55
106.73
61.45
54.23
41.89
16.20
O
N
Bn
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

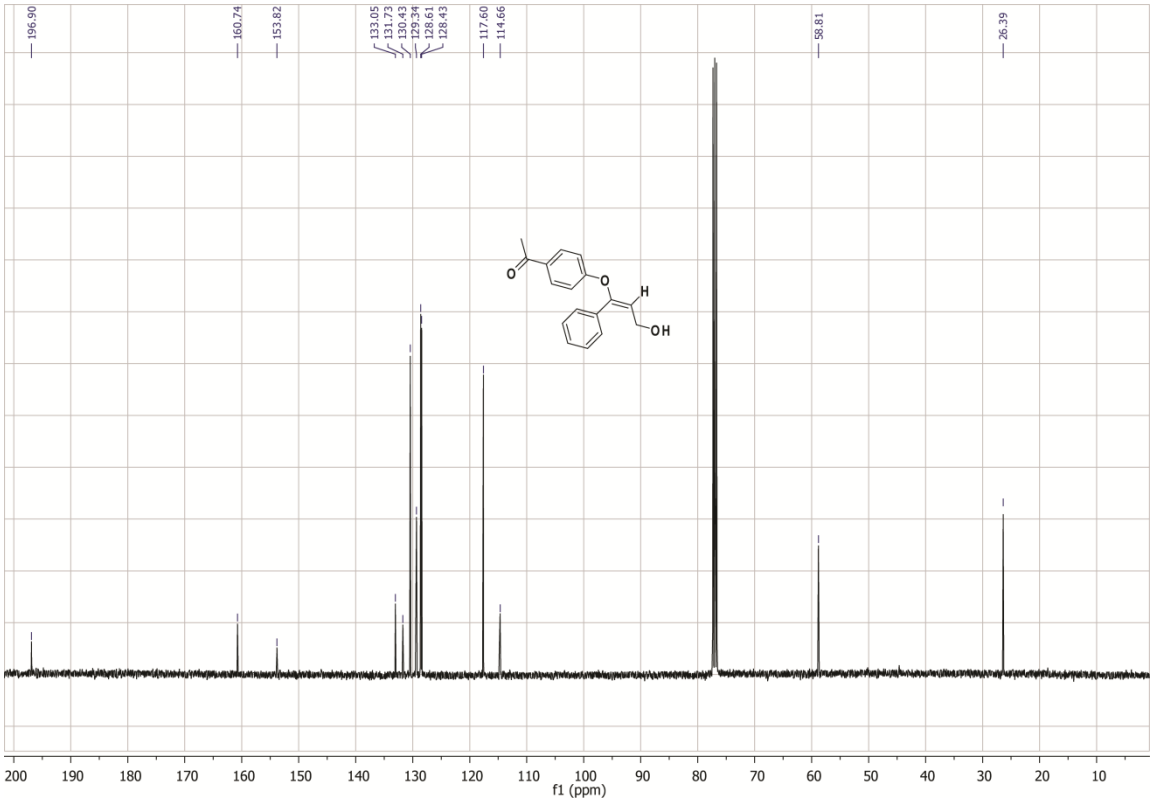
