Supporting Information for:

Synthesis and Photophysical Properties of Benzotriazole-Derived Unnatural α-Amino Acids

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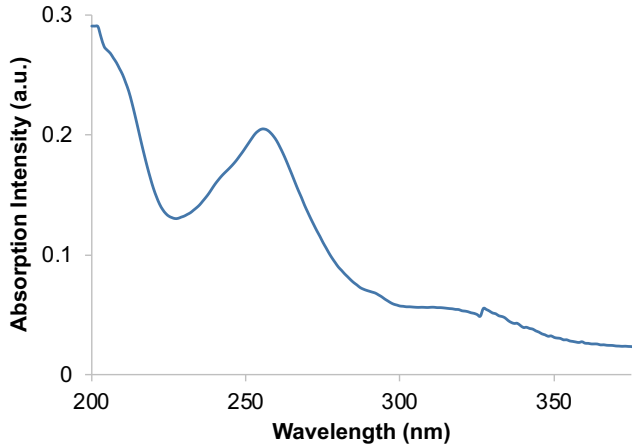
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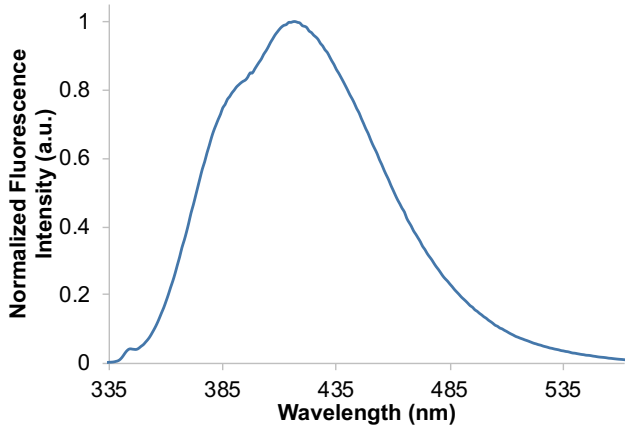
1. Absorption and Emission Spectra for α-Amino Acids **21a–c, 21e, 21f** and **24** S2–S4
2. ^{1}H and ^{13}C NMR Spectra for all Novel Compounds S5–S70

1. Absorption and Emission Spectra for Amino Acids 21a–c, 21e, 21f and 24

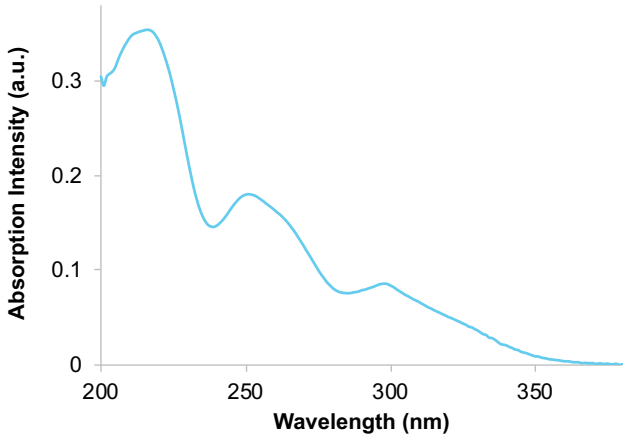
Spectra were recorded at 10 μM in methanol using an excitation and emission slit width of 3 nm.

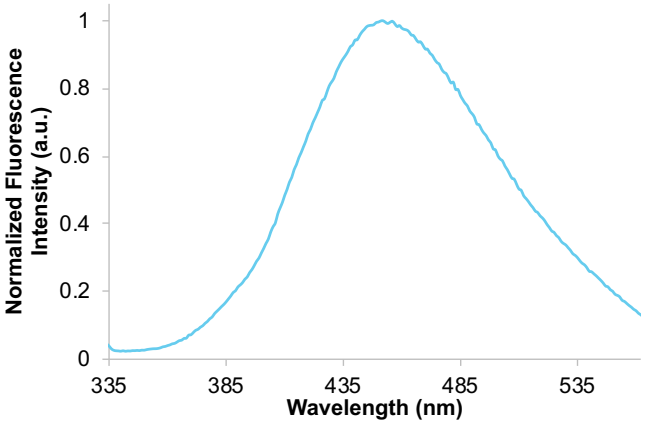
(2*S*)-2-Amino-3-[5′-(4′′-methoxyphenyl)-1*H*-benzo[*d*][1.2.3]triazol-1′-yl]propanoic acid hydrochloride (21a)



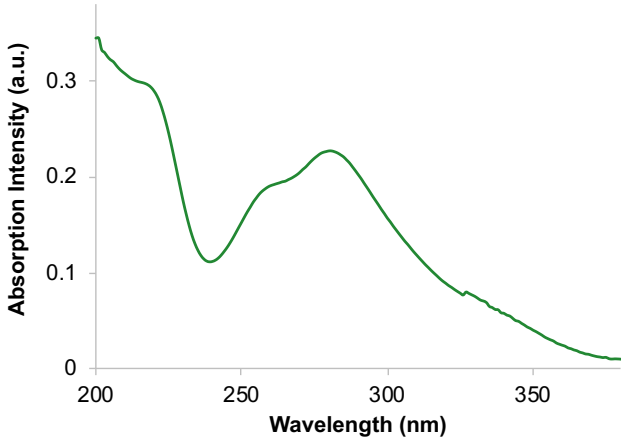


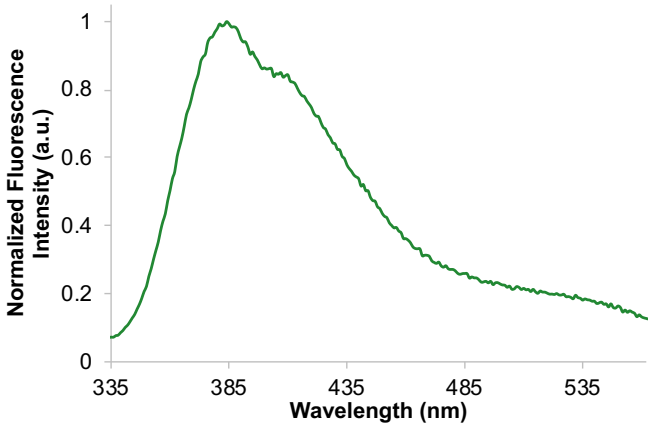
(2*S*)-2-Amino-3-[5′-(3′′,4′′-methylenedioxyphenyl)-1*H*-benzo[*d*][1.2.3]triazol-1′-yl]propanoic acid hydrochloride (21b)



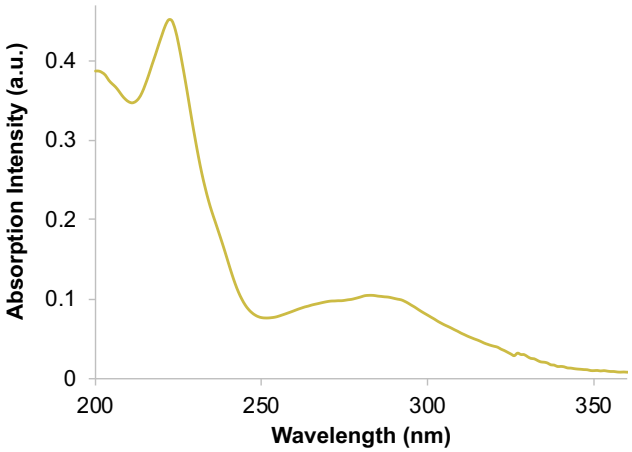


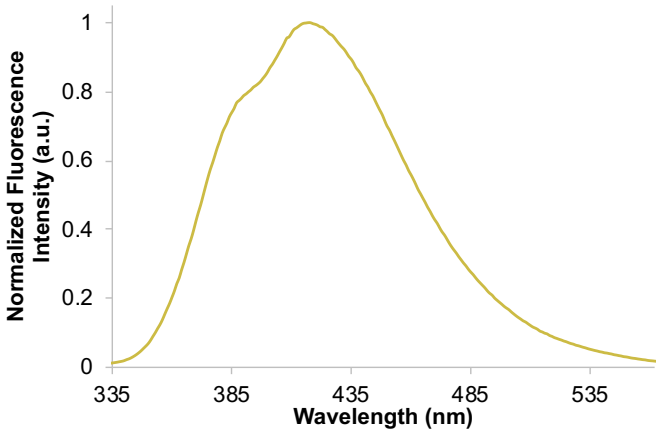
(2*S*)-2-Amino-3-[5′-(4′′-morpholinophenyl)-1*H*-benzo[*d*][1.2.3]triazol-1′-yl]propanoic acid hydrochloride (21c)



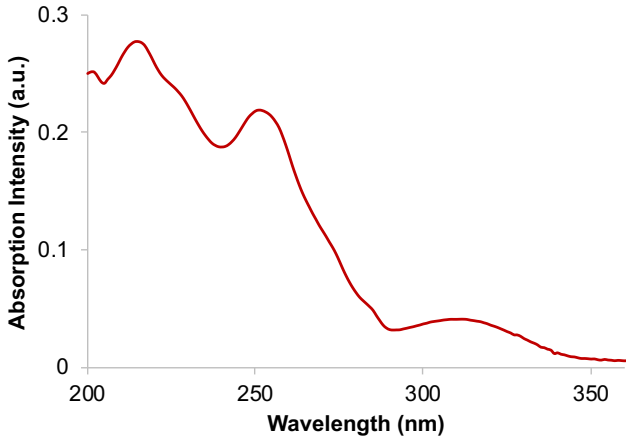


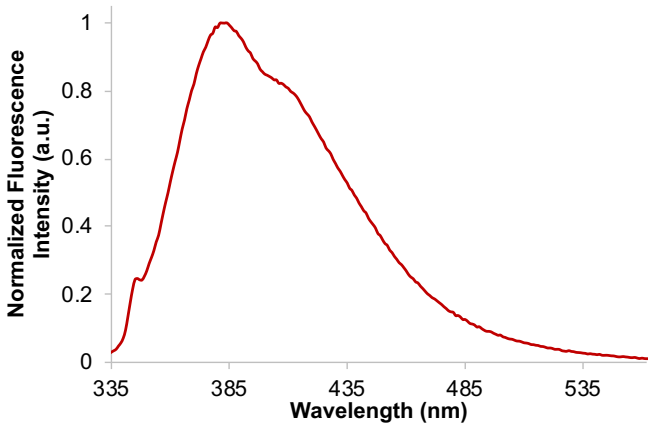
(2*S*)-2-Amino-3-[5′-(naphthalen-2′′-yl)-1*H*-benzo[*d*][1.2.3]triazol-1′-yl]propanoic acid hydrochloride (21e)



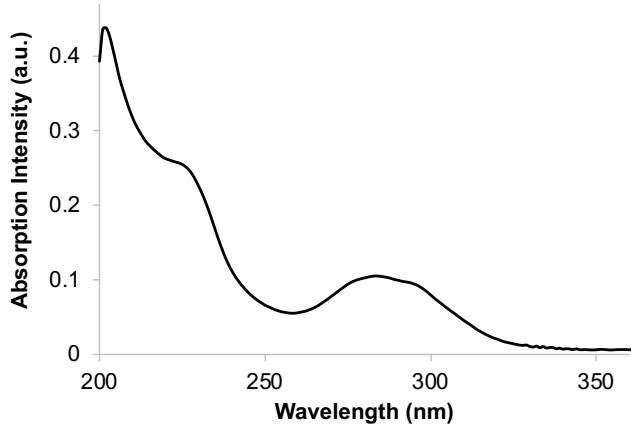


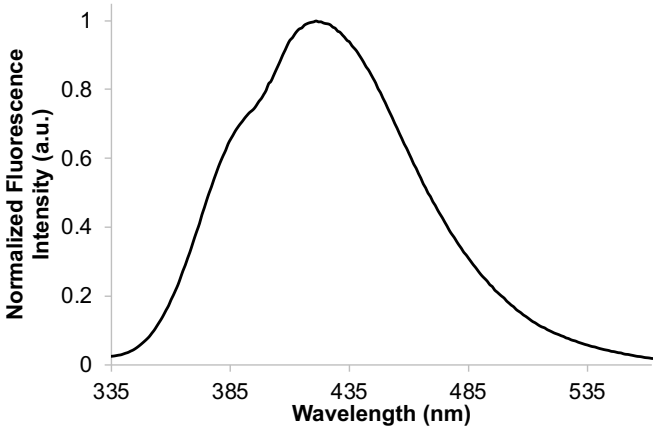
(2*S*)-2-Amino-3-[5′-(thiophen-3′′-yl)-1*H*-benzo[*d*][1.2.3]triazol-1′-yl]propanoic acid hydrochloride (21f)



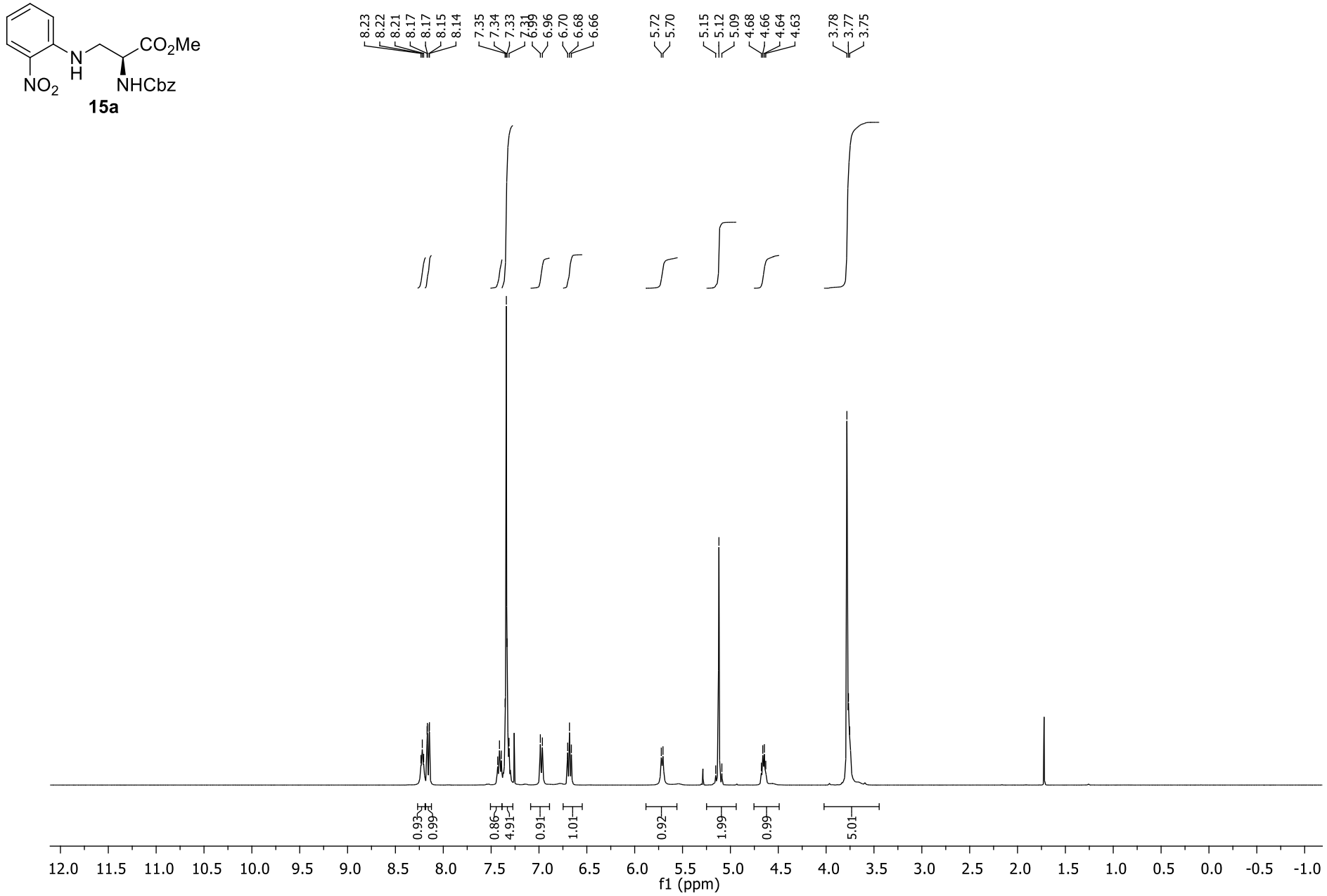


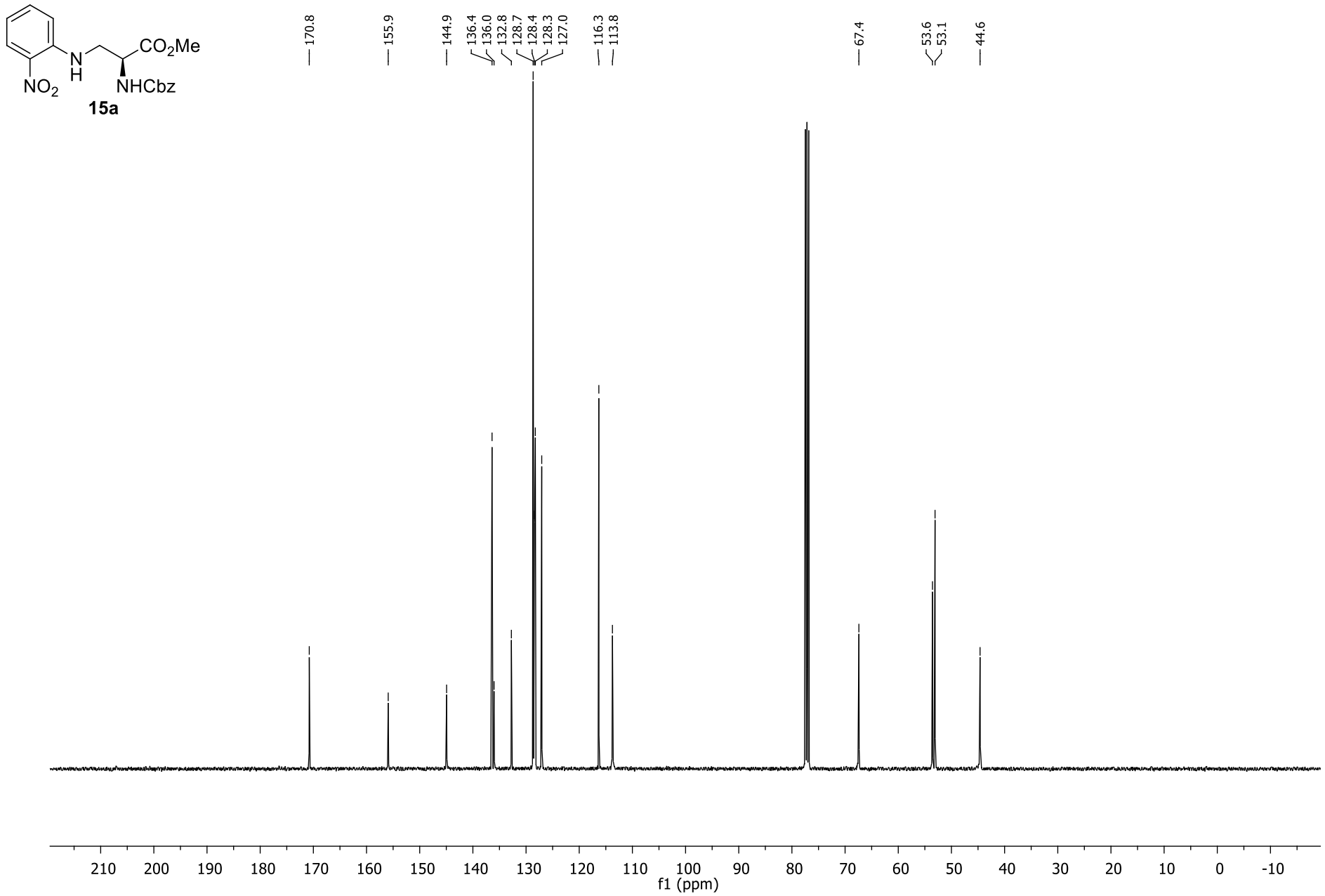
(2*S*)-2-Amino-3-(6′-methoxy-7′-(4′′-methoxyphenyl)-1*H*-benzo[*d*][1.2.3]triazol-1′-yl)propanoic acid hydrochloride (24)

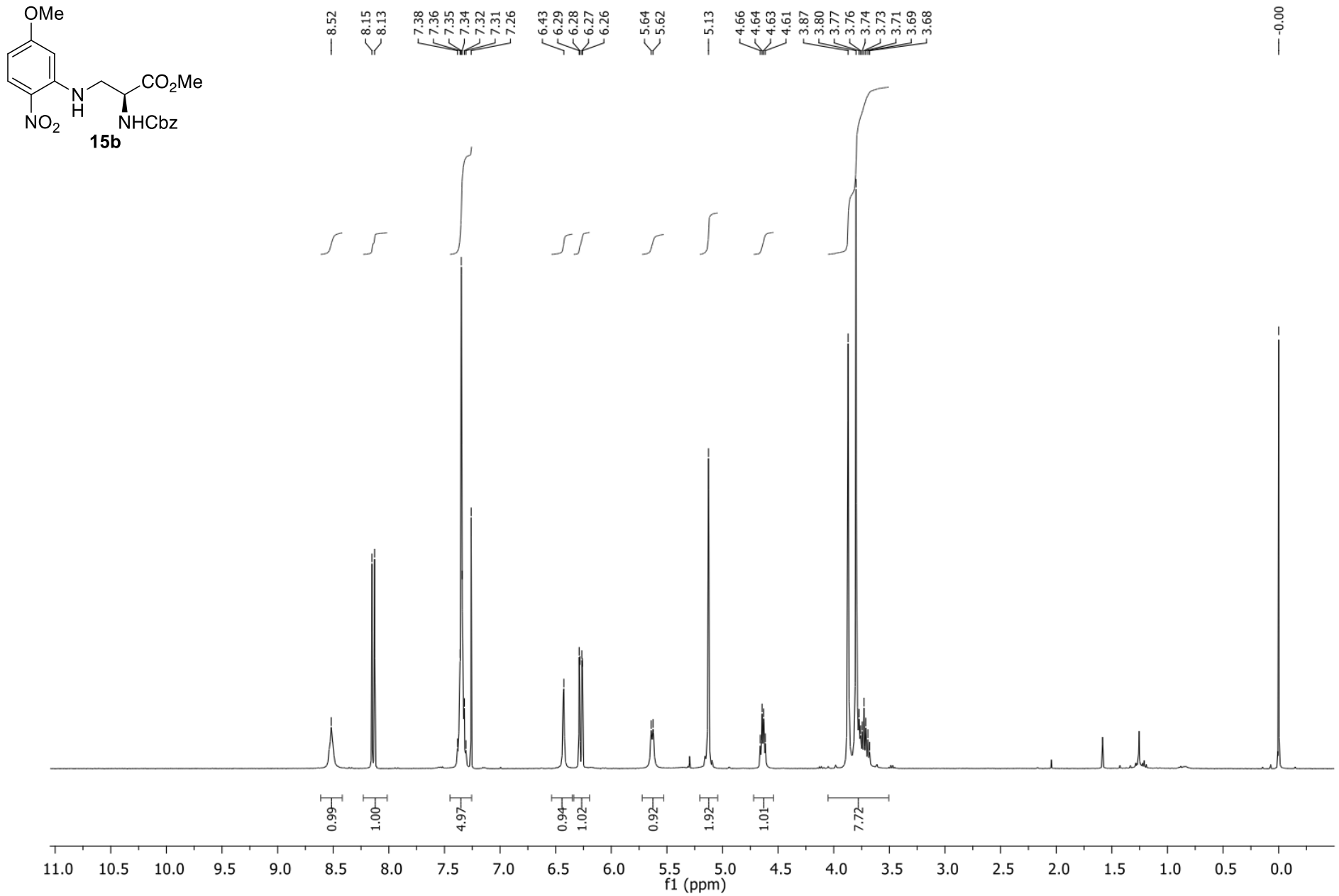


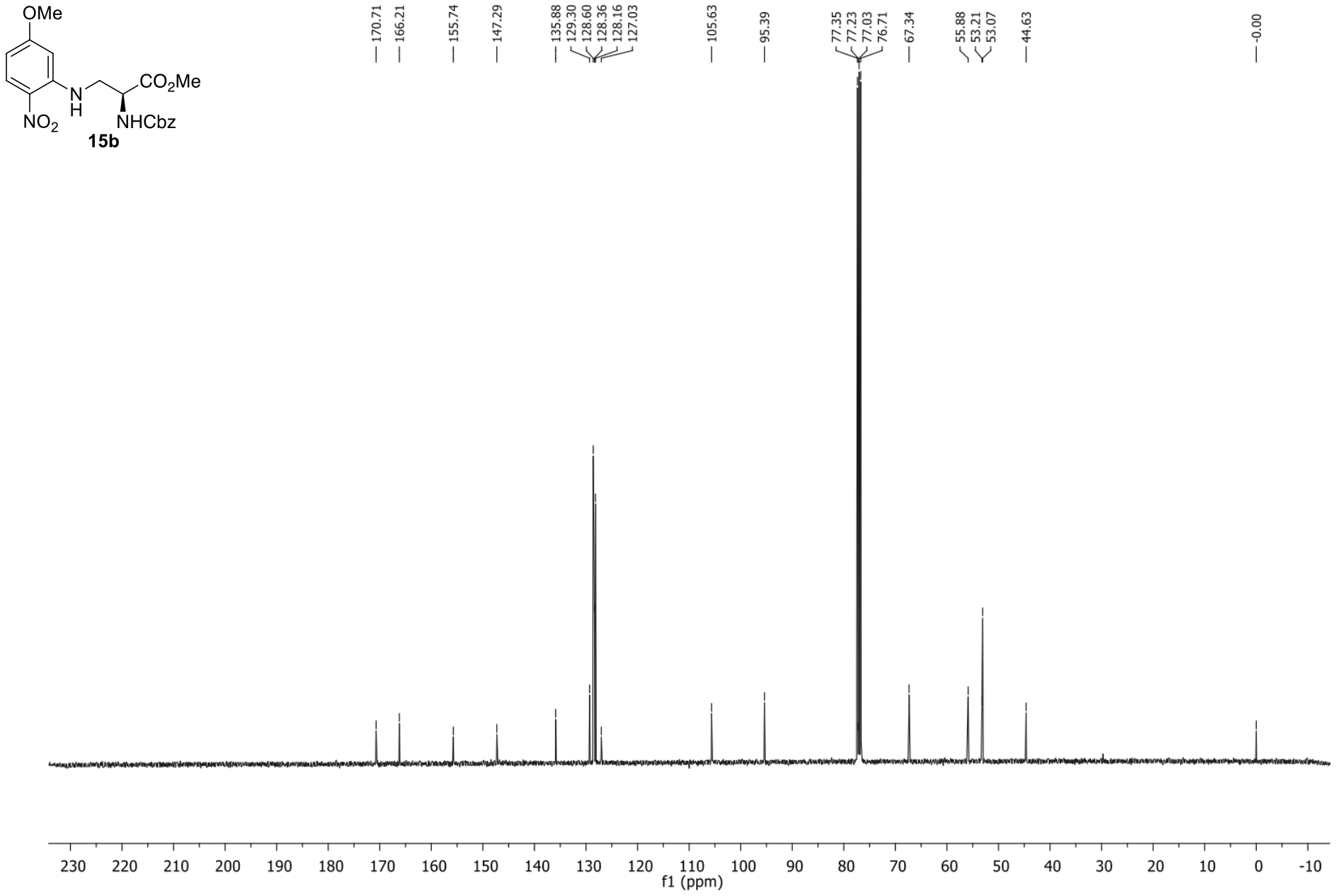


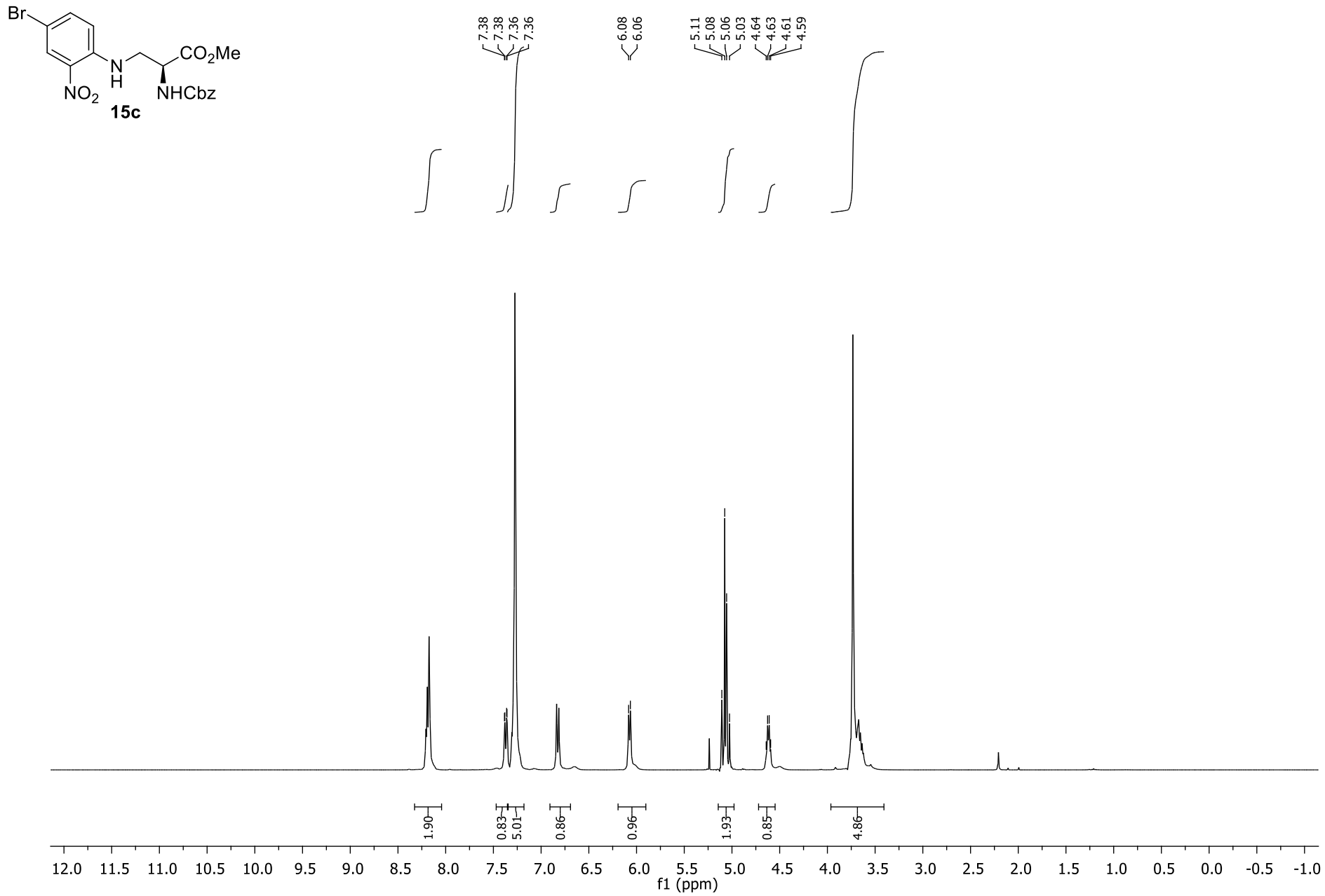
2. 1H and 13C NMR Spectra for all Novel Compounds

