Supporting Information

Design, synthesis and antimicrobial assessments of Aminoacetylenic-piperazine Nitroimidazol Hybrid Compounds

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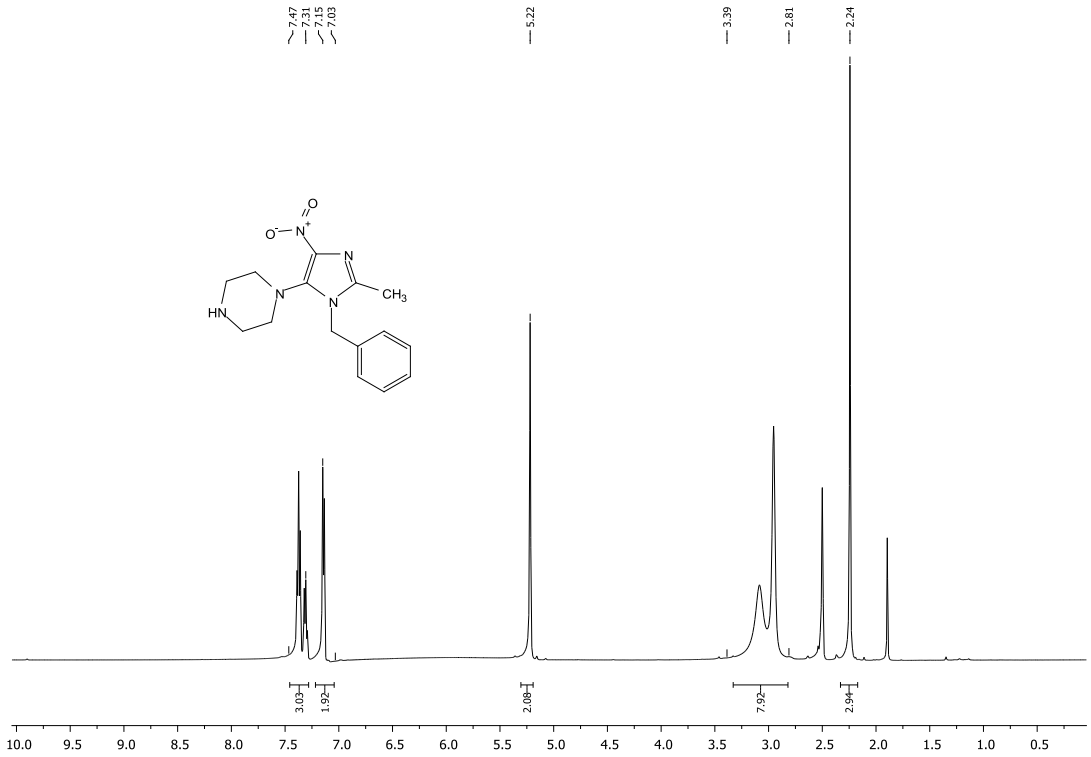
^{1}H NMR, ^{13}C NMR and DEPT 135 Spectra

Compound **6**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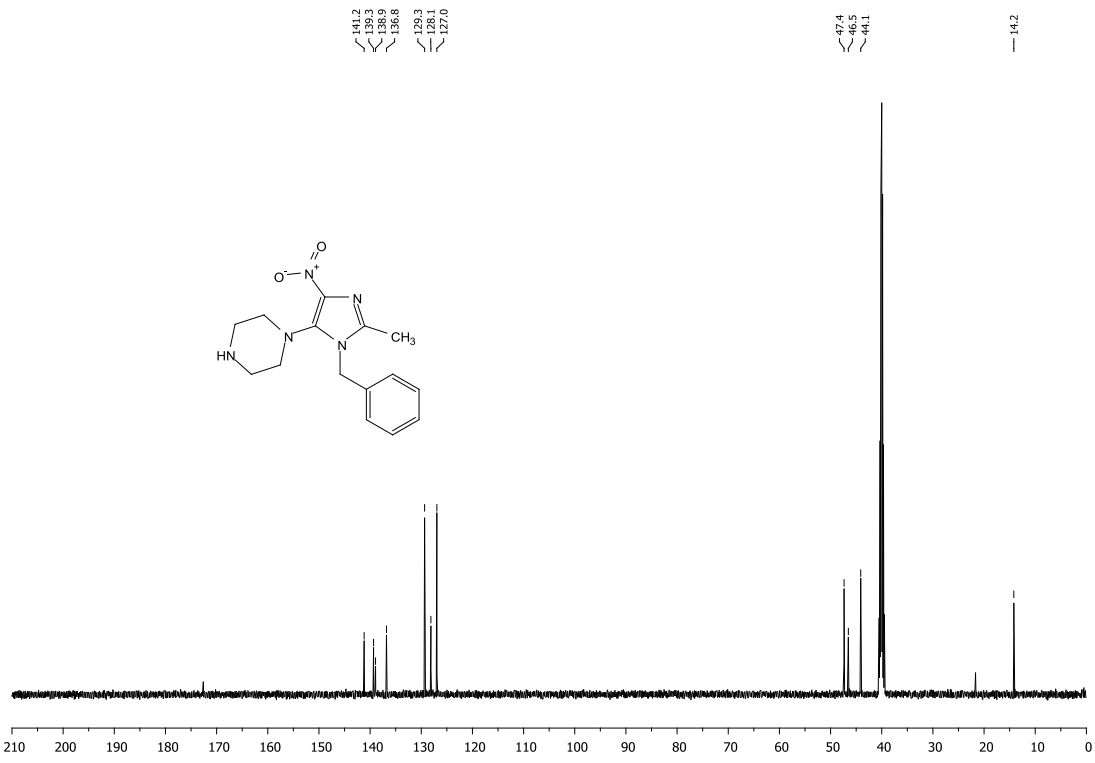
7.31
7.15
7.03
5.22
3.39
2.81
2.24
3.03
1.92
2.08
7.92
2.94
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5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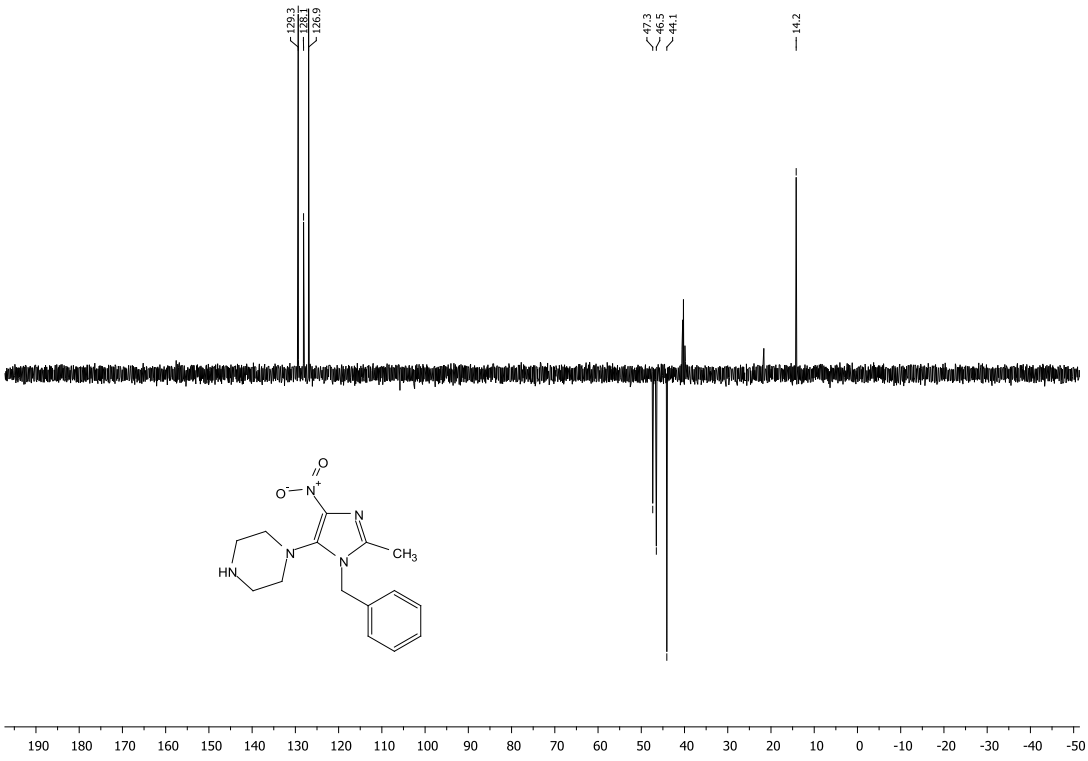
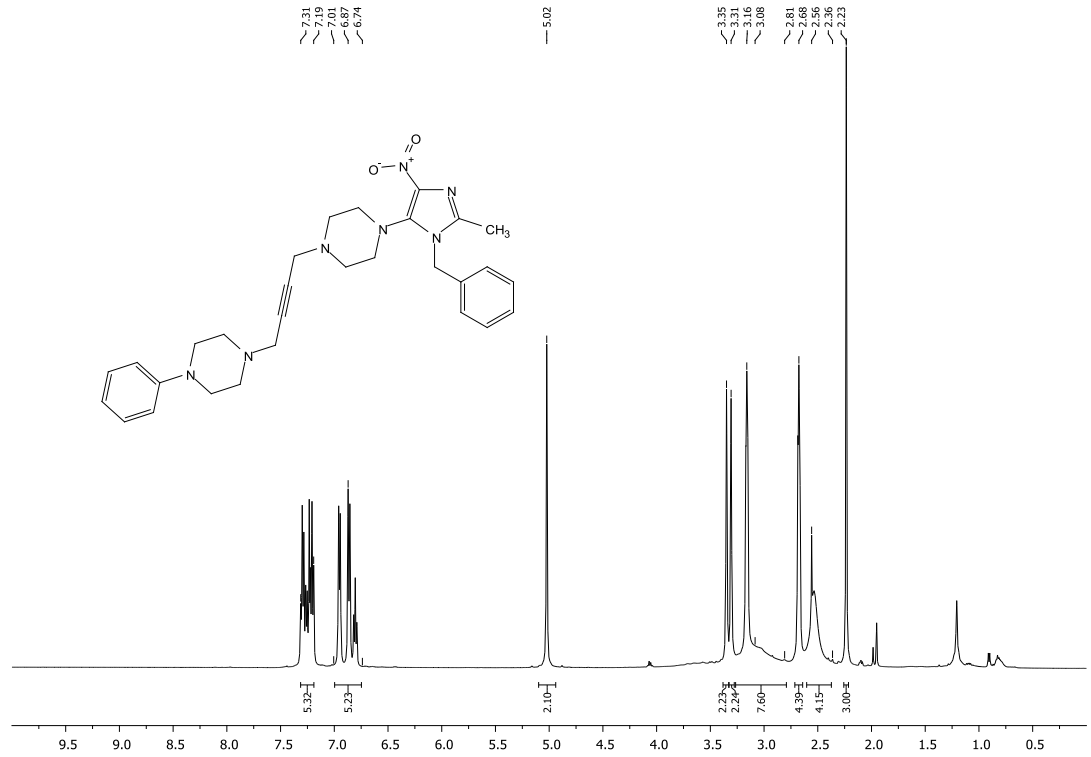
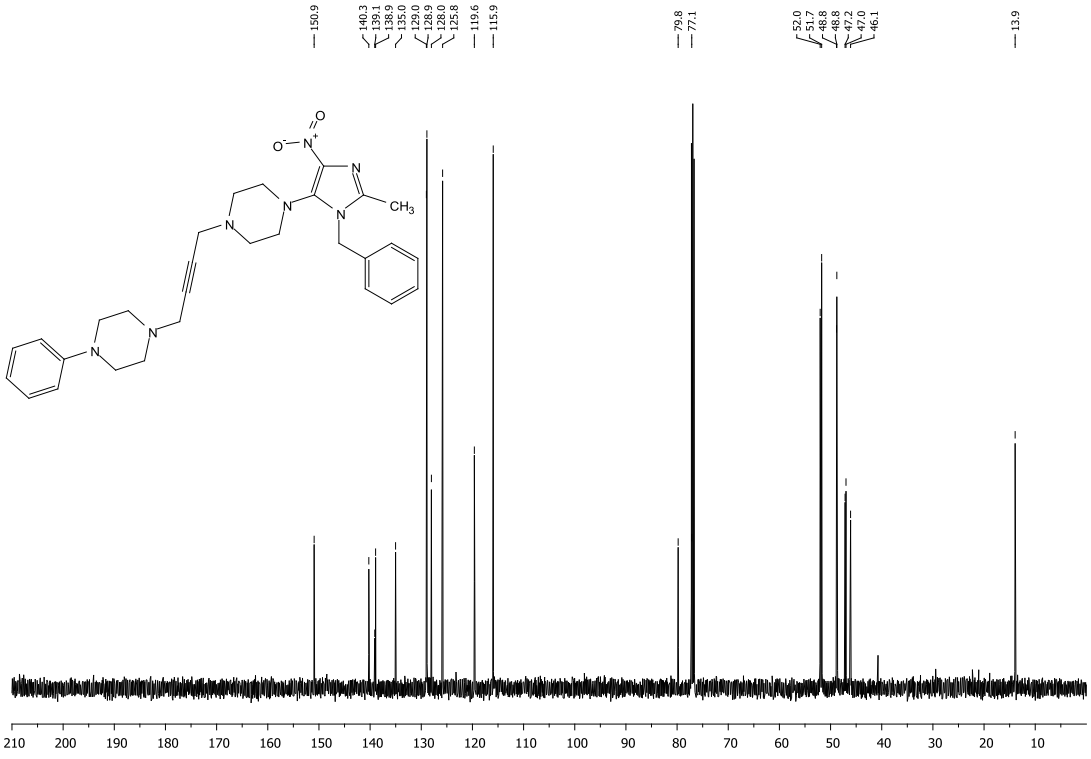
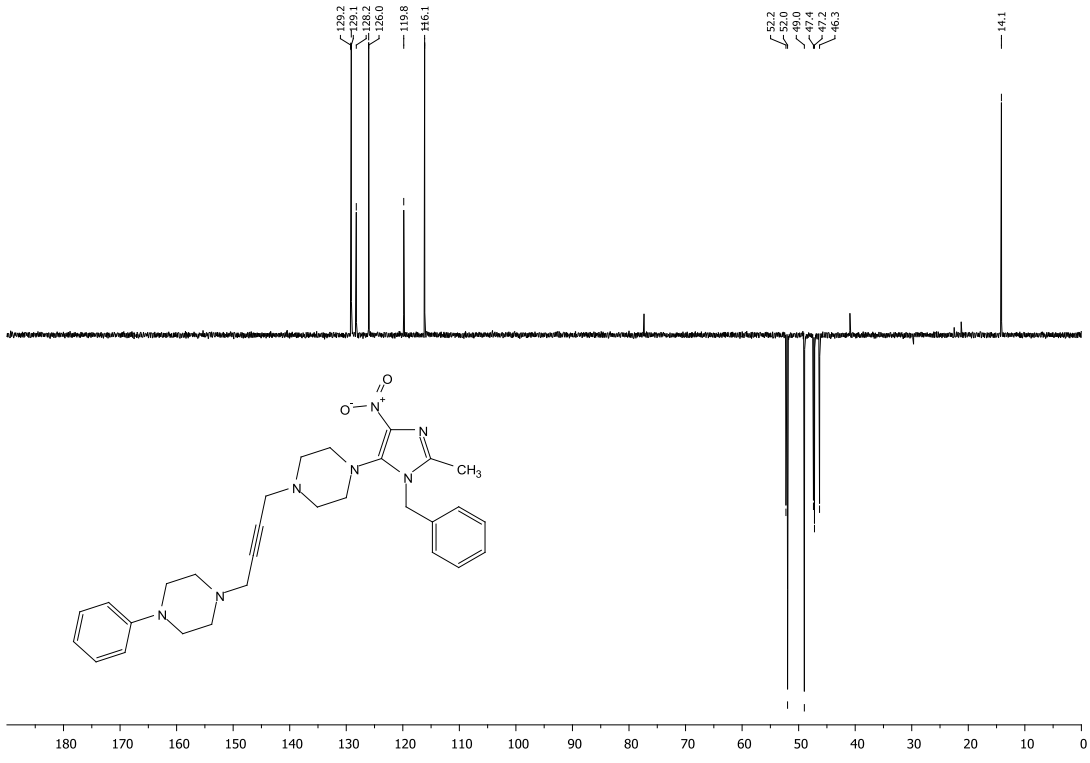
139.3
138.9
136.8
129.3
128.1
127.0
47.4
46.5
44.1
14.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


129.3
128.1
126.9
47.3
46.5
44.1
14.2
O
O⁻
N⁺
N
N
CH3
HN
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50

Compound **10a**



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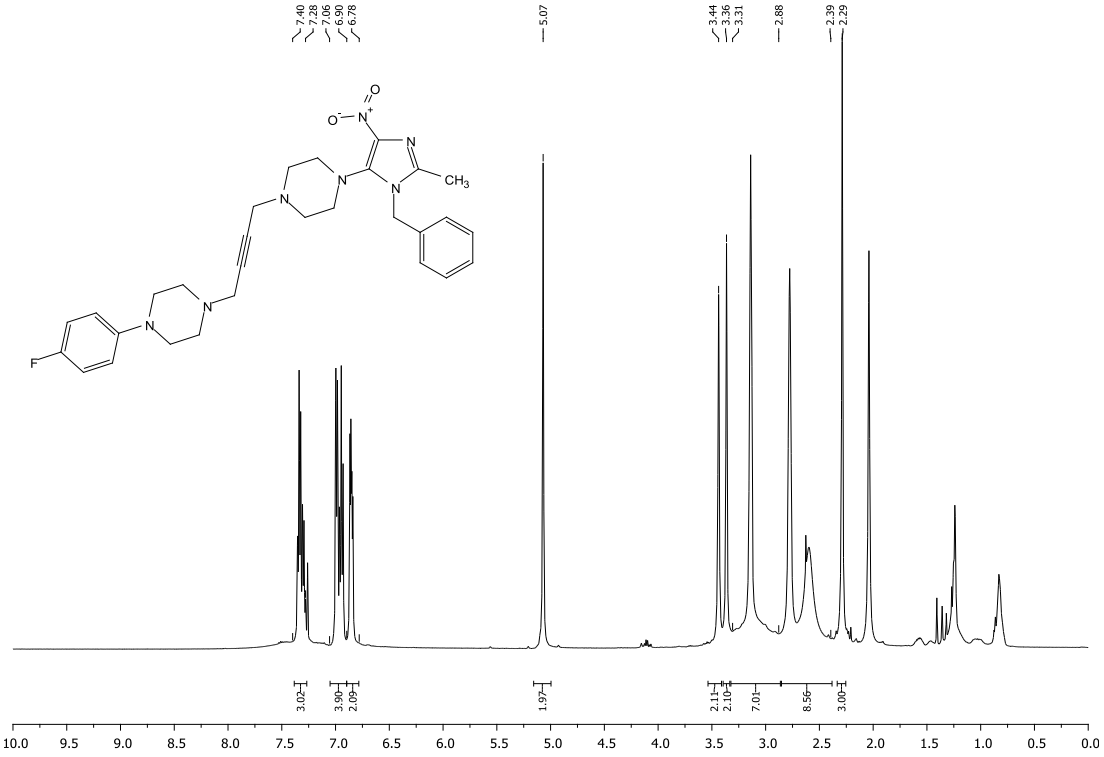
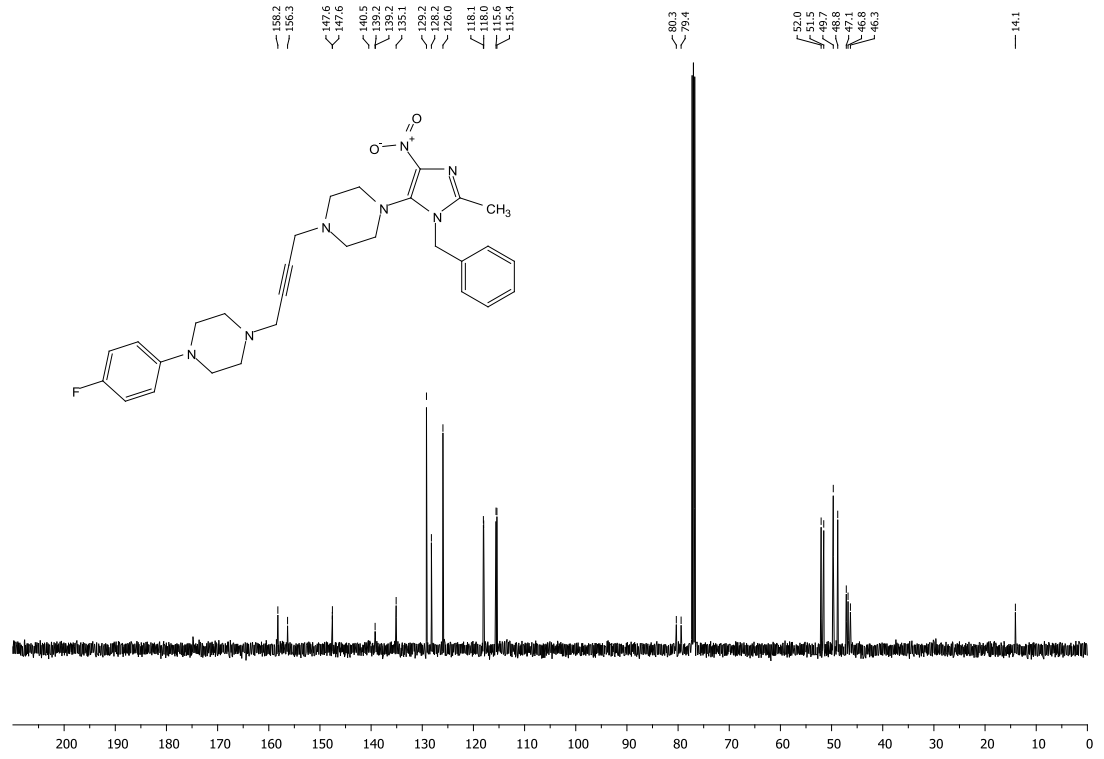
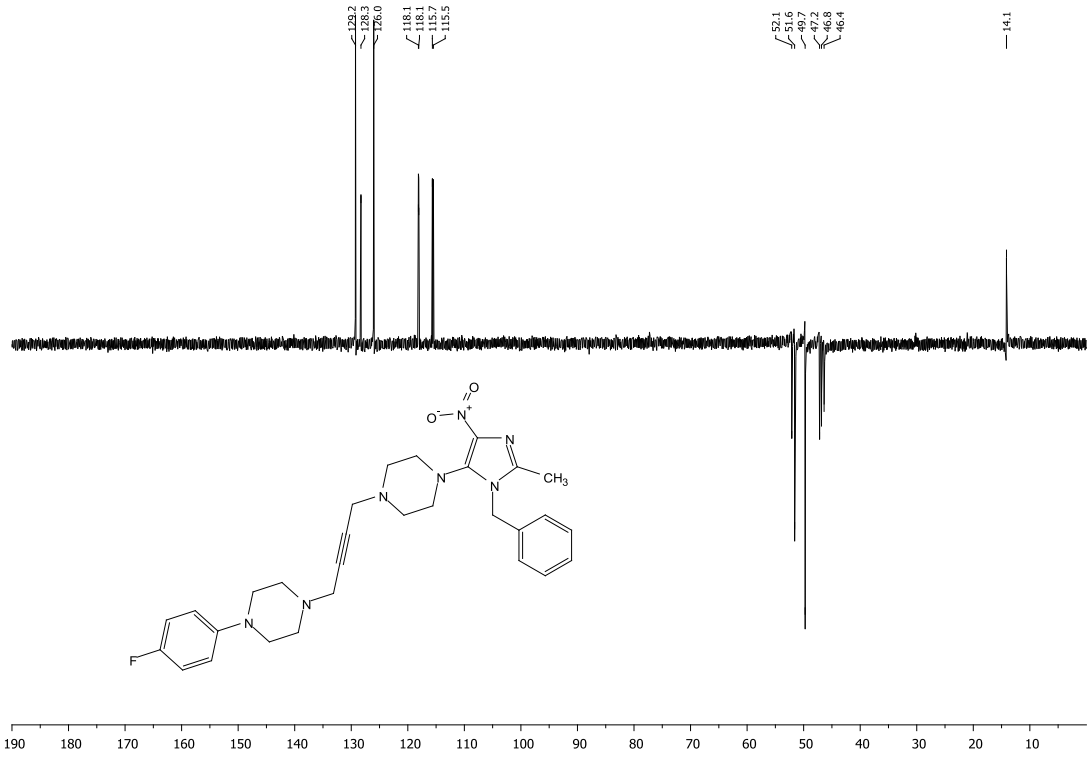
129.1
128.2
126.0
119.8
116.1
52.2
52.0
49.0
47.4
47.2
46.3
14.1
O
O
N
N
N
N
N
N
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound **10b**