Compound **9b**



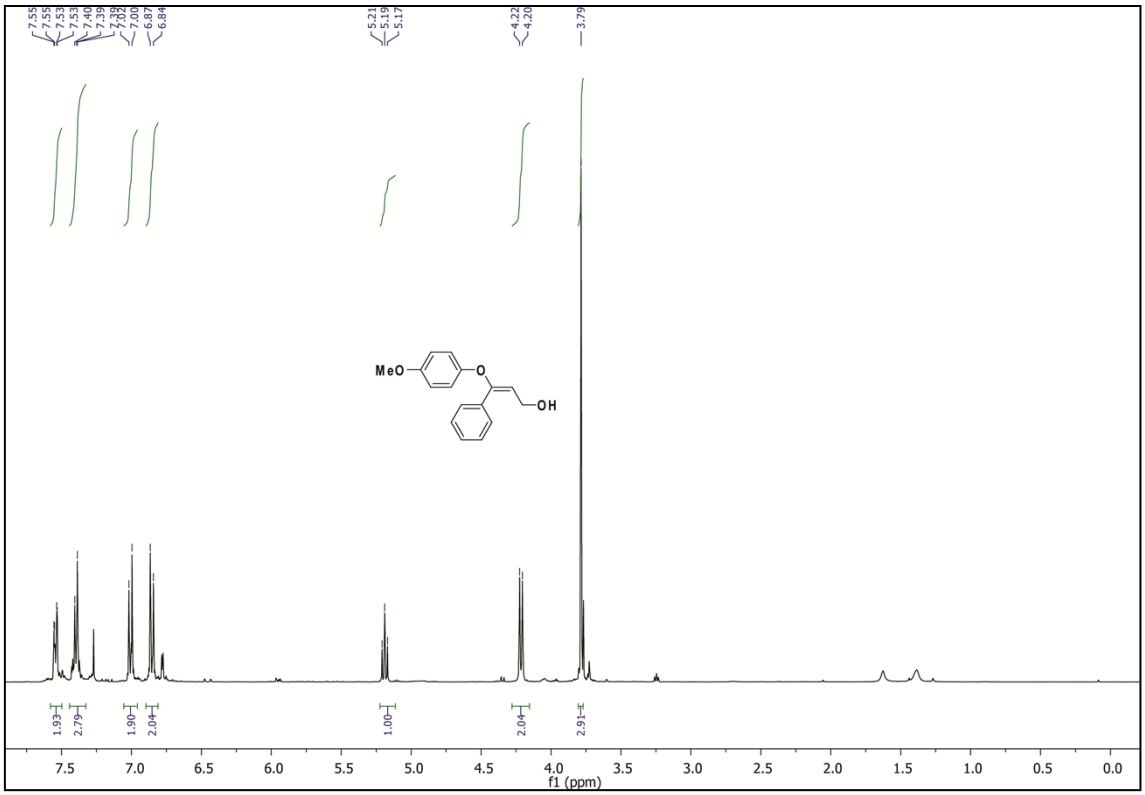


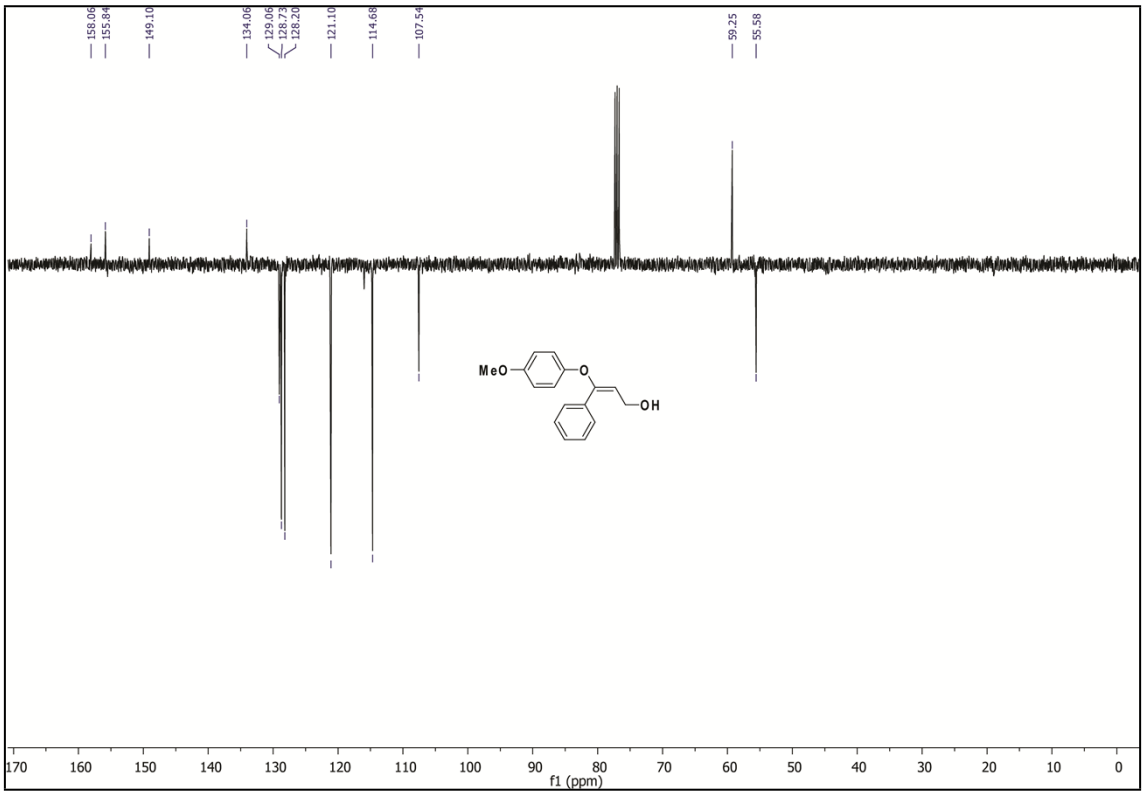
Compound **10b**