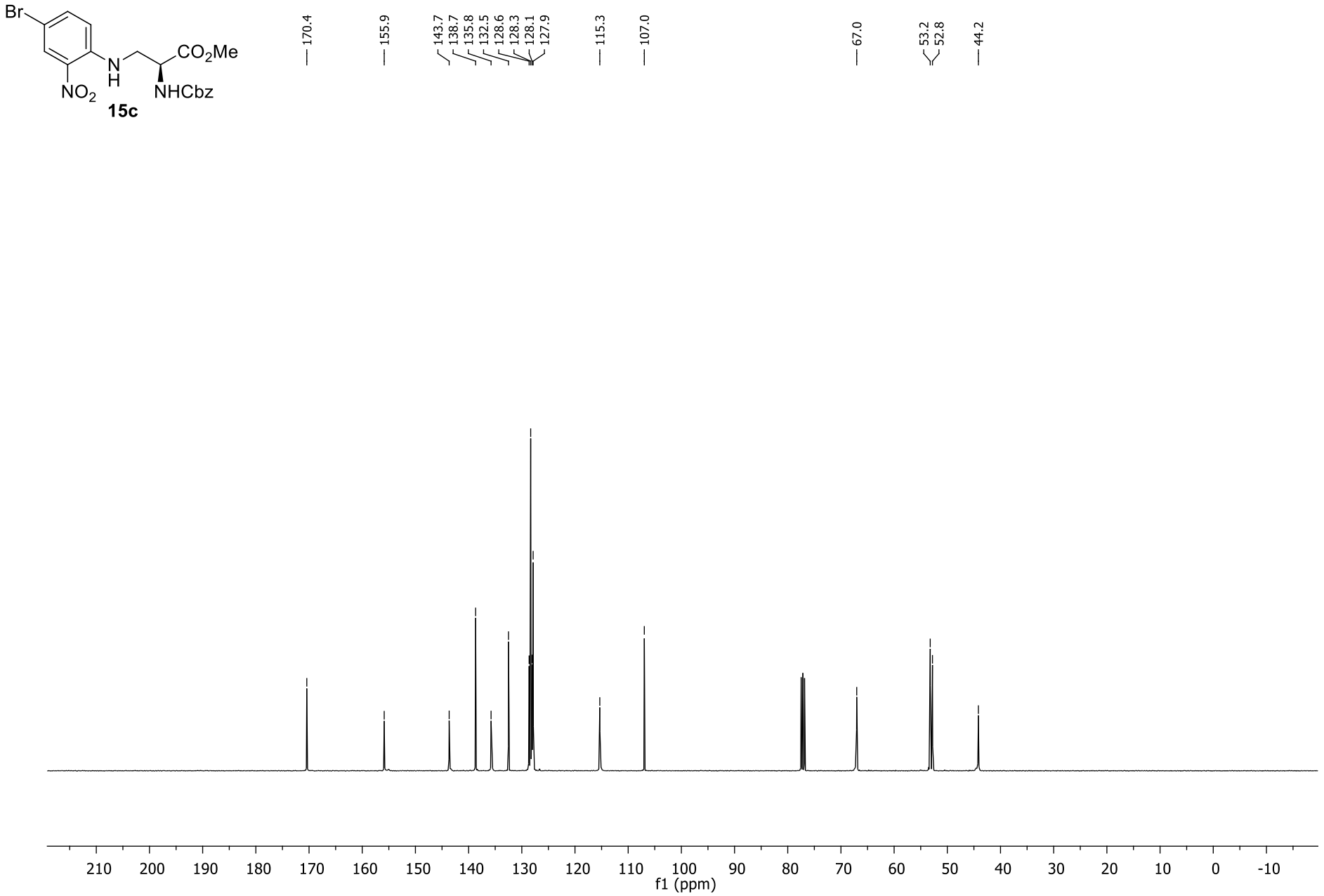


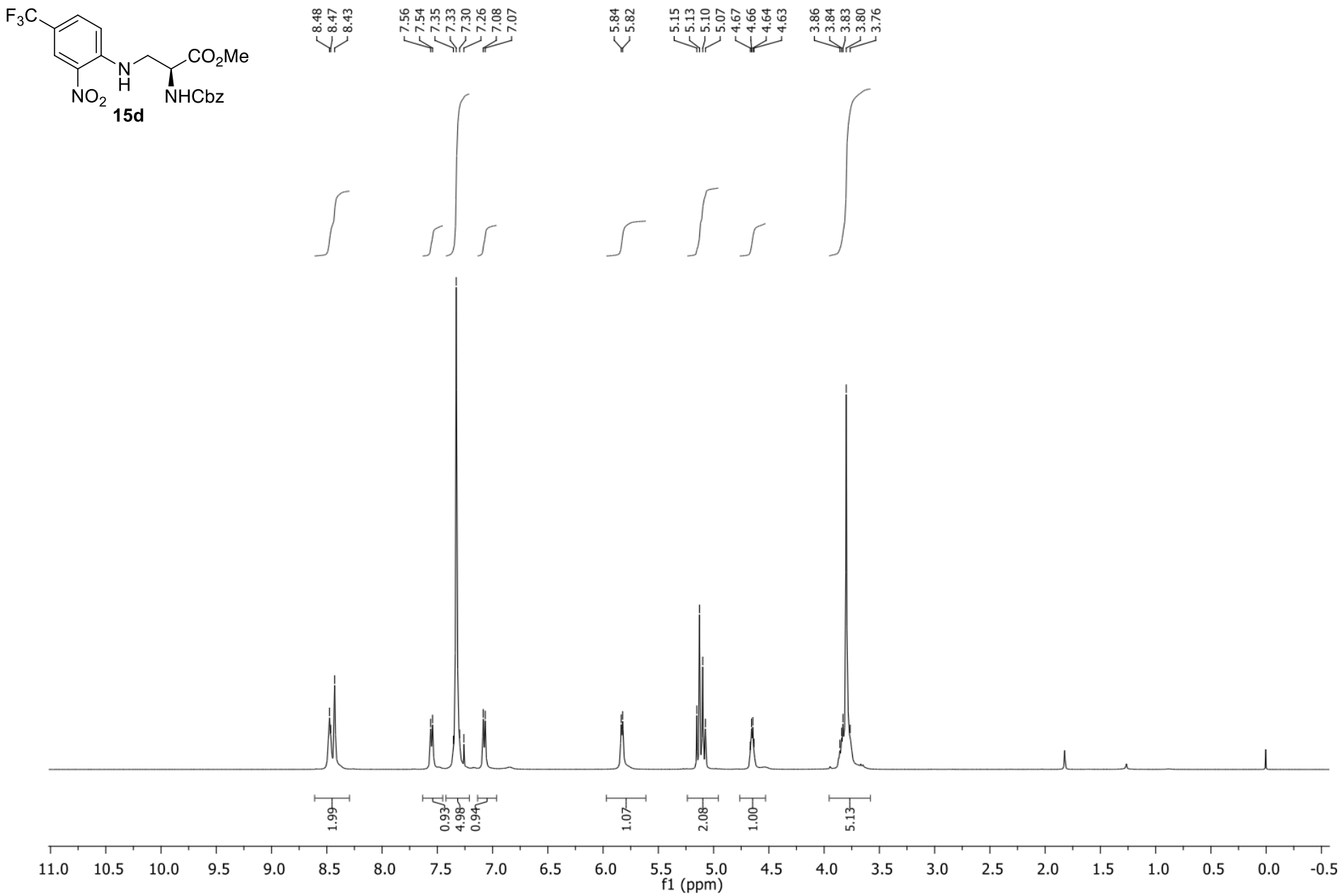

170.8
155.9
144.9
136.4
136.0
132.8
128.7
128.4
128.3
127.0
116.3
113.8
67.4
53.6
53.1
44.6
CO2Me
N
H
NO2
NHCbz
15a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

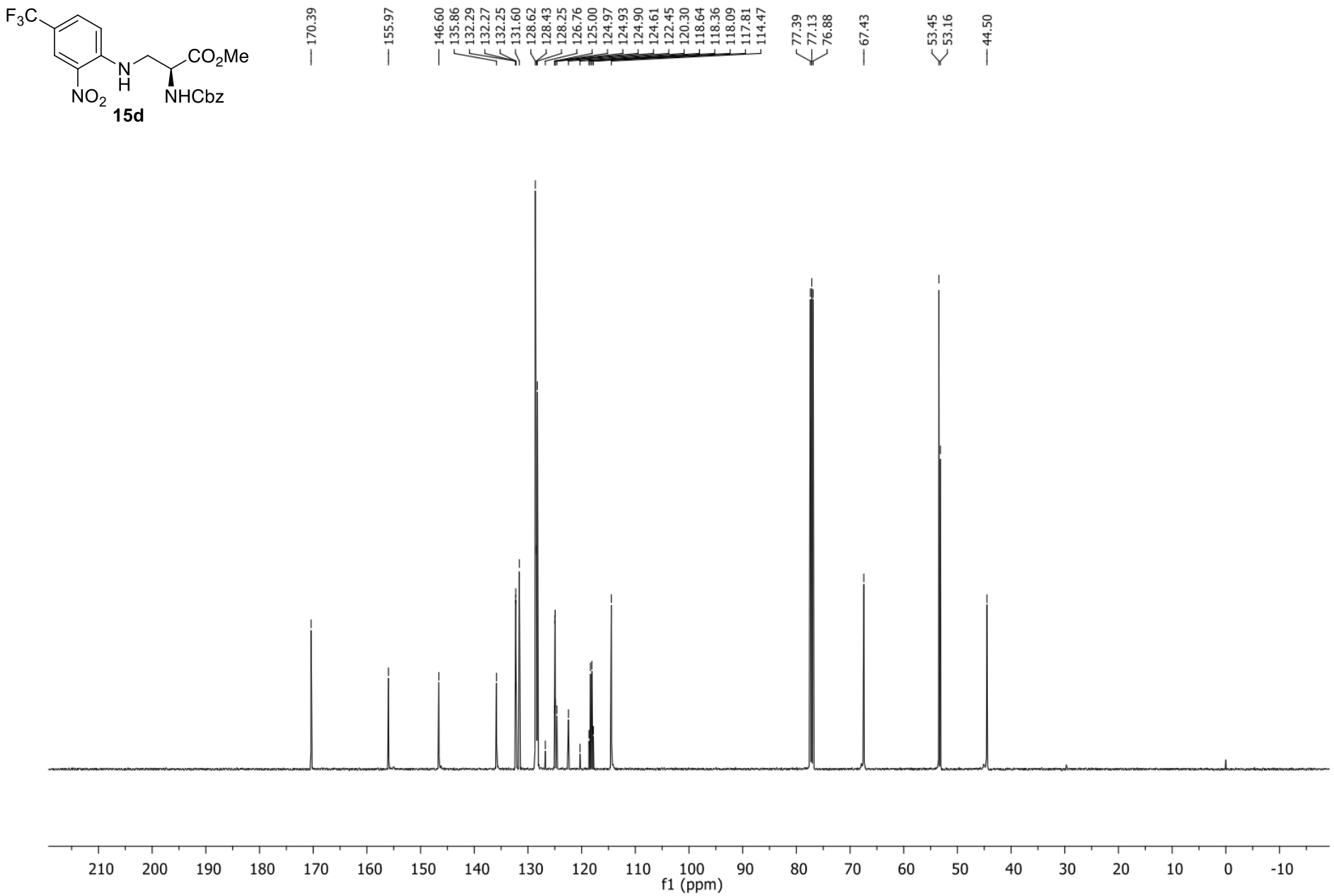

OMe
N
H
CO2Me
NO2
NHCbz
15b
8.52
8.15
8.13
7.38
7.36
7.35
7.34
7.32
7.31
7.26
6.43
6.29
6.28
6.27
6.26
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5.62
5.13
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4.63
4.61
3.87
3.80
3.77
3.76
3.74
3.73
3.71
3.69
3.68
-0.00
0.99
1.00
4.97
0.94
1.02
0.92
1.92
1.01
7.72
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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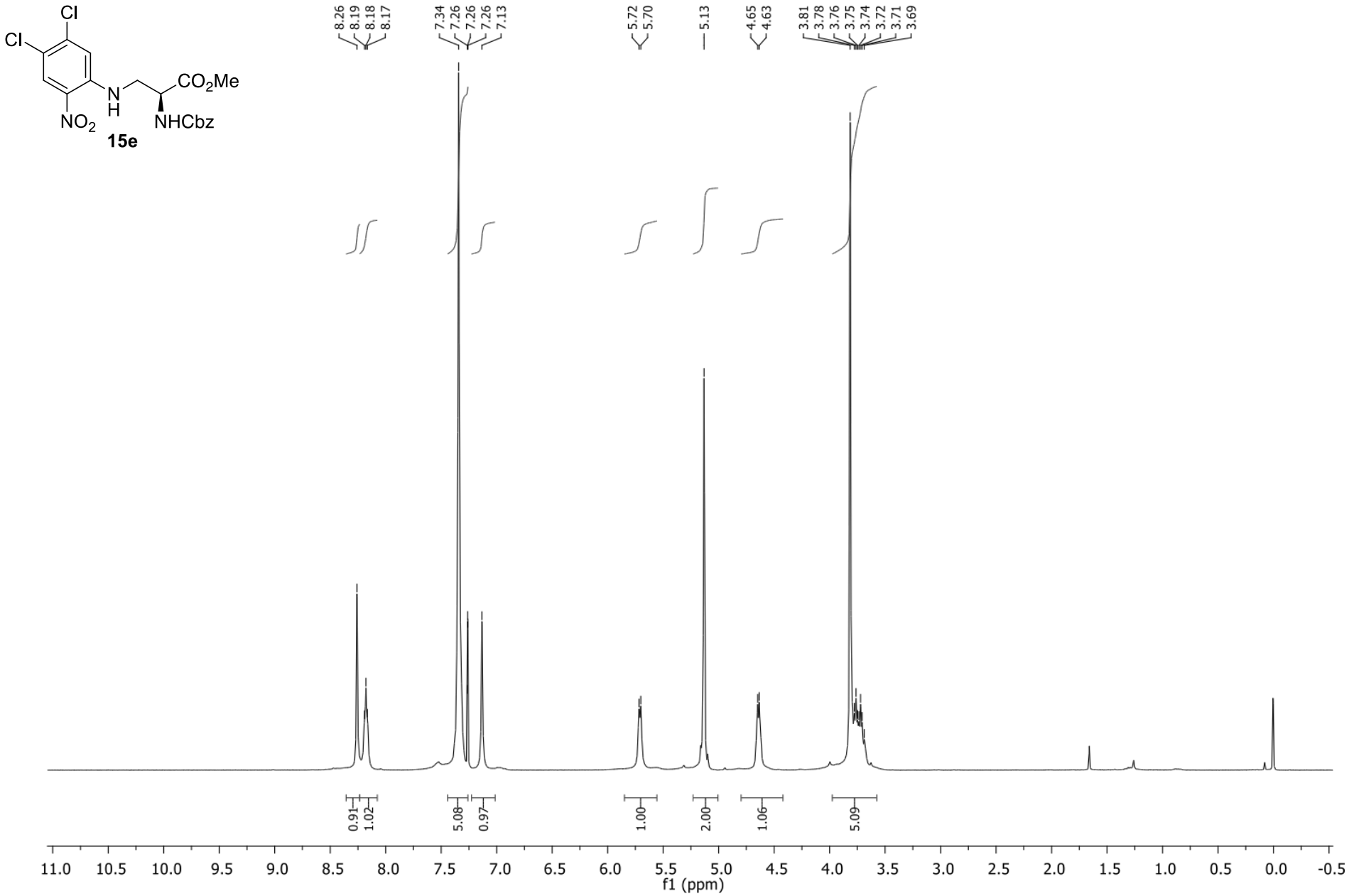

OMe
N
H
CO2Me
NO2
NHCbz
15b
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166.21
155.74
147.29
135.88
129.30
128.60
128.36
128.16
127.03
105.63
95.39
77.35
77.23
77.03
76.71
67.34
55.88
53.21
53.07
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f1 (ppm)

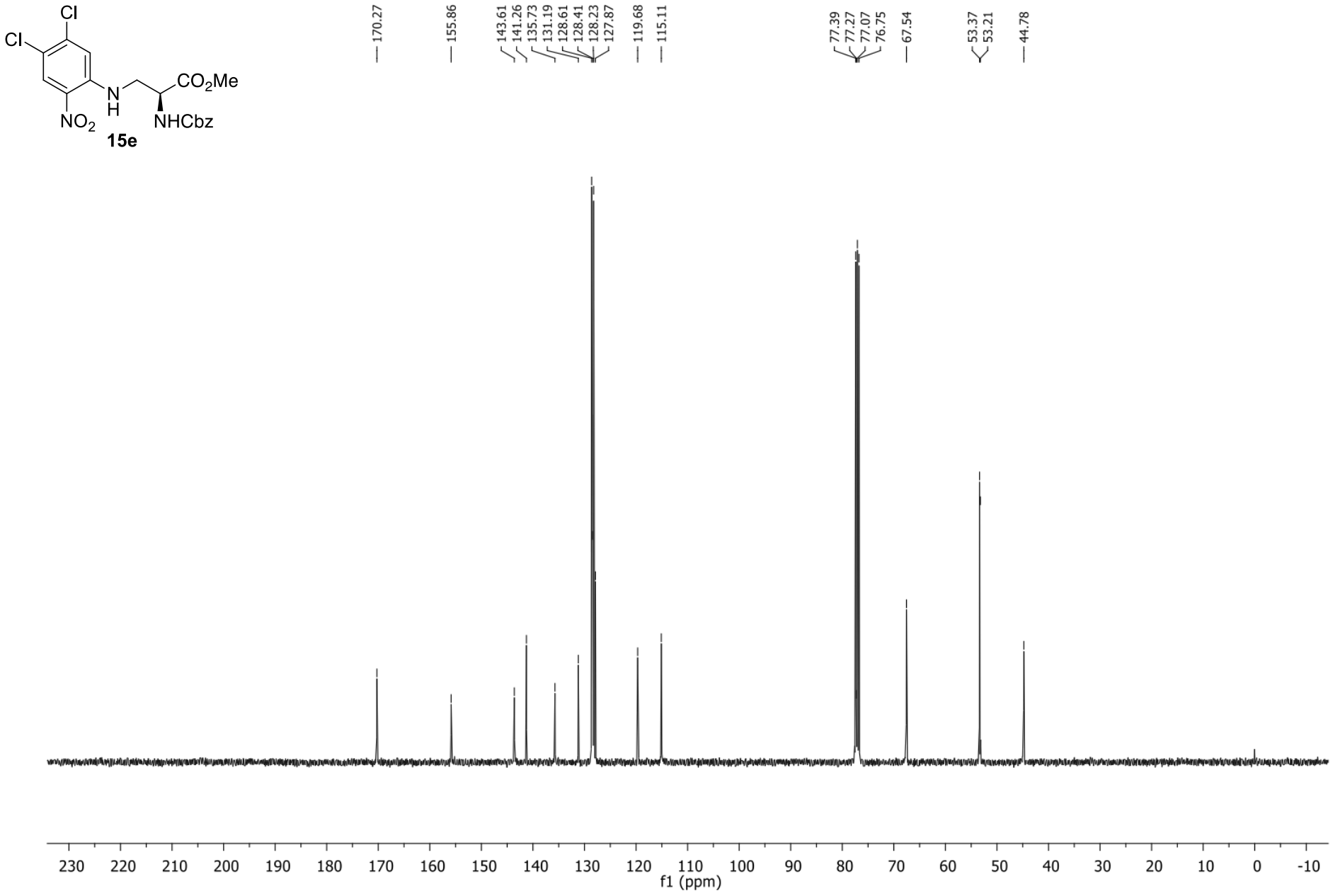

Br
N
H
CO2Me
NO2
NHCbz
15c
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7.38
7.36
7.36
6.08
6.06
5.11
5.08
5.06
5.03
4.64
4.63
4.61
4.59
1.90
0.83
5.01
0.86
0.96
1.93
0.85
4.86
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

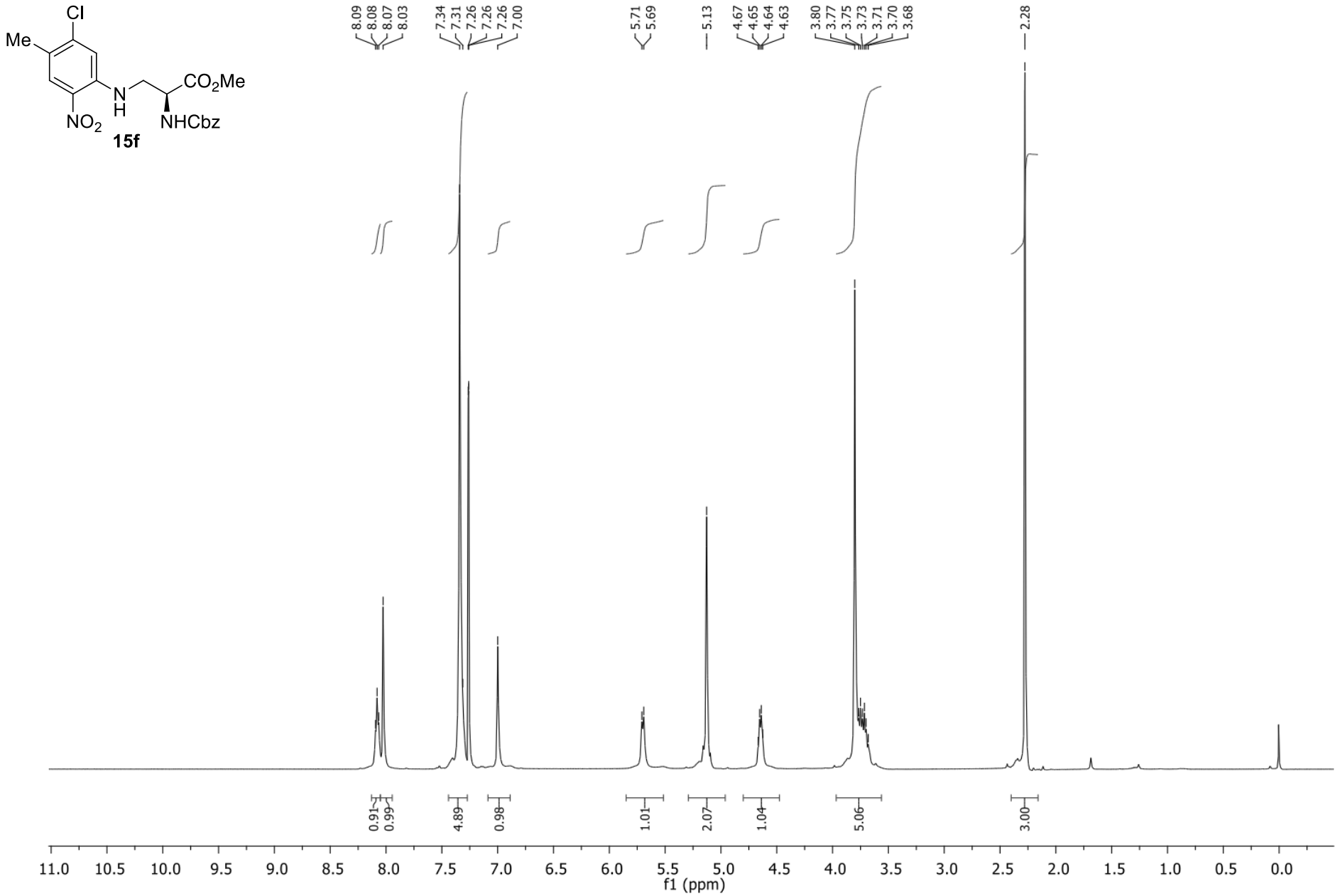

Br
N
H
CO2Me
NO2
NHCbz
15c
170.4
155.9
143.7
138.7
135.8
132.5
128.6
128.3
128.1
127.9
115.3
107.0
67.0
53.2
52.8
44.2
210
200
190
180
170
160
150
140
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120
110
100
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80
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60
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20
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0
-10
f1 (ppm)