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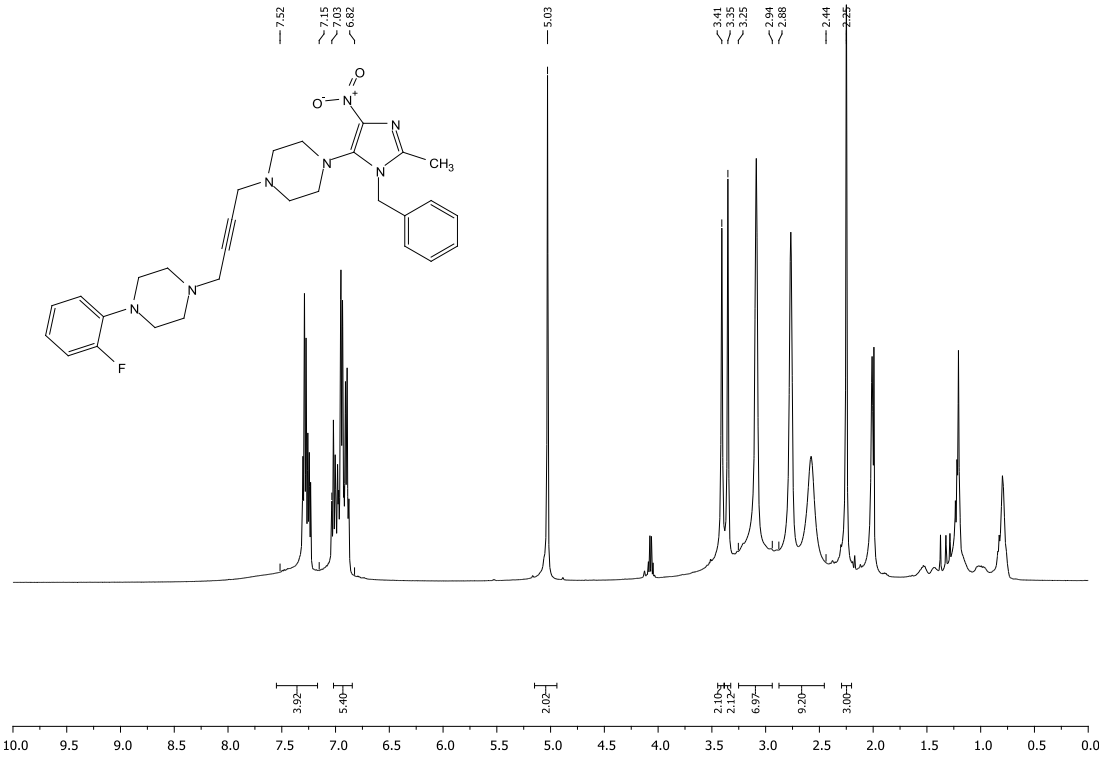
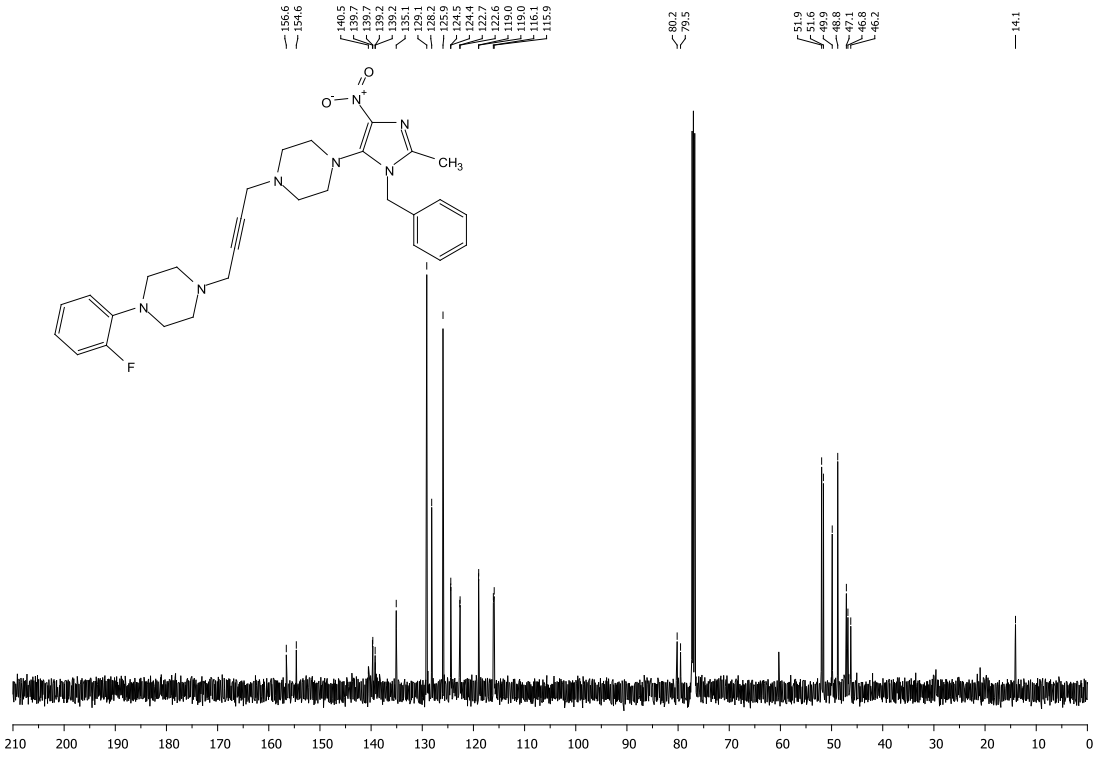
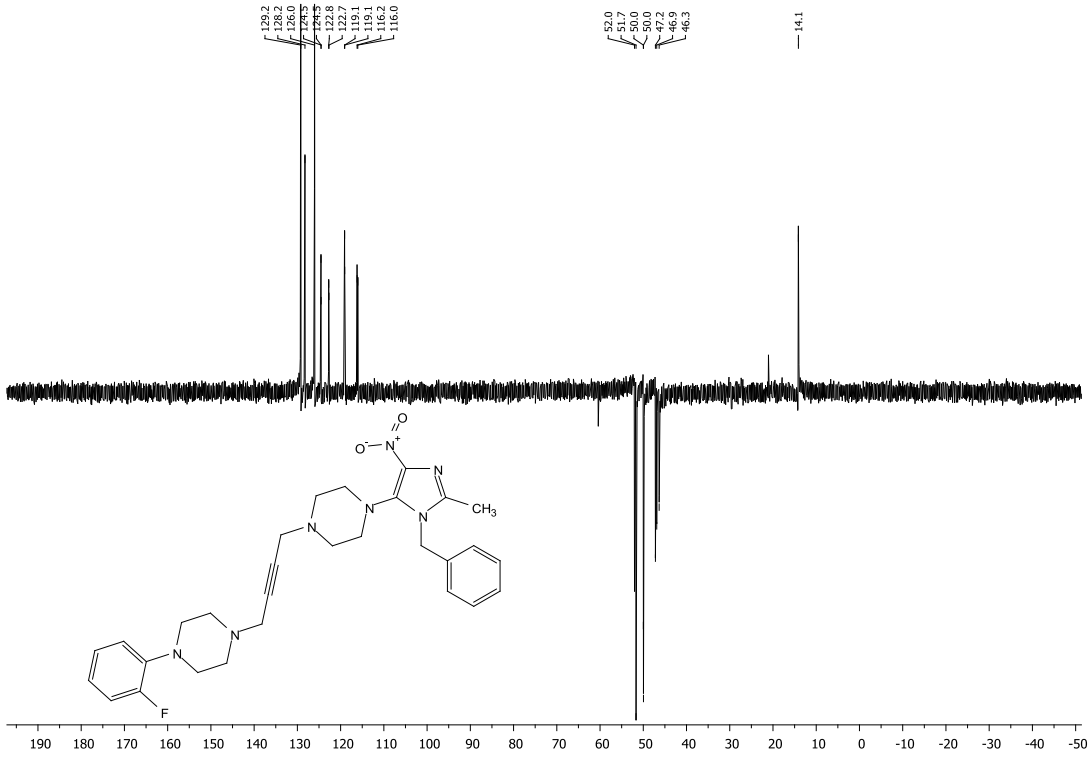
128.3
126.0
118.1
118.1
115.7
115.5
52.1
51.6
49.7
47.2
46.8
46.4
14.1
O
O
N
N
N
N
N
N
CH3
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

Compound **10c**



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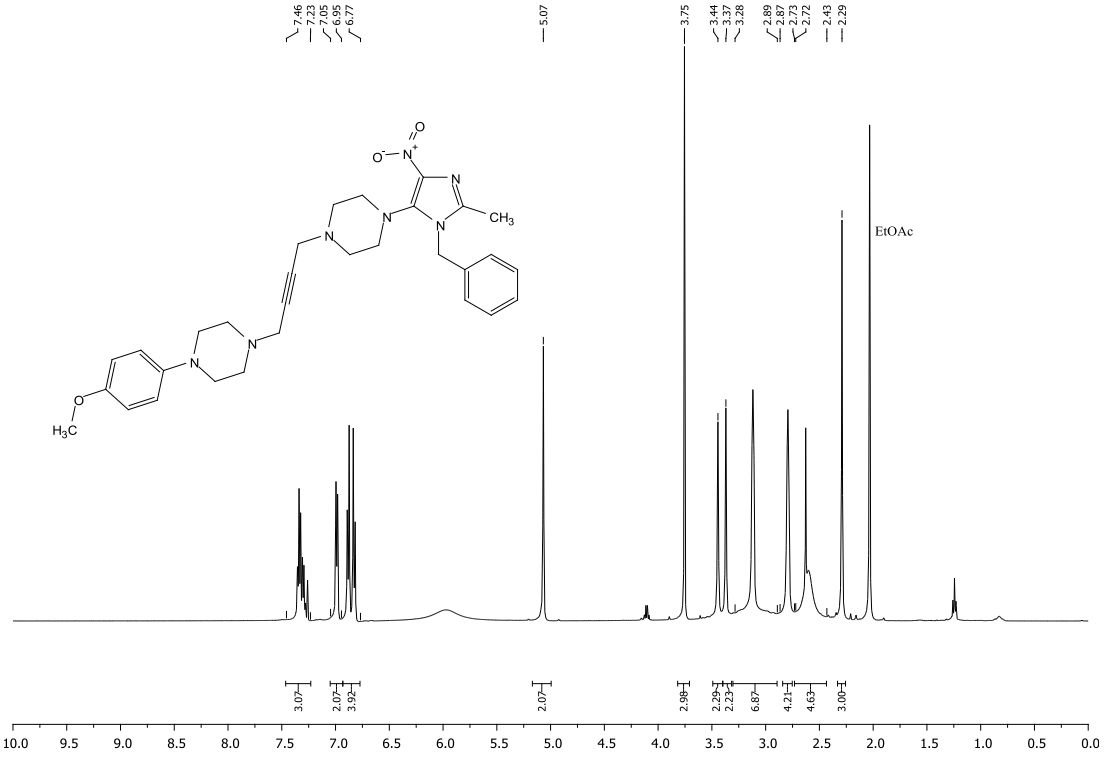
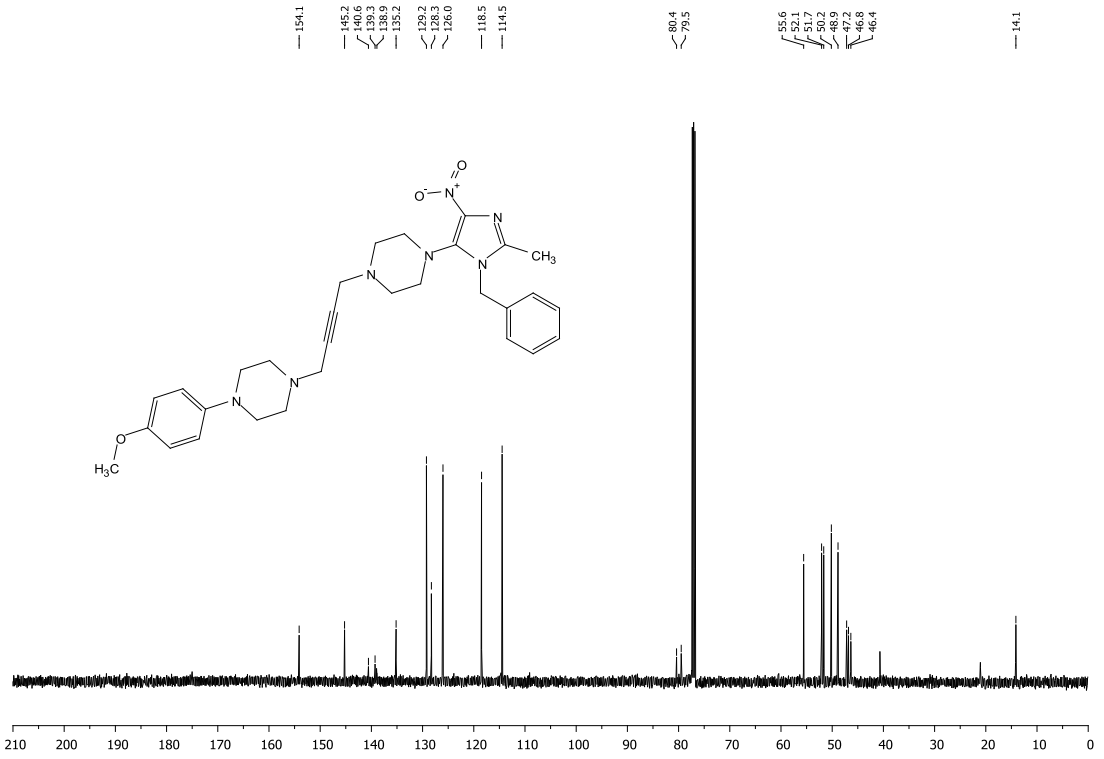
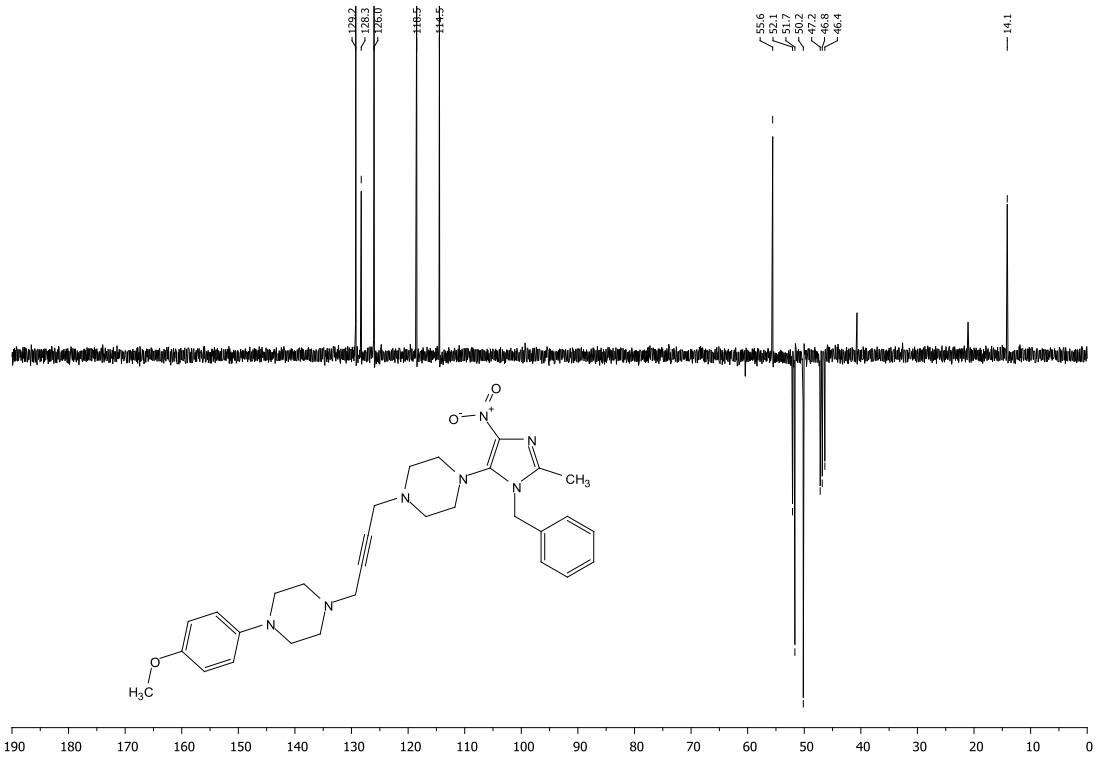
128.2
126.0
124.5
124.3
122.8
122.7
119.1
119.1
116.2
116.0
52.0
51.7
50.0
50.0
47.2
46.6
46.3
14.1
CH3
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50

Compound **10d**



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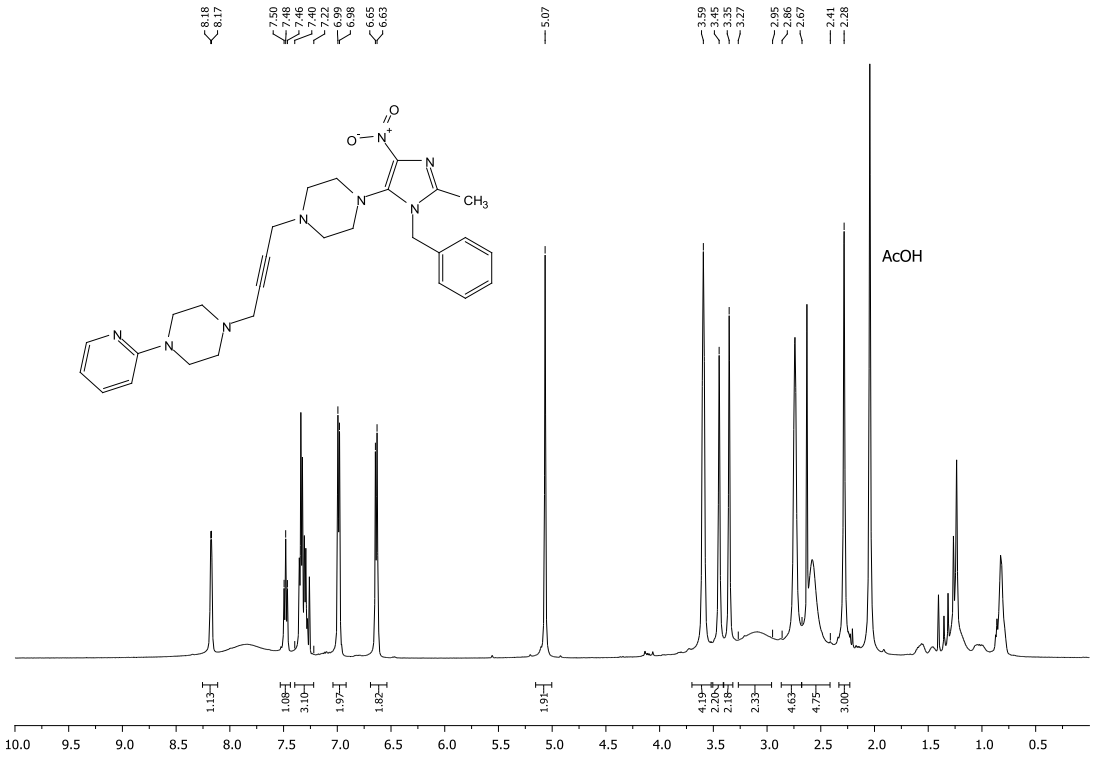
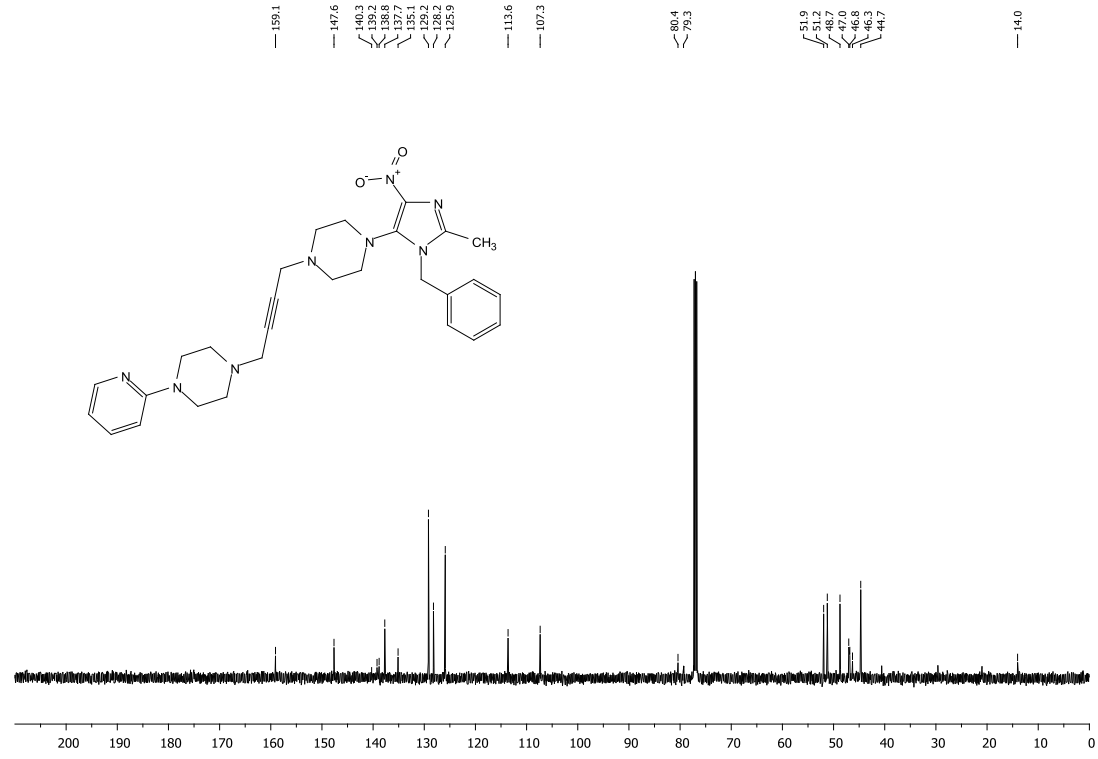
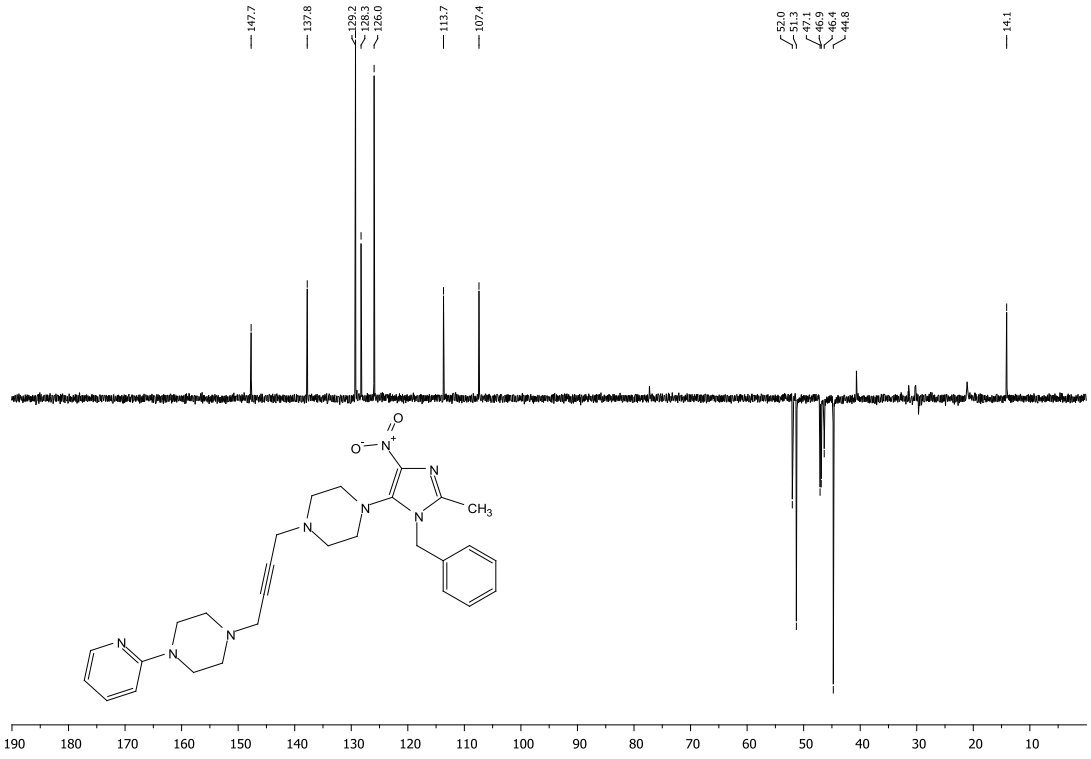
128.3
126.0
118.5
114.5
55.6
52.1
51.7
50.2
47.2
46.8
46.4
14.1
O
O
N
N
N
N
N
N
CH3
O
H3C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