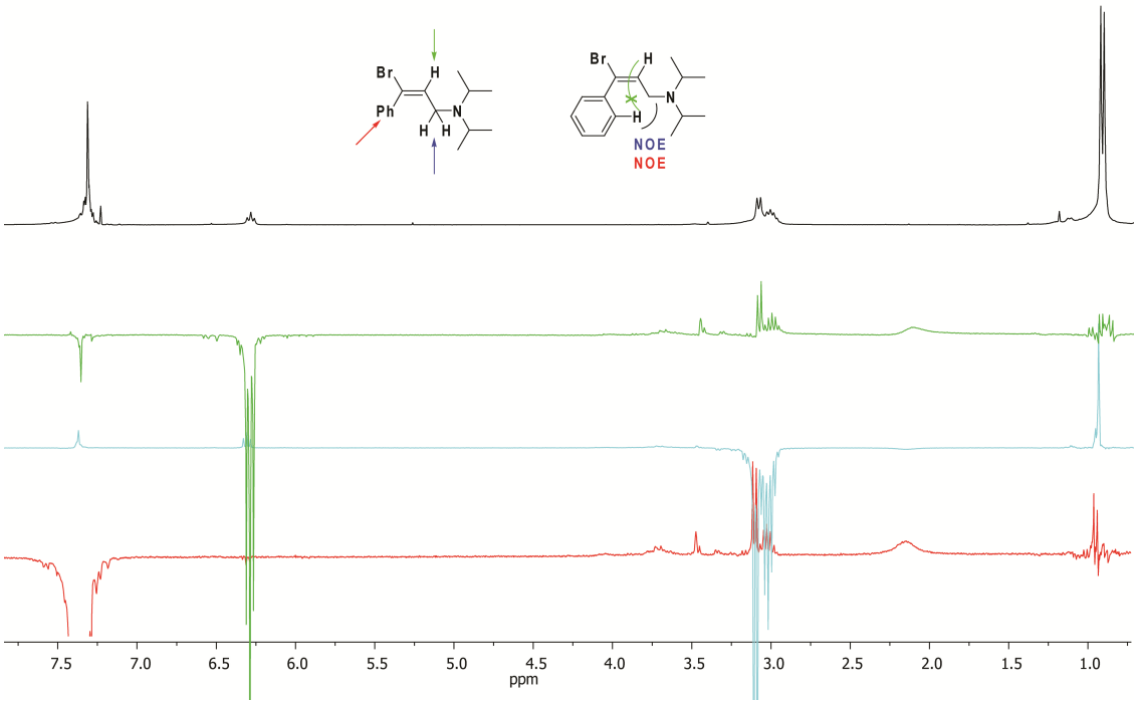
Compound **10c**



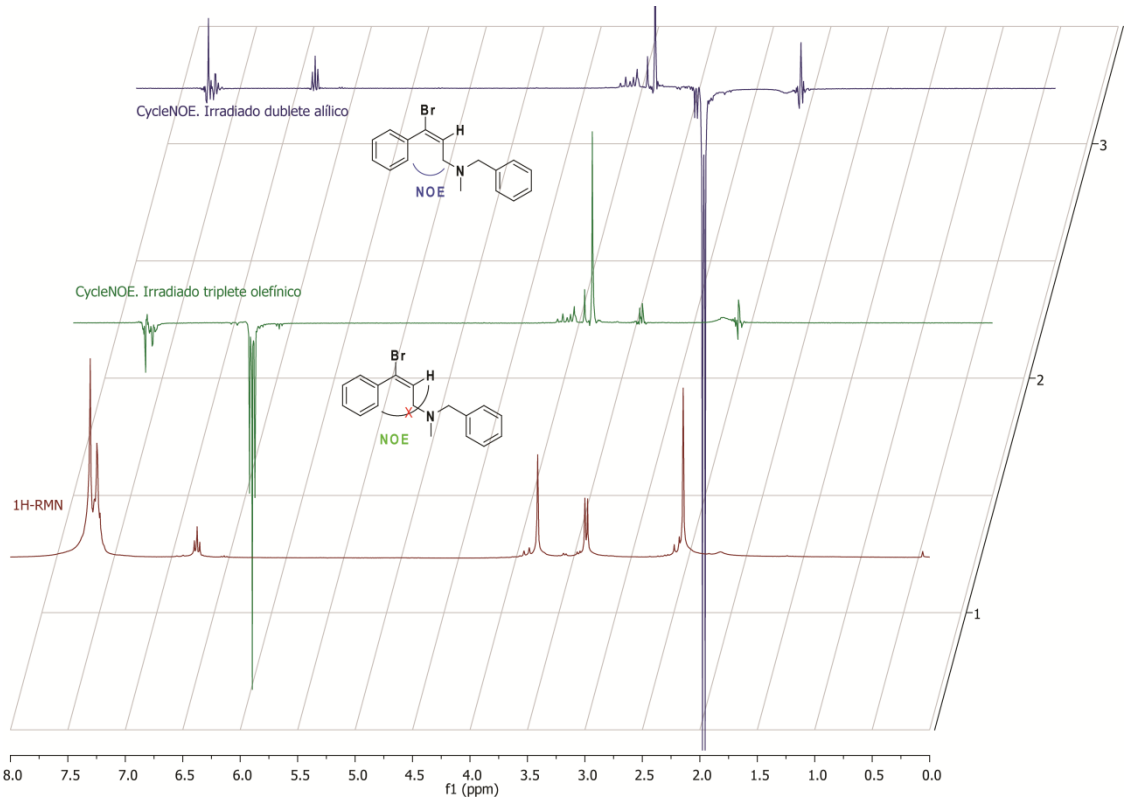


Compound **11c**