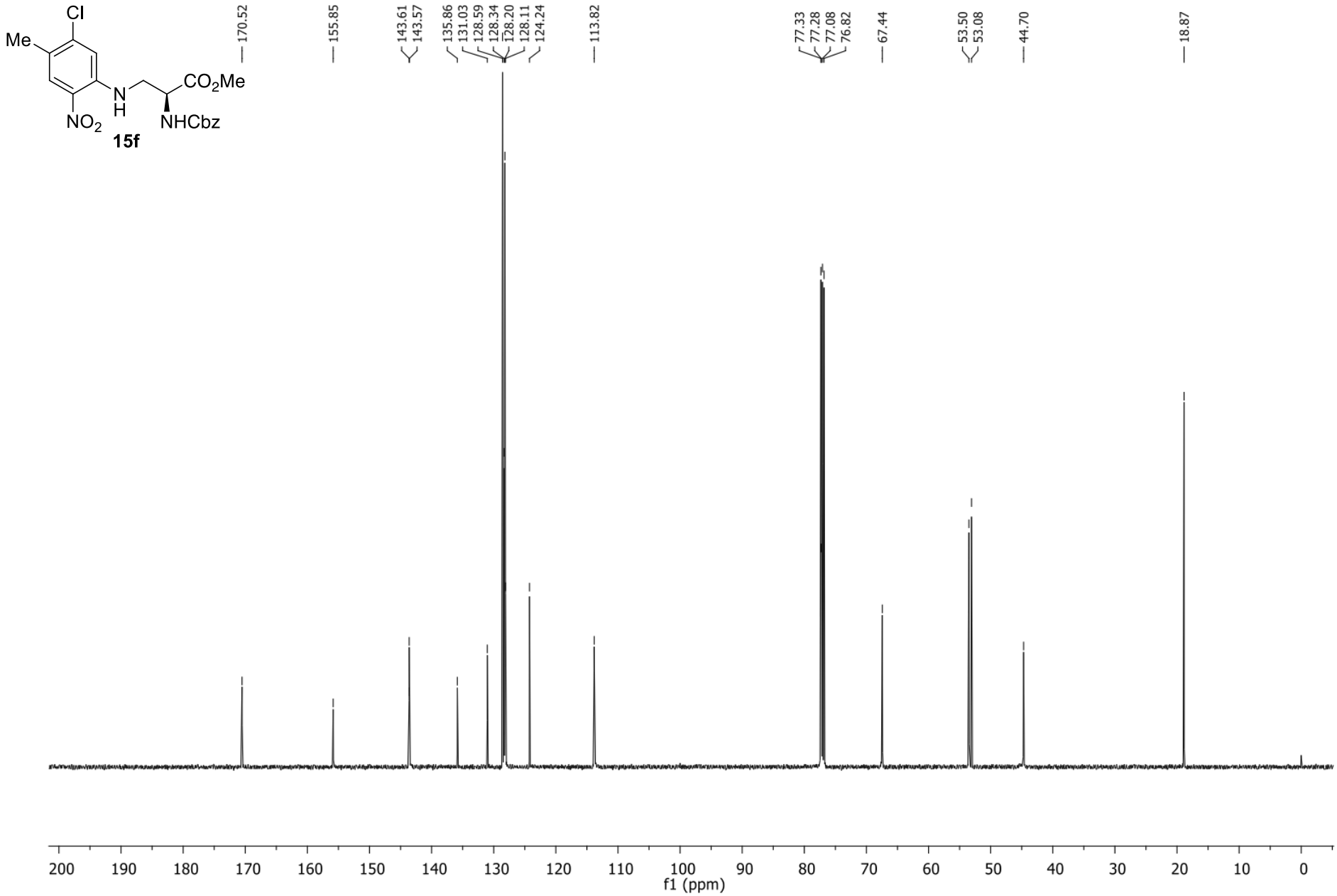

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H
NO2
NHCbz
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7.33
7.30
7.26
7.08
7.07
5.84
5.82
5.15
5.13
5.10
5.07
4.67
4.66
4.64
4.63
3.86
3.84
3.83
3.80
3.76
1.99
0.93
4.98
0.94
1.07
2.08
1.00
5.13
11.0
10.5
10.0
9.5
9.0
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8.0
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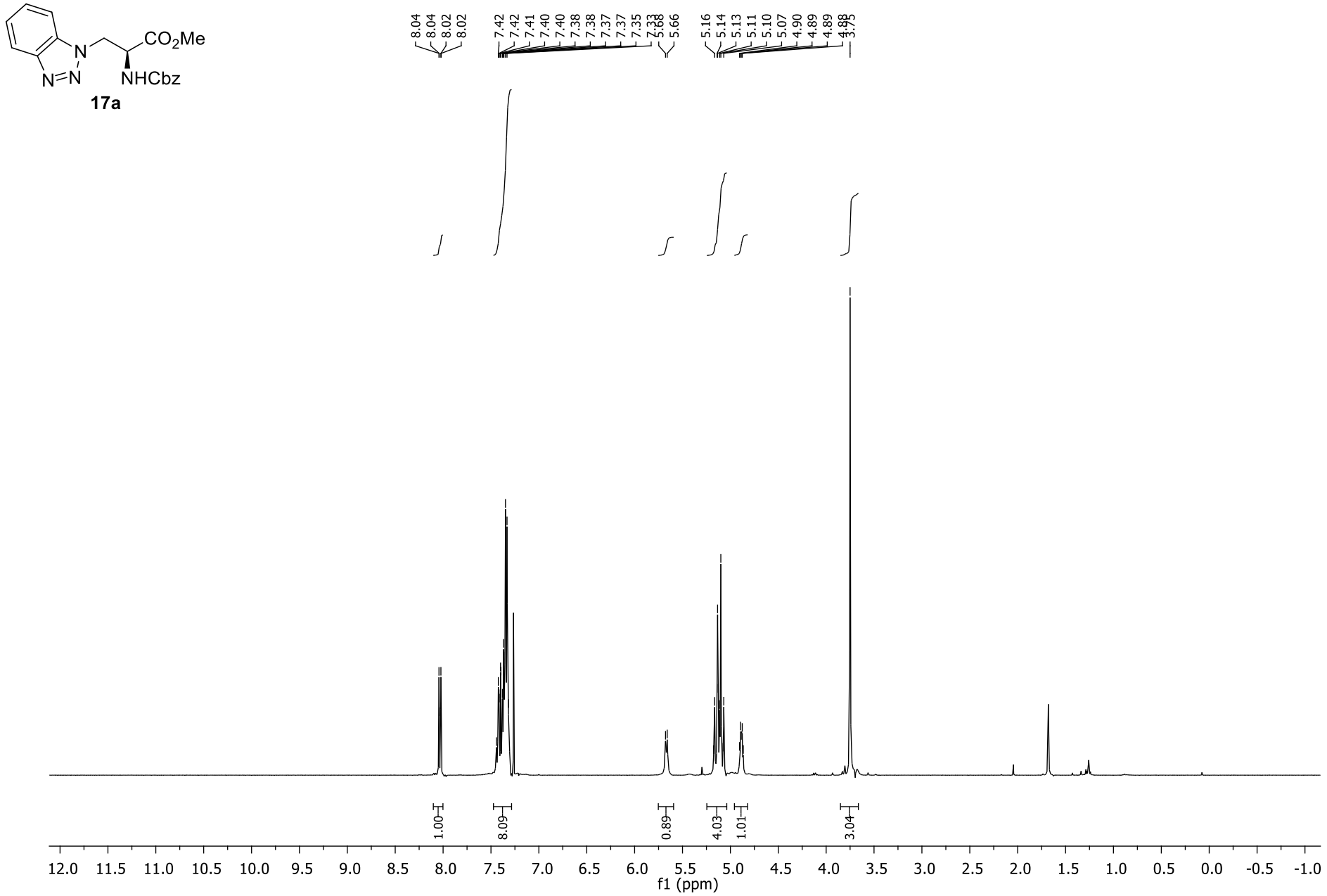

F3C
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N
H
NO2
NHCbz
15d
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135.86
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132.25
131.60
128.62
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128.25
126.76
125.00
124.97
124.93
124.90
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122.45
120.30
118.64
118.36
118.09
117.81
114.47
77.39
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210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

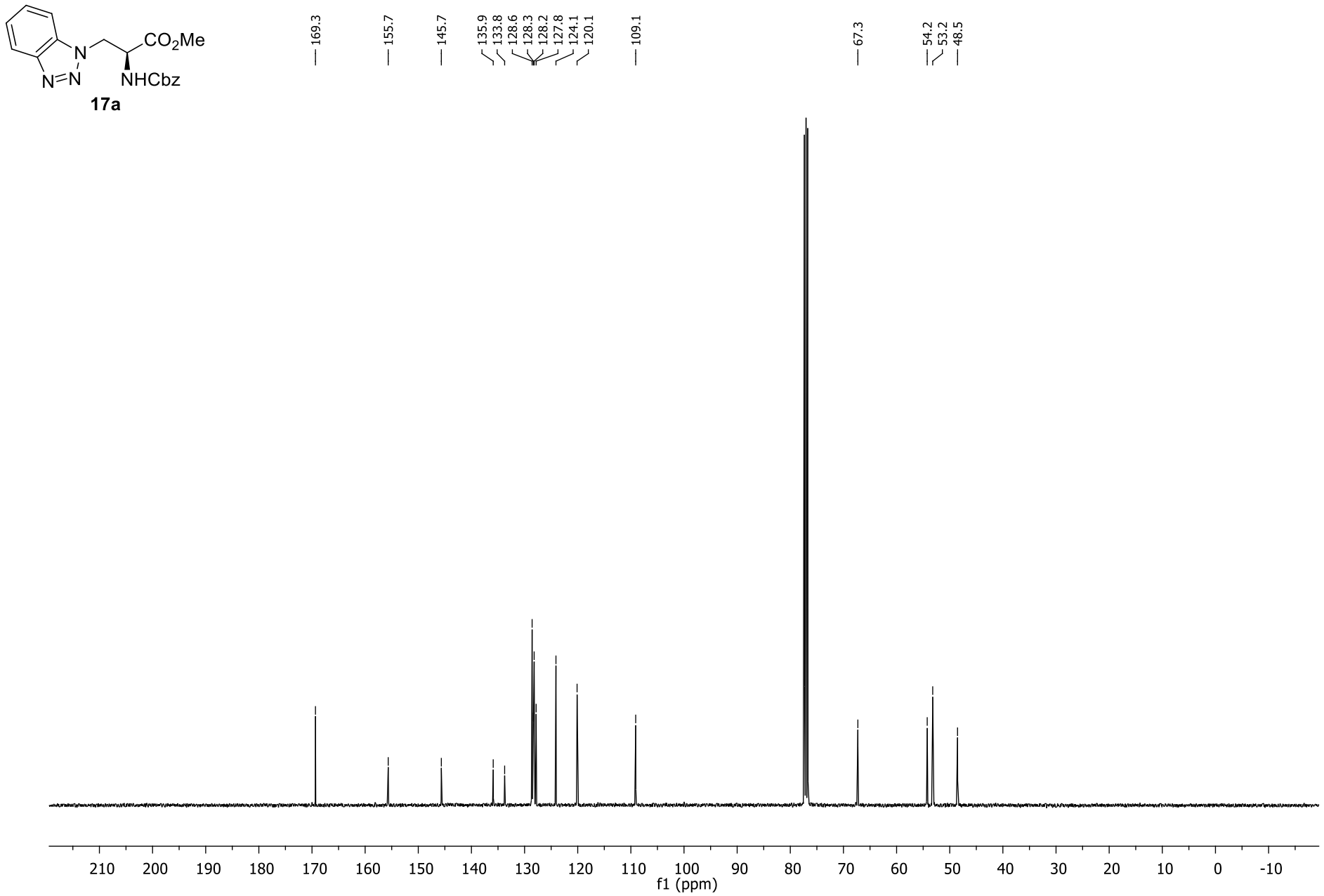

Cl
Cl
NO2
N
H
CO2Me
NHCbz
15e
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5.70
5.13
4.65
4.63
3.81
3.78
3.76
3.75
3.74
3.72
3.71
3.69
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5.08
0.97
1.00
2.00
1.06
5.09
11.0
10.5
10.0
9.5
9.0
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7.5
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6.0
5.5
5.0
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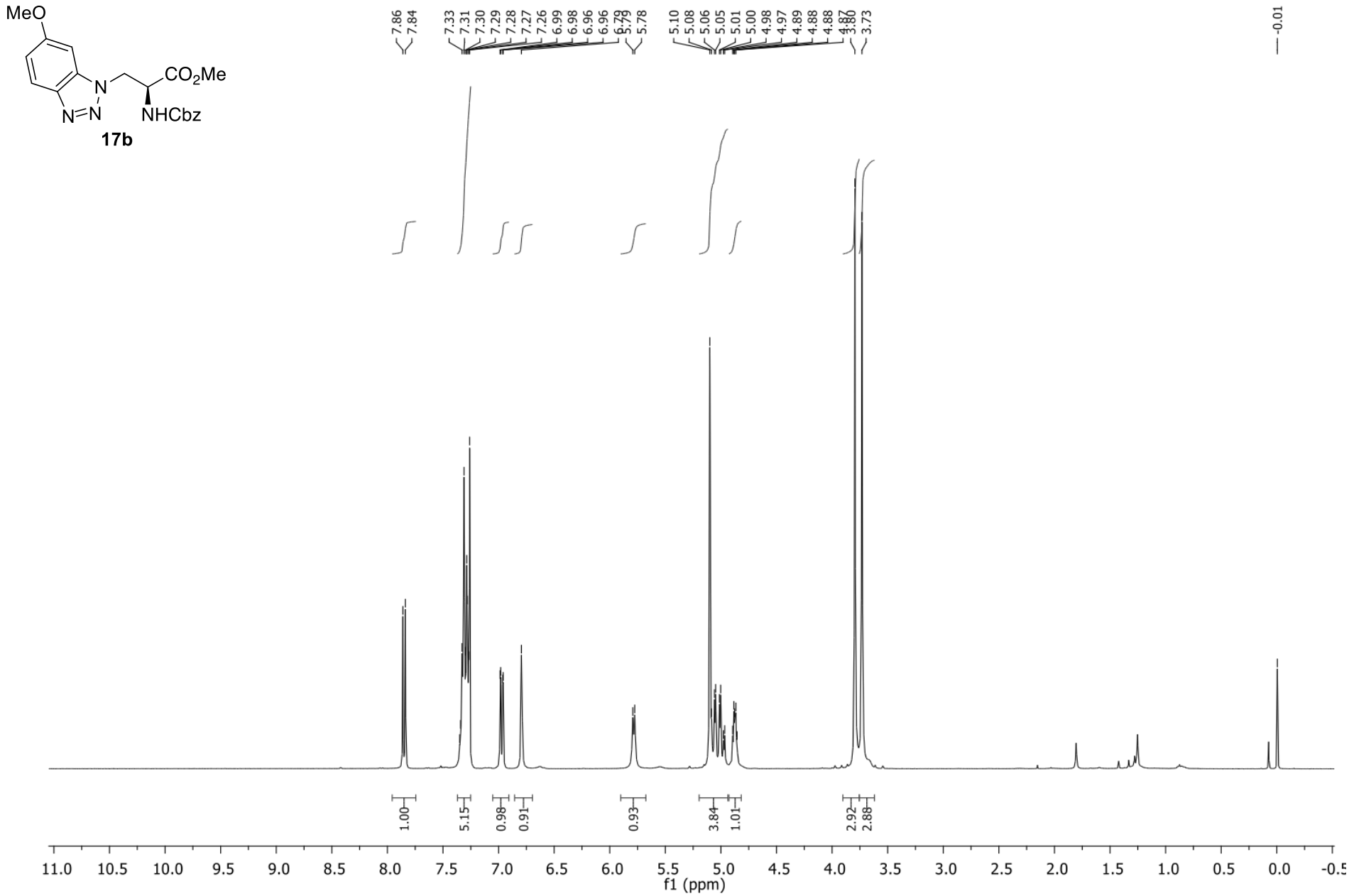

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Cl
NO2
N
H
CO2Me
NHCbz
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141.26
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128.61
128.41
128.23
127.87
119.68
115.11
77.39
77.27
77.07
76.75
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f1 (ppm)

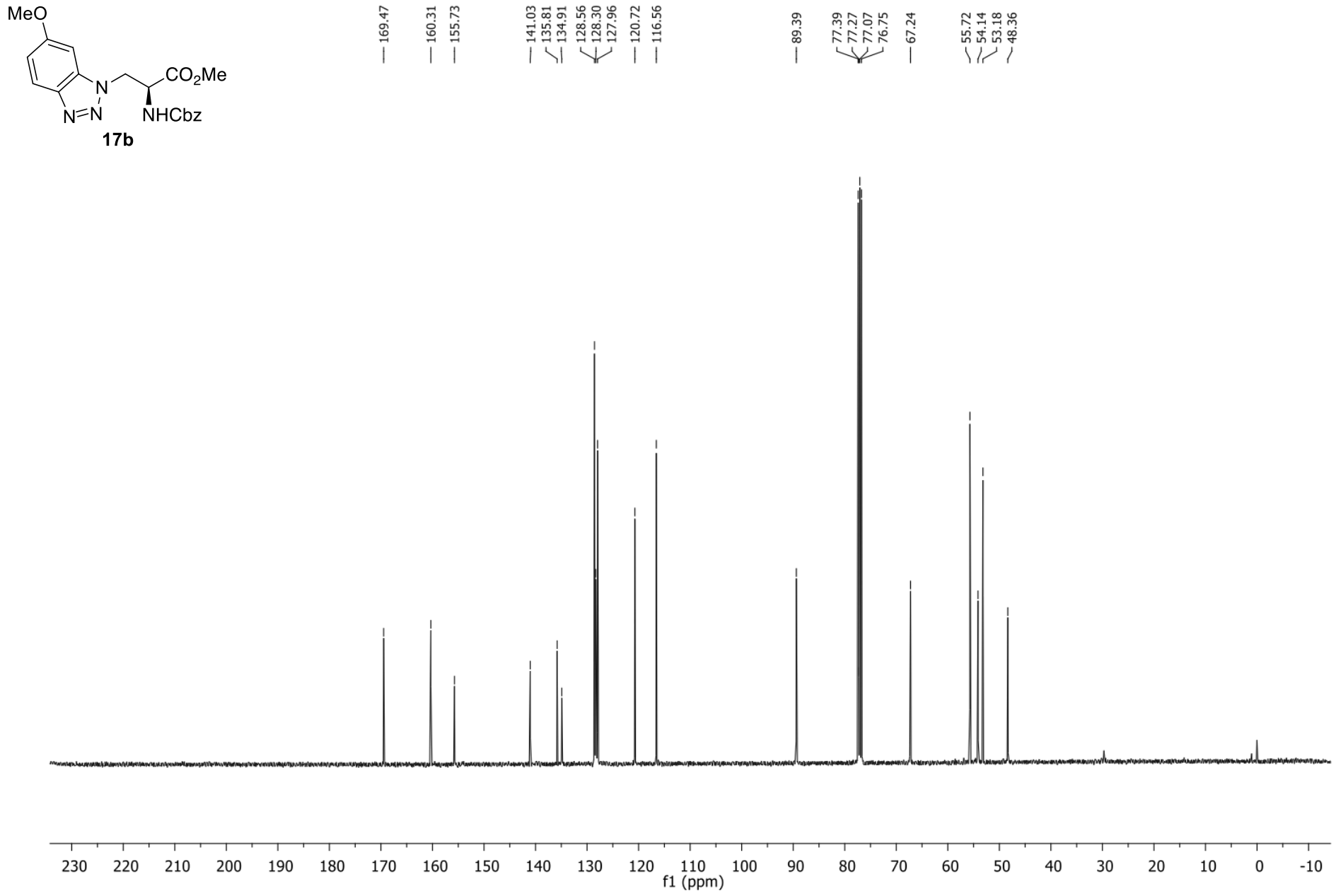

Cl
Me
N
H
CO2Me
NO2
NHCbz
15f
8.09
8.08
8.07
8.03
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7.26
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4.65
4.64
4.63
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3.77
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3.68
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3.00
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9.0
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f1 (ppm)

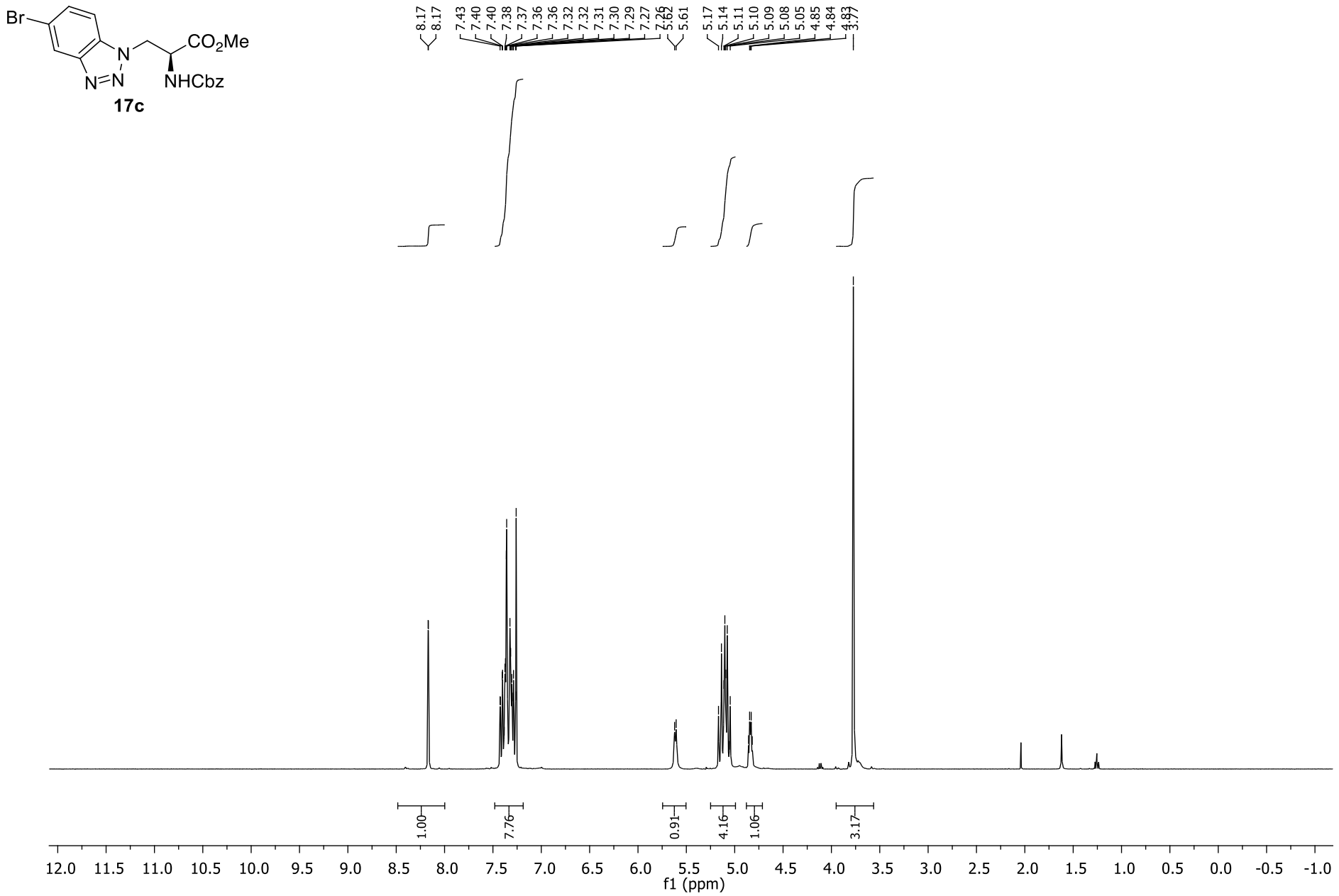

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Me
N
H
CO2Me
NHCbz
NO2
15f
170.52
155.85
143.61
143.57
135.86
131.03
128.59
128.34
128.20
128.11
124.24
113.82
77.33
77.28
77.08
76.82
67.44
53.50
53.08
44.70
18.87
200
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180
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160
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10
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f1 (ppm)

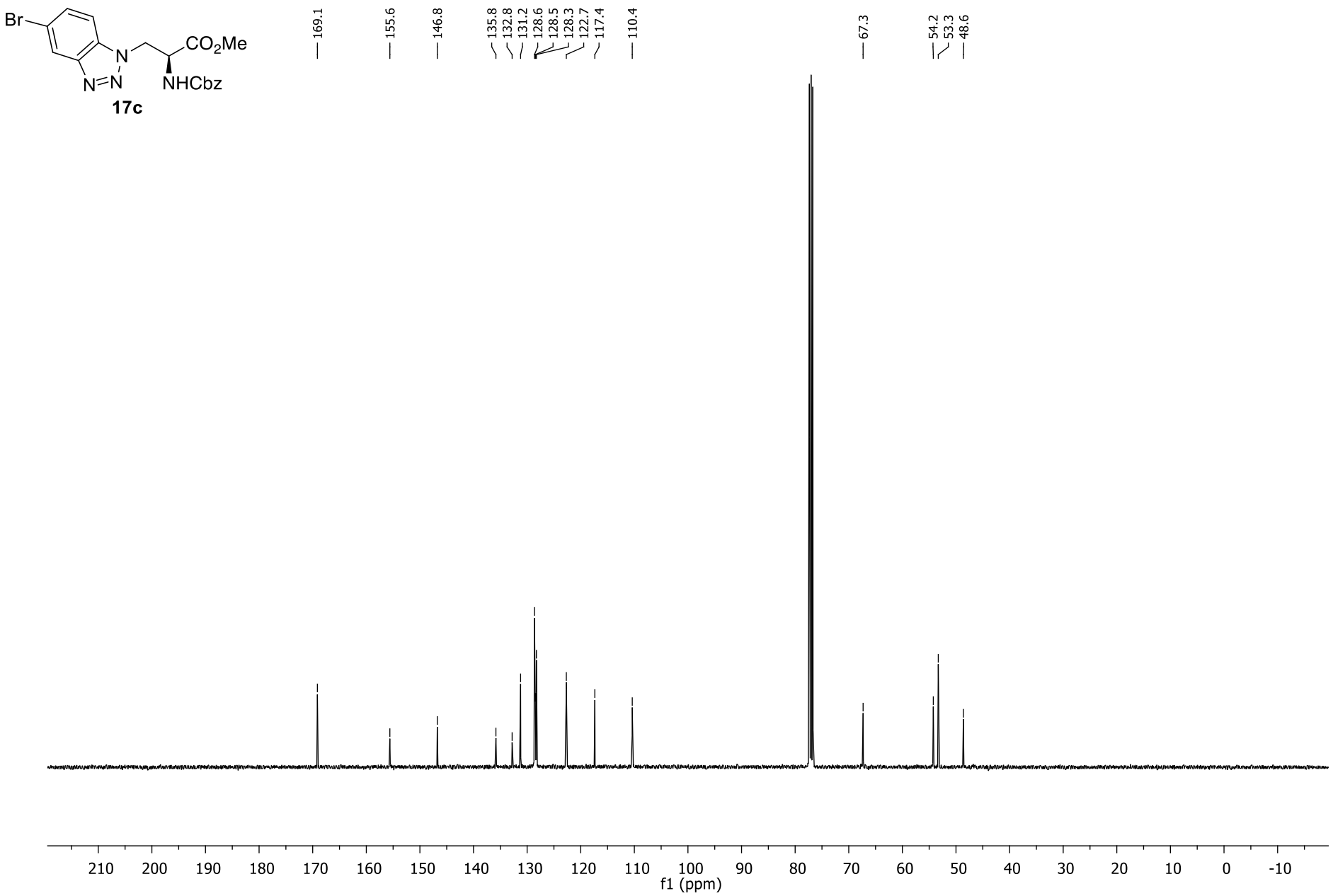

CO2Me
NHCbz
17a
8.04
8.04
8.02
8.02
7.42
7.42
7.41
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7.38
7.37
7.37
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7.33
5.68
5.66
5.16
5.14
5.13
5.11
5.10
5.07
4.90
4.89
4.89
4.88
3.75
1.00
8.09
0.89
4.03
1.01
3.04
12.0 11.5 11.0 10.5 10.0 9.5 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 0.0 -0.5 -1.0
f1 (ppm)

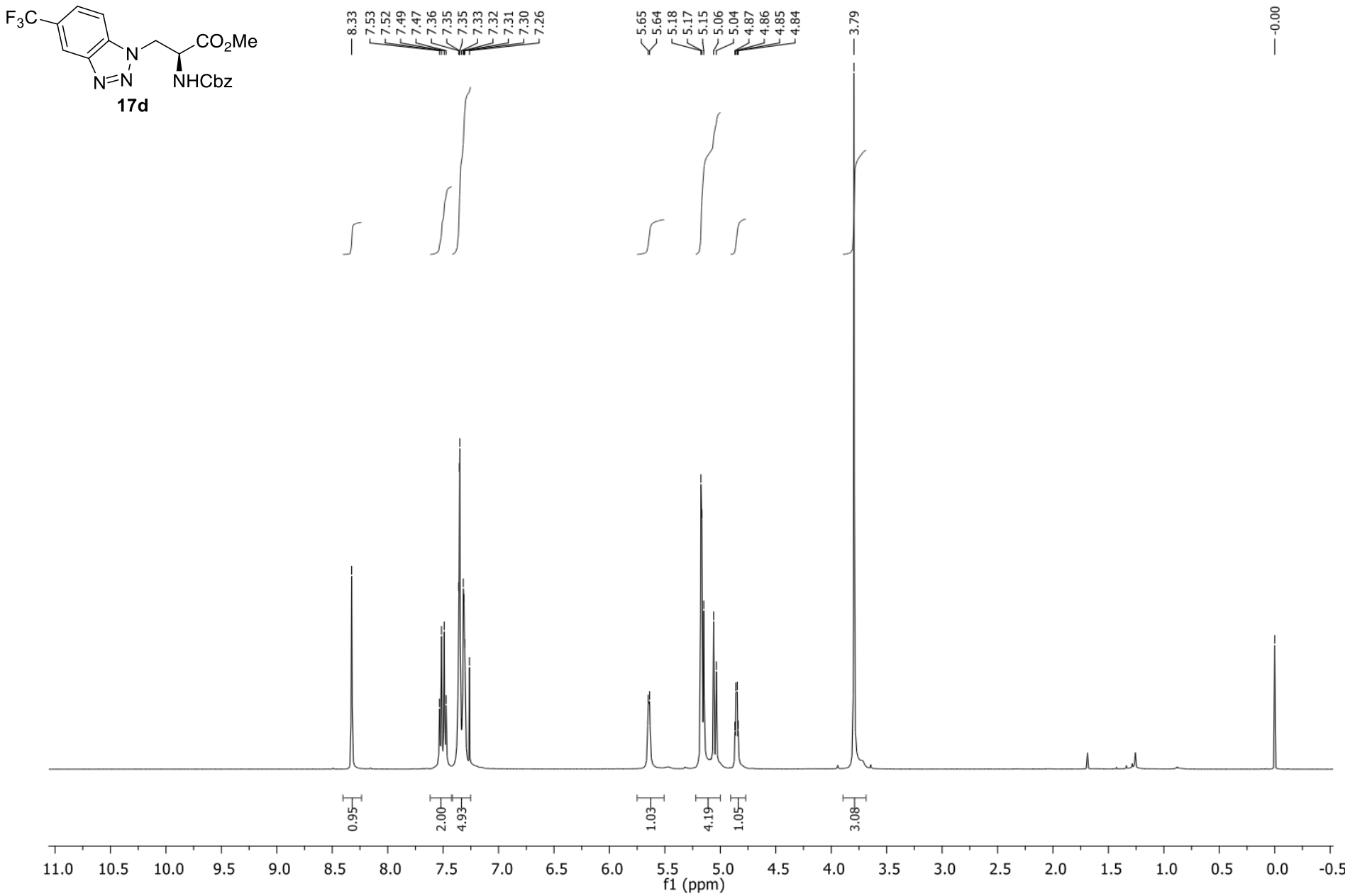

CO2Me
N
N=N
NHCbz
17a
169.3
155.7
145.7
135.9
133.8
128.6
128.3
128.2
127.8
124.1
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f1 (ppm)