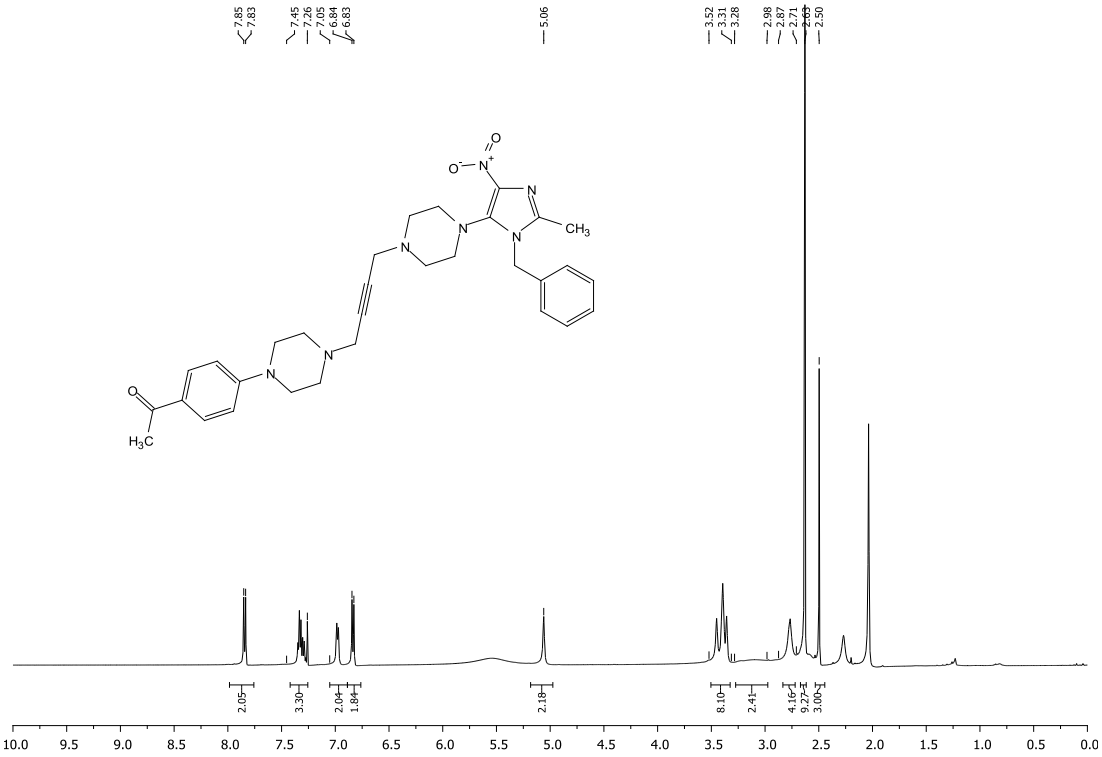
Compound **10e**

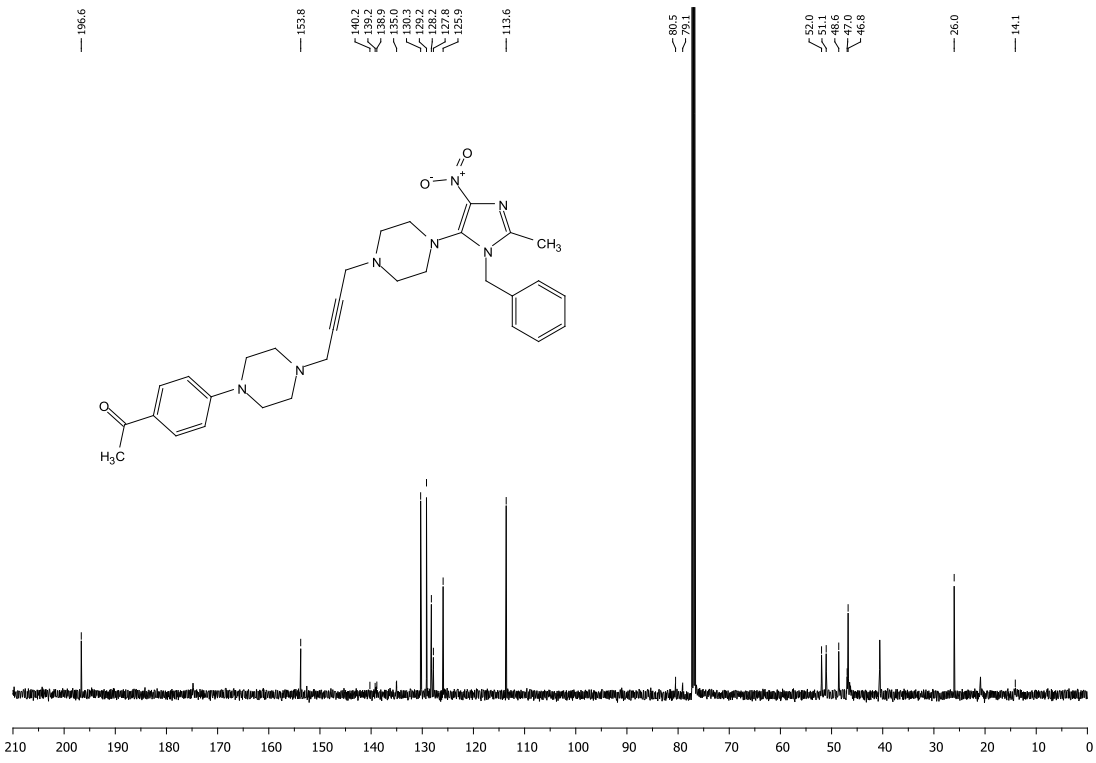


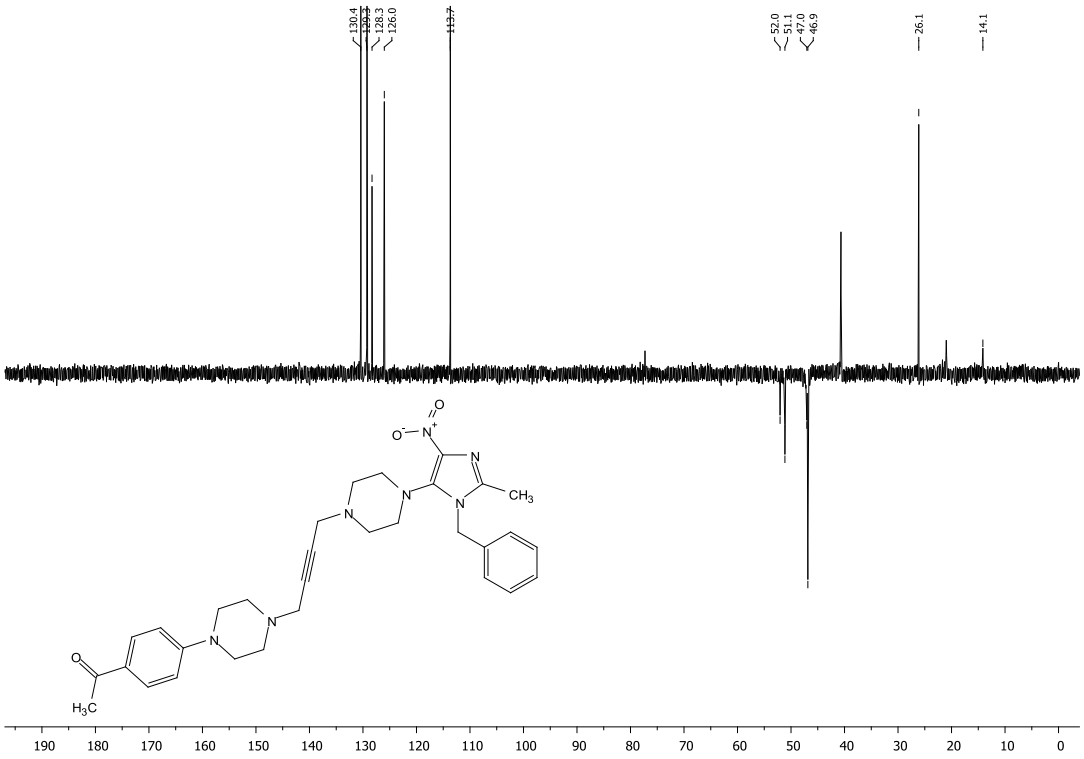



147.7
137.8
129.2
128.3
126.0
113.7
107.4
52.0
51.3
47.1
46.9
46.4
44.8
14.1
O
O-
N+
N
N
N
N
N
N
N
CH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

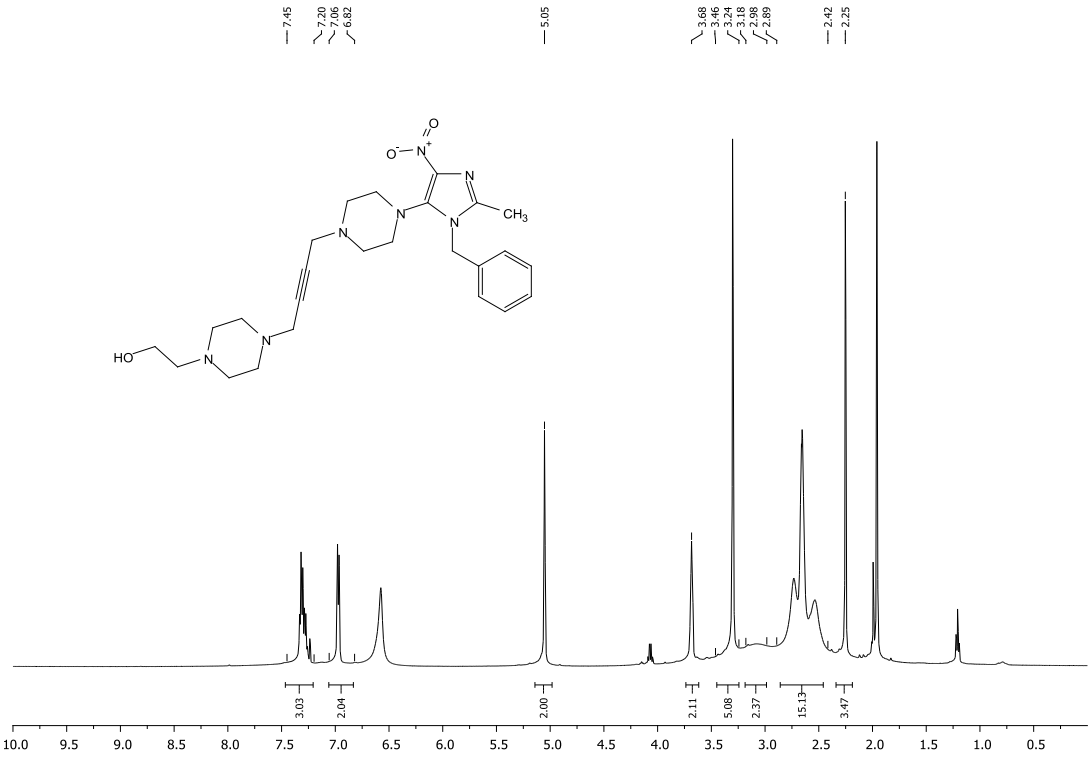
Compound **10f**

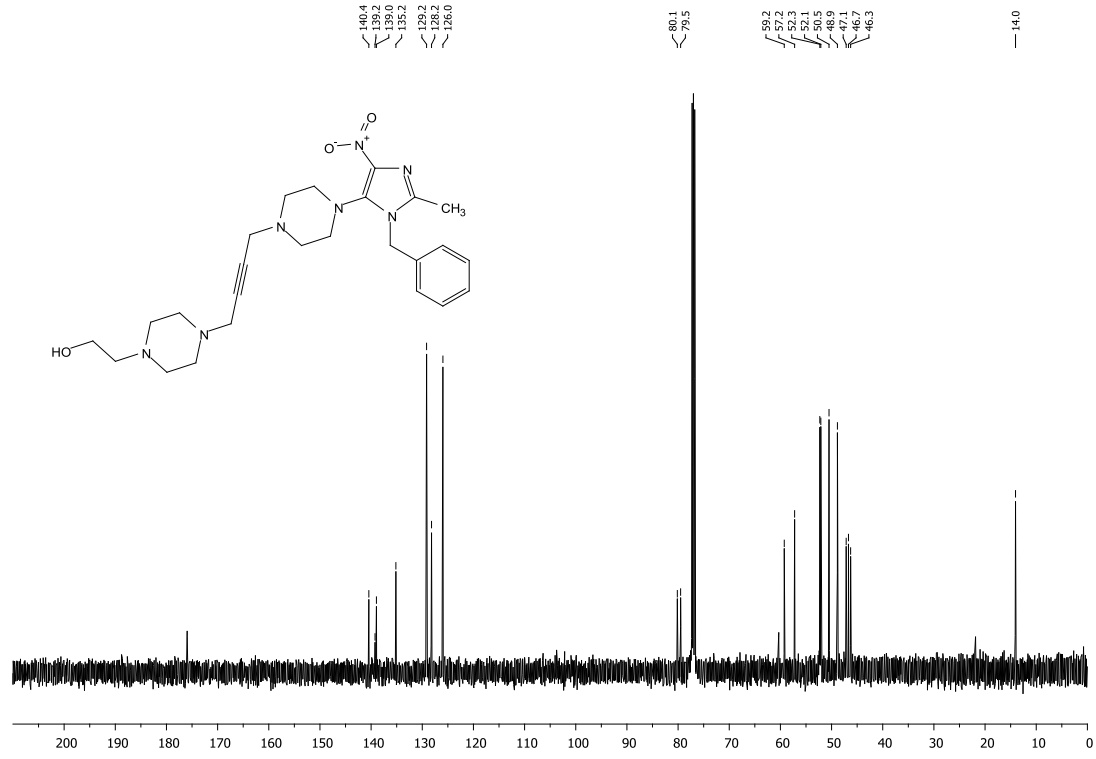


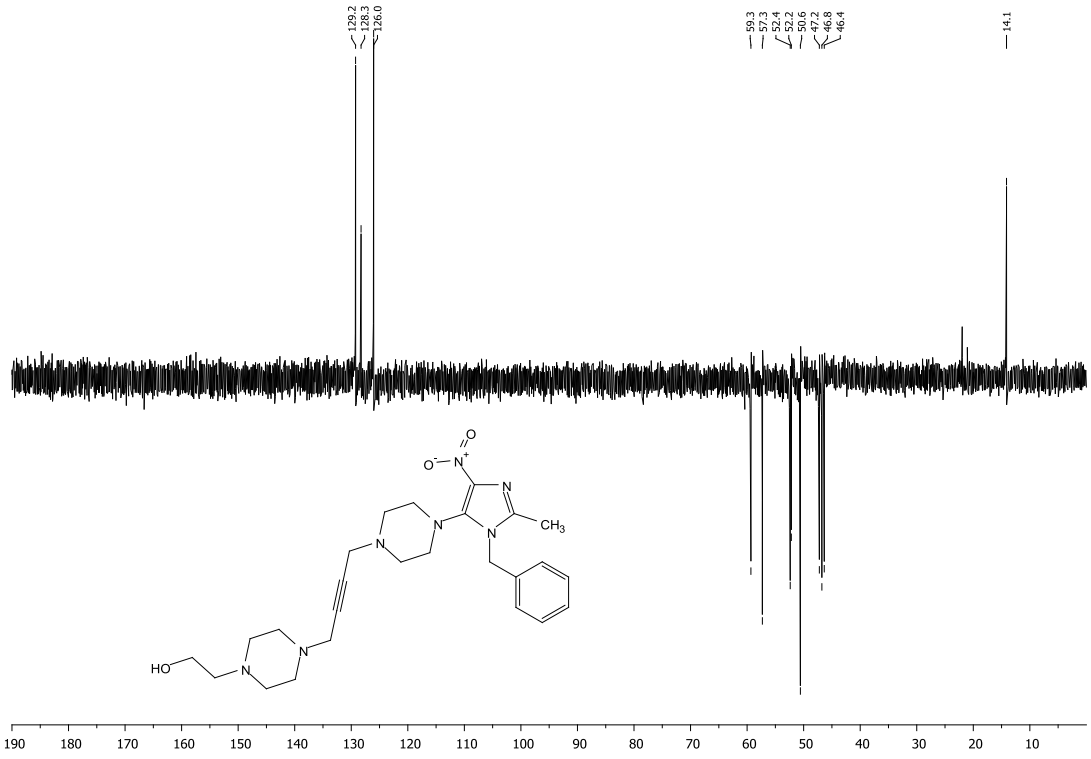



130.4
129.3
128.3
126.0
113.7
52.0
51.1
47.0
46.9
26.1
14.1
O
N+
O-
N
N
N
CH3
N
N
N
O
H3C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound **10g**



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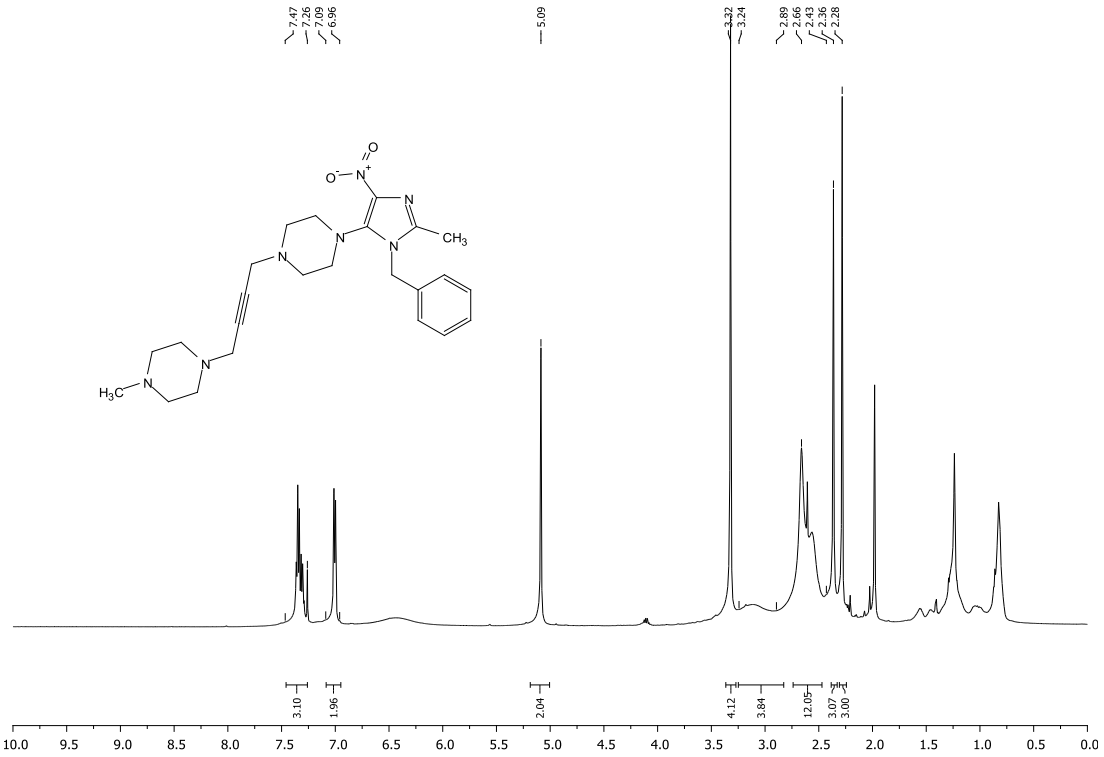
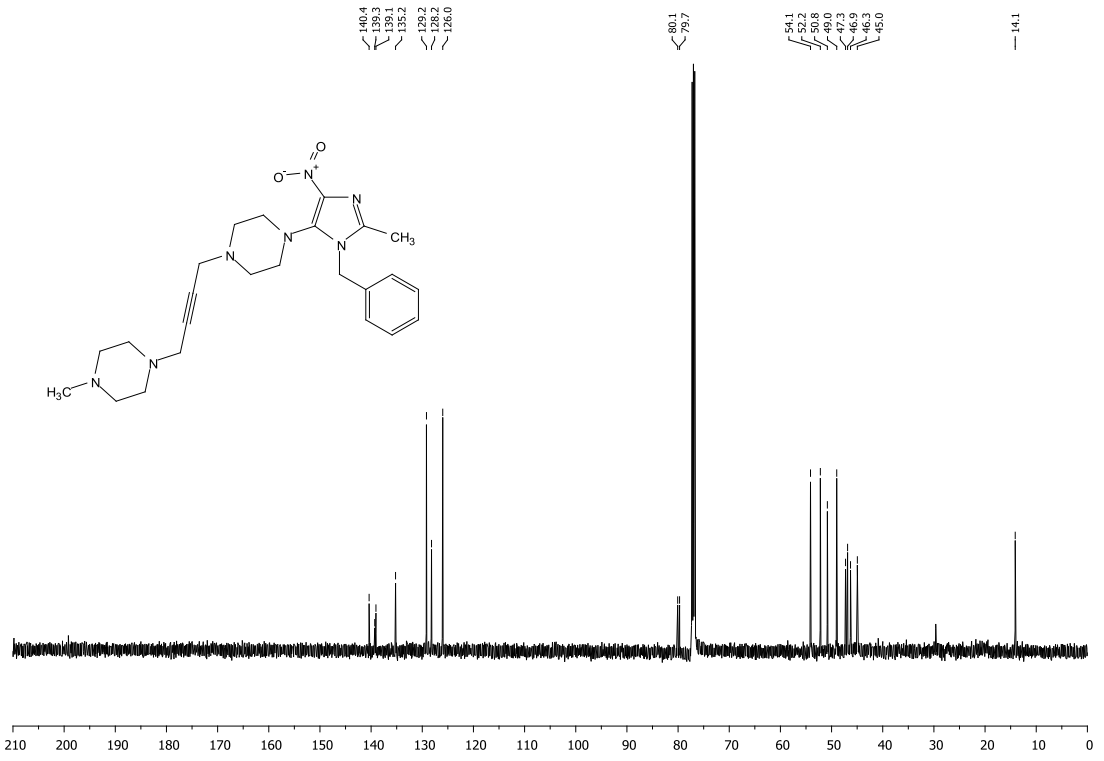
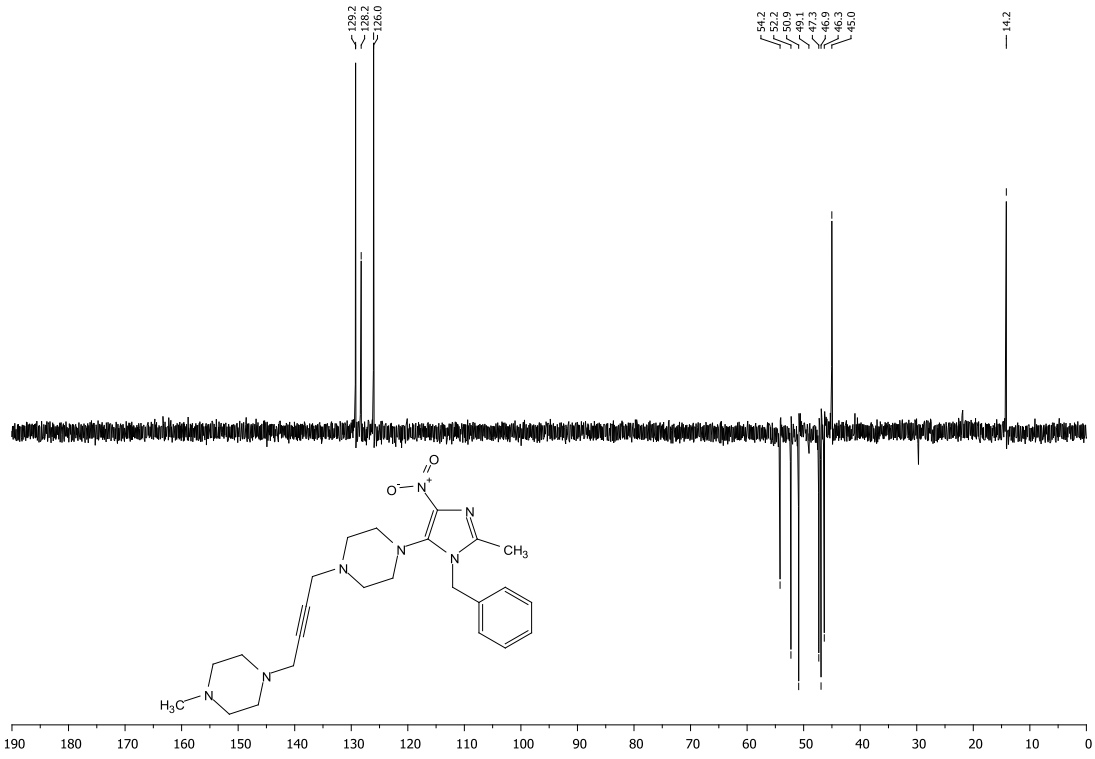
128.3
126.0
59.3
57.3
52.4
52.2
50.6
47.2
46.8
46.4
14.1
O
O
N
N
N
N
N
CH3
HO
N
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