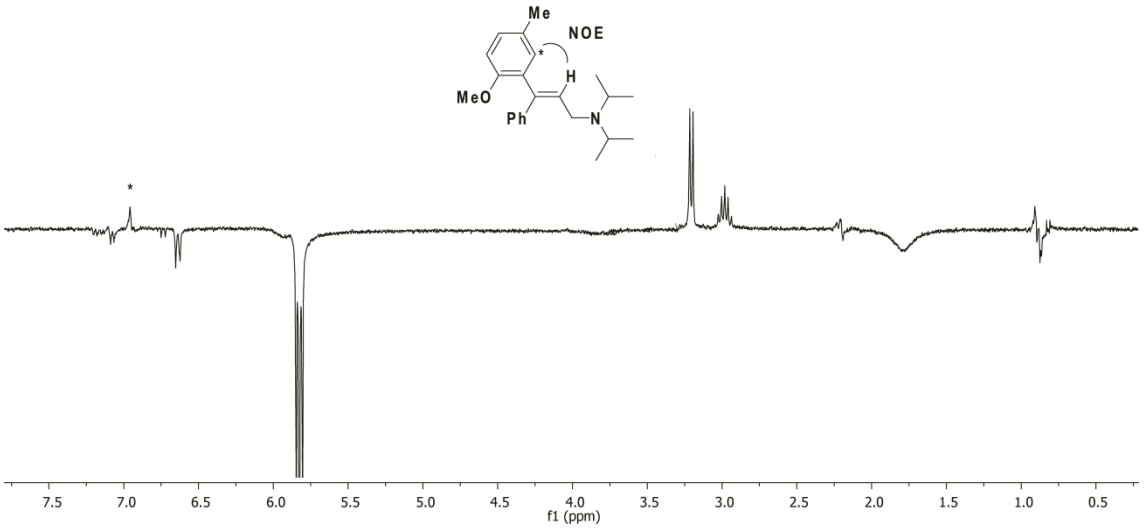
3. NOE Experiments For determination of (*E*)-Configuration of Trissubstitued Products