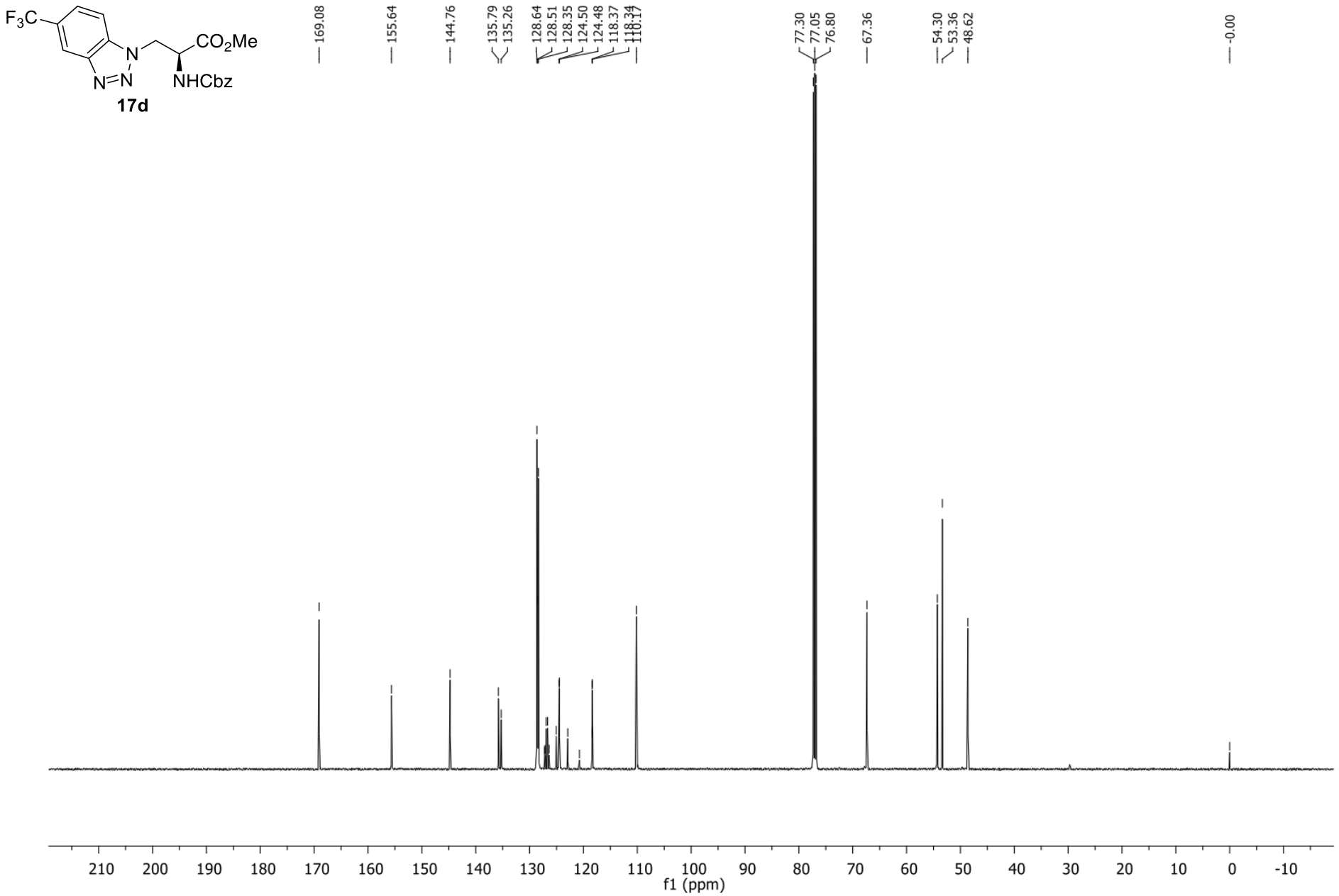

MeO
N
N=N
CO2Me
NHCbz
17b
7.86
7.84
7.33
7.31
7.30
7.29
7.28
7.27
7.26
6.99
6.98
6.96
6.96
5.78
5.10
5.08
5.06
5.05
5.01
5.00
4.98
4.97
4.89
4.88
4.88
3.80
3.73
-0.01
1.00
5.15
0.98
0.91
0.93
3.84
1.01
2.92
2.88
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

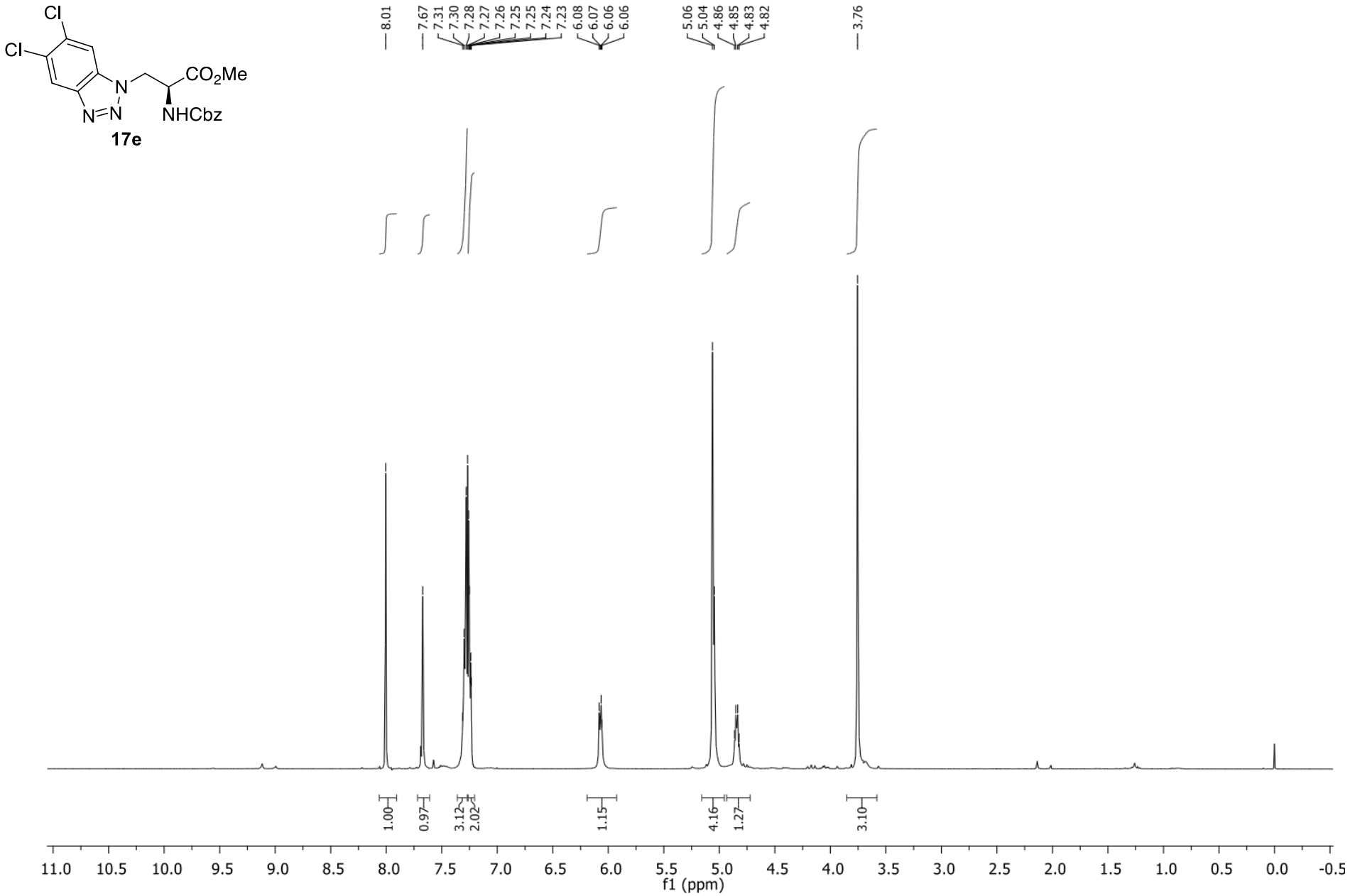

MeO
N
N=N
CO2Me
NHCbz
17b
169.47
160.31
155.73
141.03
135.81
134.91
128.56
128.30
127.96
120.72
116.56
89.39
77.39
77.27
77.07
76.75
67.24
55.72
54.14
53.18
48.36
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

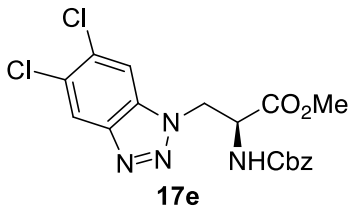

Br
N
N
N
CO2Me
NHCbz
17c
8.17
8.17
7.43
7.40
7.40
7.38
7.37
7.36
7.36
7.32
7.32
7.31
7.30
7.29
7.27
5.62
5.61
5.17
5.14
5.11
5.10
5.09
5.08
5.05
4.85
4.84
3.77
1.00
7.76
0.91
4.16
1.06
3.17
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


Br
N
N
N
CO2Me
NHCbz
17c
169.1
155.6
146.8
135.8
132.8
131.2
128.6
128.5
128.3
122.7
117.4
110.4
67.3
54.2
53.3
48.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


F3C
CO2Me
N
N
N
NHCbz
17d
8.33
7.53
7.52
7.49
7.47
7.36
7.35
7.35
7.33
7.32
7.31
7.30
7.26
5.65
5.64
5.18
5.17
5.15
5.06
5.04
4.87
4.86
4.85
4.84
3.79
-0.00
0.95
2.00
4.93
1.03
4.19
1.05
3.08
11.0
10.5
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
0.0
-0.5
f1 (ppm)

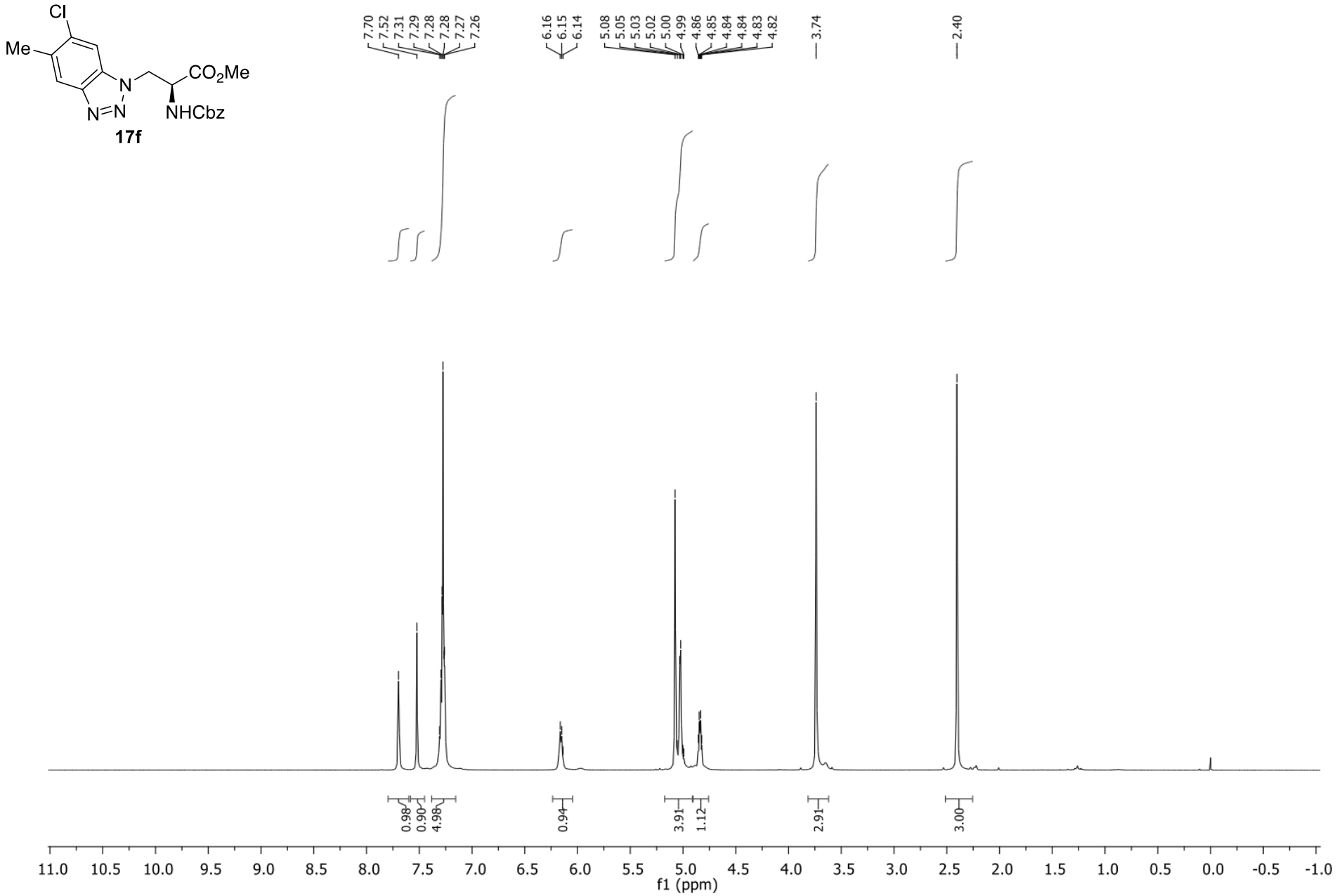

F3C
CO2Me
NHCbz
17d
169.08
155.64
144.76
135.79
135.26
128.64
128.51
128.35
124.50
124.48
118.37
77.30
77.05
76.80
67.36
54.30
53.36
48.62
-0.00
f1 (ppm)

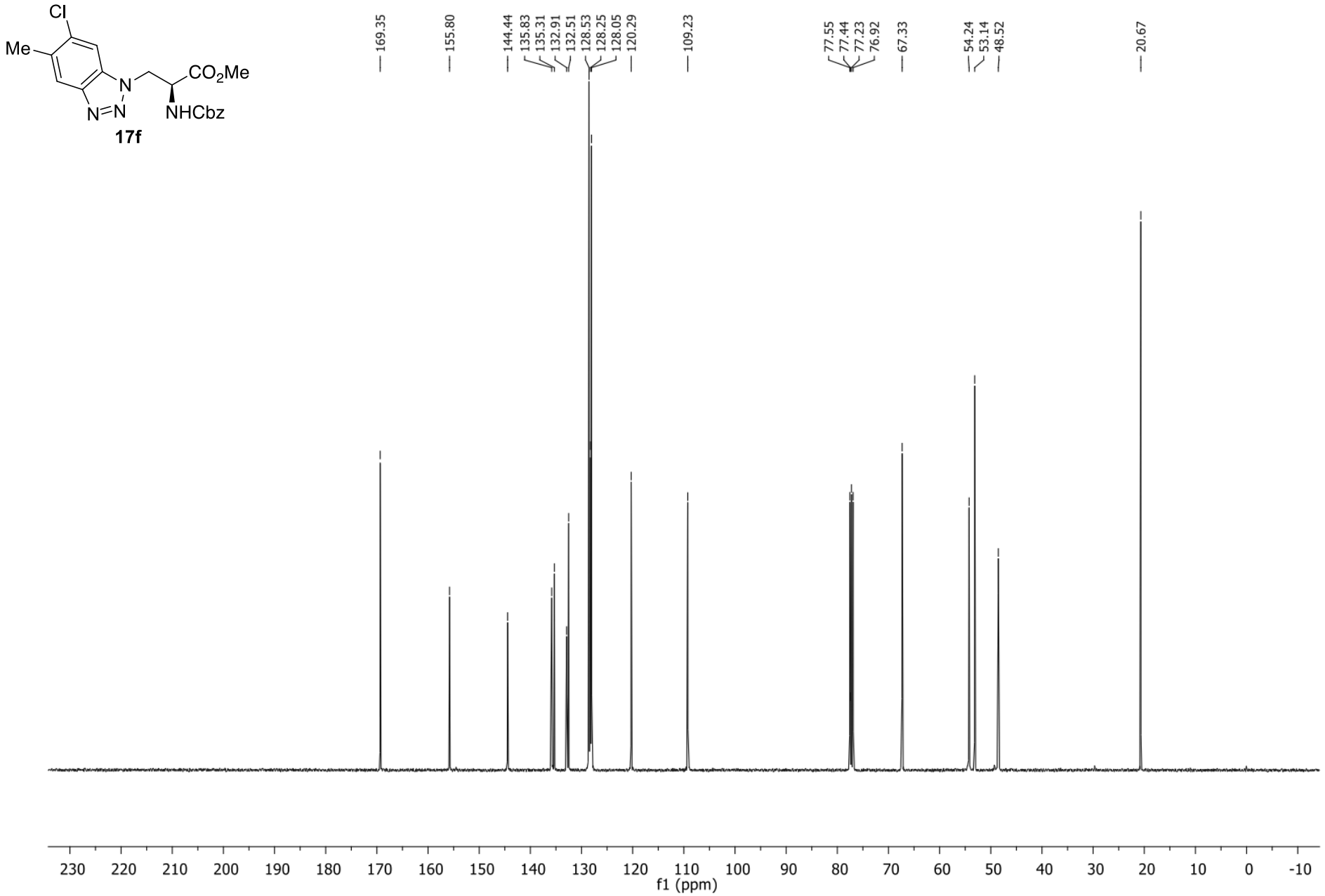

Cl
Cl
N
N=N
CO2Me
NHCbz
17e
8.01
7.67
7.31
7.30
7.28
7.27
7.26
7.25
7.24
7.23
6.08
6.07
6.06
6.06
5.06
5.04
4.86
4.85
4.83
4.82
3.76
1.00
0.97
3.12
2.02
1.15
4.16
1.27
3.10
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

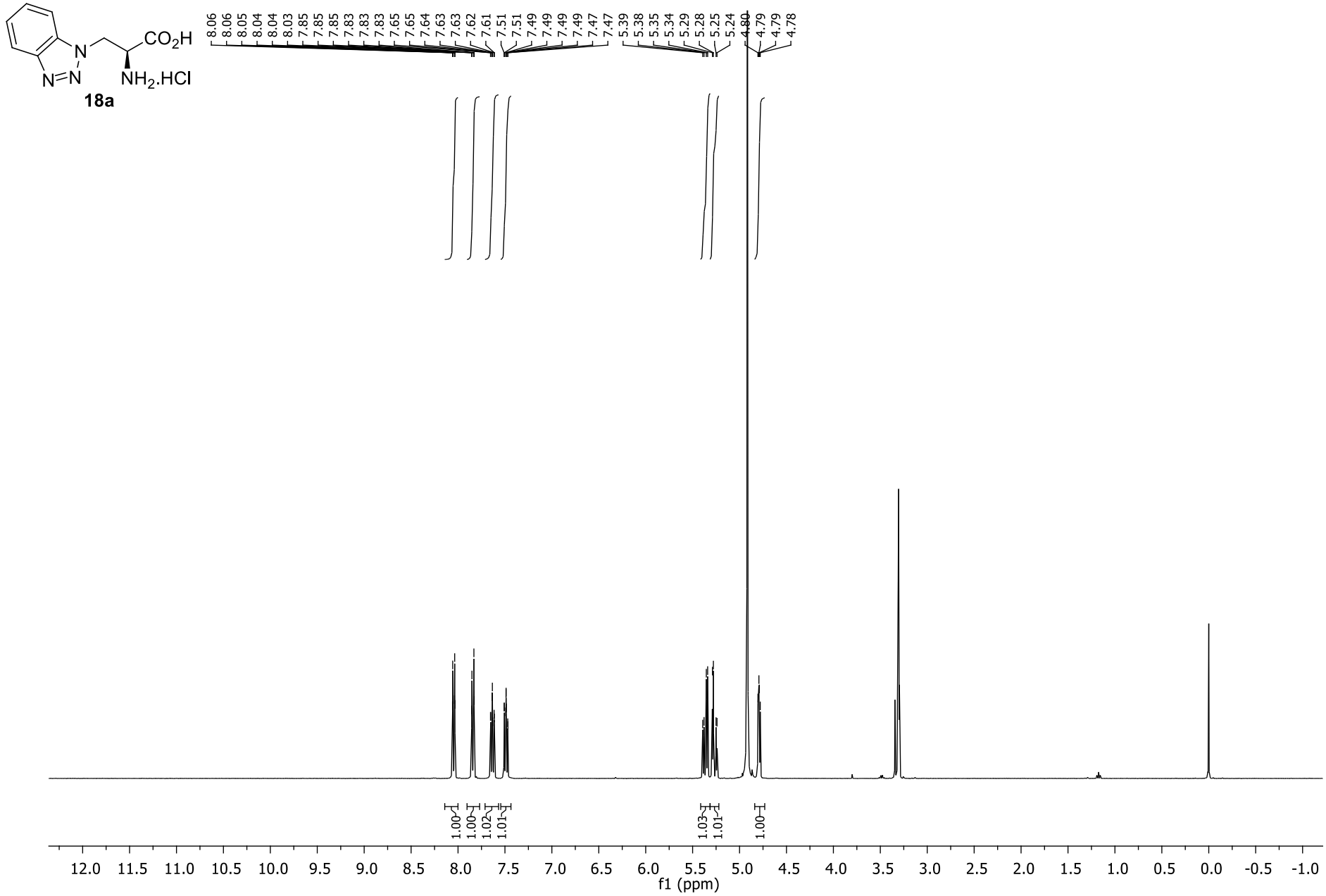

Cl
Cl
N
N
N
CO2Me
NHCbz

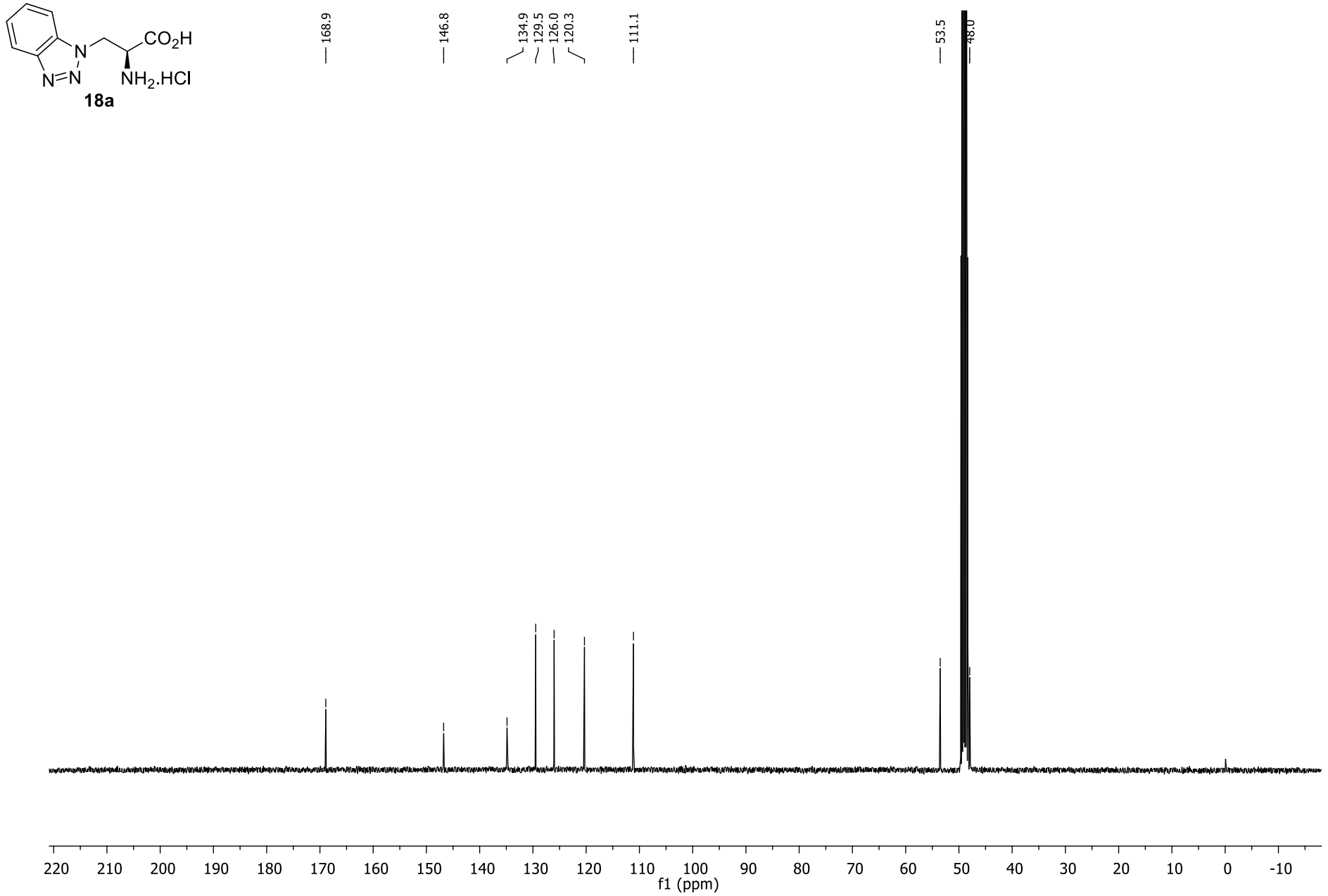
17e

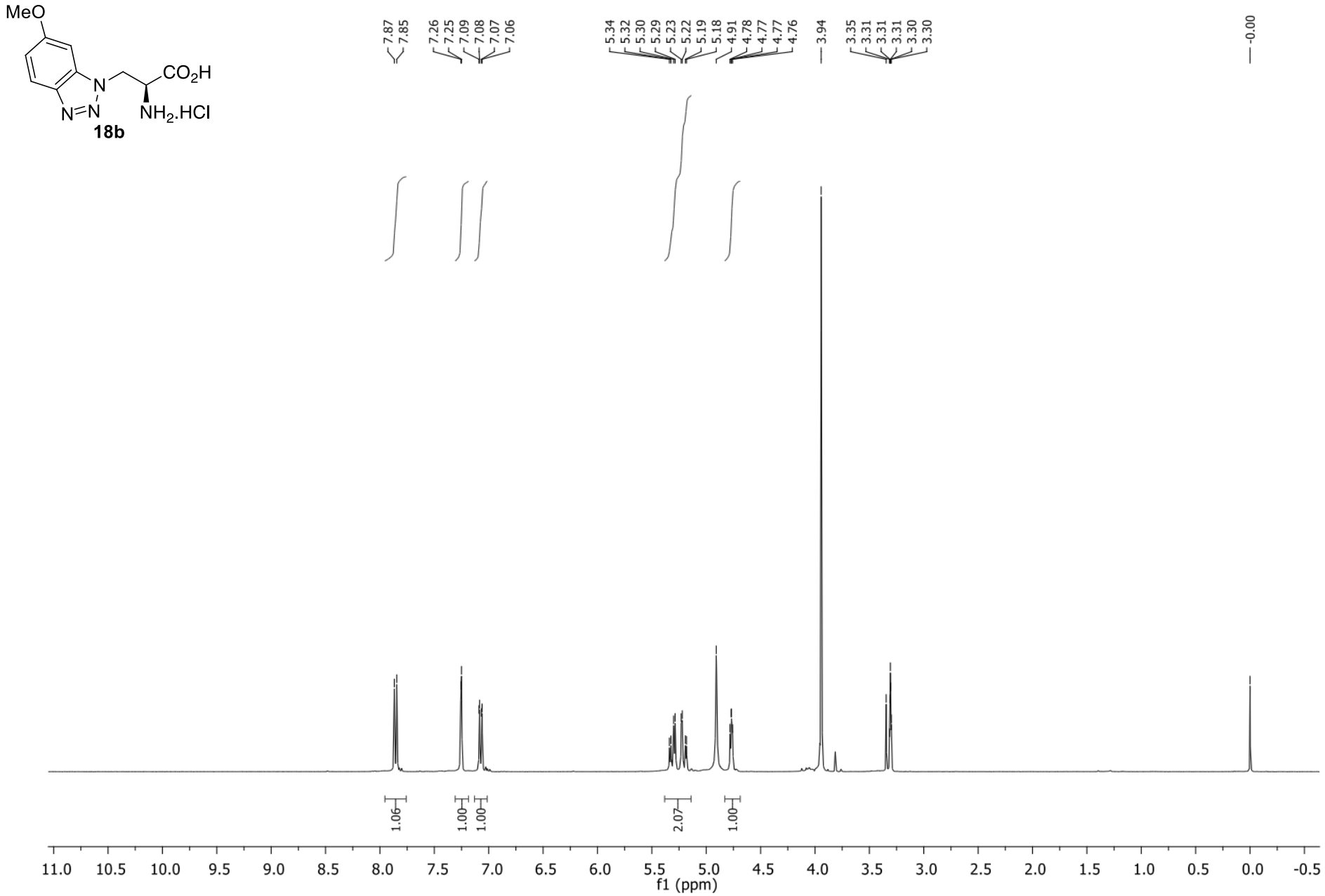
169.17
155.78
144.34
135.65
132.94
128.94
128.56
128.34
128.03
120.73
110.71
77.51
77.39
77.19
76.87
67.45
54.18
53.25
48.75
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