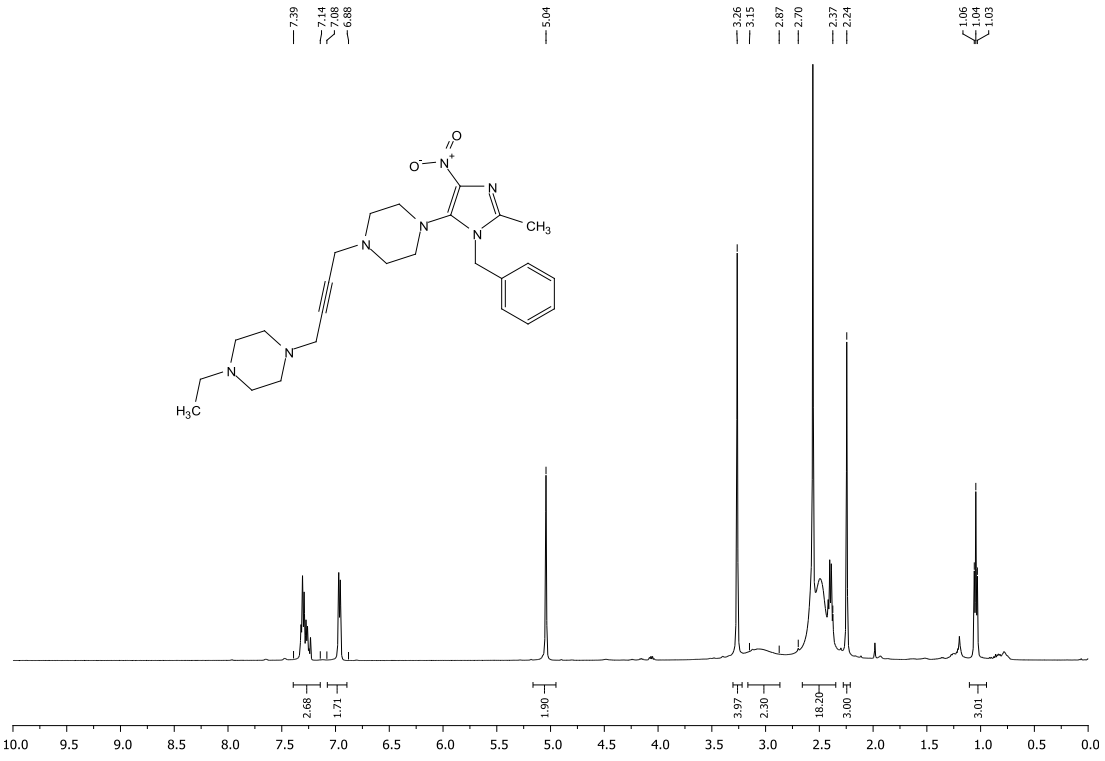
Compound **10h**

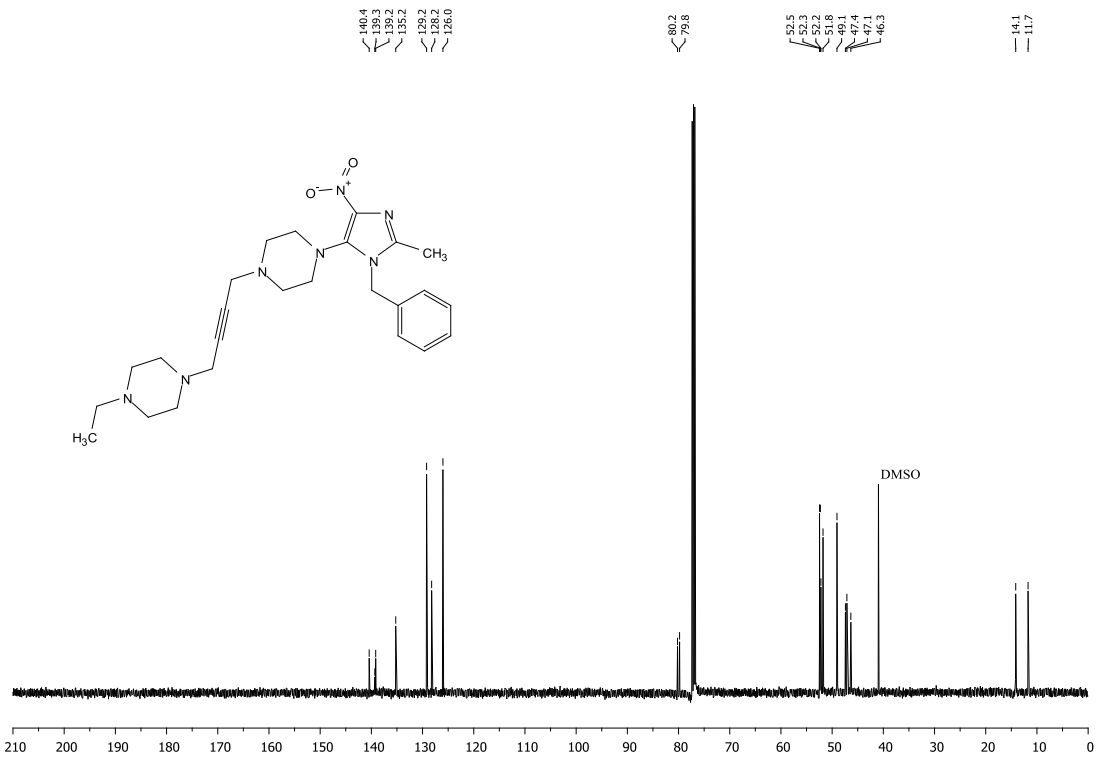


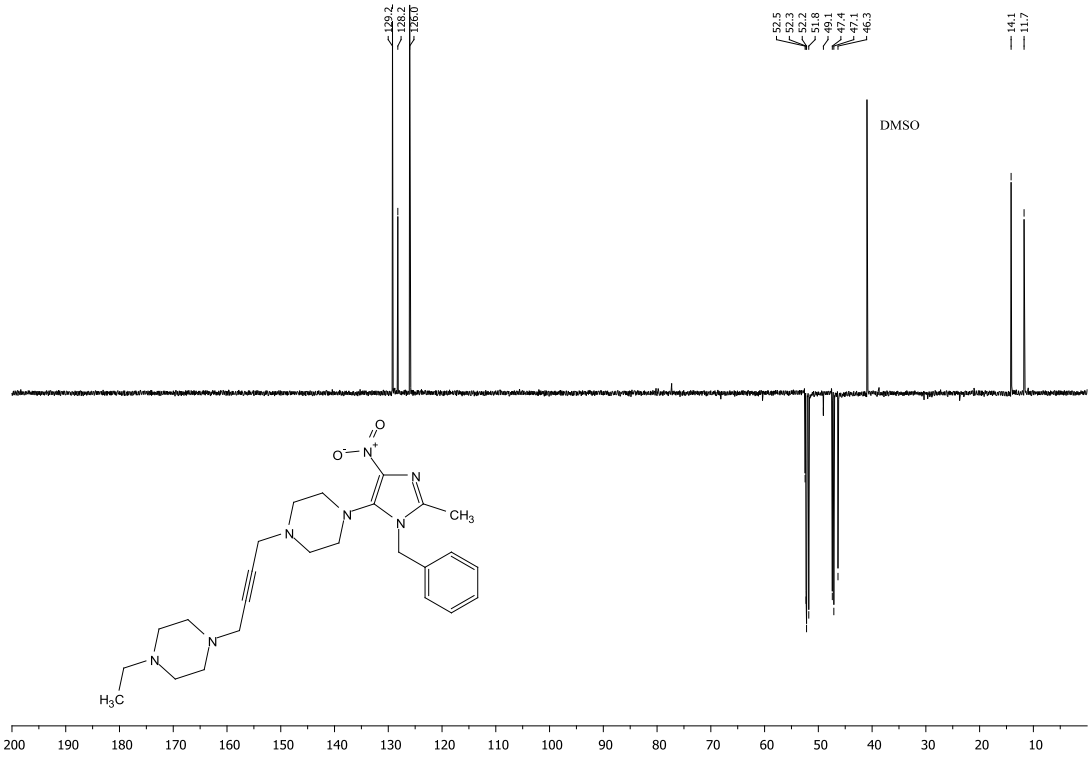



129.2
128.2
126.0
54.2
52.2
50.9
49.1
47.3
46.9
46.3
45.0
14.2
O
O⁻
N⁺
N
N
N
CH3
N
N
N
H3C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound **10i**



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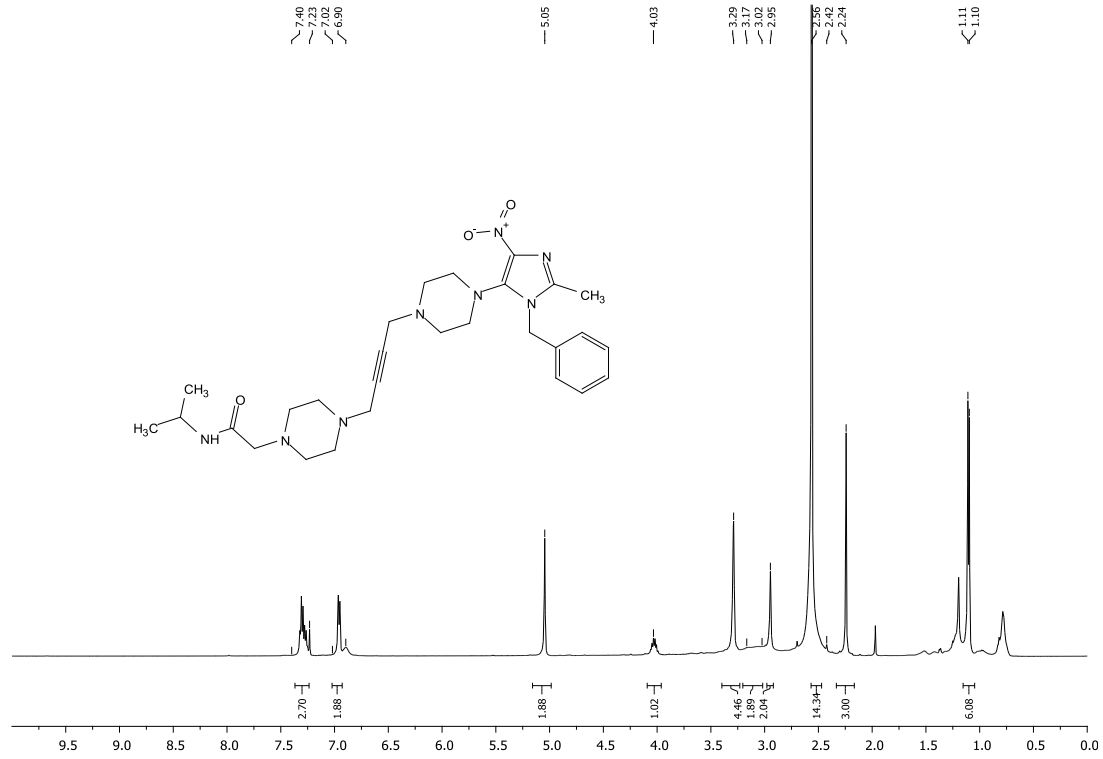
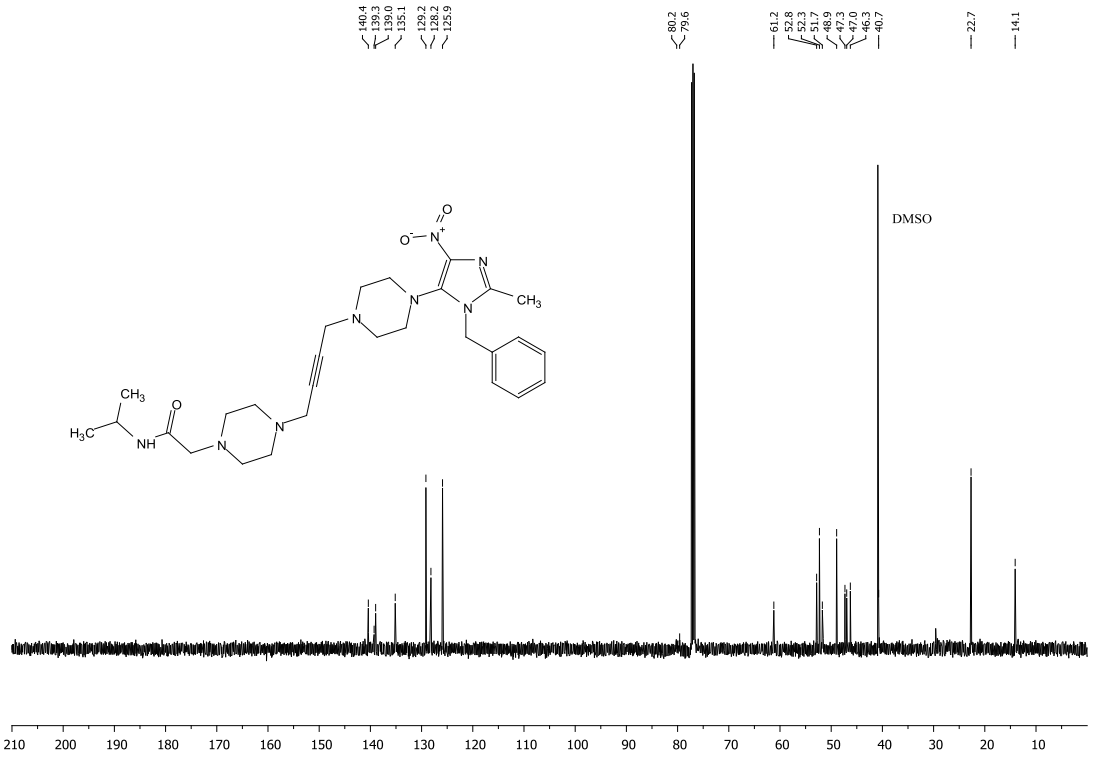
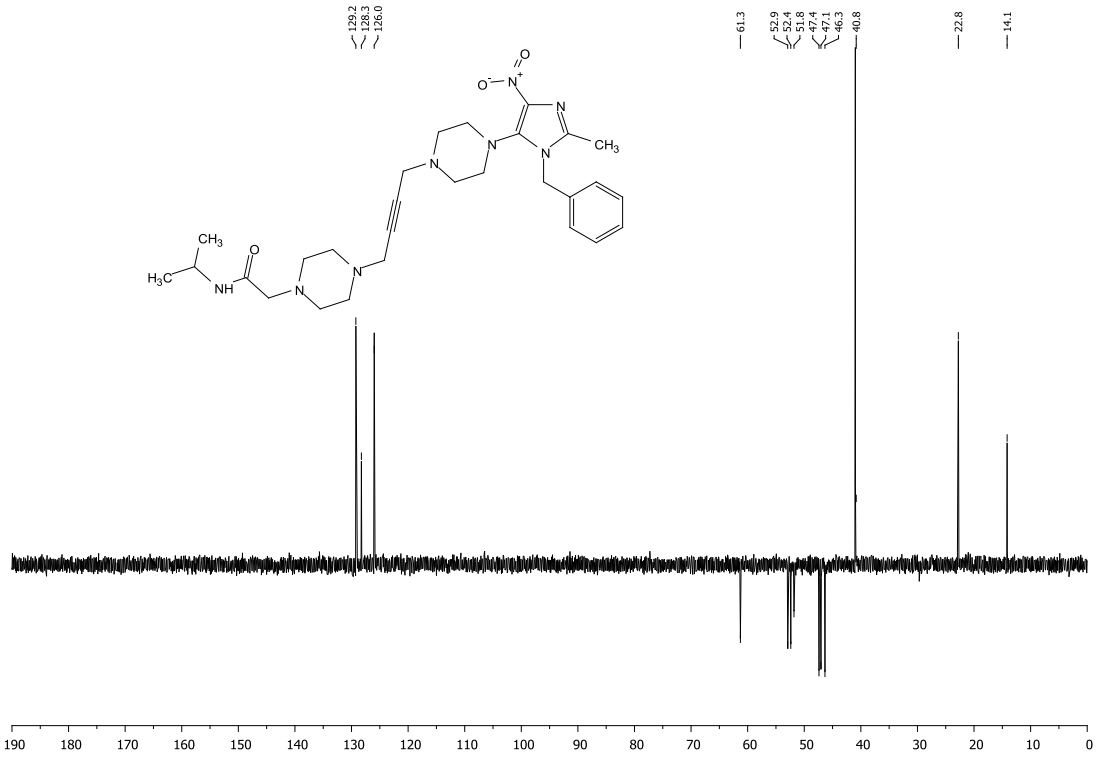
128.2
126.0
53.5
53.3
52.2
51.8
49.1
47.4
47.1
46.3
14.1
11.7
DMSO
O
O⁻
N⁺
N
CH3
N
N
N
N
H3C
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

Compound **10j**



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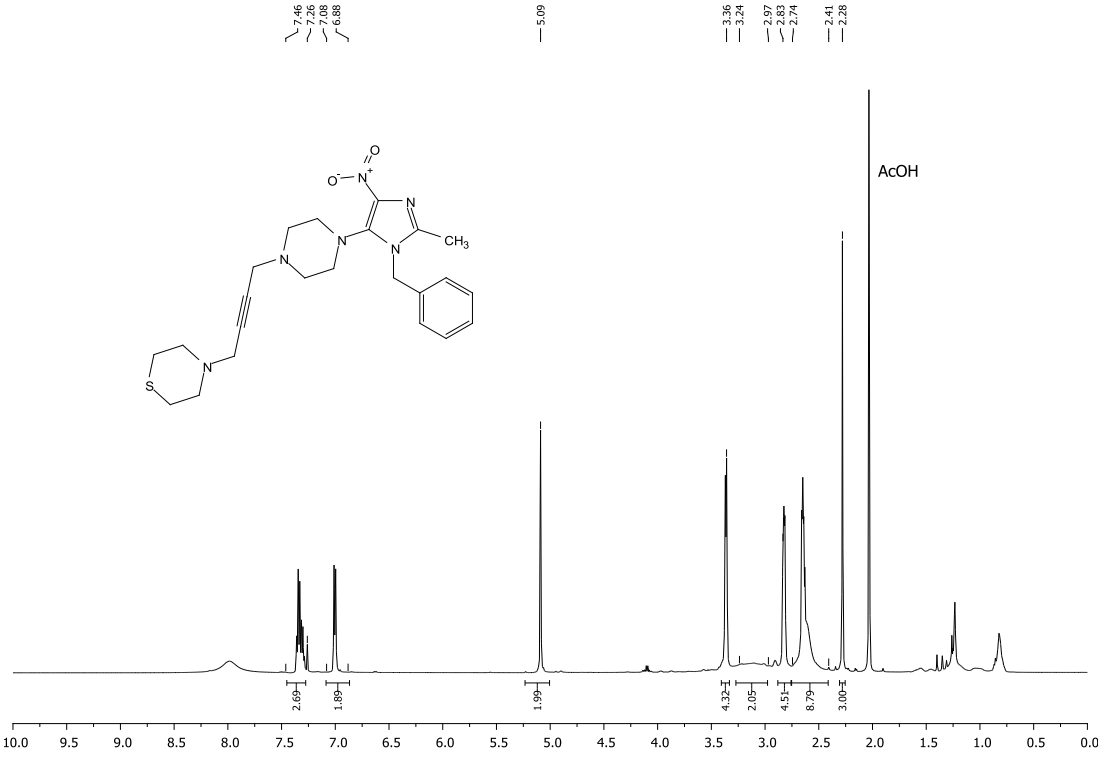
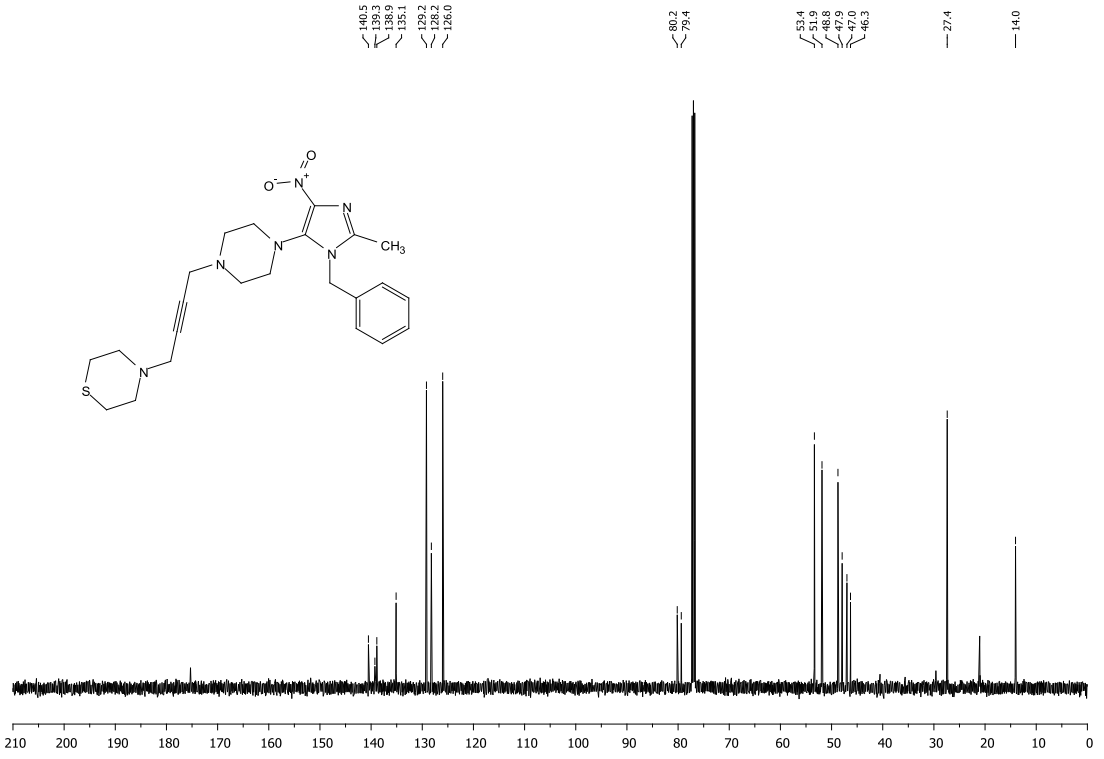
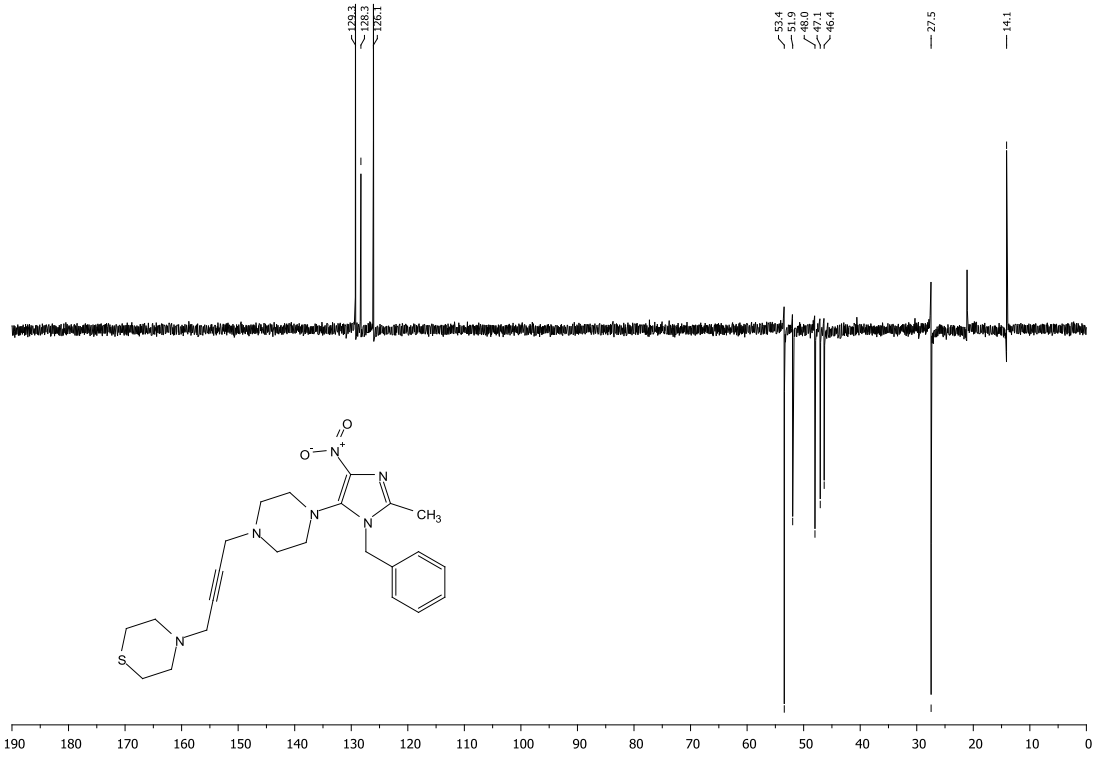
128.3
126.0
61.3
52.9
52.4
51.8
47.4
47.1
46.3
40.8
22.8
14.1
O
O⁻
N⁺
N
CH3
N
N
N
CH3
H3C
NH
O
N
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Compound **10k**