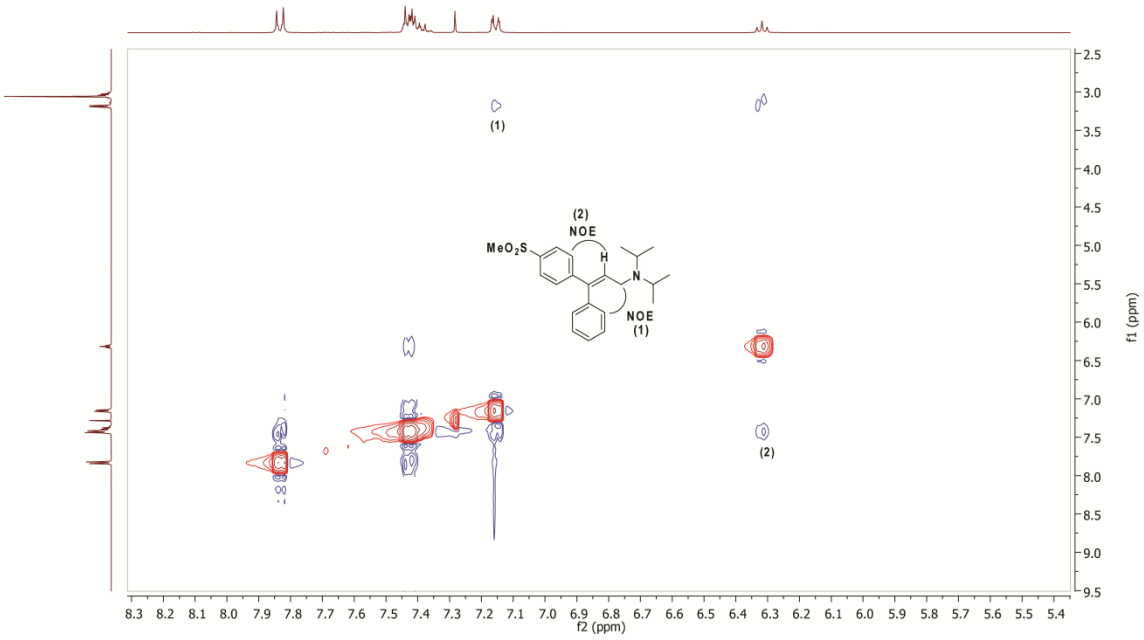
NOE-1D (CycloNoe – Varian 300MHz) Experiment to determine the *E*-configuration of vinyl bromides **5**. When the aromatic hydrogens are saturated, is possible to see NOE correlation with allylic CH_2 (red). When allylic CH_2 is saturated, is possible to see NOE correlation with aromatic hydrogens (blue). When olefinic hydrogen is saturated, no NOE correlation with aromatic is observed.



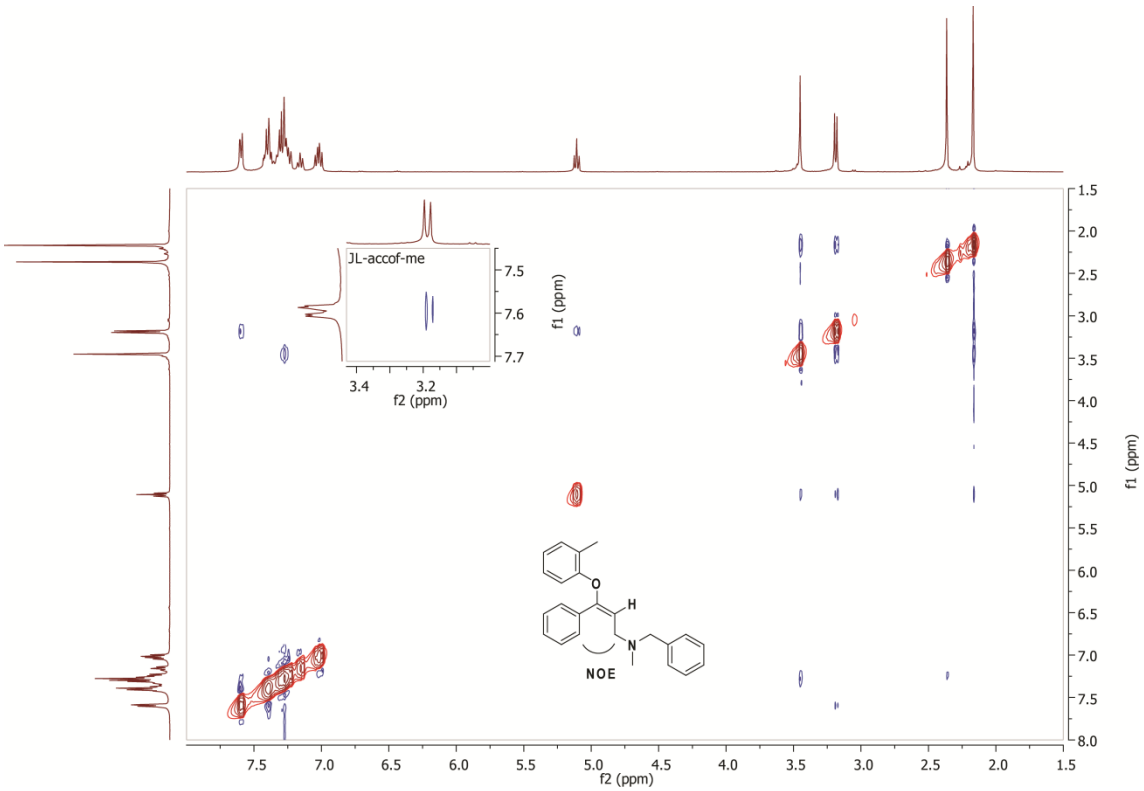
NOE-1D (CycloNoe – Varian 300 MHz) experiment to determine the *E*-configuration of the vinyl bromides **5**. With the saturation of allylic CH_2 is possible to see NOE correlation with aromatic hydrogens (blue). With saturation of olefinic hydrogens, no NOE correlation is observed with aromatics. (green).