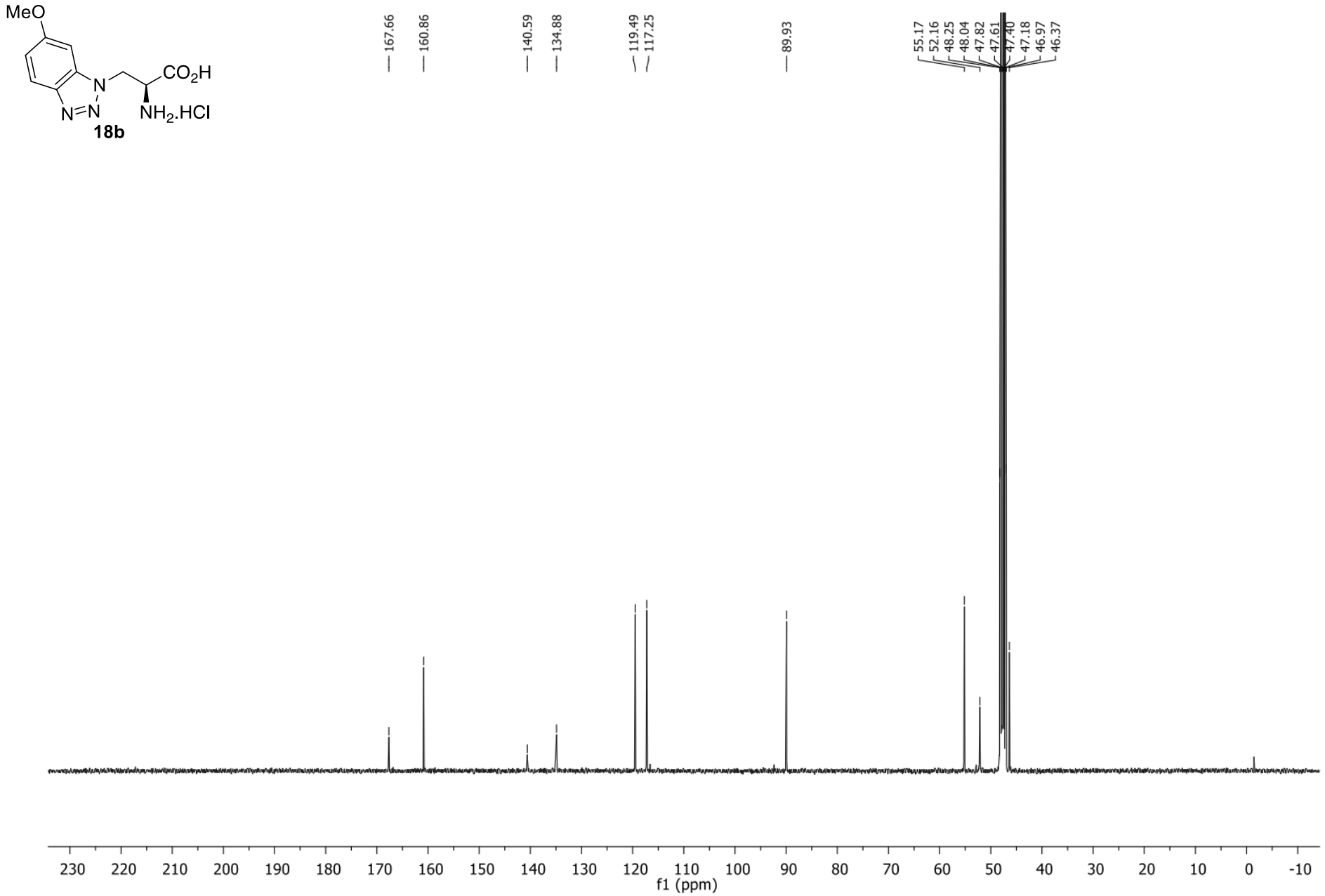

Cl
Me
N
N=N
CO2Me
NHCbz
17f
7.70
7.52
7.31
7.29
7.28
7.28
7.27
7.26
6.16
6.15
6.14
5.08
5.05
5.03
5.02
5.00
4.99
4.86
4.85
4.84
4.84
4.83
4.82
3.74
2.40
0.98
0.90
4.98
0.94
3.91
1.12
2.91
3.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

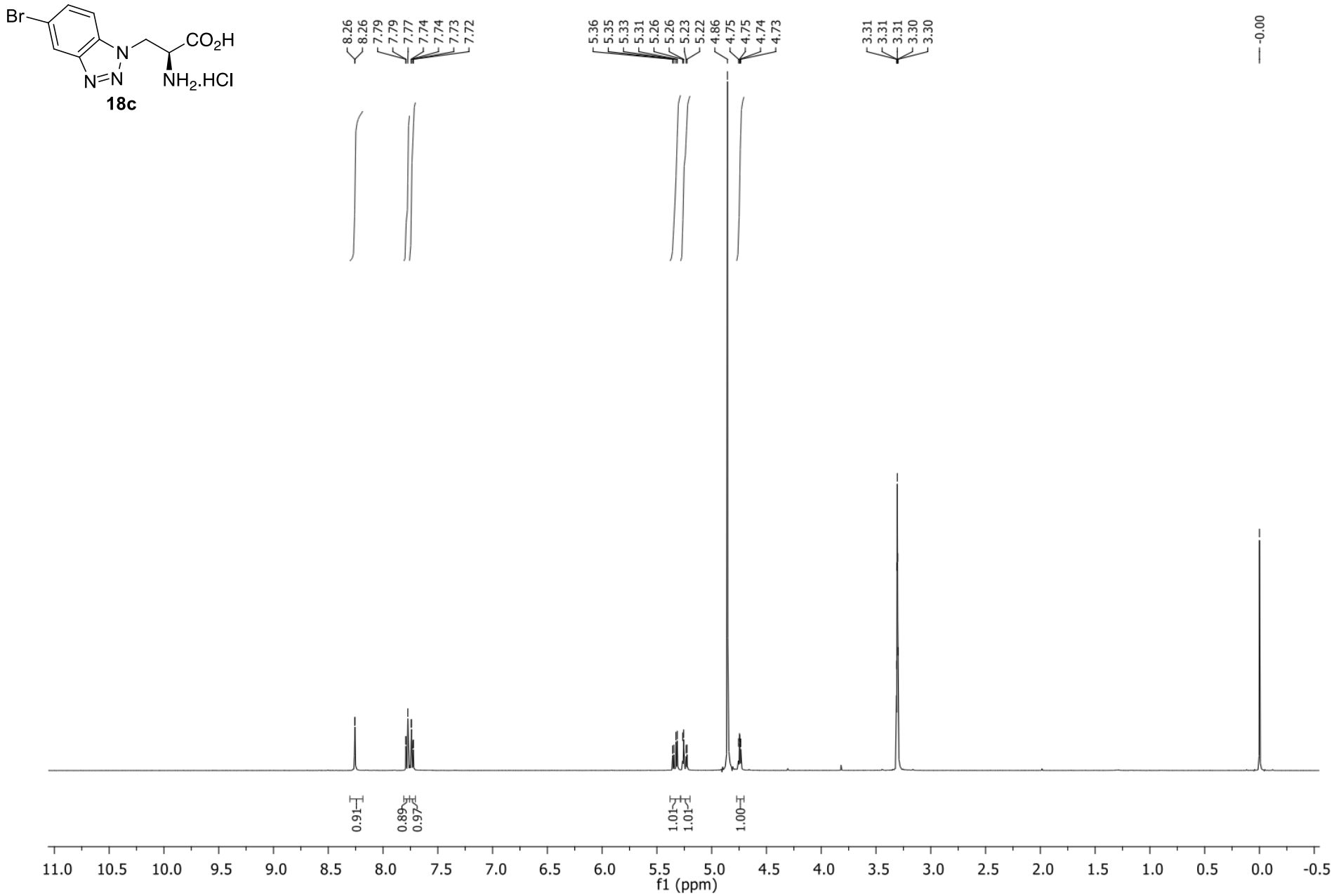

Cl
Me
N
N=N
CO2Me
NHCbz
17f
169.35
155.80
144.44
135.83
135.31
132.91
132.51
128.53
128.25
128.05
120.29
109.23
77.55
77.44
77.23
76.92
67.33
54.24
53.14
48.52
20.67
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

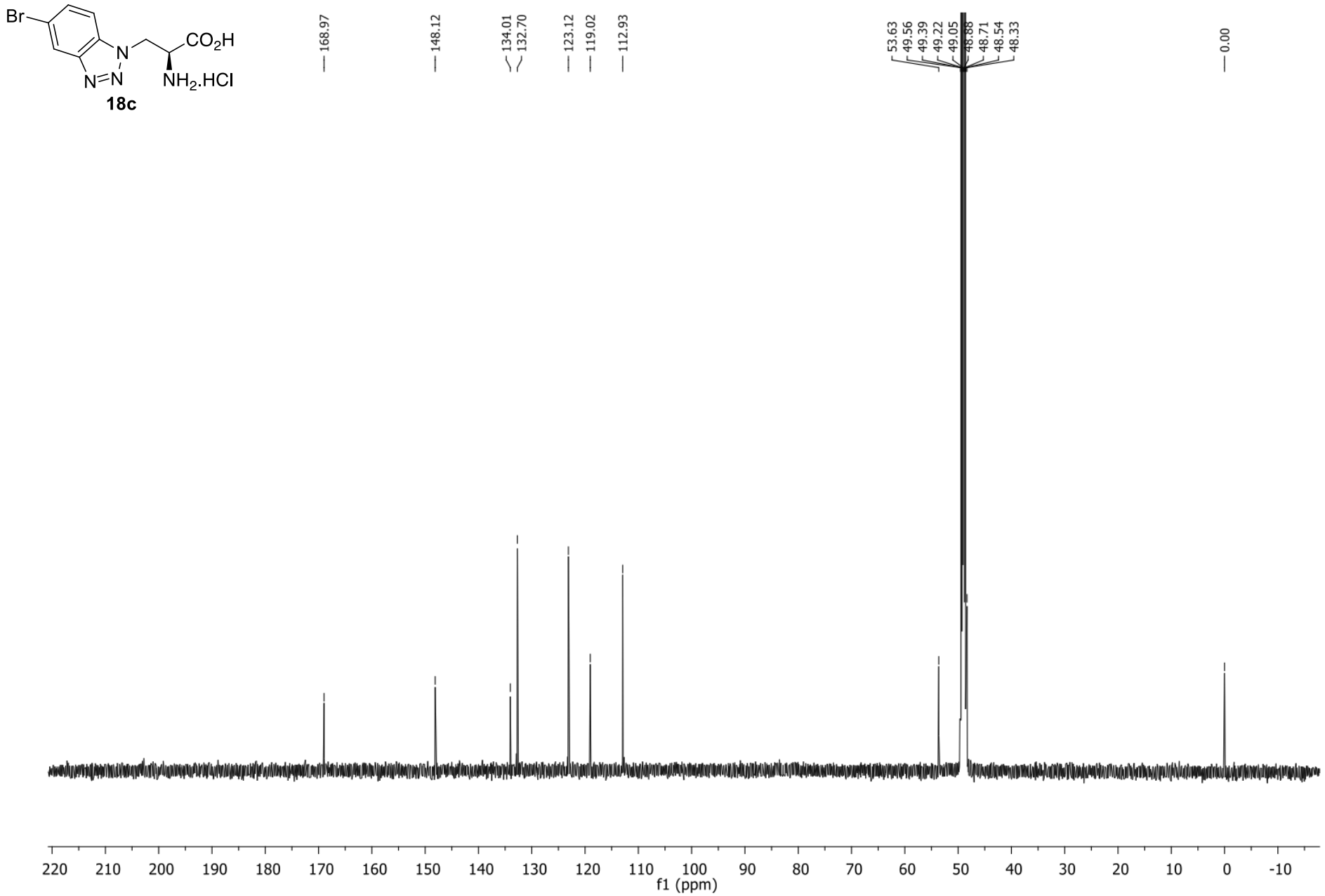

CO2H
N
N
N
NH2.HCl
18a
8.06 8.06 8.05 8.04 8.04 8.03 7.85 7.85 7.85 7.83 7.83 7.83 7.65 7.64 7.63 7.63 7.62 7.61 7.51 7.51 7.49 7.49 7.49 7.47 7.47 5.39 5.38 5.35 5.34 5.29 5.28 5.25 5.24 4.80 4.79 4.79 4.78
1.00 1.00 1.02 1.01 1.03 1.01 1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

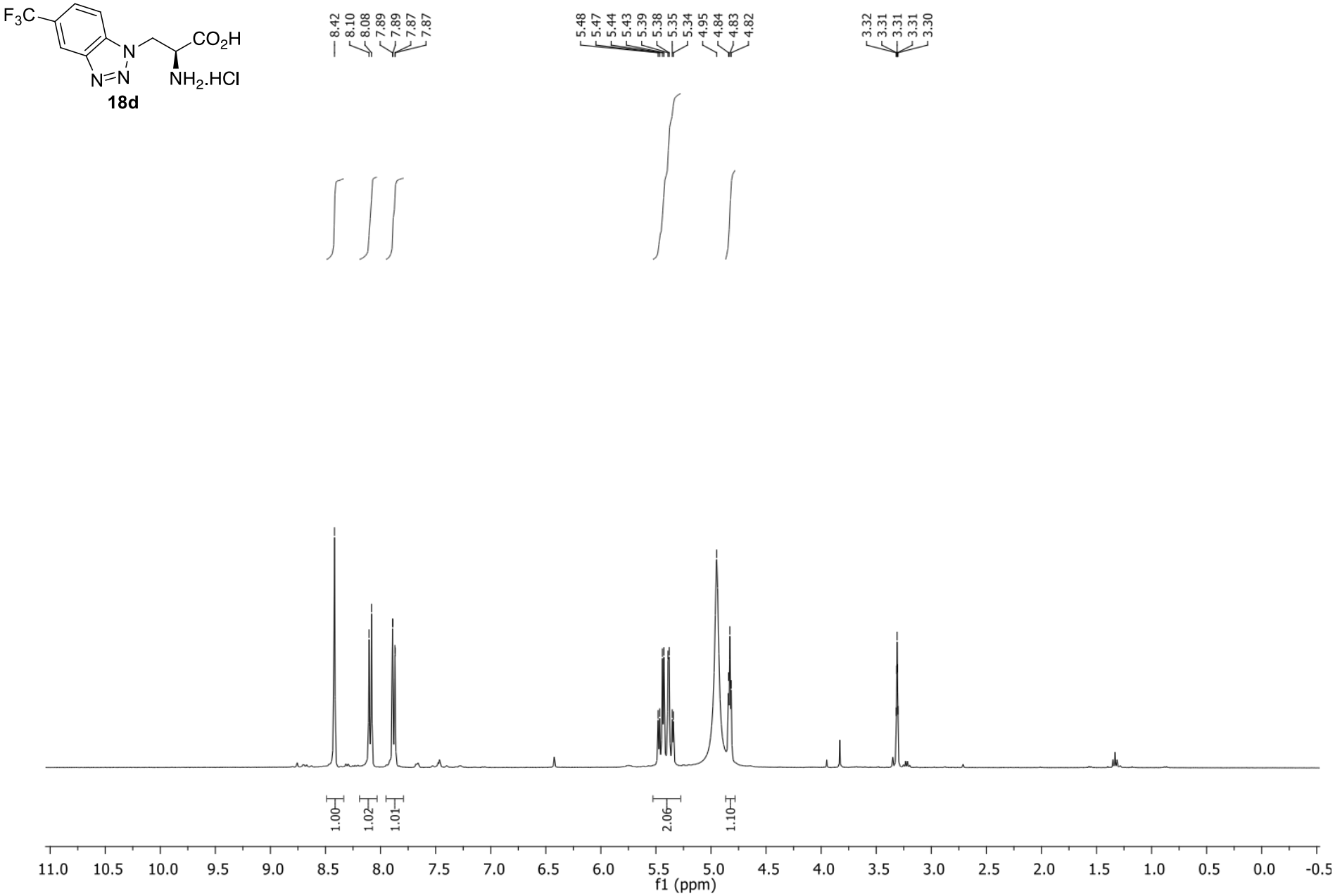

CO2H
N
N
N
NH2.HCl
18a
168.9
146.8
134.9
129.5
126.0
120.3
111.1
53.5
48.0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

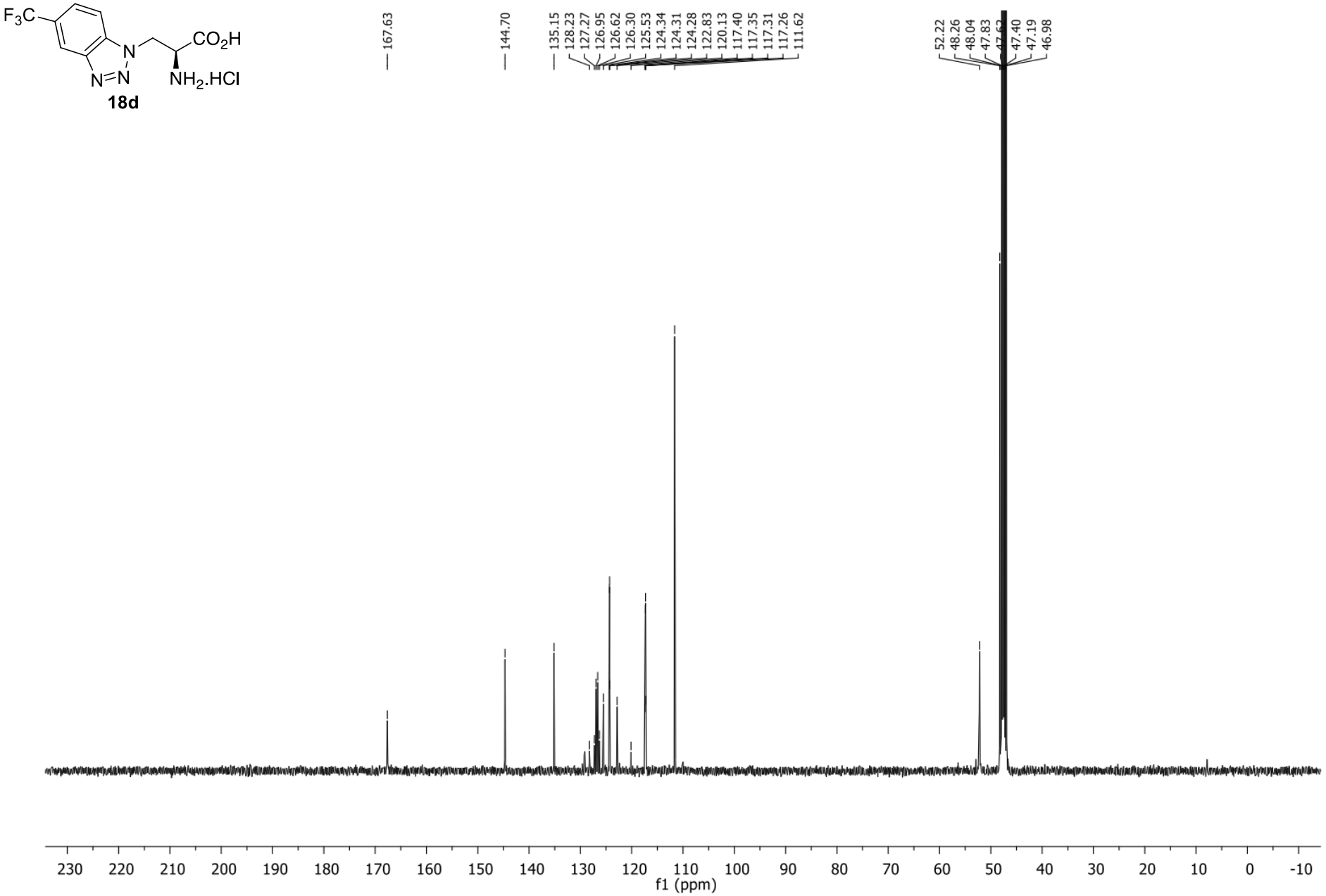

MeO
CO2H
N
N=N
NH2.HCl
18b
7.87
7.85
7.26
7.25
7.09
7.08
7.07
7.06
5.34
5.32
5.30
5.29
5.23
5.22
5.19
5.18
4.91
4.78
4.77
4.77
4.76
3.94
3.35
3.31
3.31
3.31
3.30
3.30
-0.00
1.06
1.00
1.00
2.07
1.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

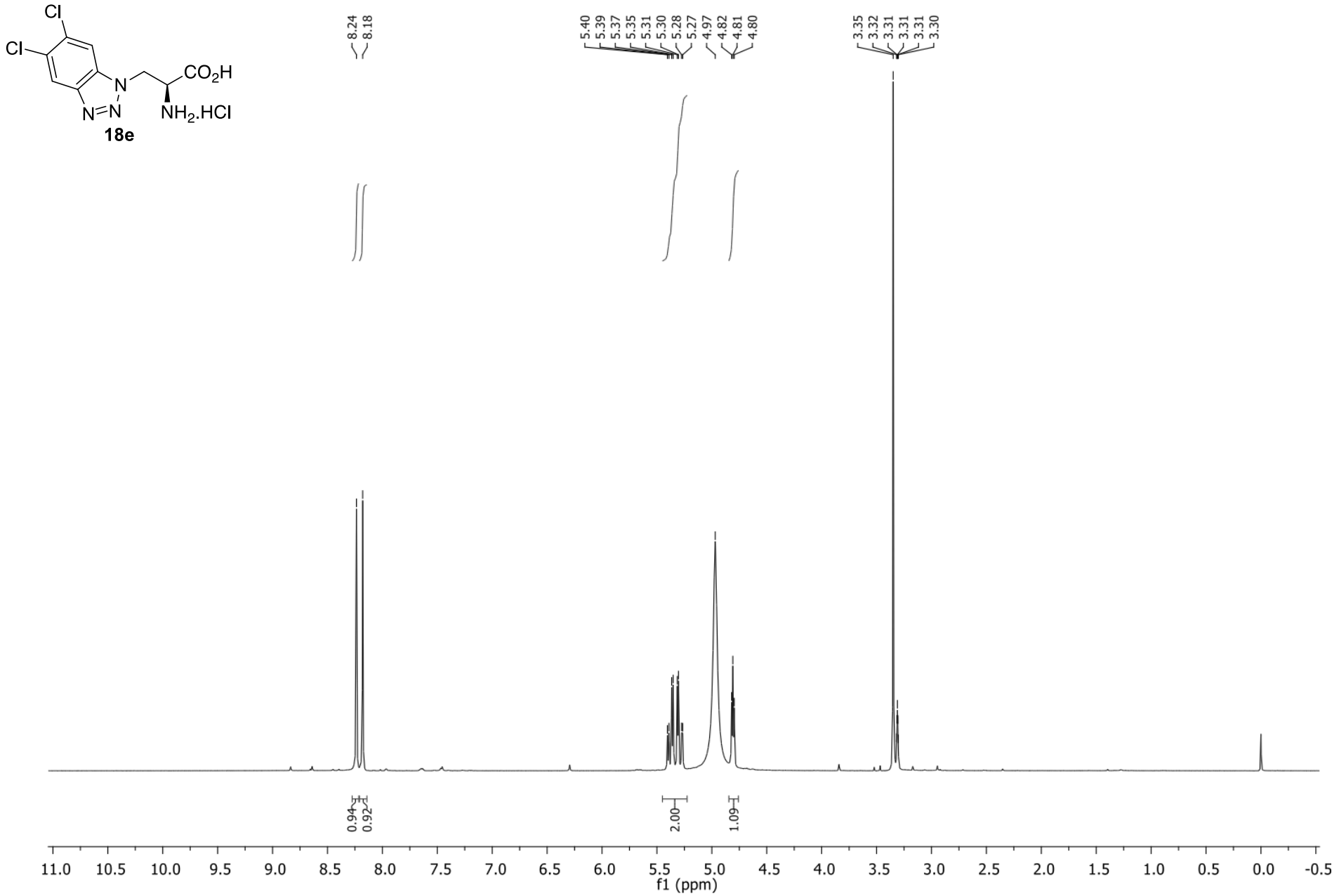

MeO
CO2H
N
N=N
NH2.HCl
18b
167.66
160.86
140.59
134.88
119.49
117.25
89.93
55.17
52.16
48.25
48.04
47.82
47.61
47.40
47.18
46.97
46.37
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

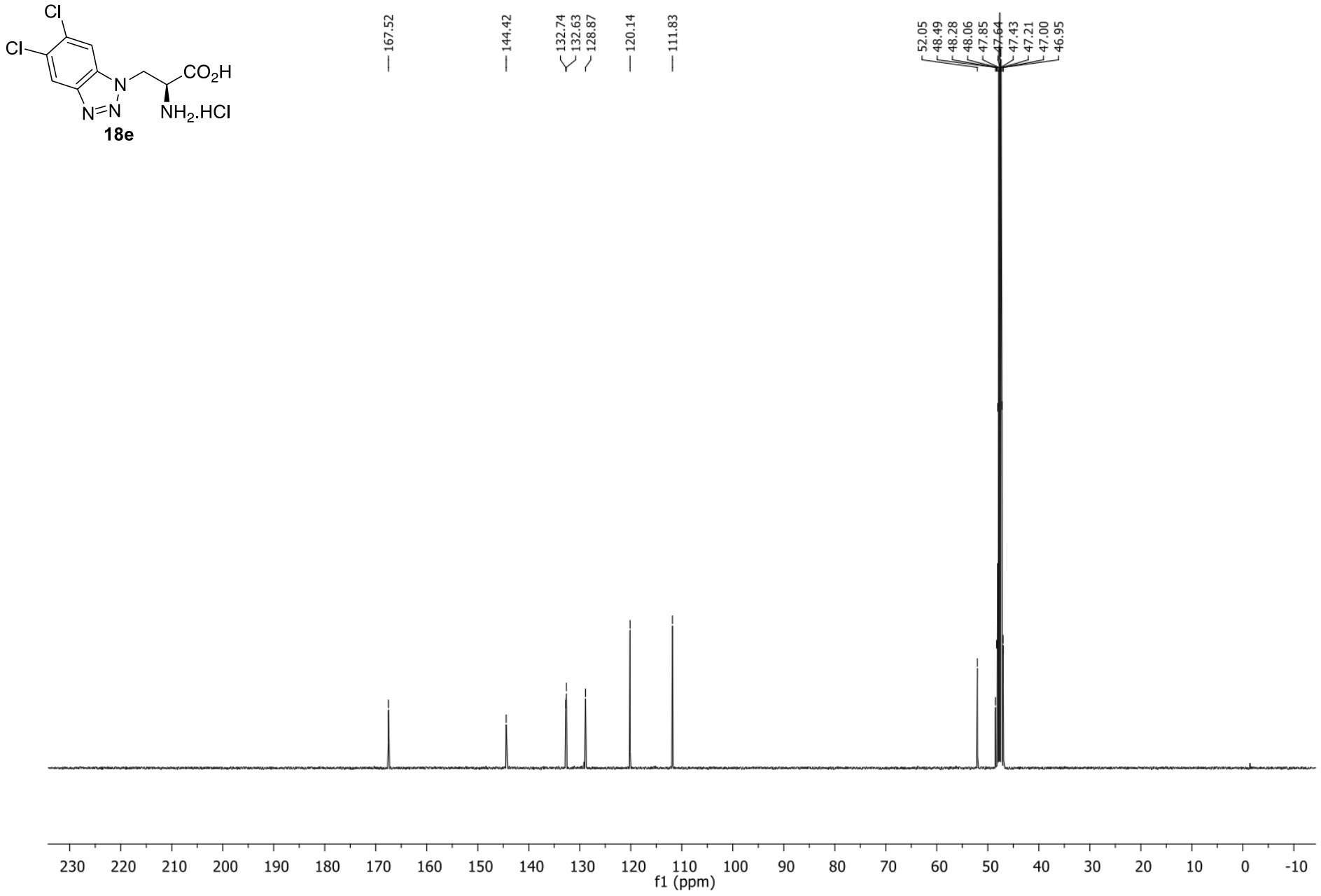

Br
CO2H
NH2.HCl
18c
8.26
8.26
7.79
7.79
7.77
7.74
7.74
7.73
7.72
5.36
5.35
5.33
5.31
5.26
5.26
5.23
5.22
4.86
4.75
4.75
4.74
4.73
3.31
3.31
3.31
3.30
3.30
-0.00
0.91
0.89
0.97
1.01
1.01
1.00
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