129.3
128.3
126.1
53.4
51.9
49.0
47.1
46.4
27.5
14.1
O
O
N
N
CH3
N
N
N
S
190
180
170
160
150
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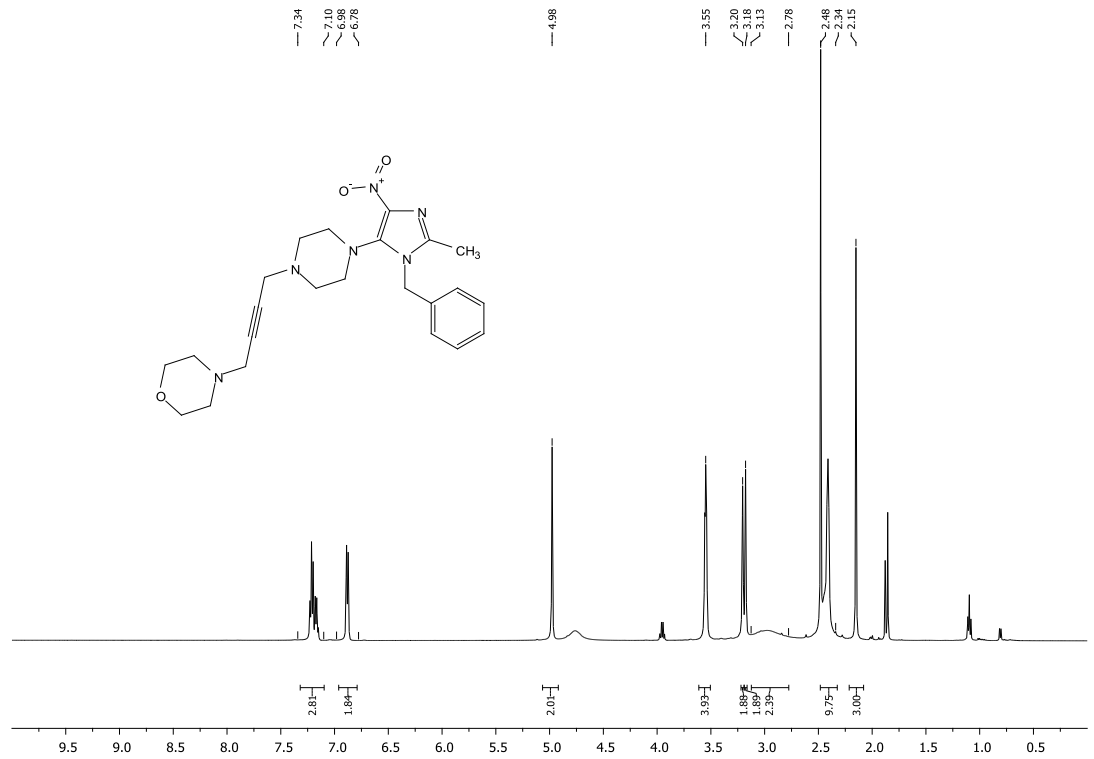
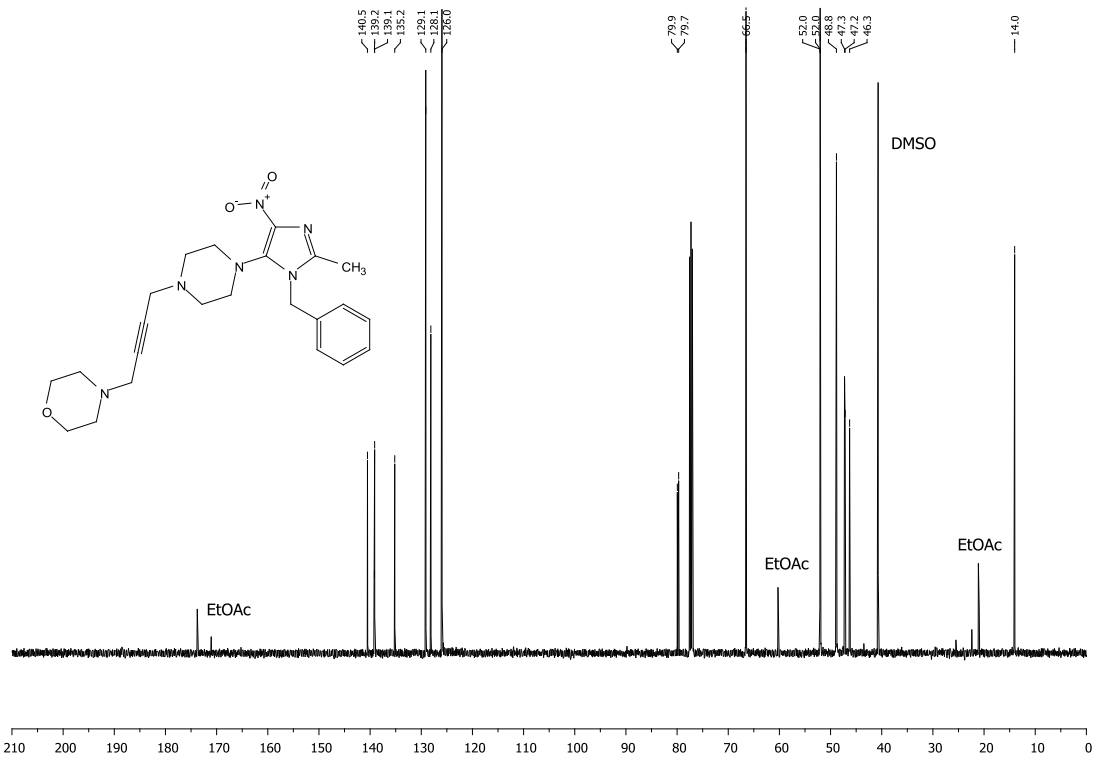
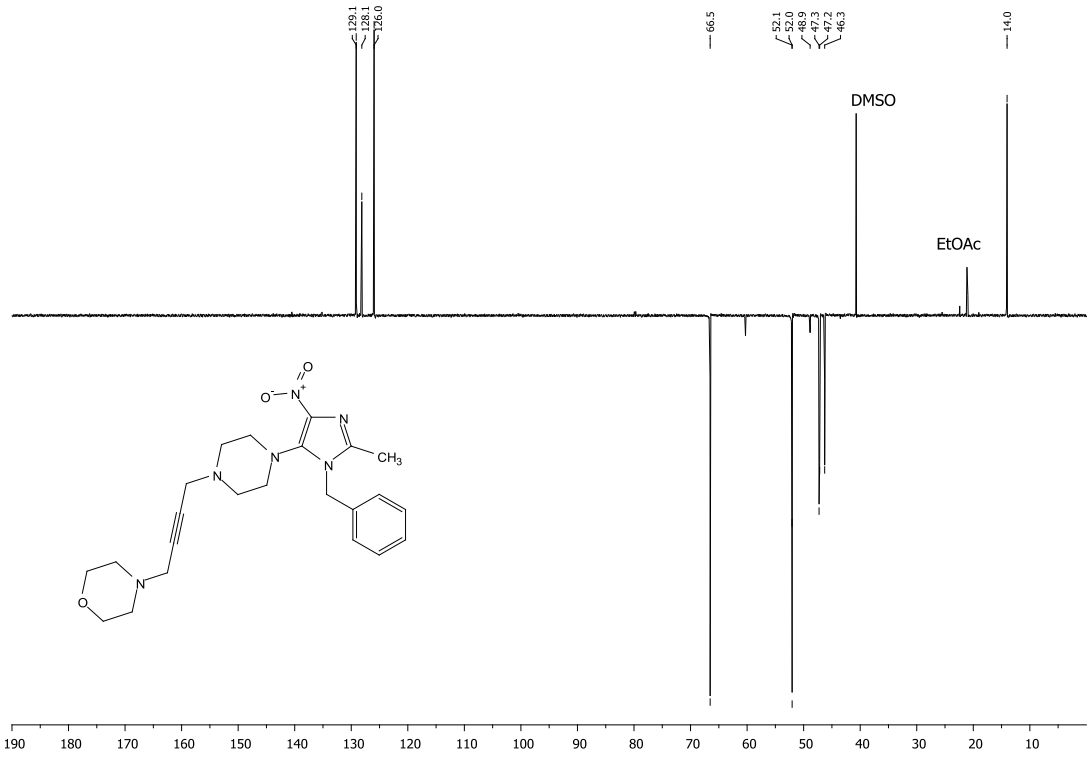
120
110
100
90
80
70
60
50
40
30
20
10
0

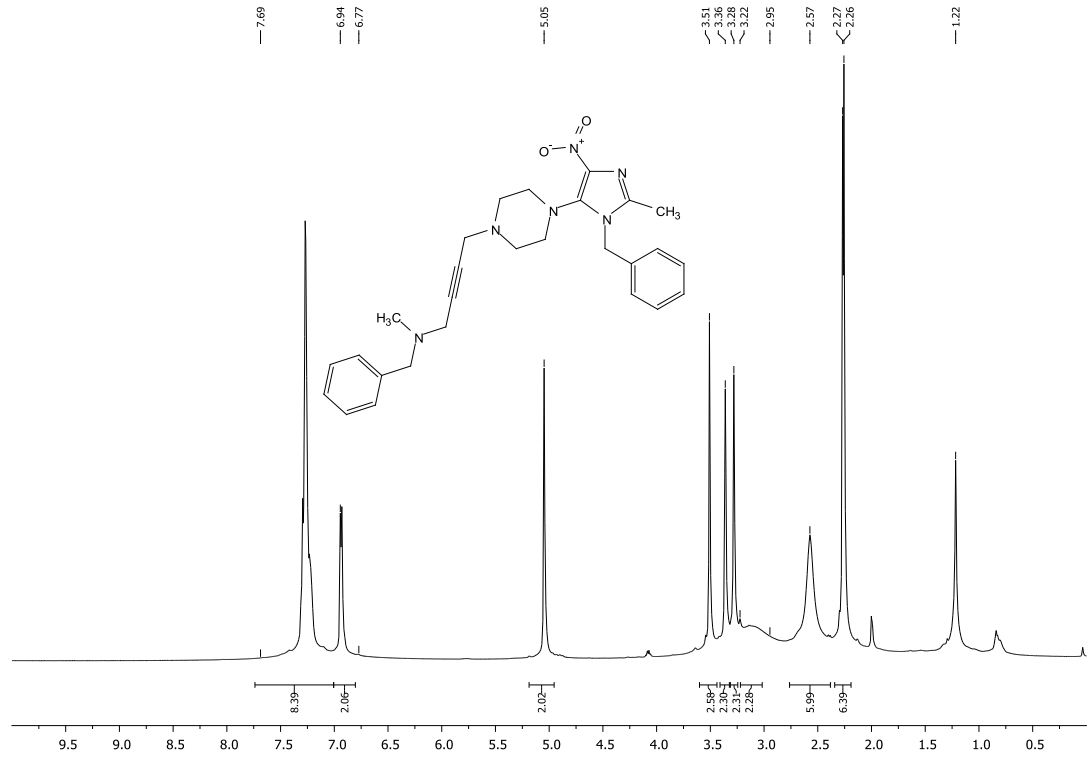
Compound **10l**

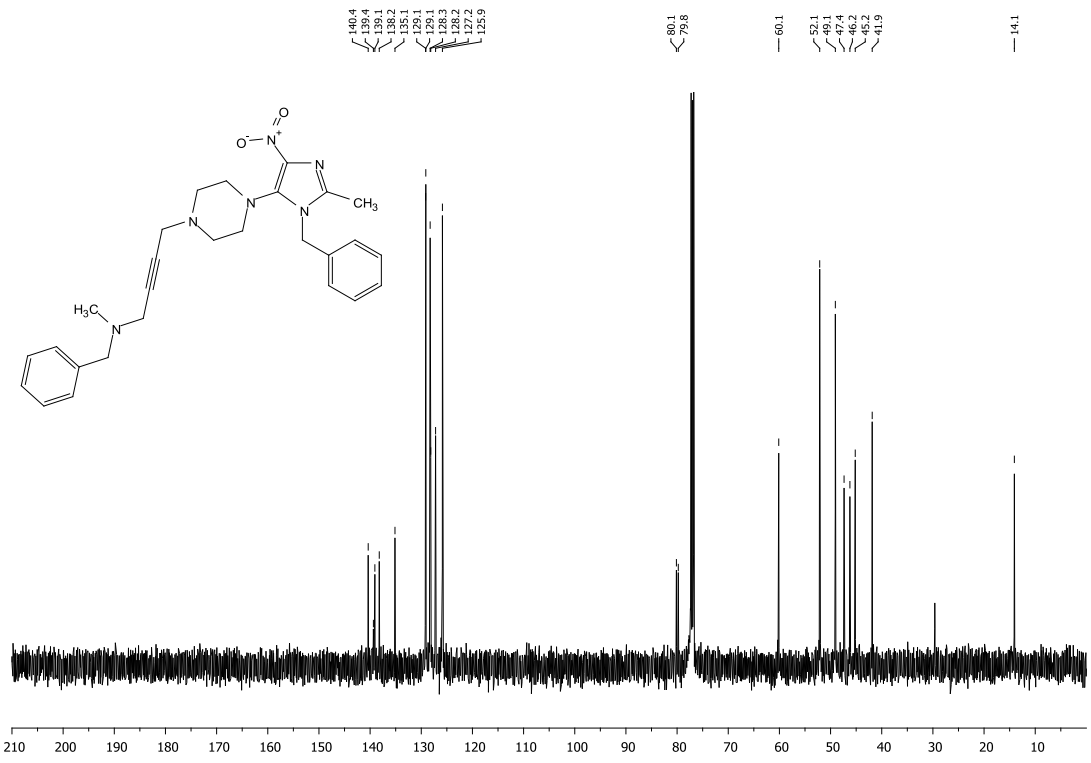




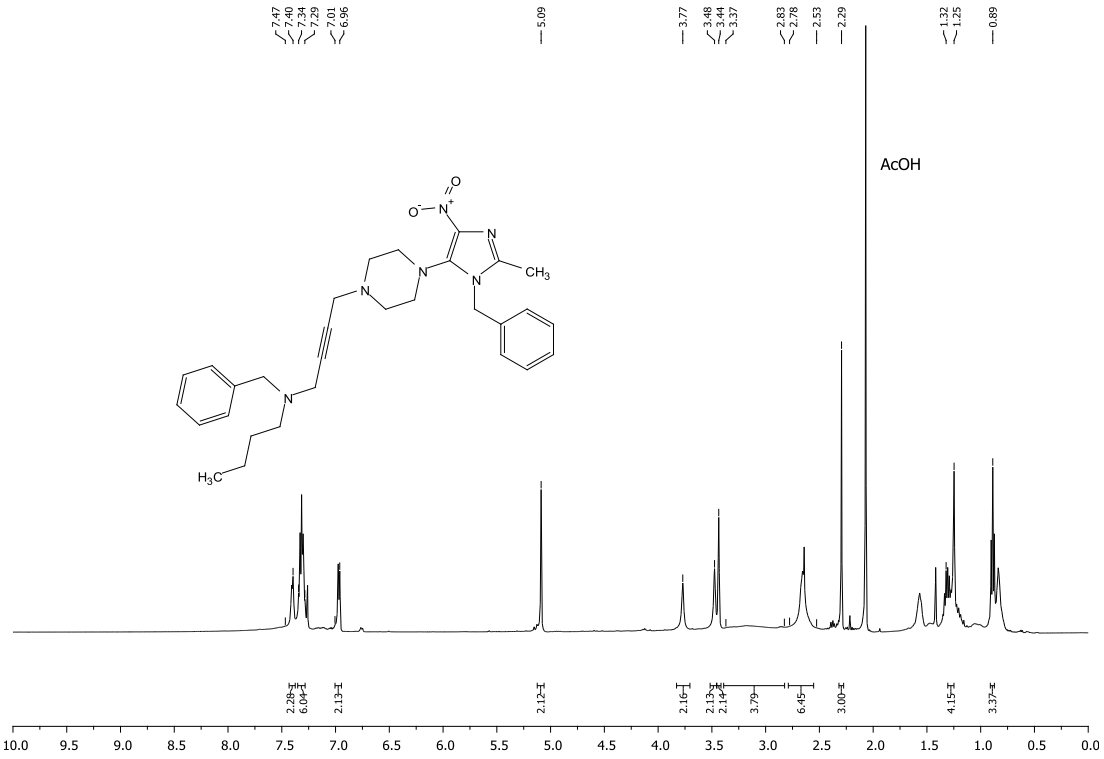

129.1
128.1
126.0
66.5
52.1
51.0
48.9
47.3
47.2
46.3
14.0
DMSO
EtOAc
O
O
N
N
N
N
N
CH3
N
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