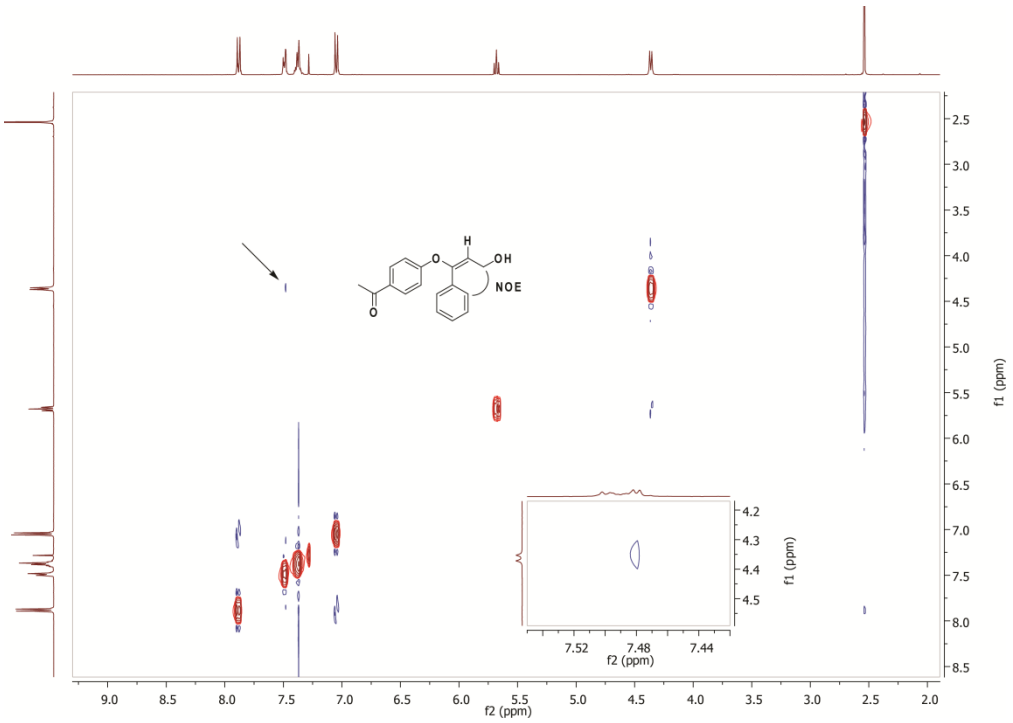
NOE-1D (CycloNoe – Varian 300 MHz) experiment to determine the *E*-configuration of the trissubstitued olefins. With the saturation of the olefinic hydrogen it is possible to note NOE correlation with the aromatic hydrogen singlet orto-methyl.



NOE-2D (Varian 400, mixing time 600 ms) experiment to determine the *E*-configuration of the trissubstitued olefins. It is possible to observe NOE correlation between the hydrogens of the SO_2Me substituted aryl group with the olefinic hydrogen **(2).** It is also possible to note NOE correlation of phenyl hydrogens and allylic CH_2 **(1)**.



NOE-2D (Varian 400, mixing time 600 ms) experiment to determine the *E*-configuration of the trisubstitued vinyl-ethers. It is possible to observe NOE correlation between allylic CH_2 and hydrogens of the phenyl ring near to oxygen.



NOE-2D (Varian 400, mixing time 600 ms) experiment to determine the *E*-configuration of the trisubstitued vinyl-ethers. It is possible to observe NOE correlation between allylic CH_2 and hydrogens of the unsubstitued phenyl ring.