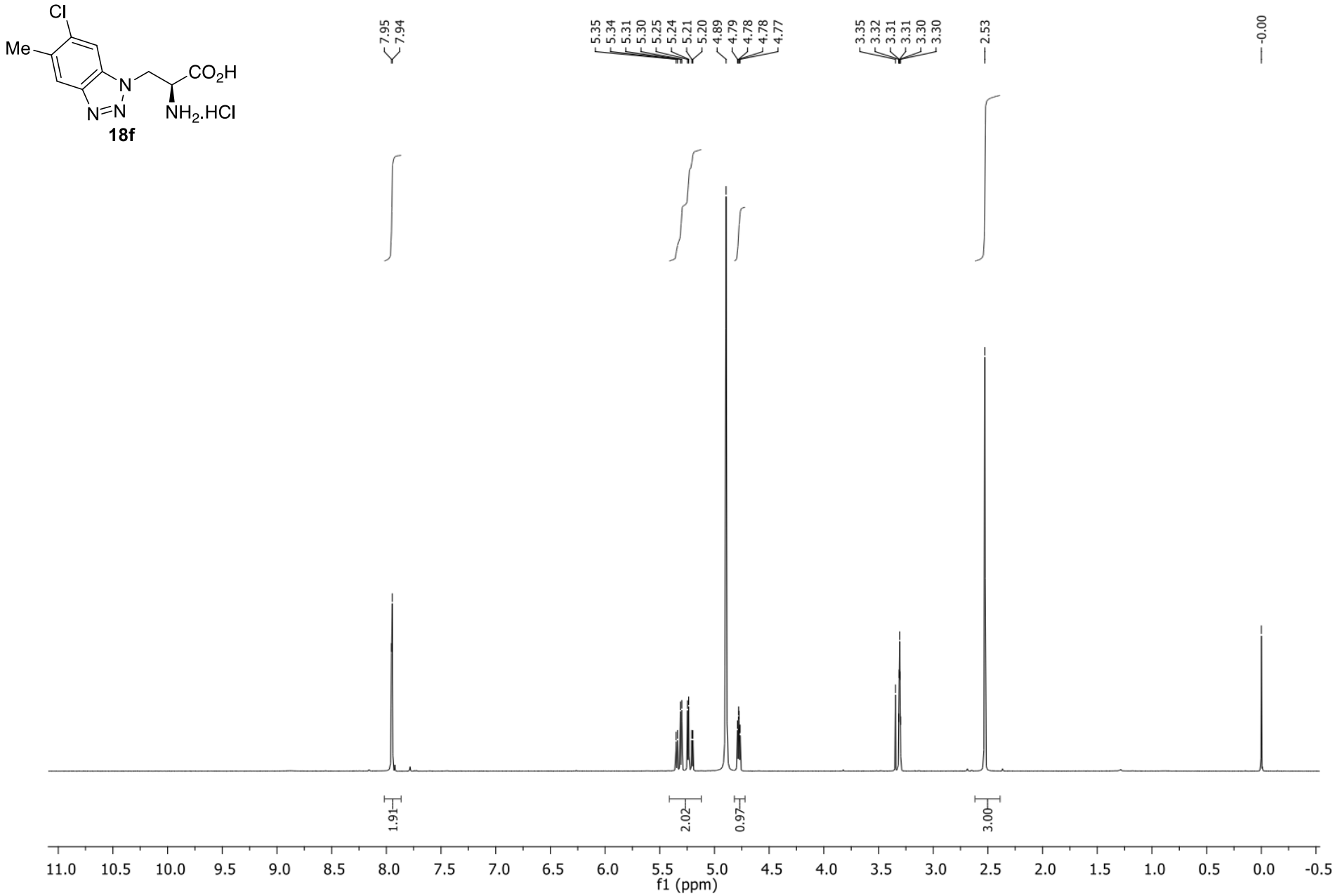

Br
CO2H
N
N=N
NH2.HCl
18c
168.97
148.12
134.01
132.70
123.12
119.02
112.93
53.63
49.56
49.39
49.22
49.05
48.88
48.71
48.54
48.33
0.00
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

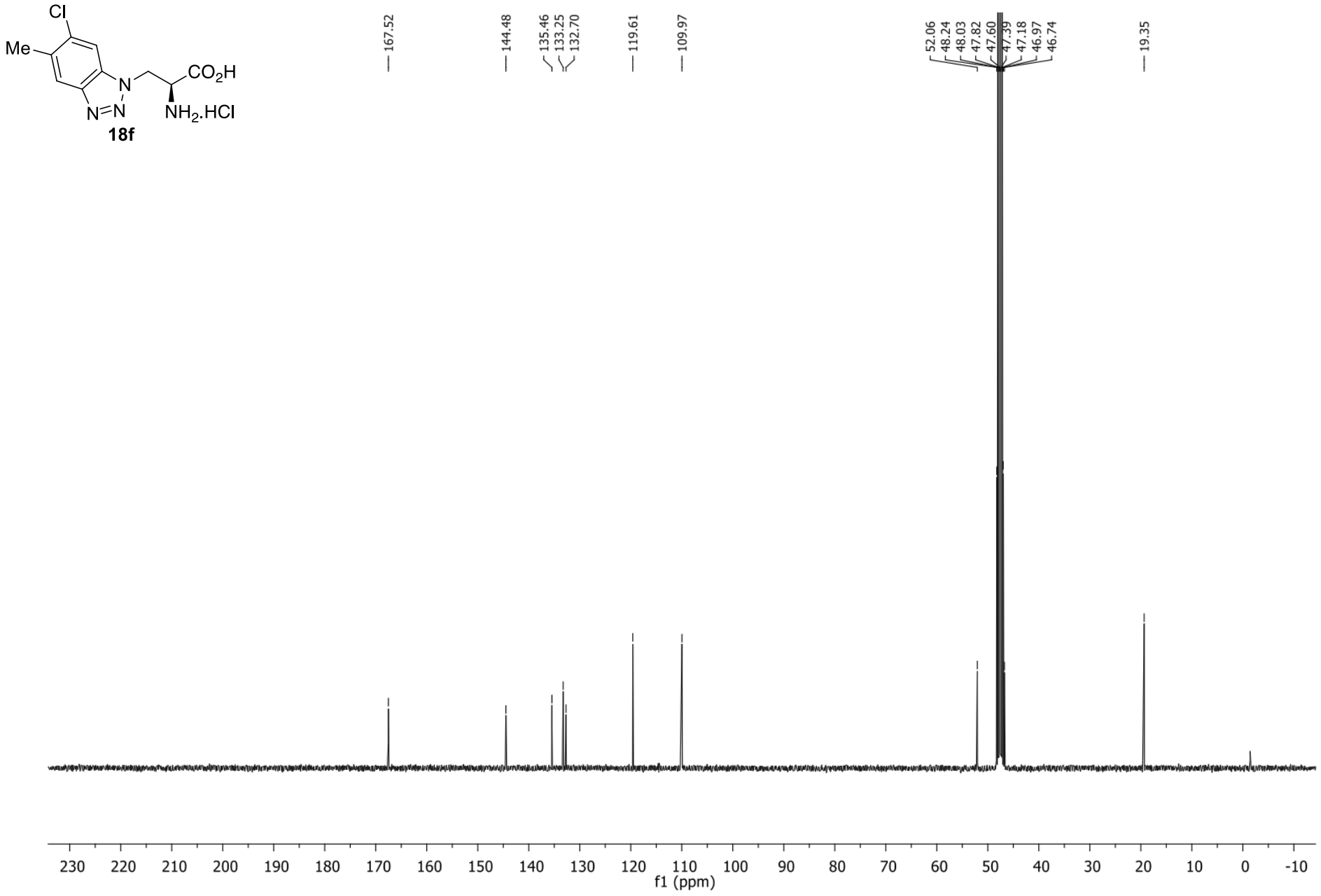

F3C
CO2H
N
N=N
NH2.HCl
18d
8.42
8.10
8.08
7.89
7.89
7.87
7.87
5.48
5.47
5.44
5.43
5.39
5.38
5.35
5.34
4.95
4.84
4.83
4.82
3.32
3.31
3.31
3.31
3.30
1.00
1.02
1.01
2.06
1.10
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

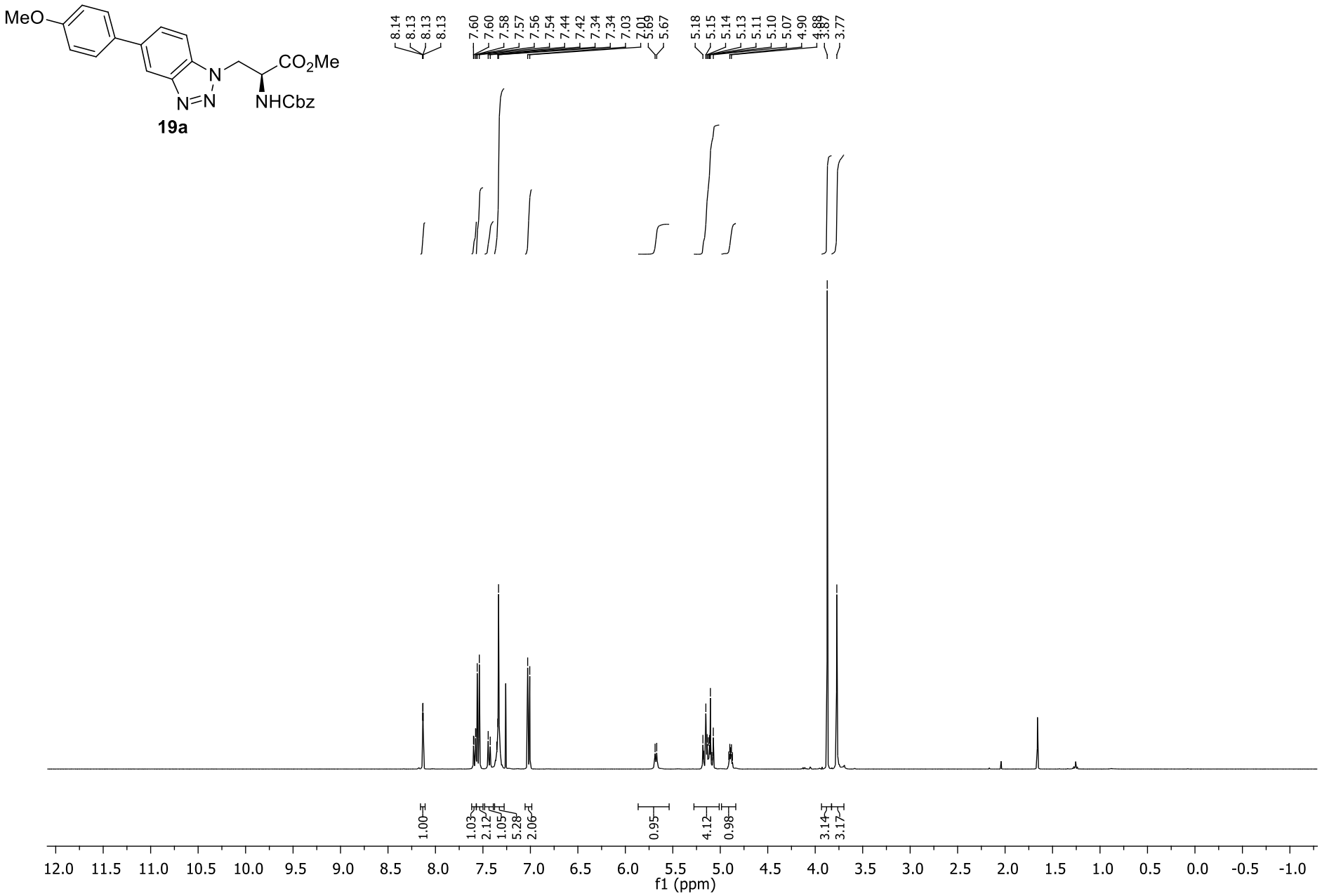

F3C
CO2H
N
N
N
NH2.HCl
18d
167.63
144.70
135.15
128.23
127.27
126.95
126.62
126.30
125.53
124.34
124.31
124.28
122.83
120.13
117.40
117.35
117.31
117.26
111.62
52.22
48.26
48.04
47.83
47.62
47.40
47.19
46.98
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

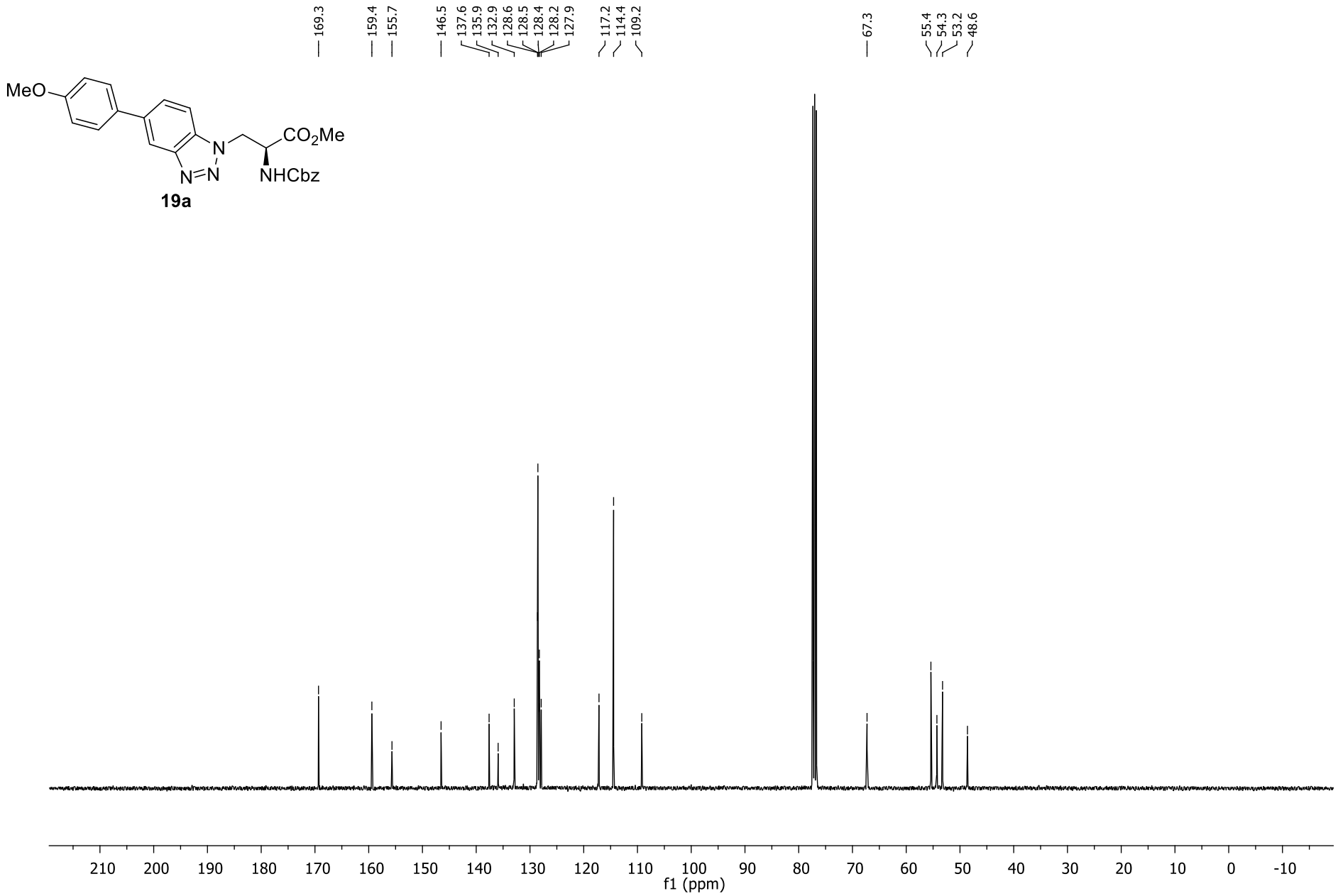

Cl
Cl
N
N=N
CO2H
NH2.HCl
18e
8.24
8.18
5.40
5.39
5.37
5.35
5.31
5.30
5.28
5.27
4.97
4.82
4.81
4.80
3.35
3.32
3.31
3.31
3.31
3.30
0.94
0.92
2.00
1.09
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

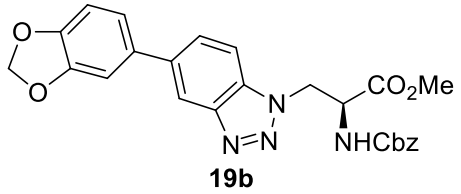

Cl
Cl
N
N=N
CO2H
NH2.HCl
18e
167.52
144.42
132.74
132.63
128.87
120.14
111.83
52.05
48.49
48.28
48.06
47.85
47.64
47.43
47.21
47.00
46.95
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Cl
Me
N
N=N
CO2H
NH2.HCl
18f
7.95
7.94
5.35
5.34
5.31
5.30
5.25
5.24
5.21
5.20
4.89
4.79
4.78
4.78
4.77
3.35
3.32
3.31
3.31
3.30
3.30
2.53
-0.00
1.91
2.02
0.97
3.00
11.0
10.5
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
0.0
-0.5
f1 (ppm)


Cl
Me
N
N=N
CO2H
NH2.HCl
18f
167.52
144.48
135.46
133.25
132.70
119.61
109.97
52.06
48.24
48.03
47.82
47.60
47.39
47.18
46.97
46.74
19.35
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

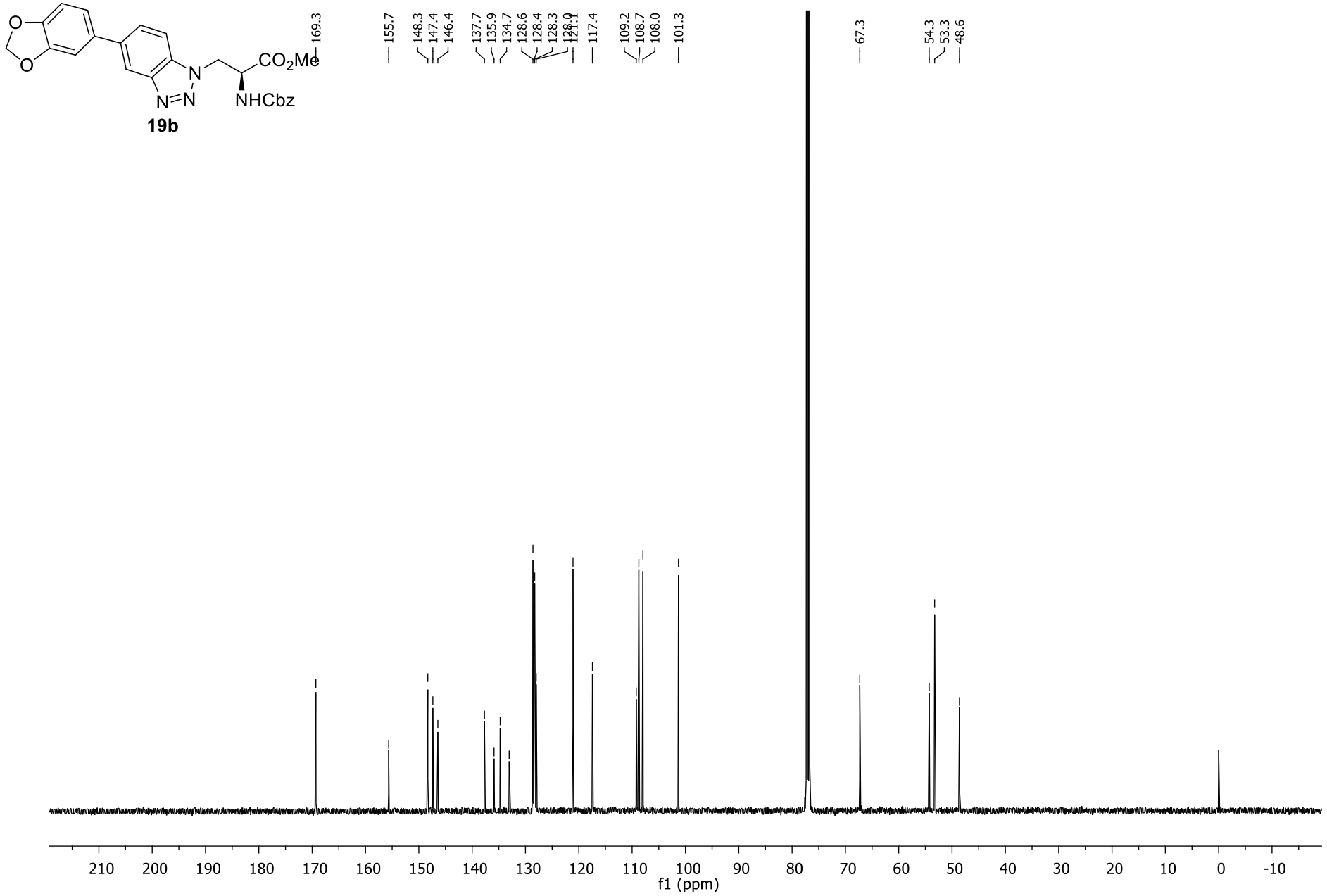

MeO
N
N=N
CO2Me
NHCbz
19a
8.14
8.13
8.13
8.13
7.60
7.60
7.58
7.57
7.56
7.54
7.44
7.42
7.34
7.34
7.03
7.01
7.00
5.69
5.67
5.18
5.15
5.14
5.13
5.11
5.10
5.07
4.90
4.88
4.87
3.87
3.77
1.00
1.03
2.12
1.05
5.28
2.06
0.95
4.12
0.98
3.14
3.17
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

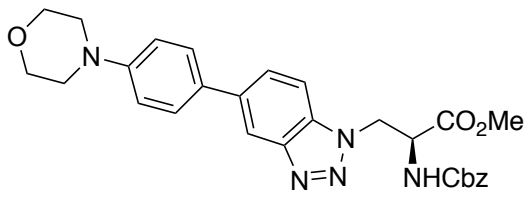

169.3
159.4
155.7
146.5
137.6
135.9
132.9
128.6
128.5
128.4
128.2
127.9
117.2
114.4
109.2
67.3
55.4
54.3
53.2
48.6
MeO
N
N=N
CO2Me
NHCbz
19a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
N
N=N
CO2Me
NHCbz

19b

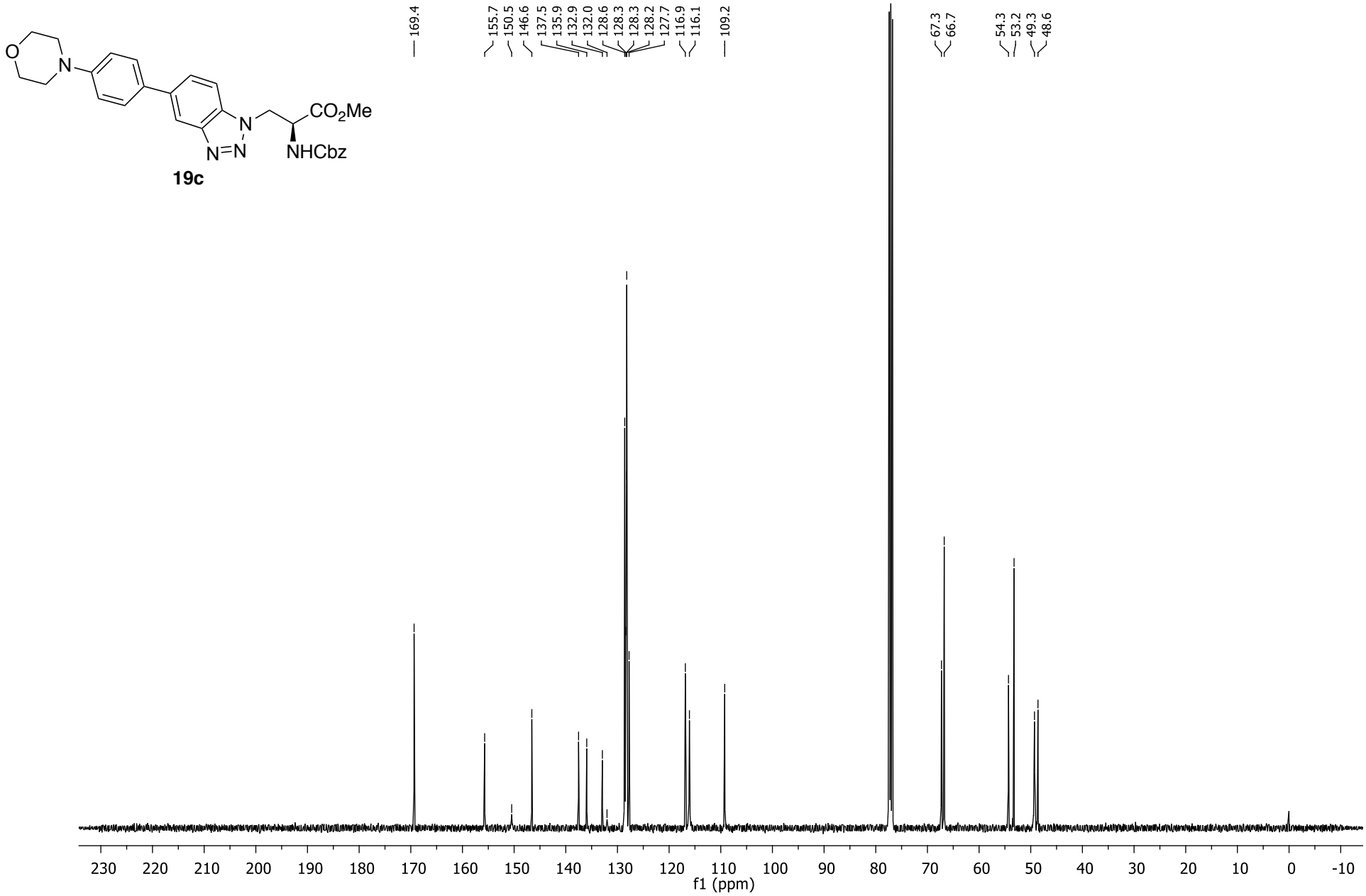
8.10
8.10
8.10
8.10
7.34
7.34
7.33
7.26
7.08
7.07
7.06
6.93
6.92
6.91
6.03
5.66
5.65
5.18
5.16
5.15
5.14
5.12
5.12
5.10
5.08
4.89
4.88
3.78
1.00
1.04
0.93
5.02
1.97
1.03
2.06
0.93
4.08
0.95
3.14
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


O
O
N
N=N
CO2Me
NHCbz
19b
169.3
155.7
148.3
147.4
146.4
137.7
135.9
134.7
128.6
128.4
128.3
128.0
121.1
117.4
109.2
108.7
108.0
101.3
67.3
54.3
53.3
48.6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