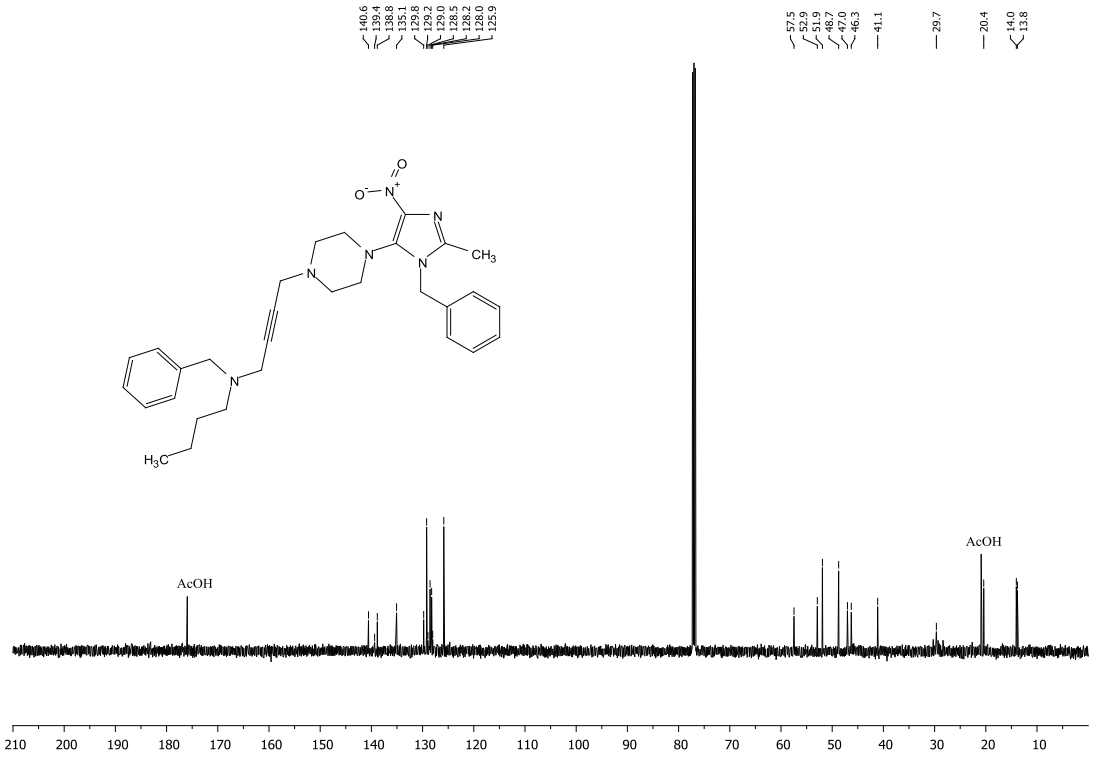
Compound **10m**

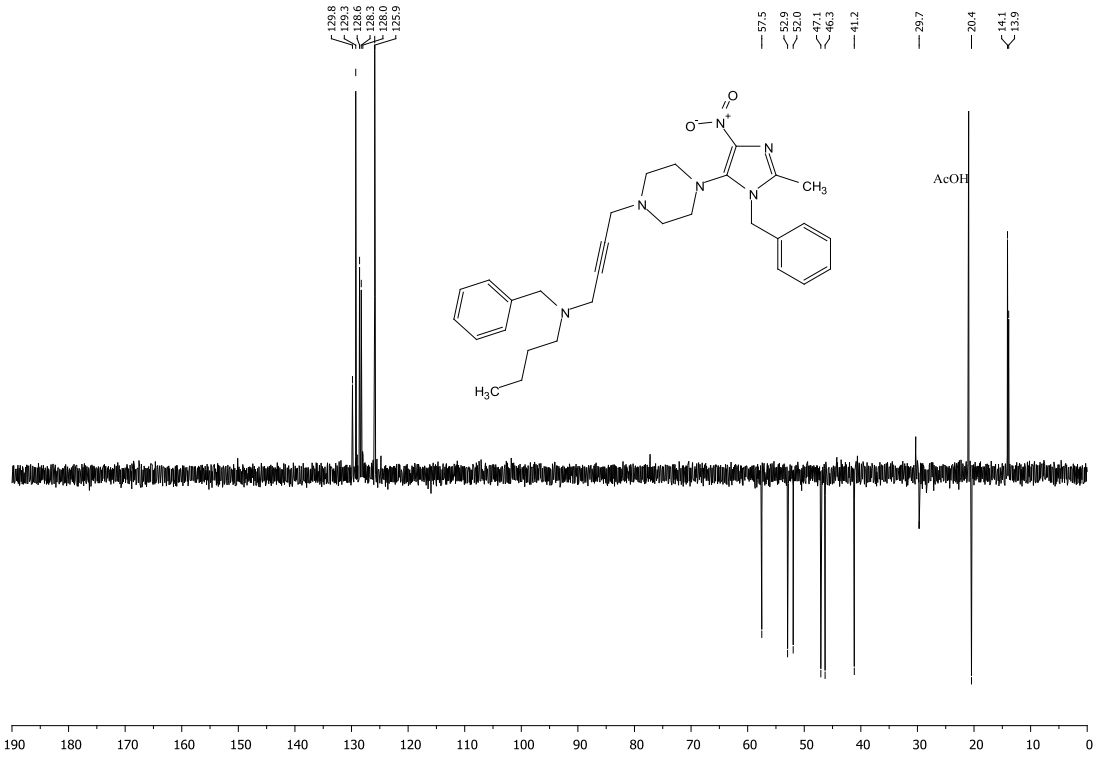




Compound **10n**



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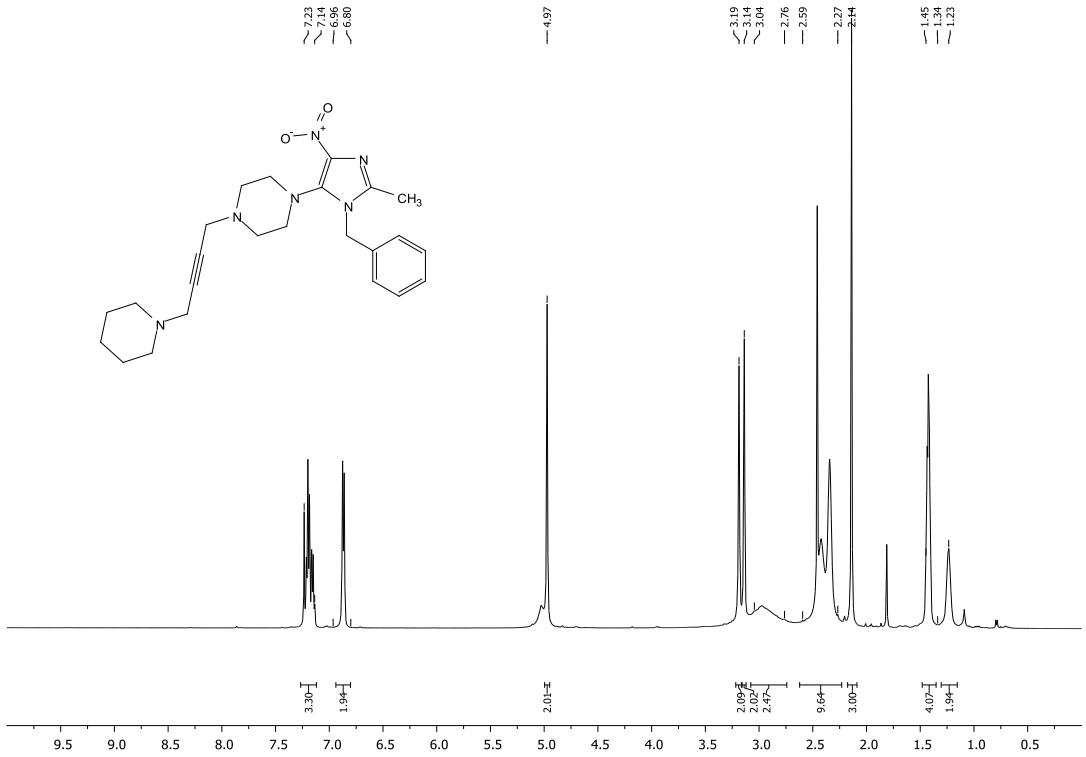
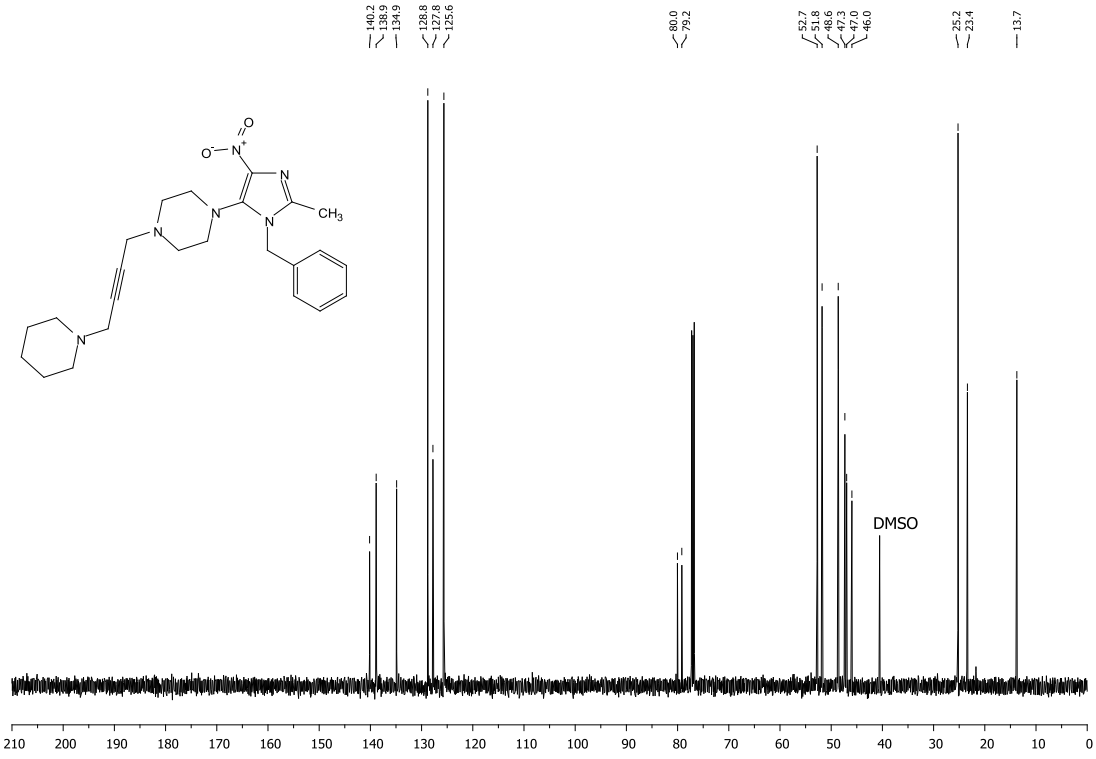
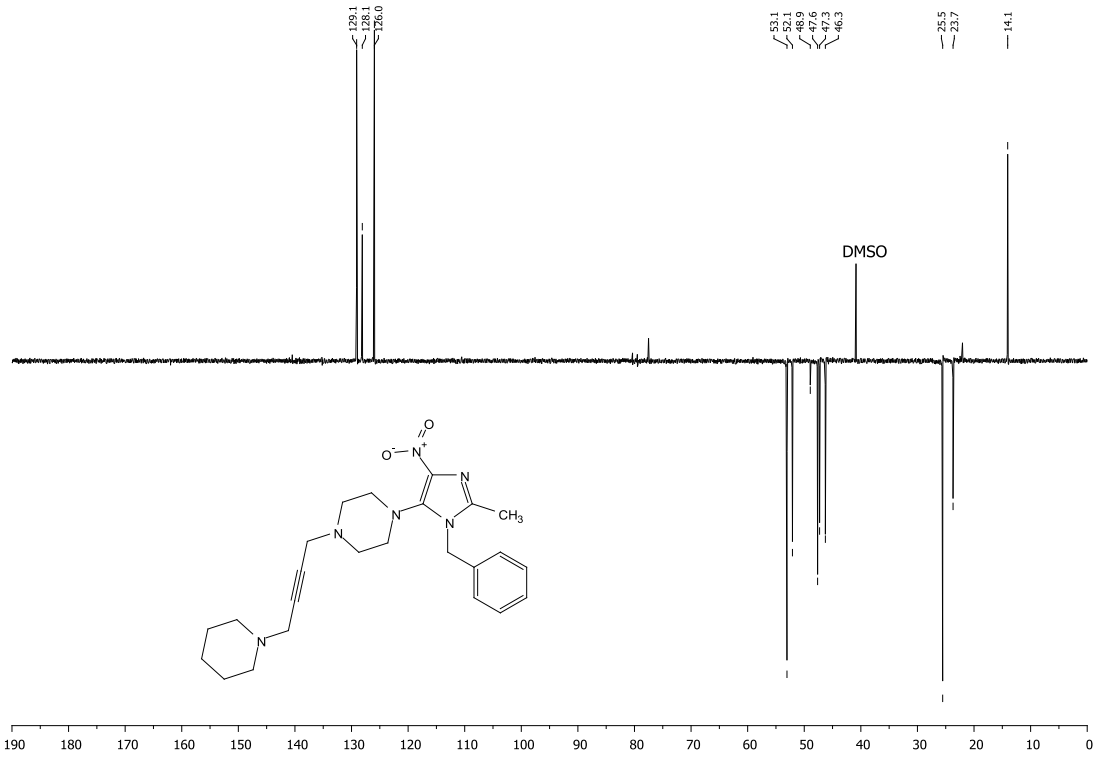
128.3
128.0
125.9
57.5
52.9
52.0
47.1
46.3
41.2
29.7
20.4
14.1
13.9
AcOH
O
O
N
N
N
N
N
CH3
N
H3C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

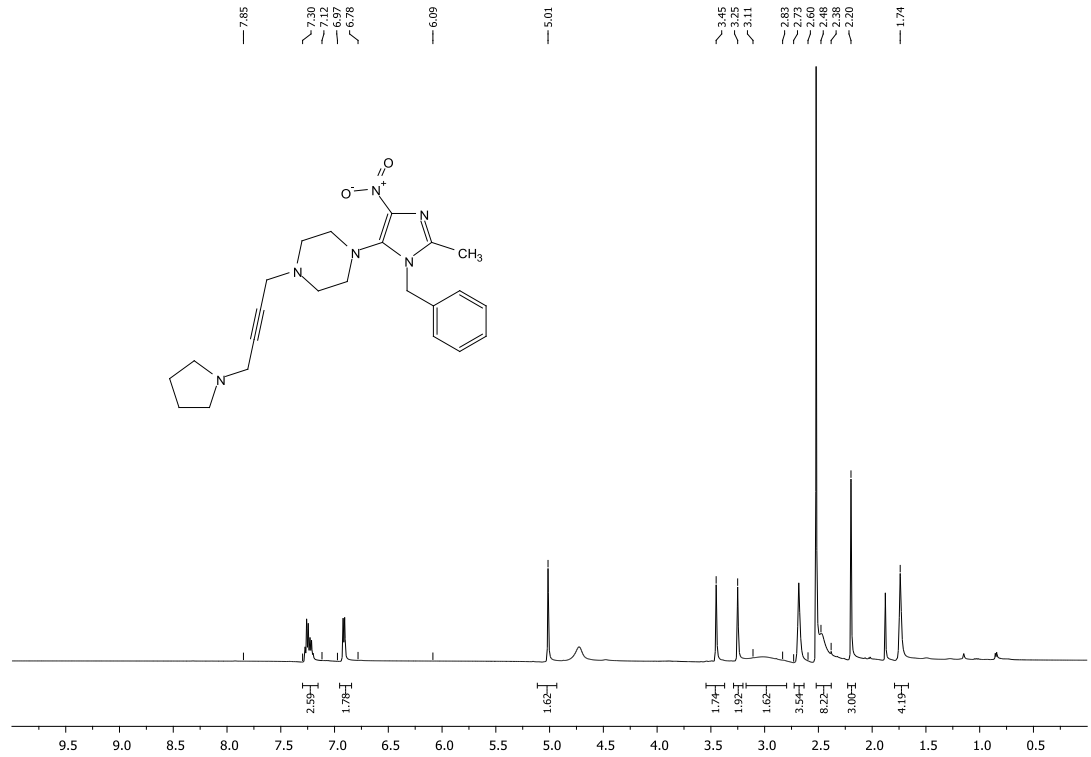
Compound **10o**

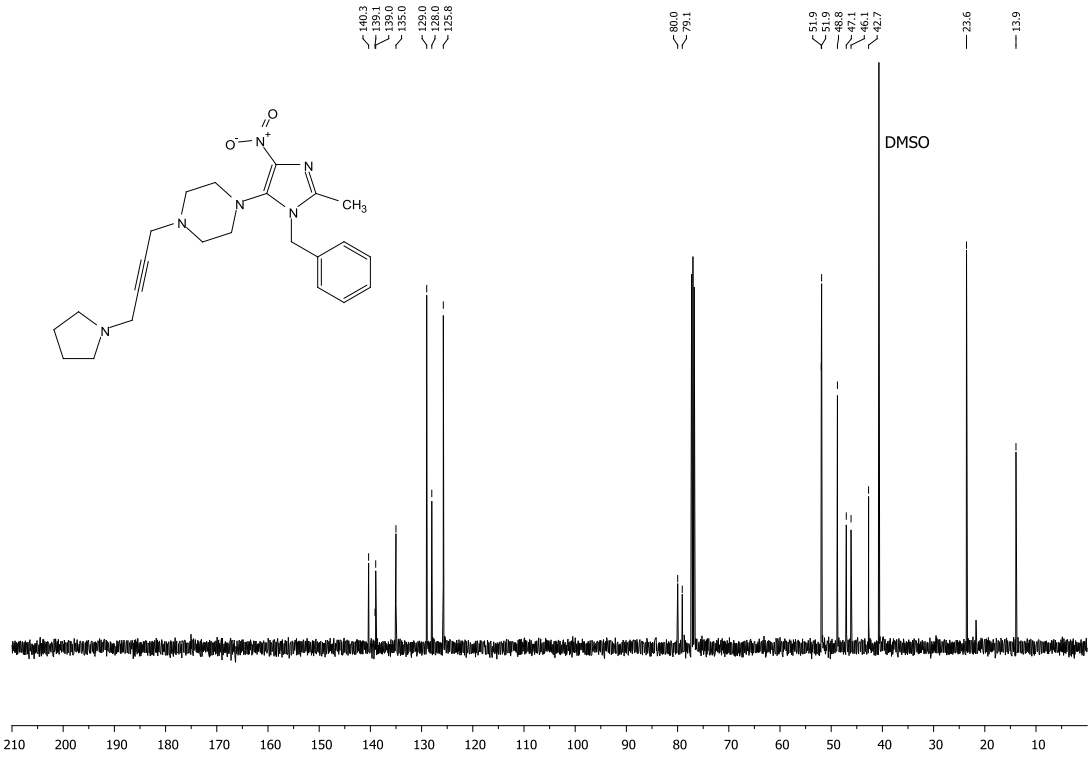


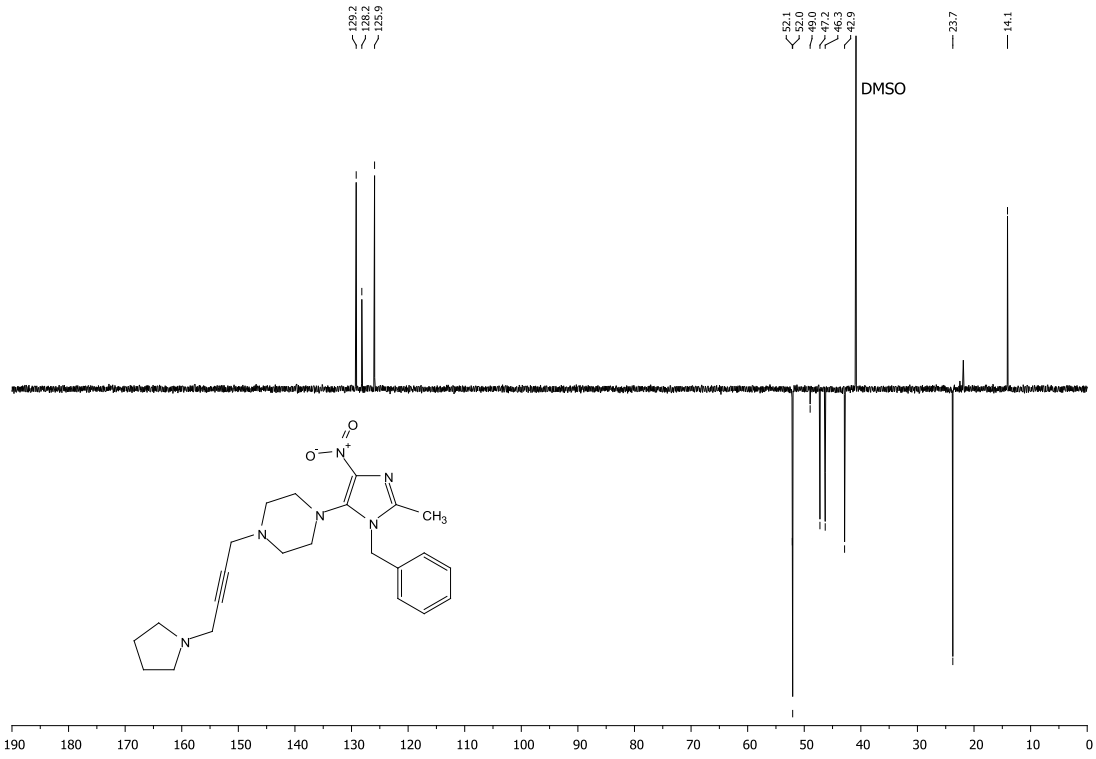



129.1
128.1
126.0
53.1
52.1
48.9
47.6
47.3
46.3
25.5
23.7
14.1
DMSO
O
O
N
N
N
N
N
CH3
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

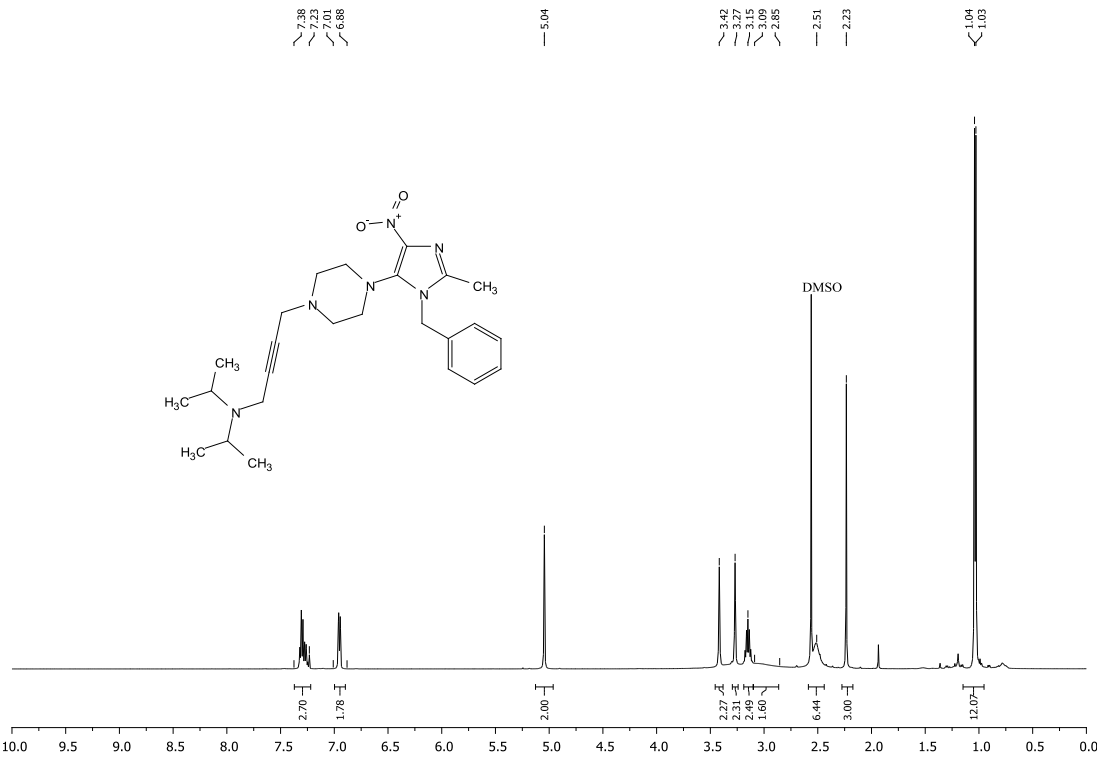
Compound **10p**

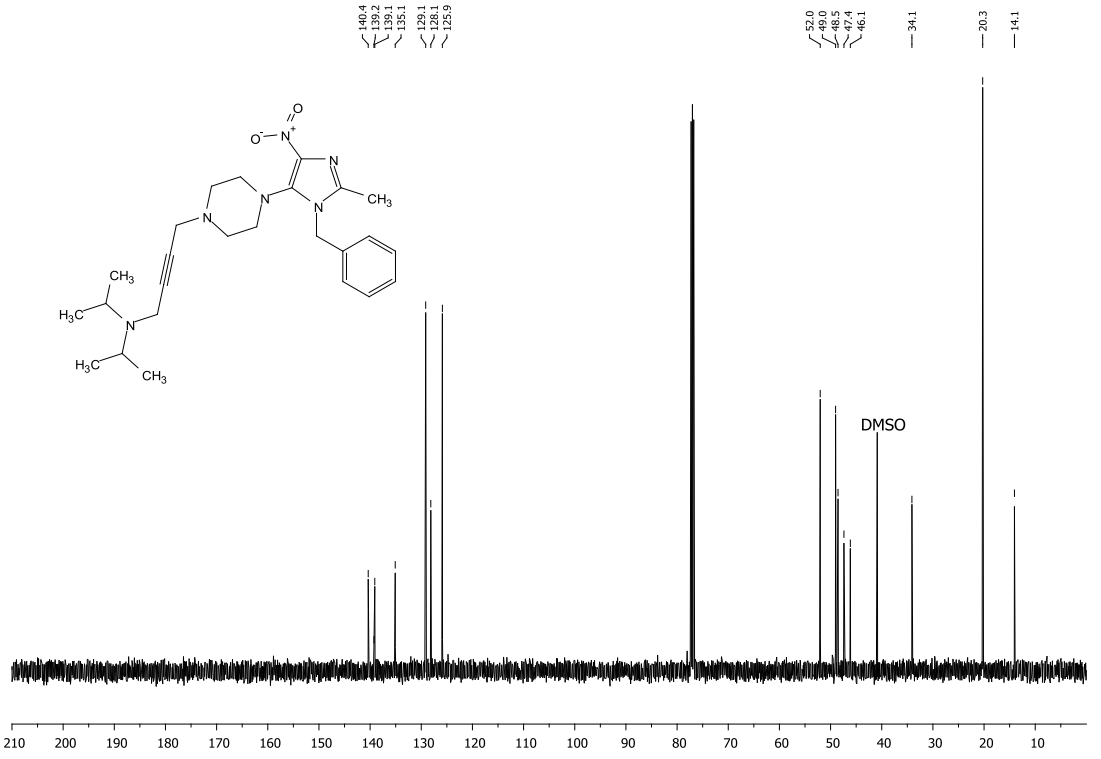


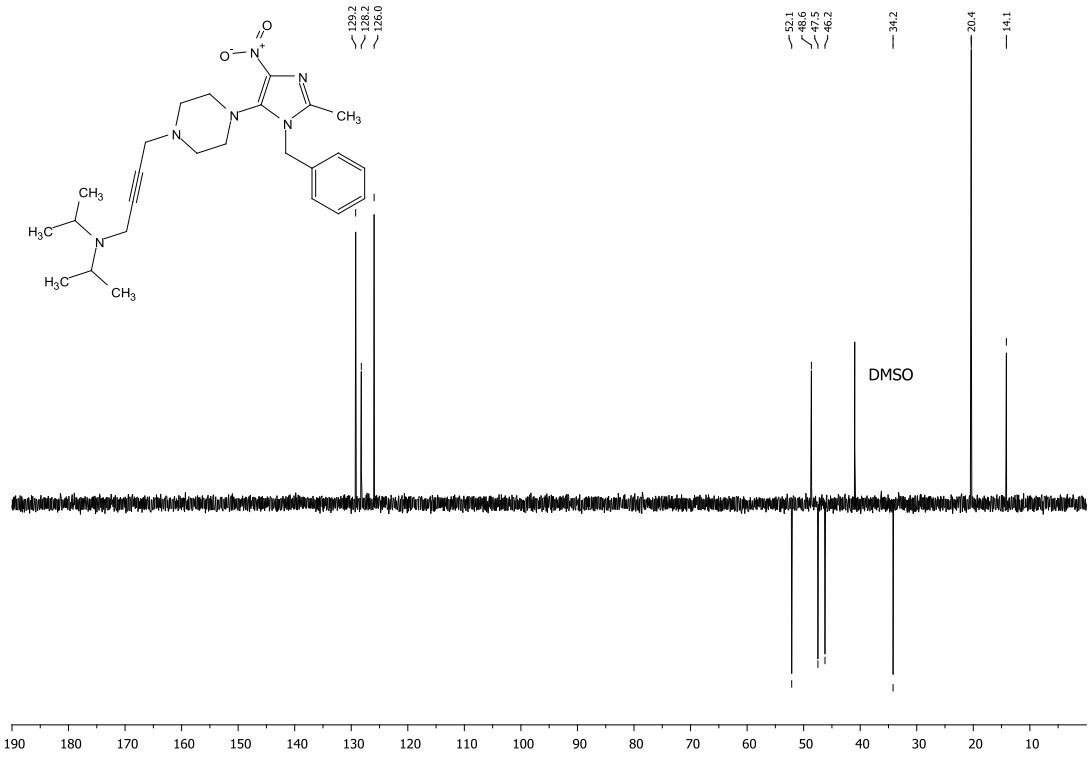



129.2
128.2
125.9
52.1
52.0
49.0
47.2
46.3
42.9
23.7
14.1
DMSO
O
O⁻
N⁺
N
N
N
N
CH3
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