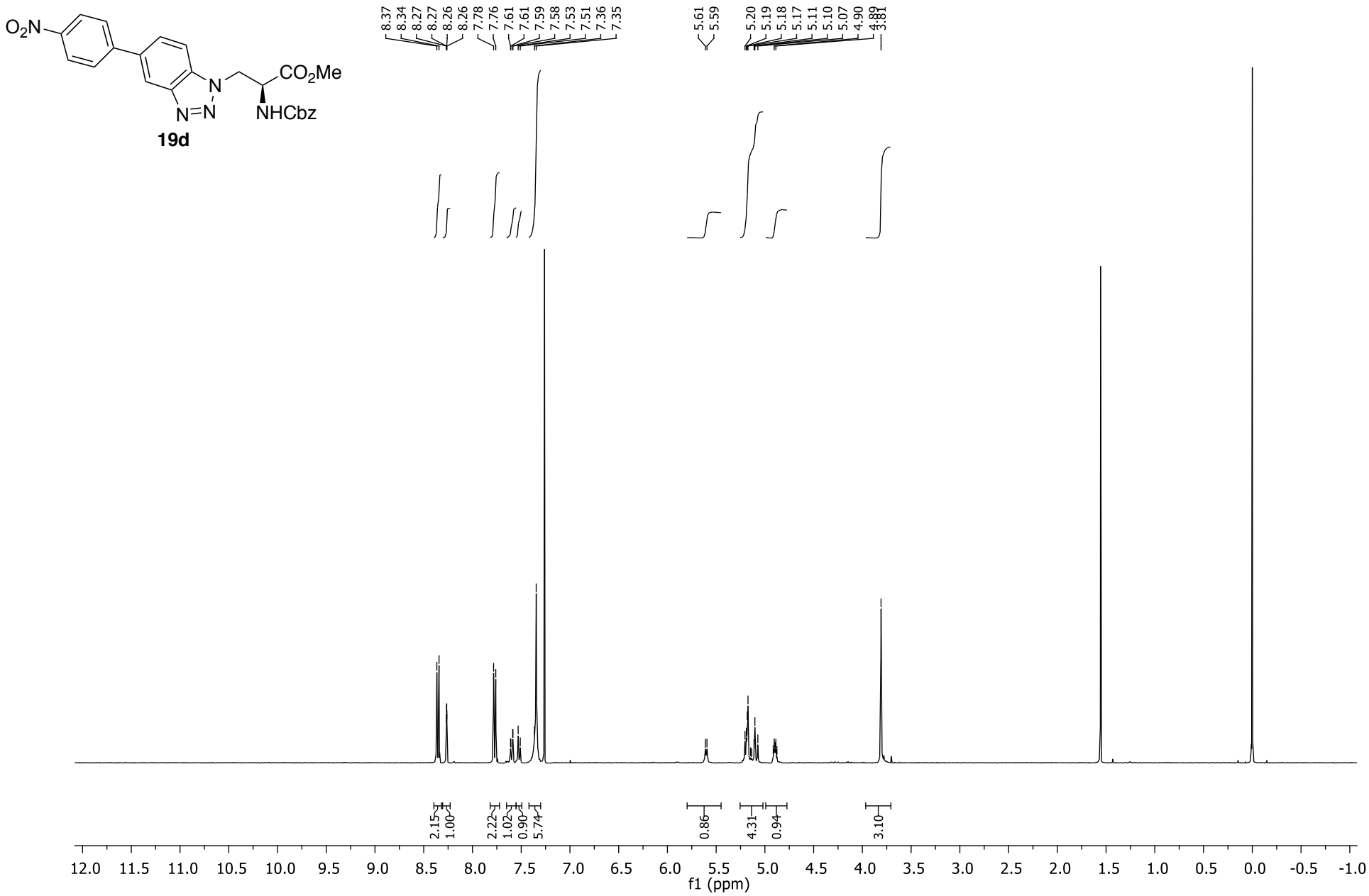

O
N
N
N=N
CO2Me
NHCbz

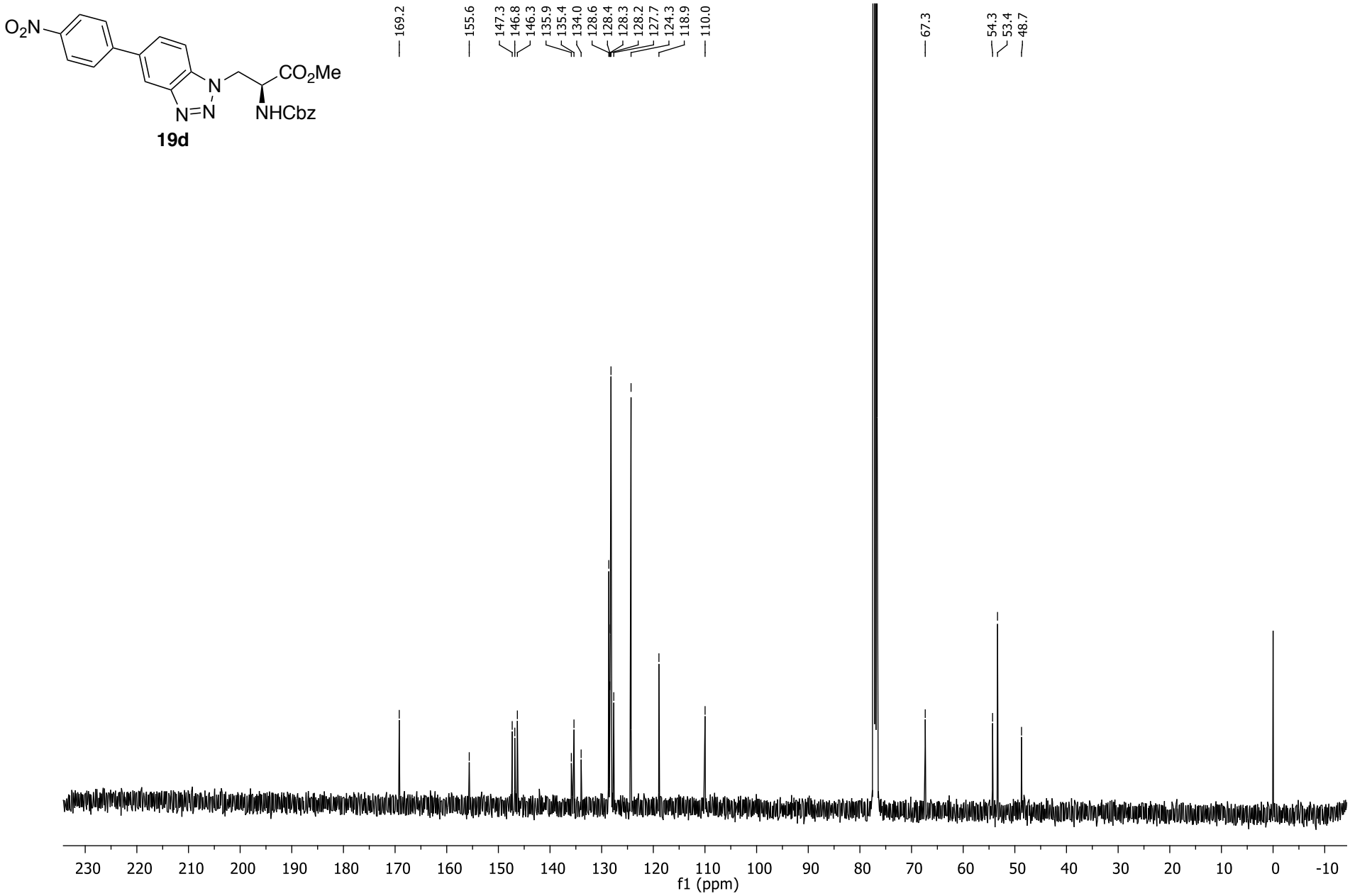
19c

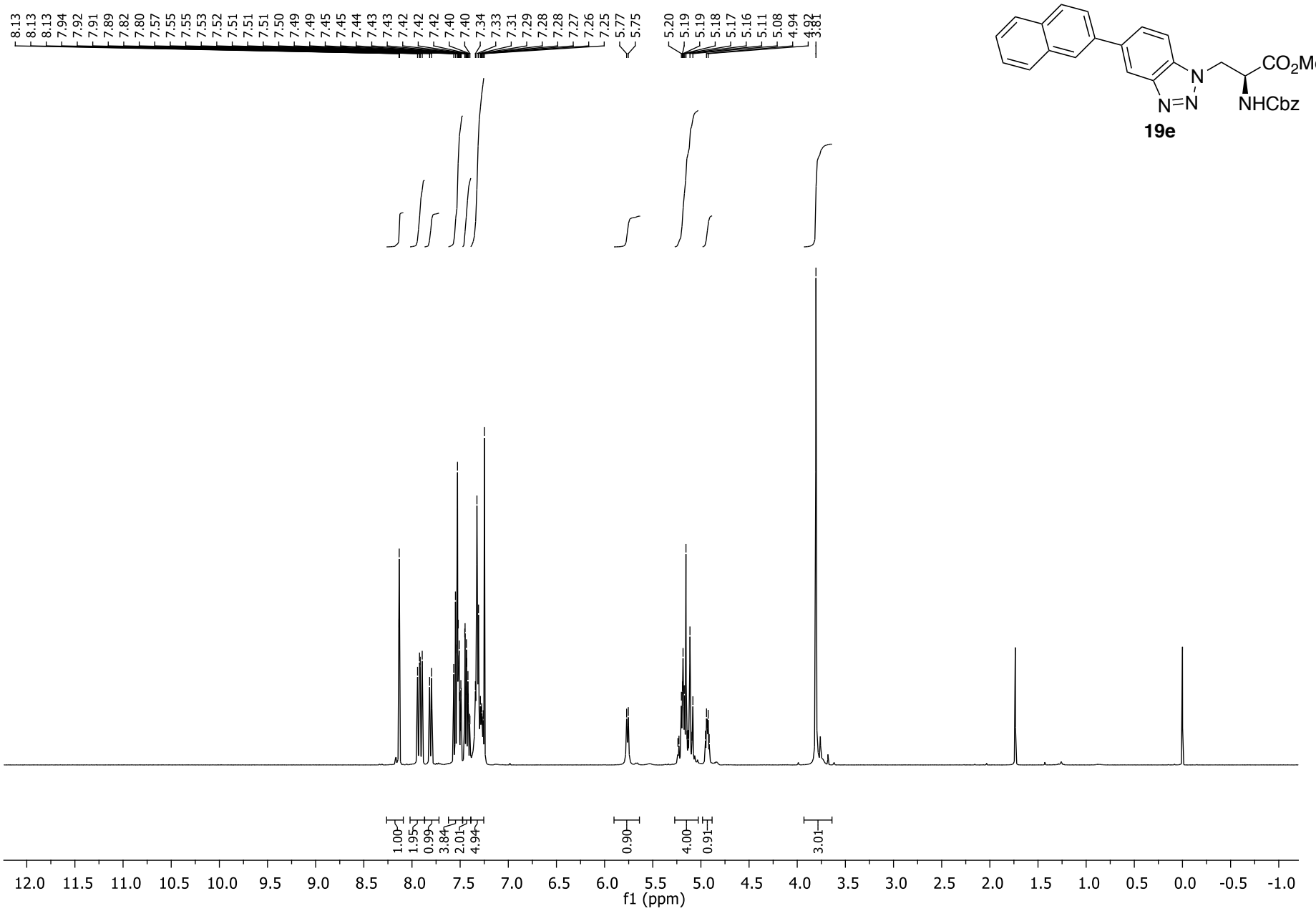
8.13
7.61
7.60
7.59
7.58
7.56
7.54
7.44
7.42
7.33
7.26
7.26
7.05
5.76
5.75
5.17
5.14
5.13
5.11
5.10
5.09
5.06
4.89
3.91
3.90
3.89
3.76
3.24
3.23
3.22
1.00
1.16
1.94
1.01
5.17
1.96
0.91
4.02
1.02
4.17
3.04
4.08
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


O
N
N
N=N
CO2Me
NHCbz
169.4
155.7
150.5
146.6
137.5
135.9
132.9
132.0
128.6
128.3
128.3
128.2
127.7
116.9
116.1
109.2
67.3
66.7
54.3
53.2
49.3
48.6
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

19c

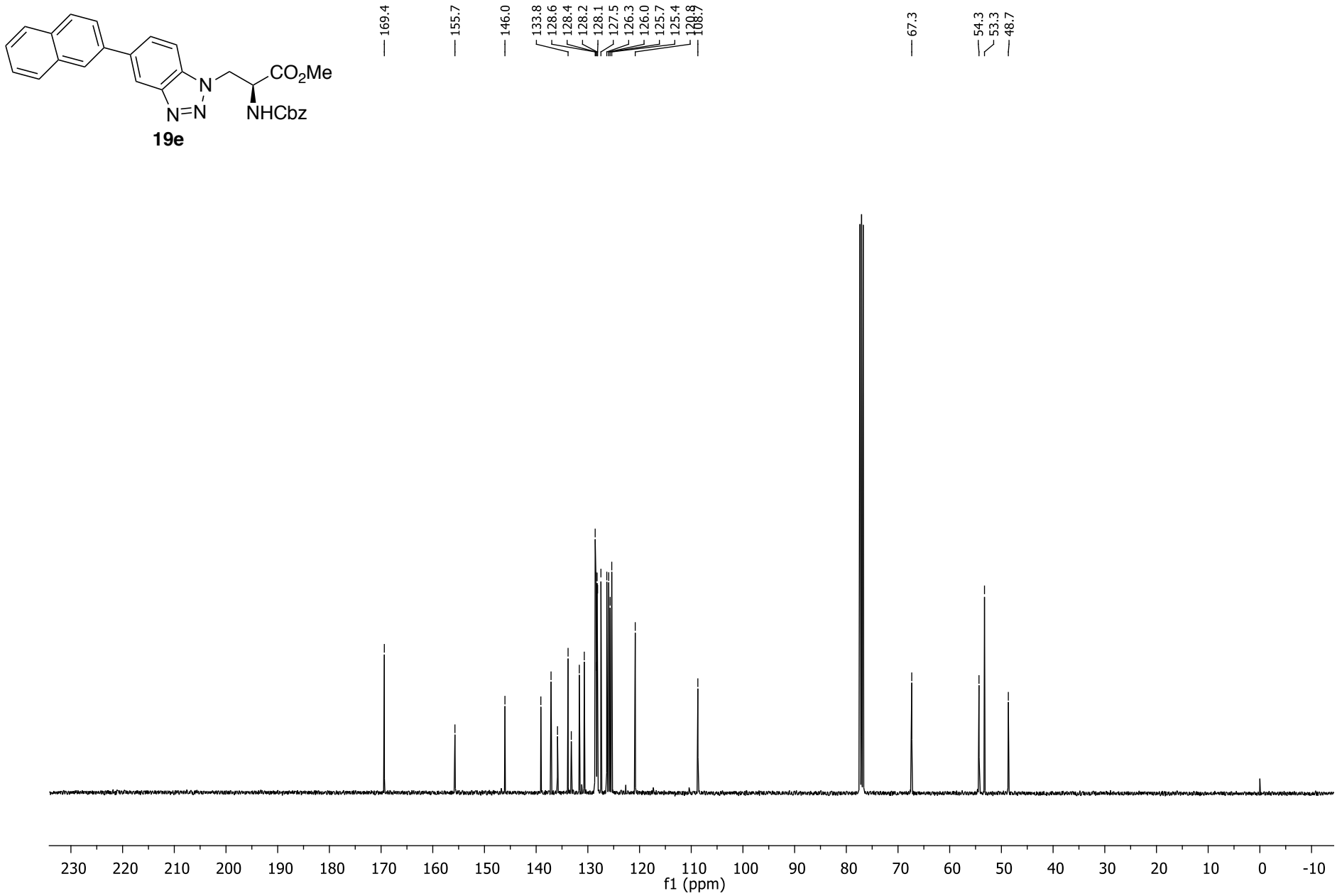

O2N
CO2Me
N
N=N
NHCbz
19d
8.37
8.34
8.27
8.27
8.26
8.26
7.78
7.76
7.61
7.61
7.59
7.58
7.53
7.51
7.36
7.35
5.61
5.59
5.20
5.19
5.18
5.17
5.11
5.10
5.07
4.90
3.81
2.15
1.00
2.22
1.02
0.90
5.74
0.86
4.31
0.94
3.10
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

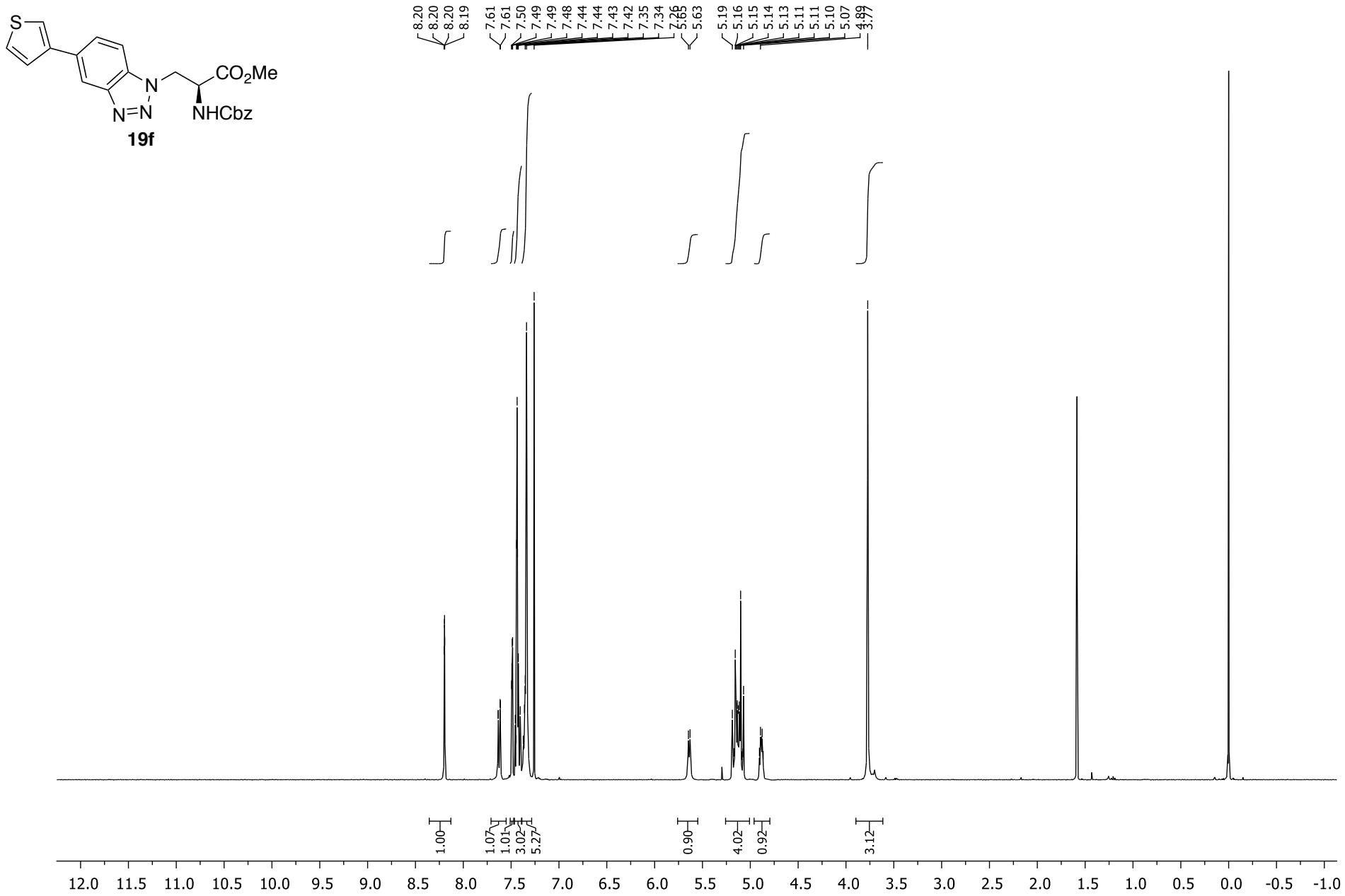

O2N
CO2Me
N
N=N
NHCbz
19d
169.2
155.6
147.3
146.8
146.3
135.9
135.4
134.0
128.6
128.4
128.3
128.2
127.7
124.3
118.9
110.0
67.3
54.3
53.4
48.7
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

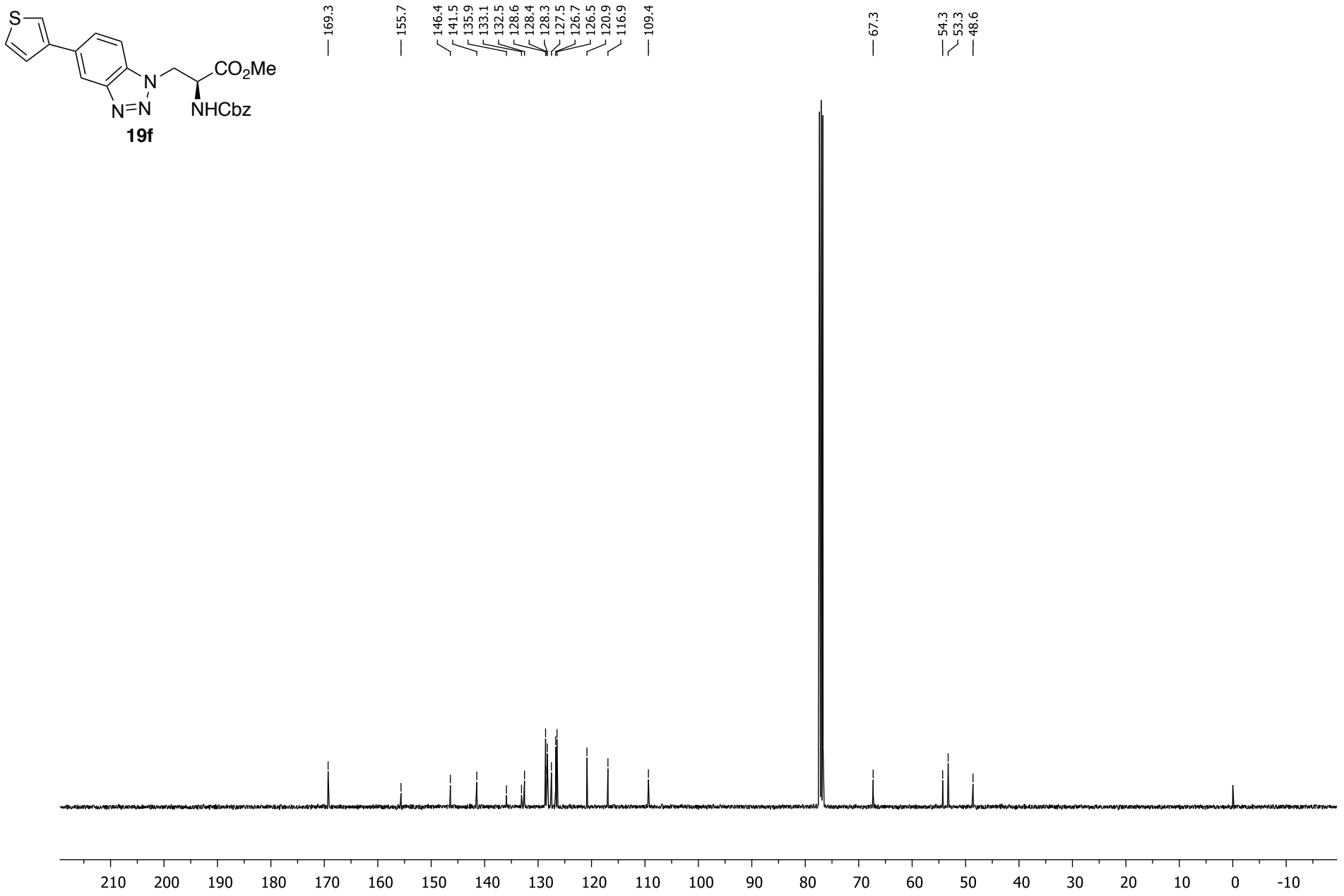

8.13
8.13
8.13
7.94
7.92
7.91
7.89
7.82
7.80
7.57
7.55
7.55
7.53
7.52
7.51
7.51
7.51
7.50
7.49
7.49
7.45
7.45
7.44
7.43
7.43
7.42
7.42
7.42
7.40
7.40
7.34
7.33
7.31
7.29
7.28
7.28
7.27
7.26
7.25
5.77
5.75
5.20
5.19
5.19
5.18
5.17
5.16
5.11
5.08
4.94
4.92
3.81
1.00
1.95
0.99
3.84
2.01
4.94
0.90
4.00
0.91
3.01
12.0
11.5
11.0
10.5
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
0.0
-0.5
-1.0
f1 (ppm)

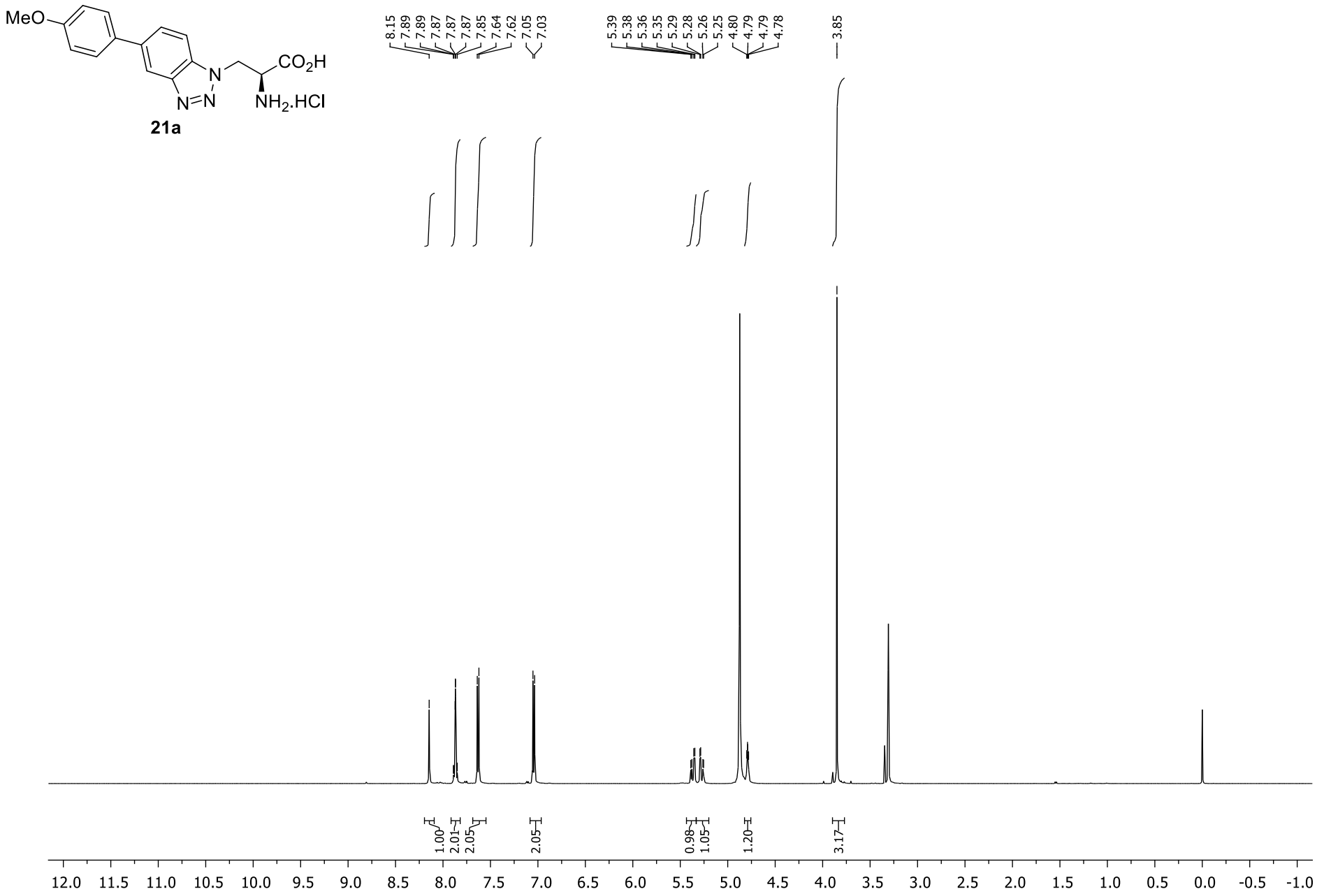
CO2Me
N
N=N
NHCbz

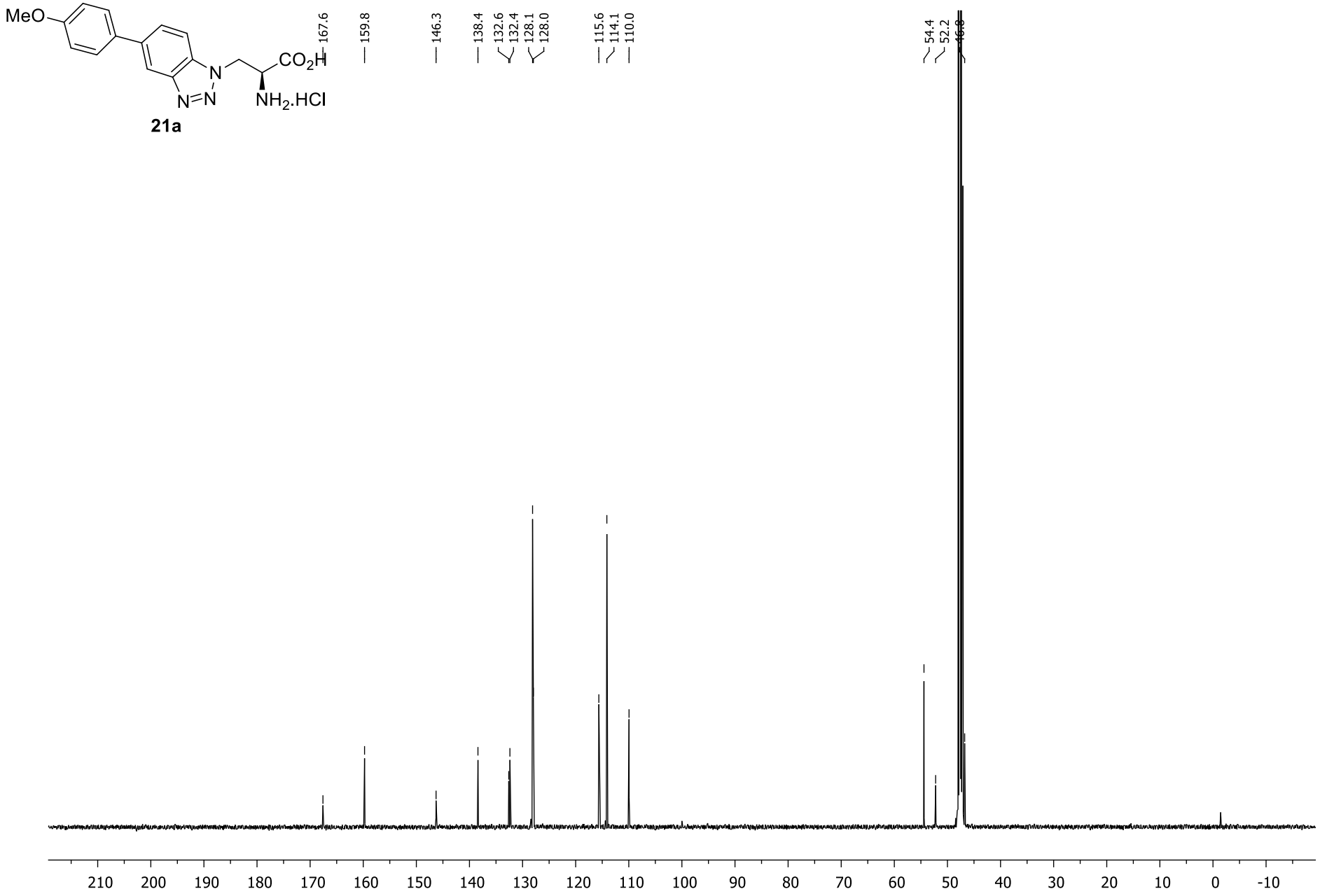
19e

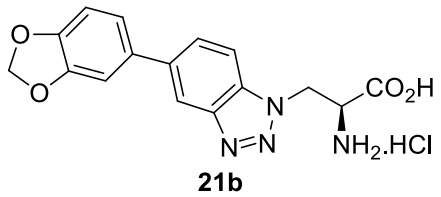

169.4
155.7
146.0
133.8
128.6
128.4
128.2
128.1
127.5
126.3
126.0
125.7
125.4
120.8
108.7
67.3
54.3
53.3
48.7
CO2Me
N
N=N
NHCbz
19e
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