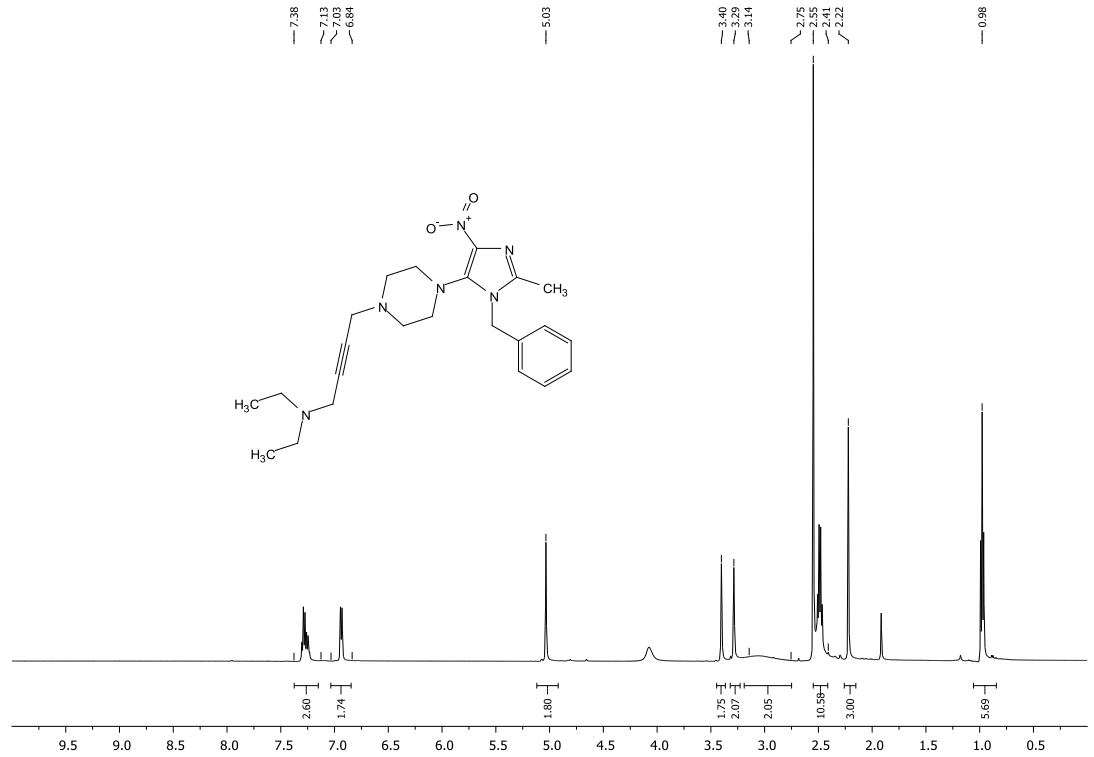
Compound **10q**

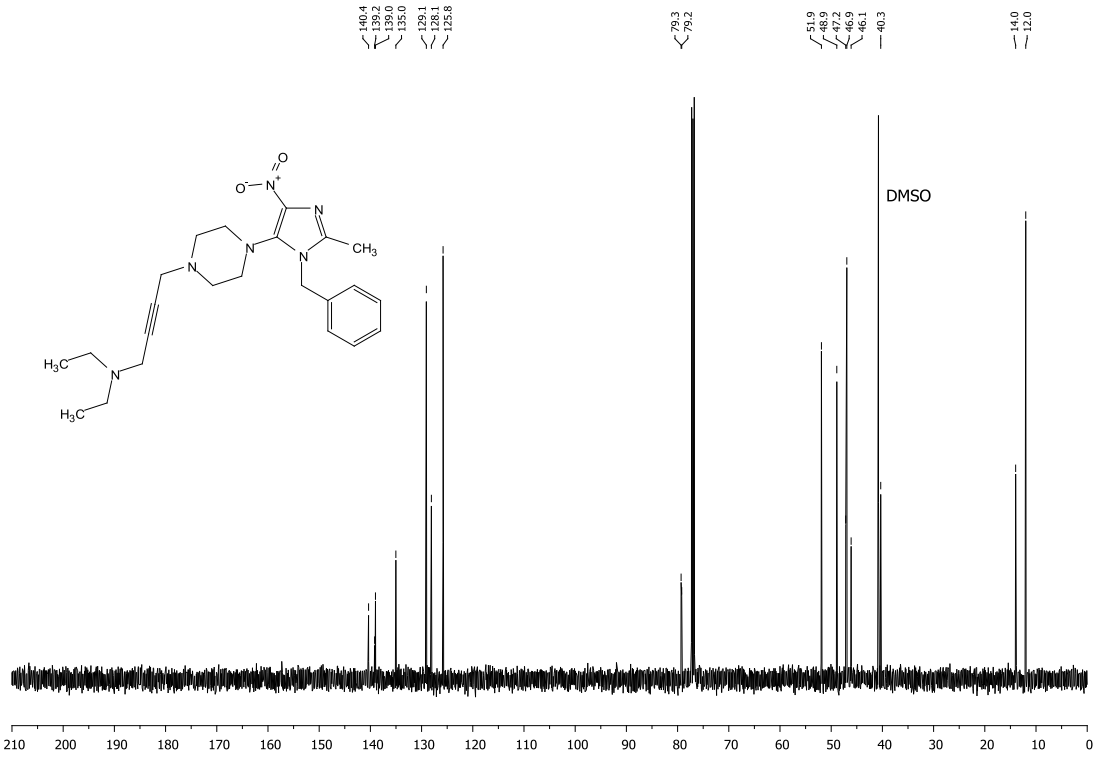


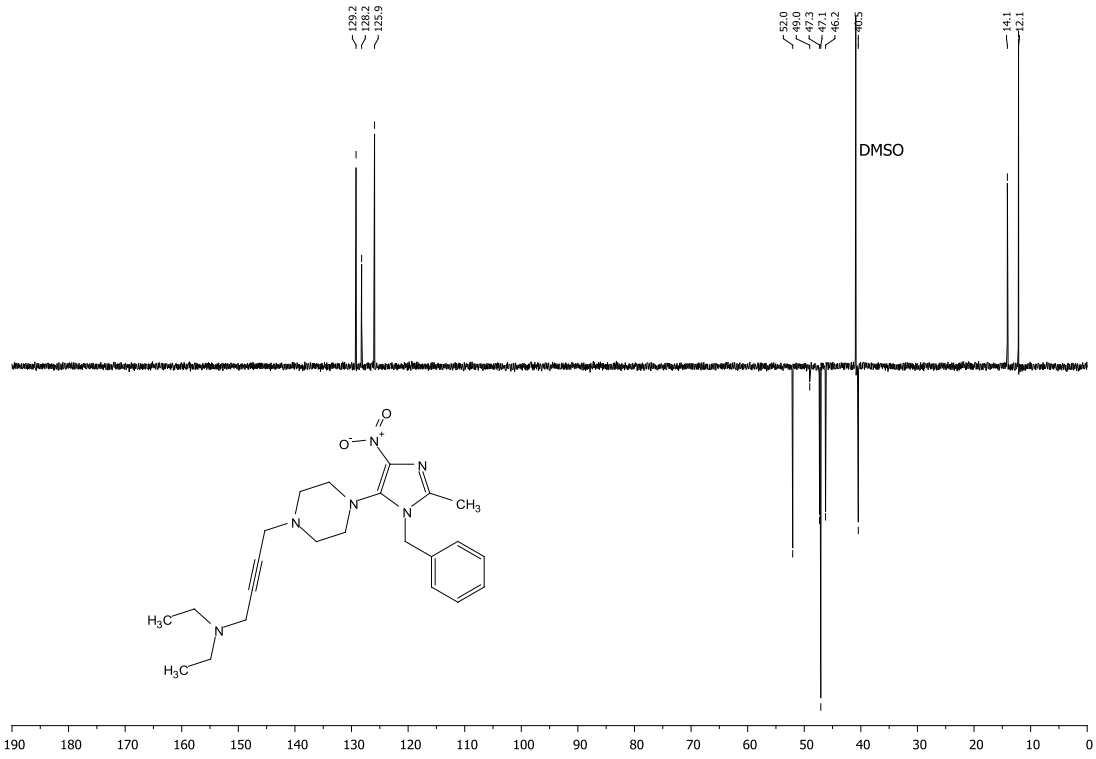



129.2
128.2
126.0
52.1
48.6
47.5
46.2
34.2
20.4
14.1
DMSO
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

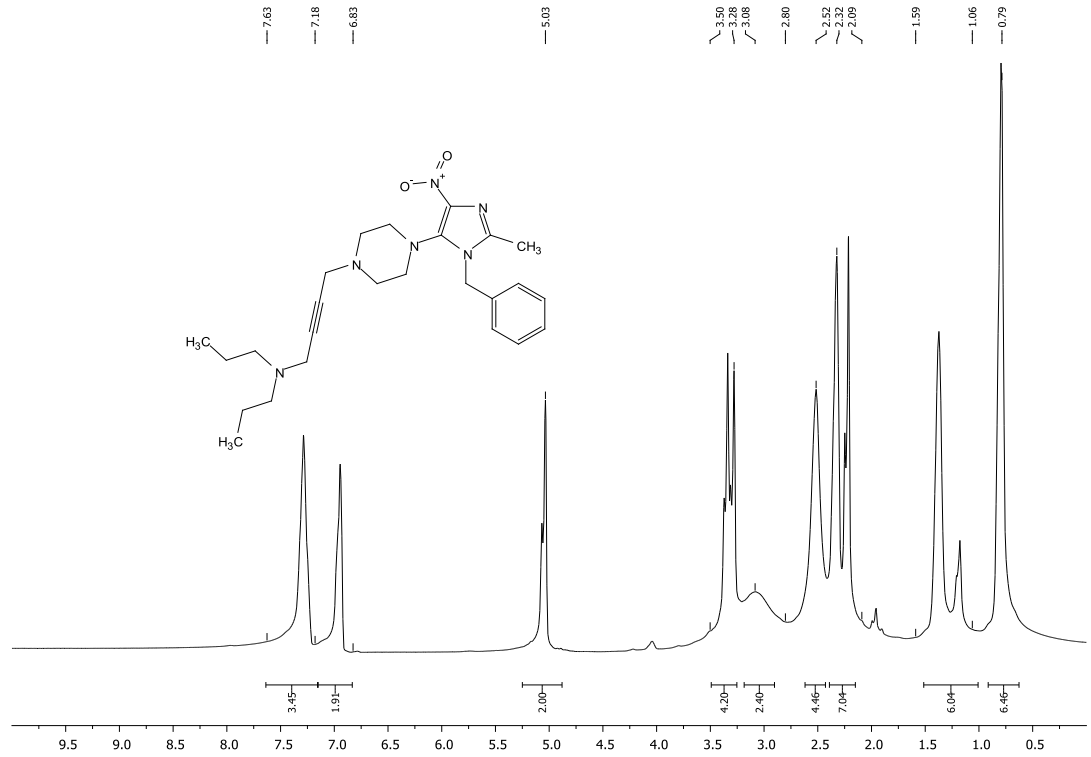
Compound **10r**

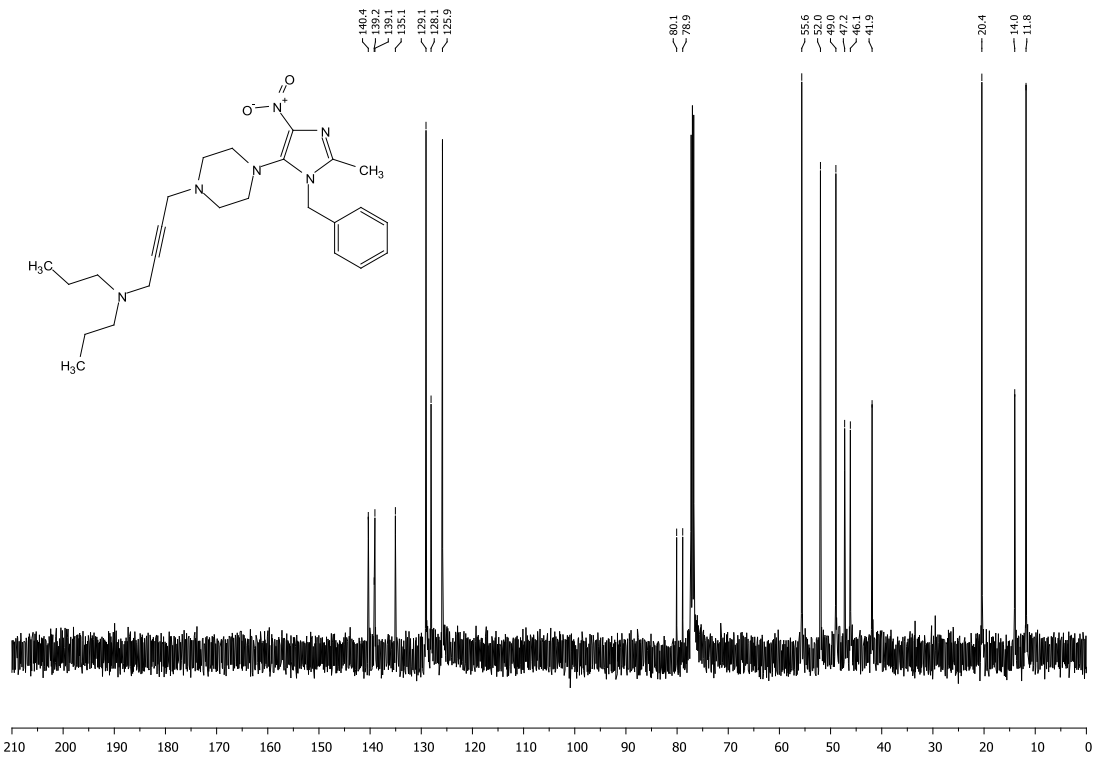


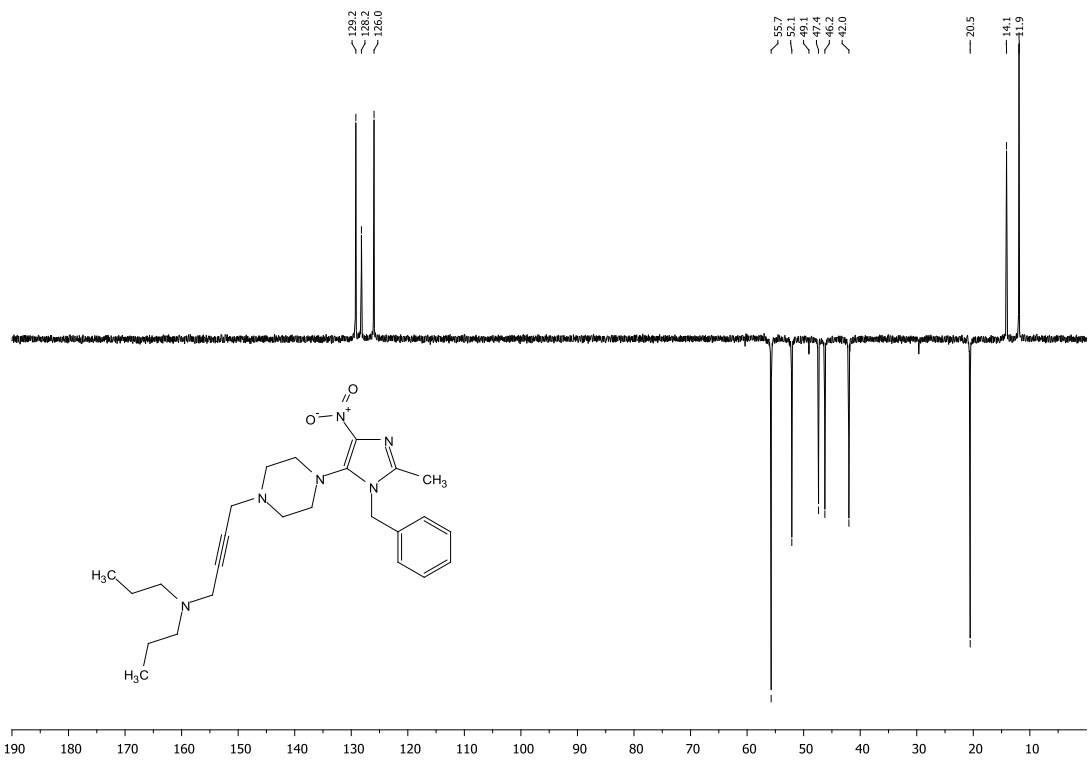



129.2
128.2
125.9
52.0
49.0
47.3
47.1
46.2
40.5
14.1
12.1
DMSO
O
O
N
N
N
N
N
CH3
H3C
H3C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

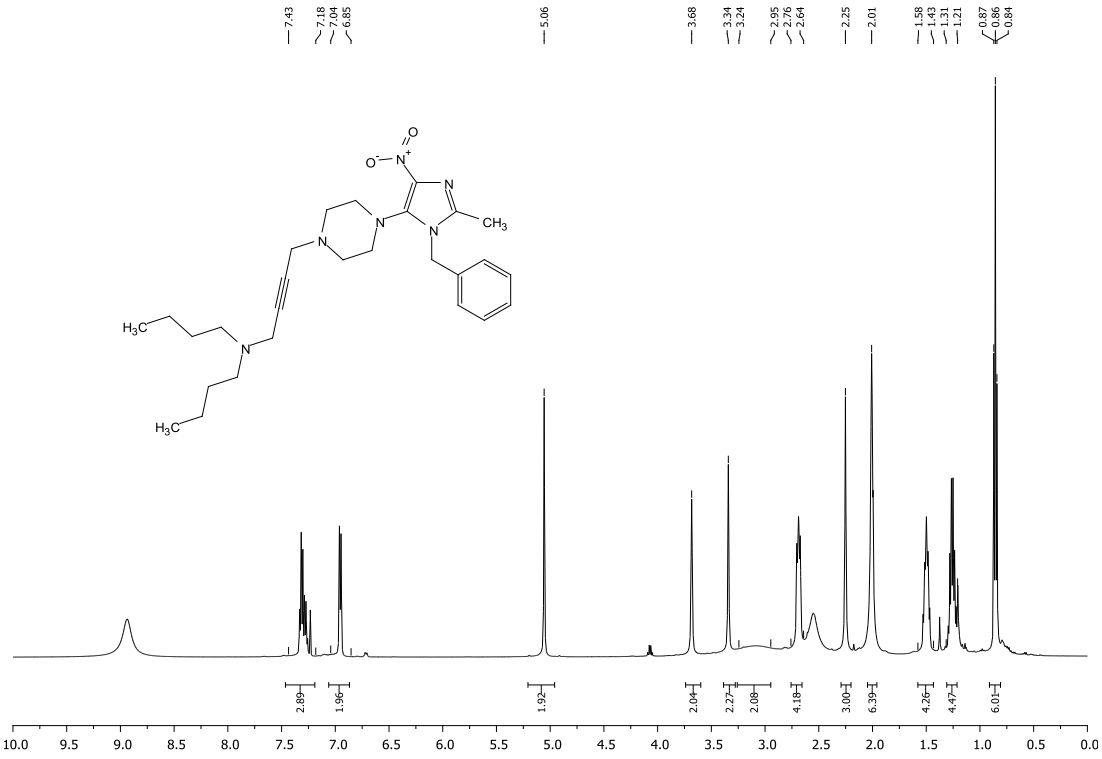
Compound **10s**

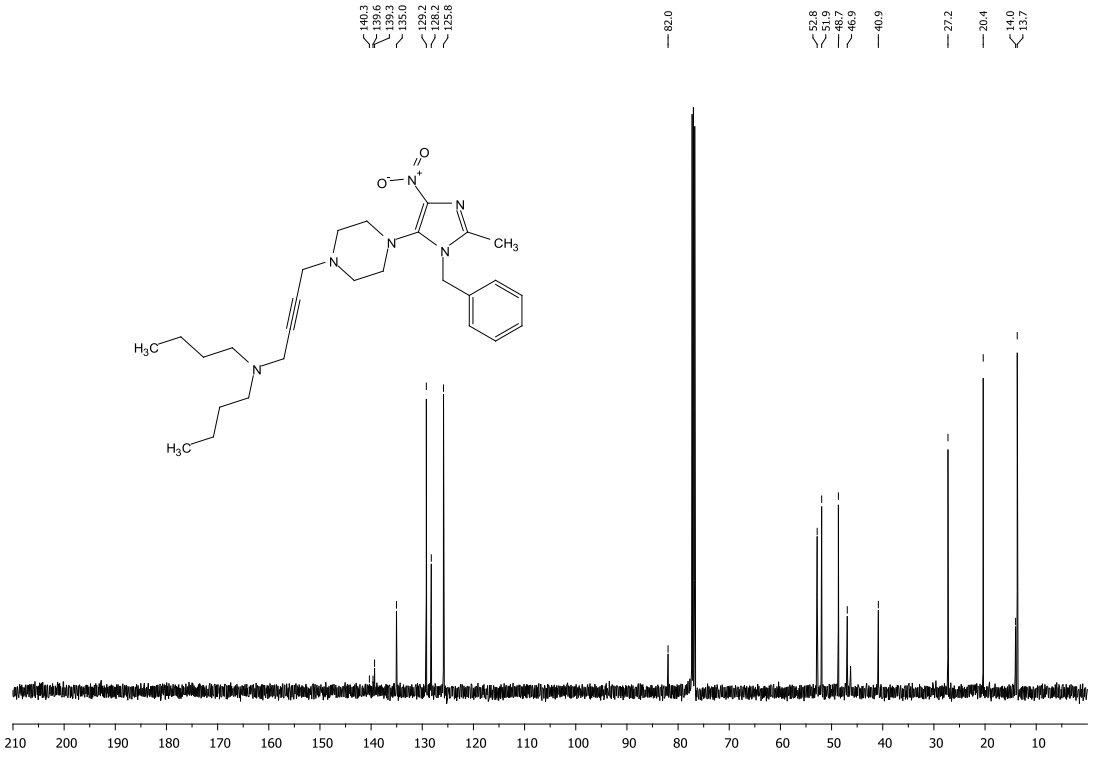


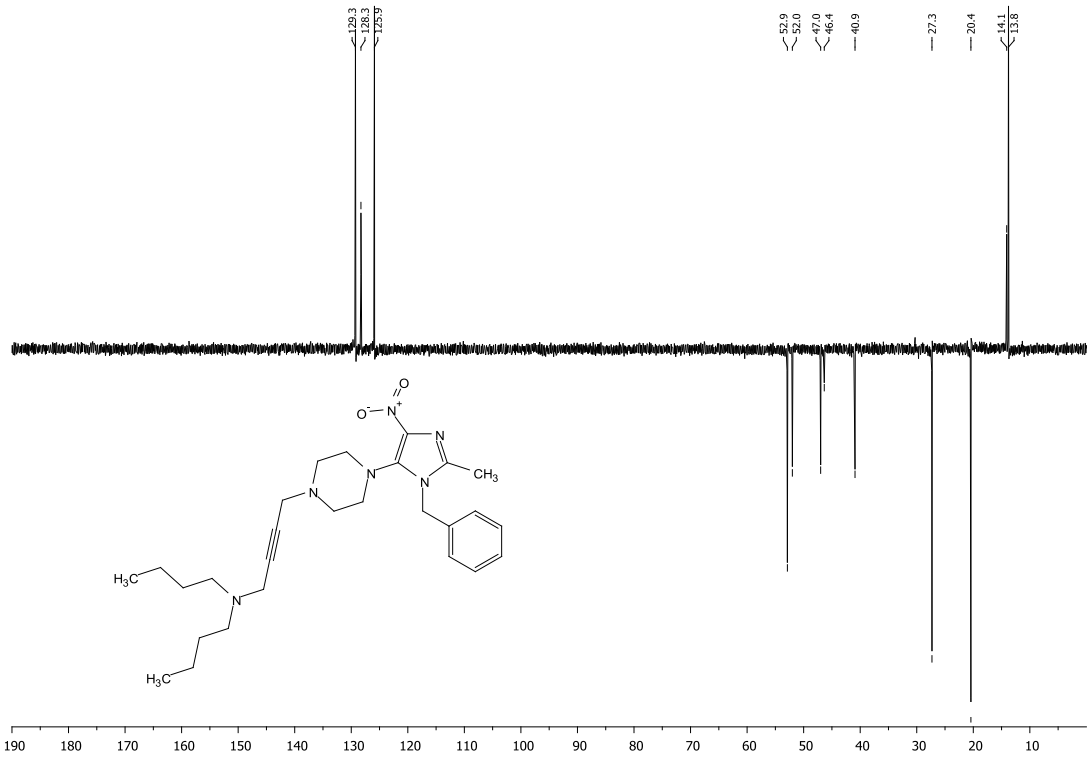



129.2
128.2
126.0
55.7
52.1
49.1
47.4
46.2
42.0
20.5
14.1
11.9
O
O⁻
N⁺
N
N
N
N
CH3
H3C
N
H3C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

Compound **10t**



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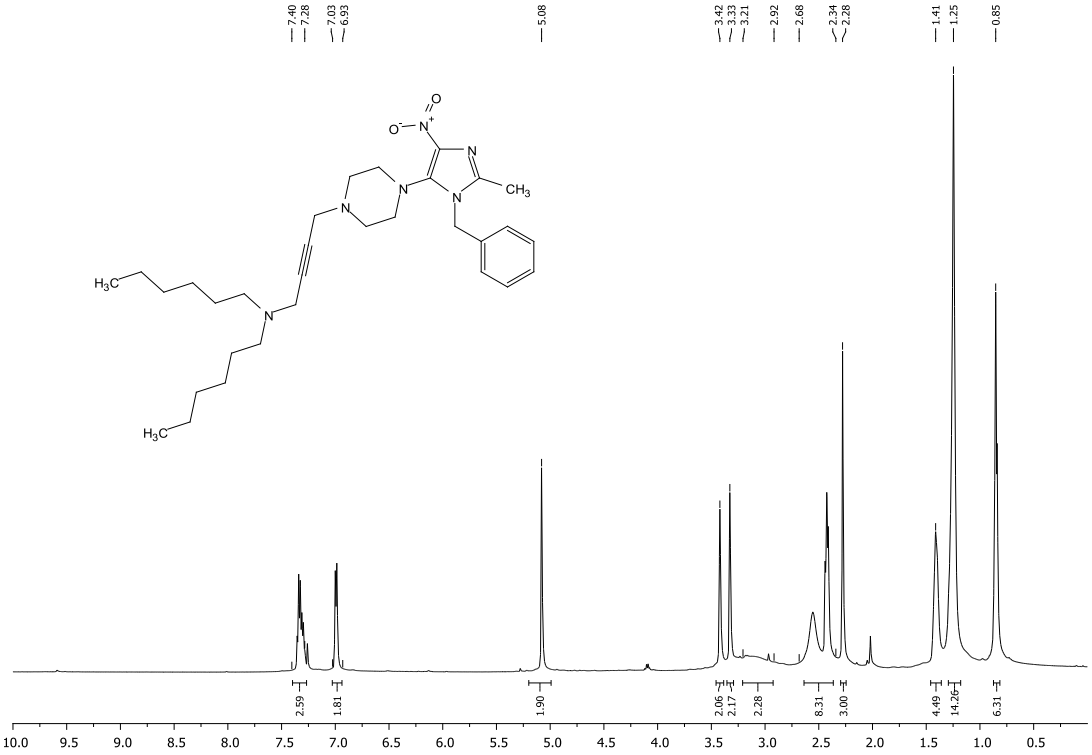
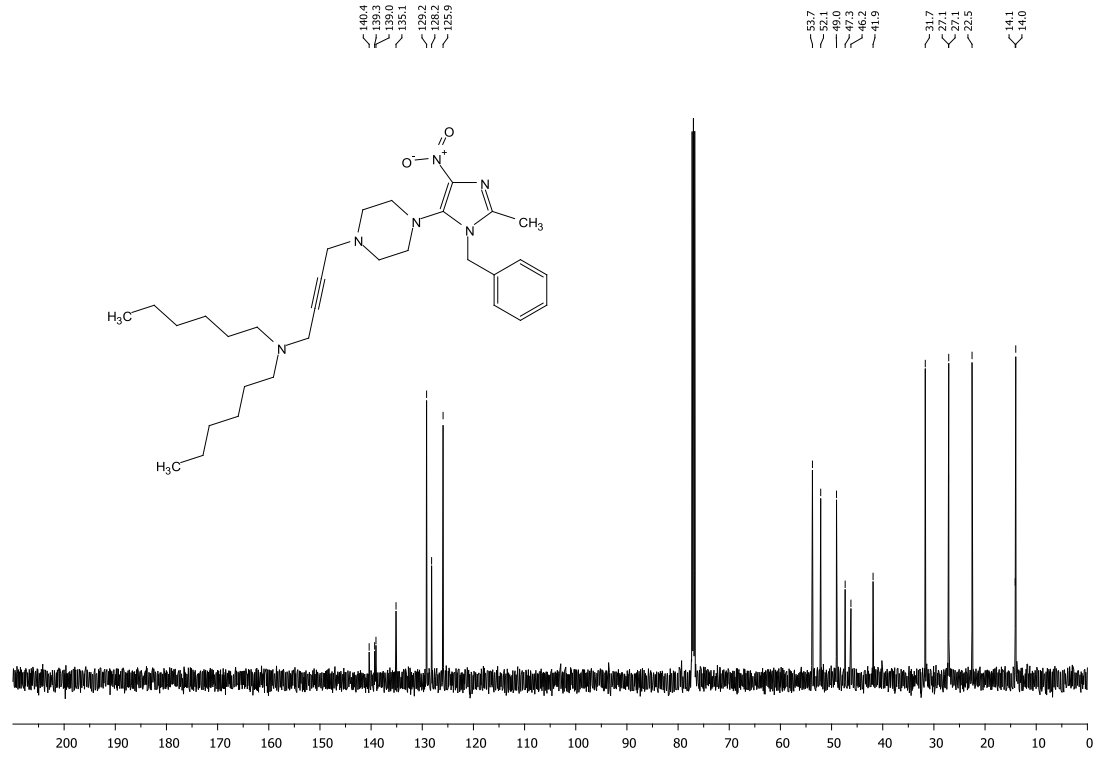
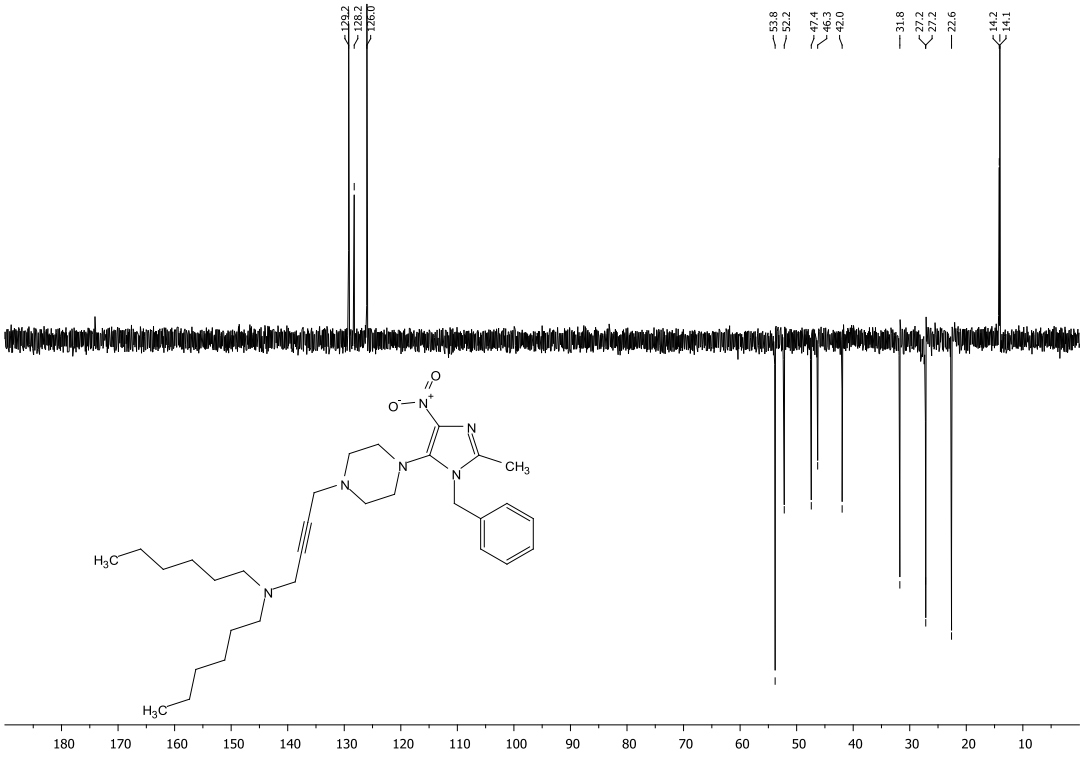
128.3
125.9
52.9
52.0
47.0
46.4
40.9
27.3
20.4
14.1
13.8
O
O⁻
N⁺
N
N
N
N
CH3
H3C
N
H3C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

Compound **10u**



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128.2
126.0
53.8
52.2
47.4
46.3
42.0
31.8
27.2
27.2
22.6
14.2
14.1
180
170
160
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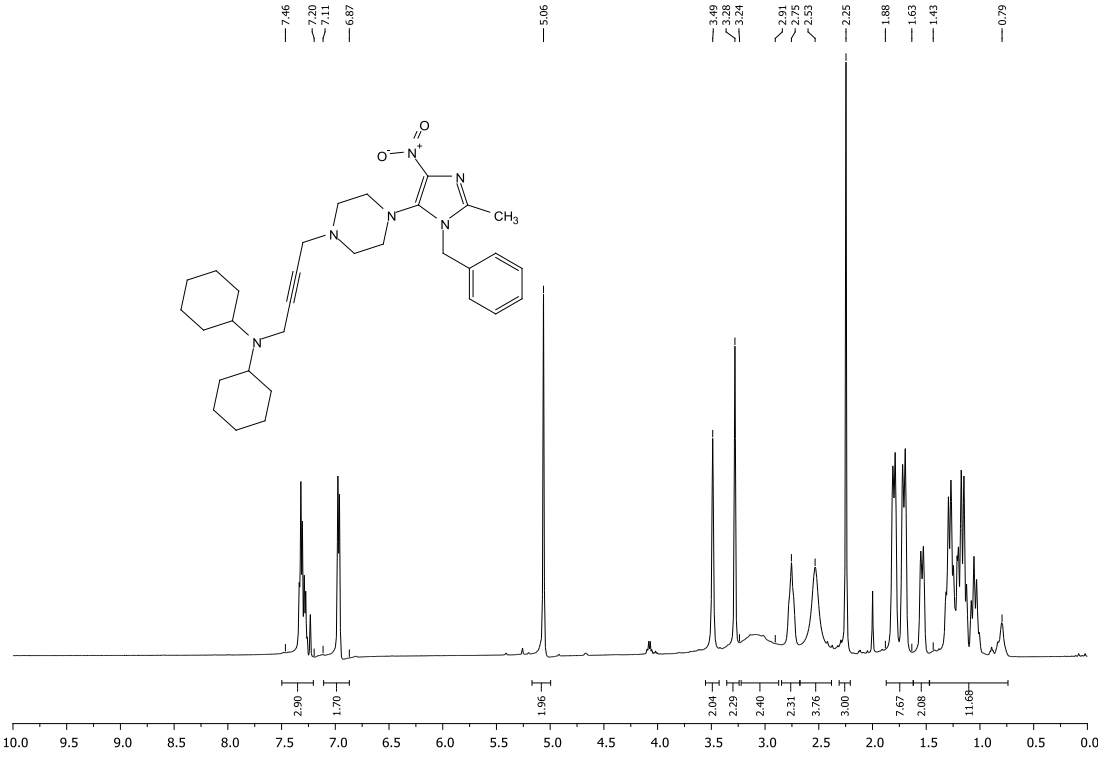
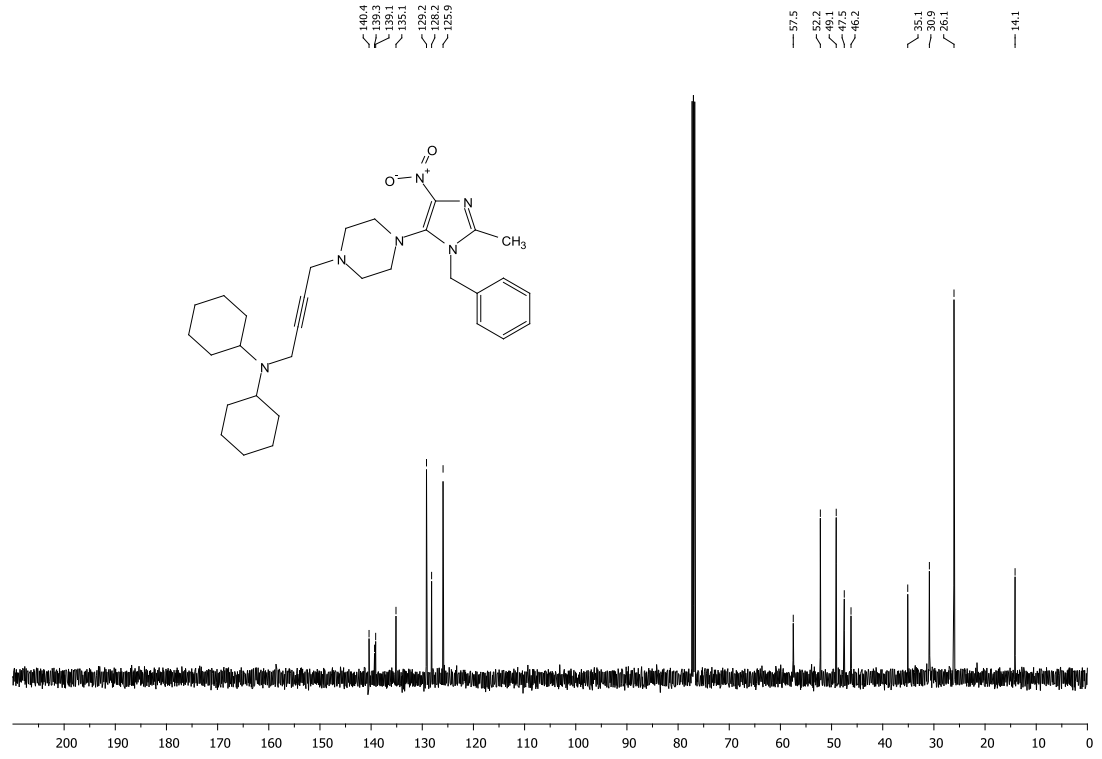
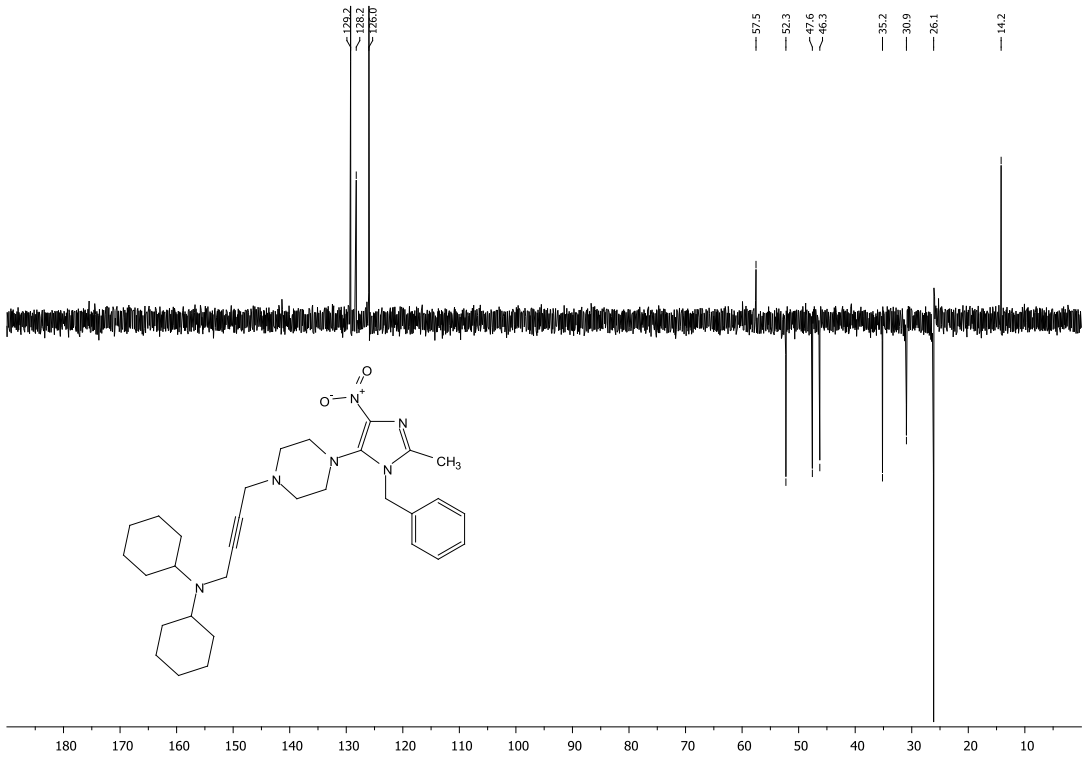
140
130
120
110
100
90
80
70
60
50
40
30
20
10

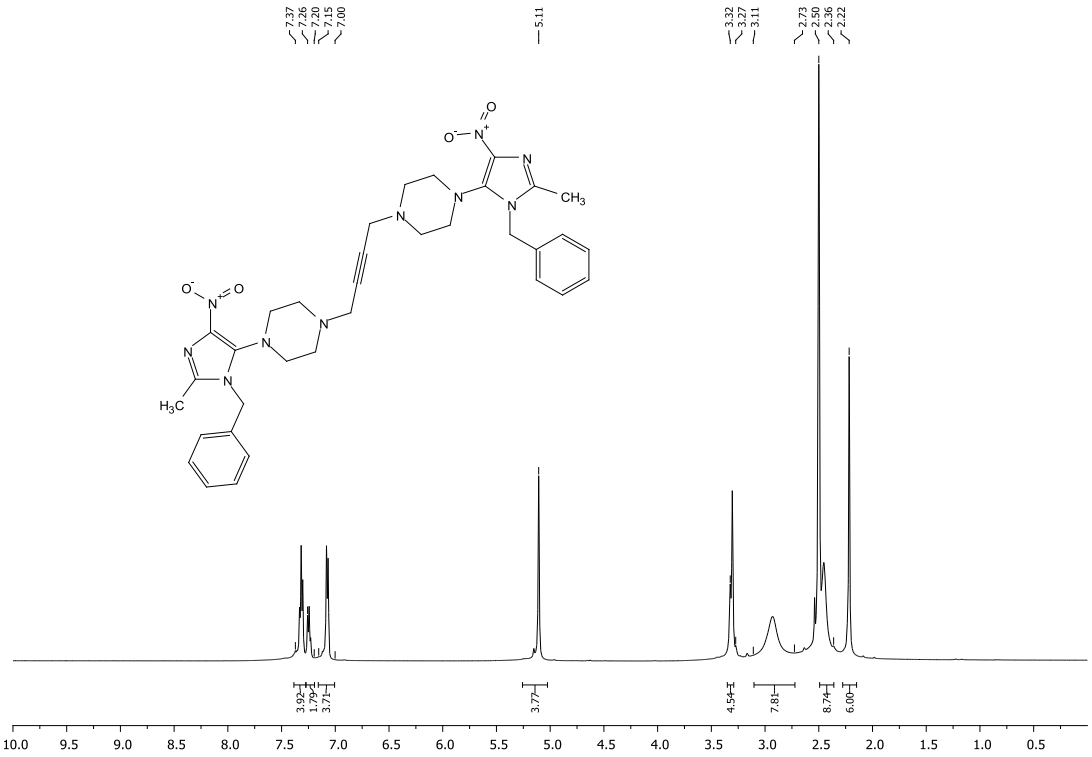
Compound **10v**

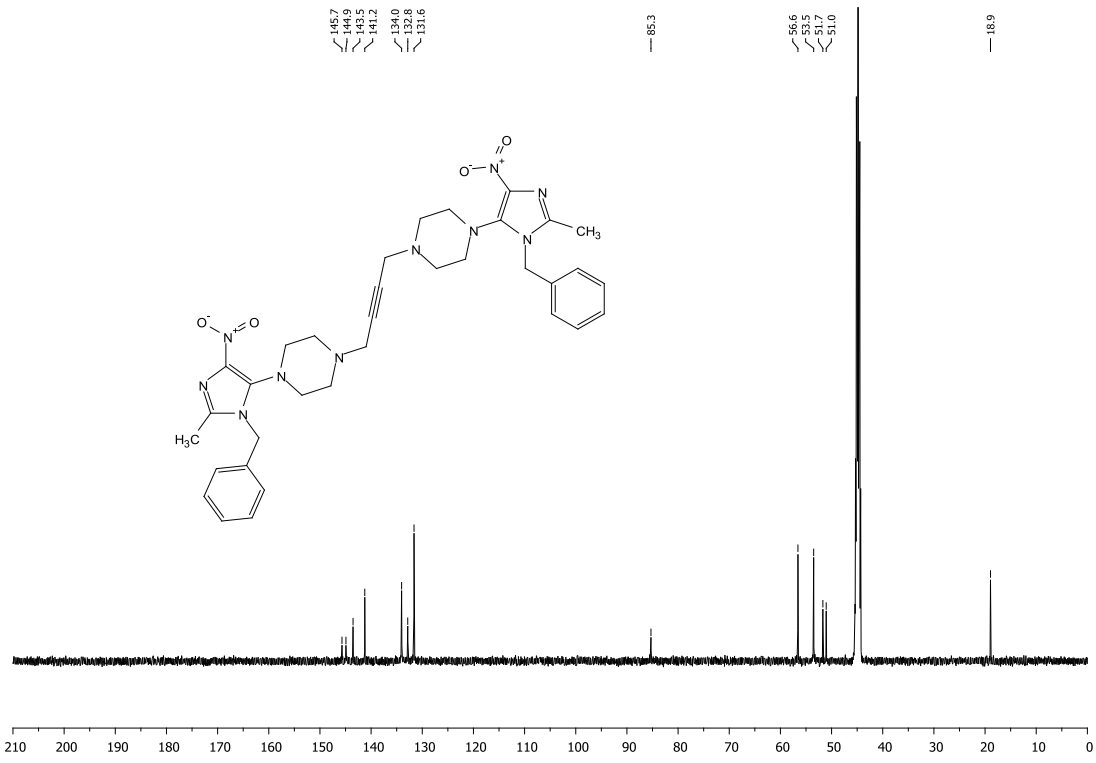


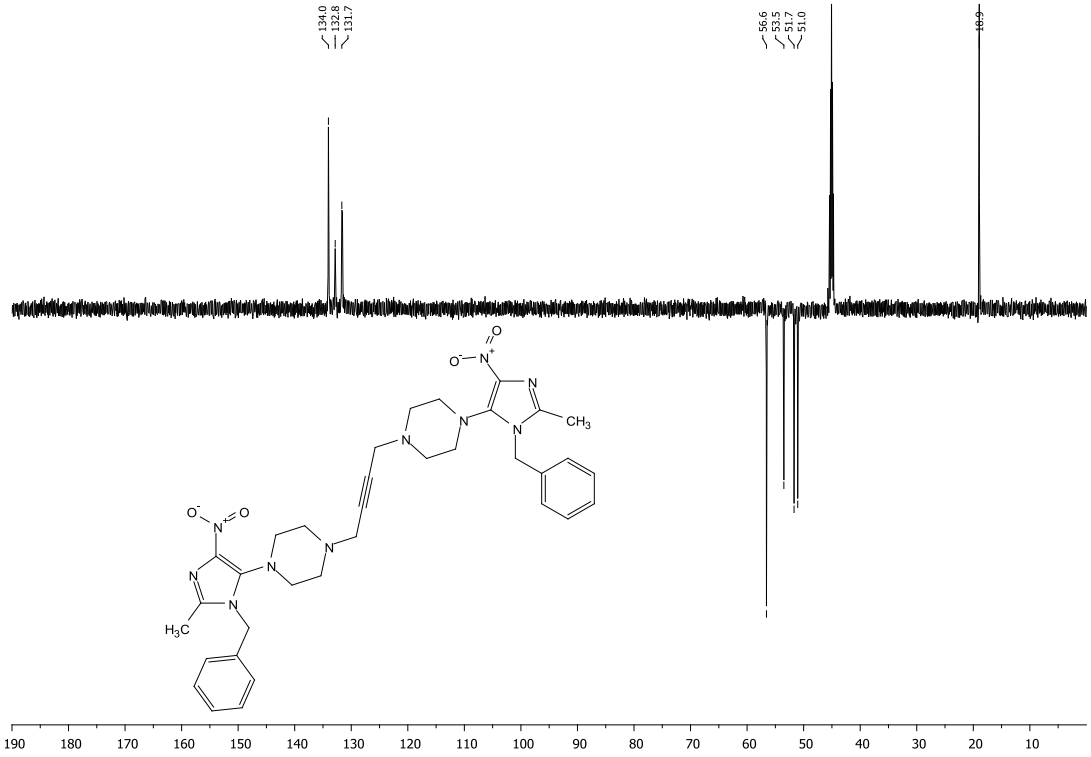



129.2
128.2
126.0
57.5
52.3
47.6
46.3
35.2
30.9
26.1
14.2
O
O⁻
N⁺
N
N
N
N
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

Compound **10w**



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132.8
131.7
56.6
55.5
51.7
51.0
18.9
190
180
170
160
150
140
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120
110
100
90
80
70
60
50
40
30
20
10