S
N
N=N
CO2Me
NHCbz
19f
8.20
8.20
8.20
8.19
7.61
7.61
7.50
7.49
7.49
7.48
7.44
7.44
7.43
7.42
7.35
7.34
5.65
5.63
5.19
5.16
5.15
5.14
5.13
5.11
5.11
5.10
5.07
4.89
3.77
1.00
1.07
1.01
3.02
5.27
0.90
4.02
0.92
3.12
12.0
11.5
11.0
10.5
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
0.0
-0.5
-1.0


S
N
N=N
CO2Me
NHCbz
19f
169.3
155.7
146.4
141.5
135.9
133.1
132.5
128.6
128.4
128.3
127.5
126.7
126.5
120.9
116.9
109.4
67.3
54.3
53.3
48.6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

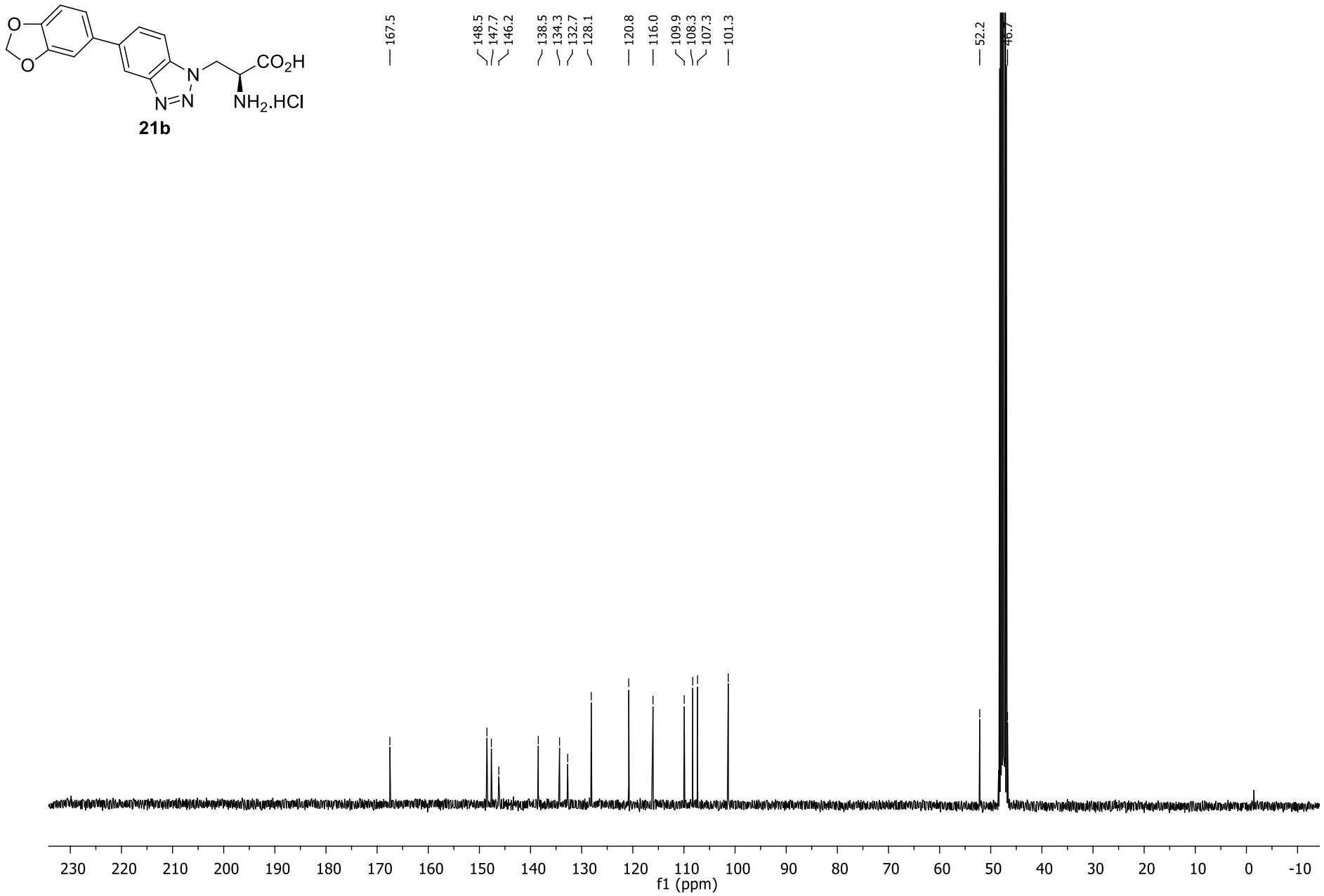

MeO
N
N=N
CO2H
NH2.HCl
21a
8.15
7.89
7.89
7.87
7.87
7.87
7.85
7.64
7.62
7.05
7.03
5.39
5.38
5.36
5.35
5.29
5.28
5.26
5.25
4.80
4.79
4.79
4.78
3.85
1.00
2.01
2.05
2.05
0.98
1.05
1.20
3.17
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0

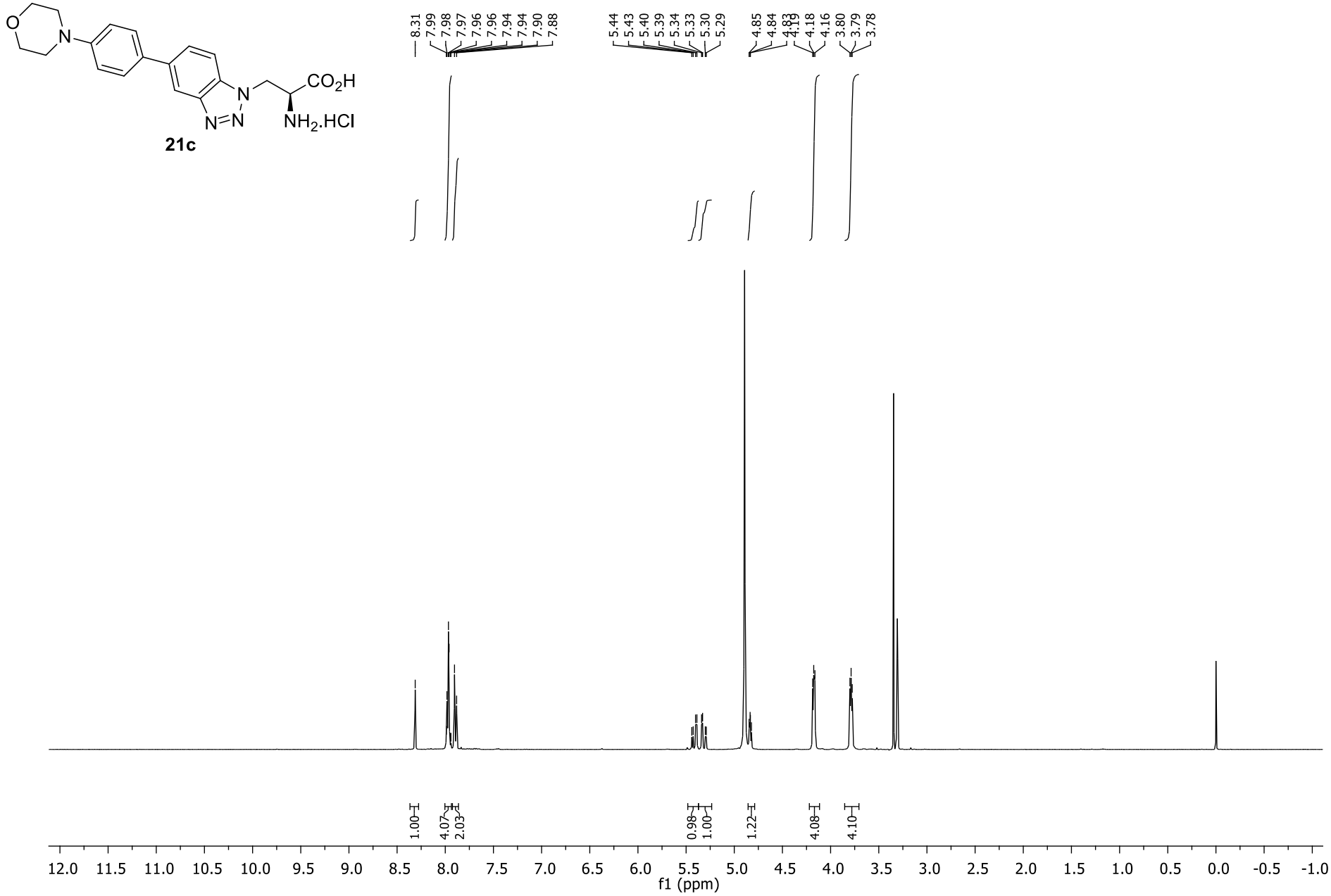

MeO
N
N=N
CO2H
NH2.HCl
21a
167.6
159.8
146.3
138.4
132.6
132.4
128.1
128.0
115.6
114.1
110.0
54.4
52.2
46.8
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

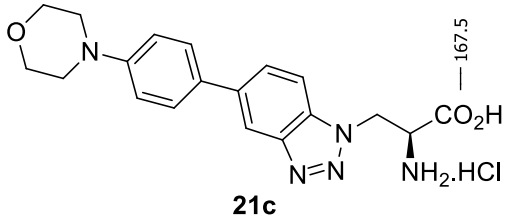

O
O
N
N=N
CO2H
NH2.HCl

21b

8.14
8.14
8.13
7.85
7.85
7.83
7.19
7.19
7.19
7.17
7.16
6.95
6.95
6.93
6.93
6.01
5.39
5.36
5.35
5.30
4.82
4.81
4.80
4.79
1.00
2.10
2.06
0.93
2.03
1.04
0.99
1.05
12.0 11.5 11.0 10.5 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 0.0 -0.5 -1.0
f1 (ppm)

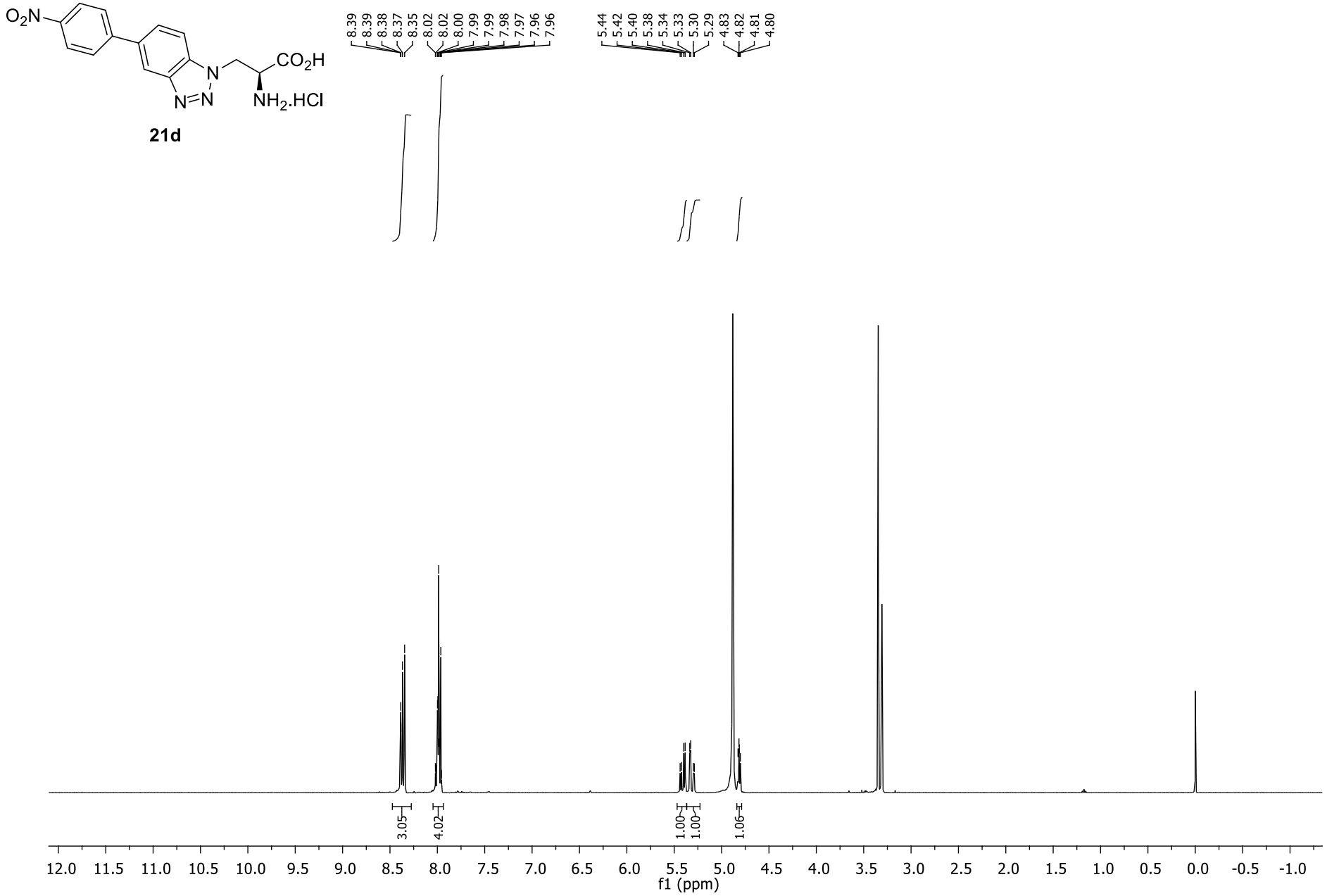

O
O
N
N=N
CO2H
NH2.HCl
21b
167.5
148.5
147.7
146.2
138.5
134.3
132.7
128.1
120.8
116.0
109.9
108.3
107.3
101.3
52.2
46.7
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

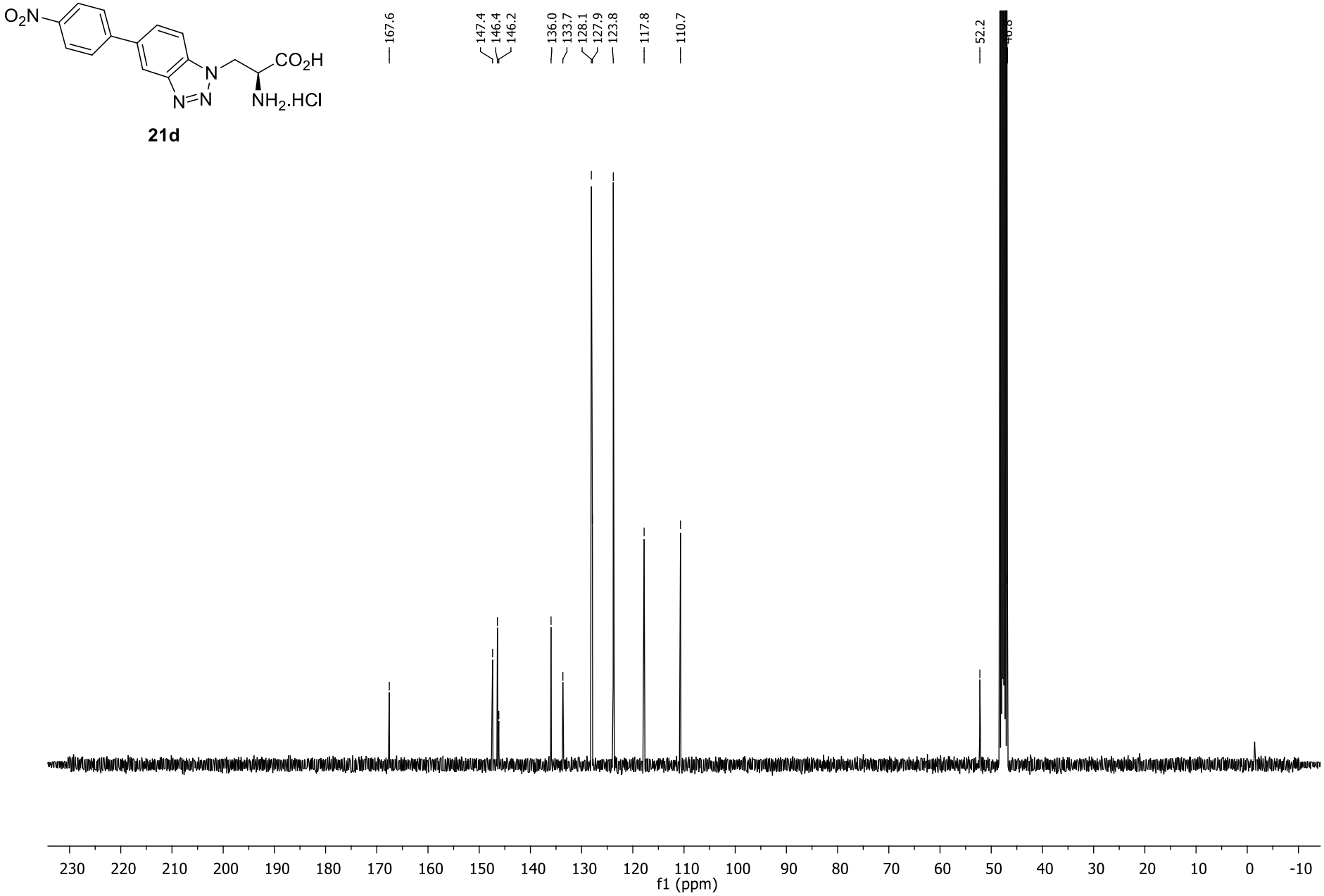

21c
8.31
7.99
7.98
7.97
7.96
7.96
7.94
7.94
7.90
7.88
5.44
5.43
5.40
5.39
5.34
5.33
5.30
5.29
4.85
4.84
4.83
4.19
4.18
4.16
3.80
3.79
3.78
1.00
4.07
2.03
0.98
1.00
1.22
4.08
4.10
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

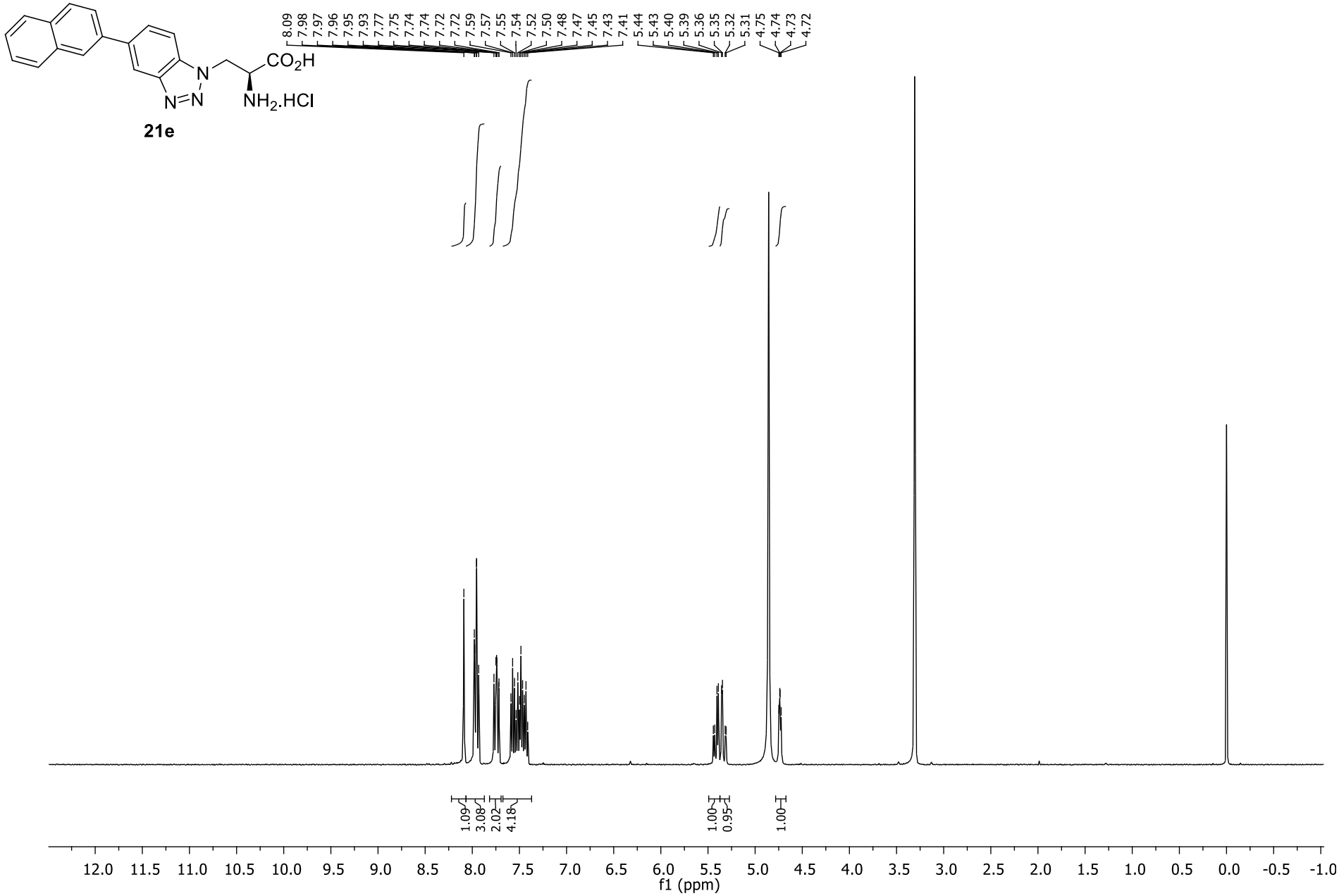

O
N
N
N=N
CO2H
NH2.HCl

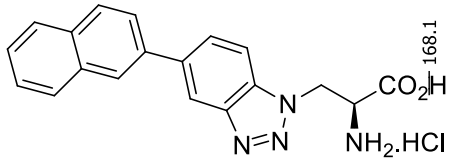
21c

167.5
146.2
141.9
141.3
136.3
133.4
129.1
127.9
121.5
117.2
110.6
64.1
54.9
52.1
46.8
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O2N
CO2H
N
N=N
NH2.HCl
21d
8.39
8.39
8.38
8.37
8.35
8.02
8.02
8.00
7.99
7.99
7.98
7.97
7.96
7.96
5.44
5.42
5.40
5.38
5.34
5.33
5.30
5.29
4.83
4.82
4.81
4.80
3.05
4.02
1.00
1.00
1.06
12.0 11.5 11.0 10.5 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 0.0 -0.5 -1.0
f1 (ppm)

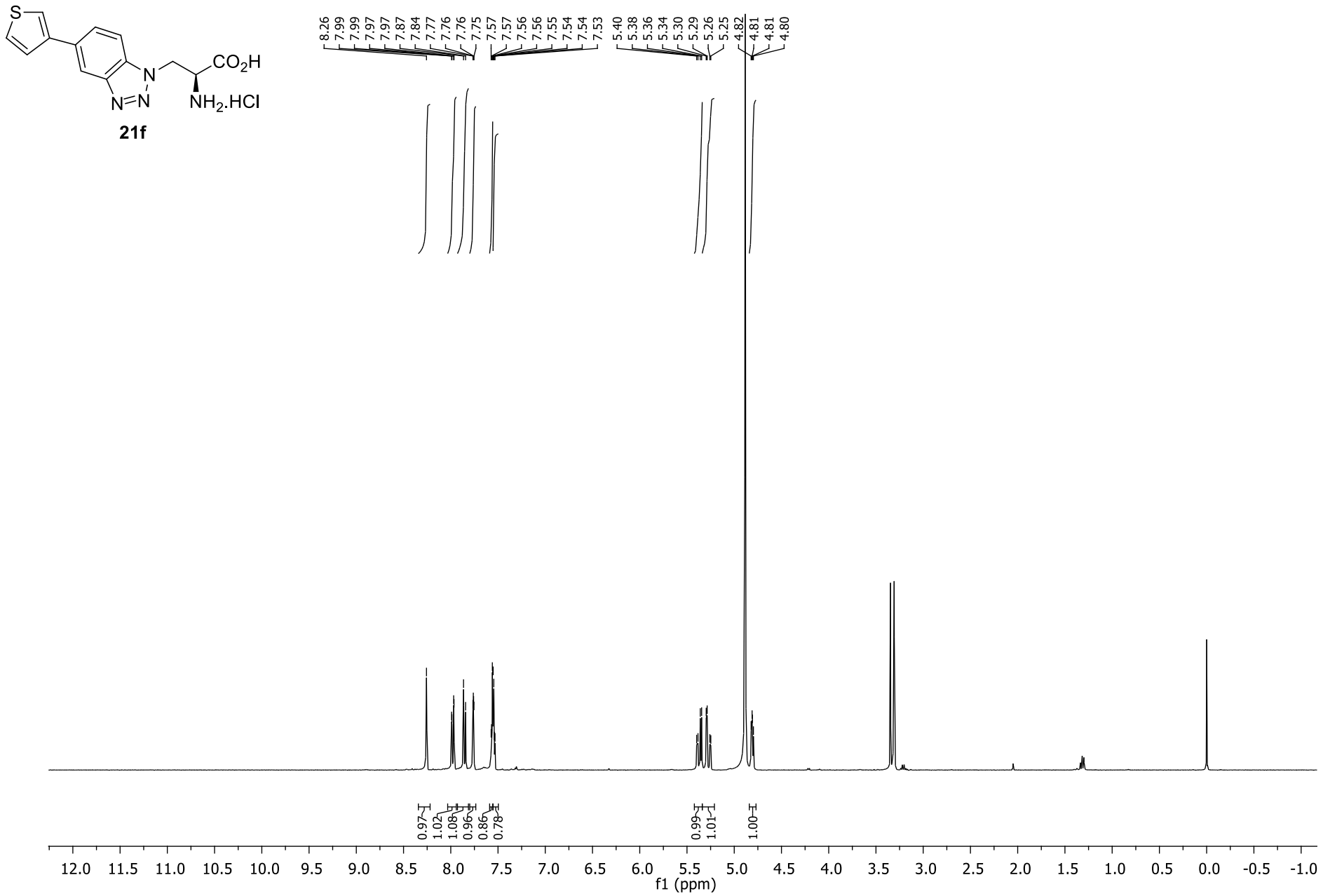

O2N
CO2H
NH2.HCl
N
N=N
21d
167.6
147.4
146.4
146.2
136.0
133.7
128.1
127.9
123.8
117.8
110.7
52.2
46.8
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

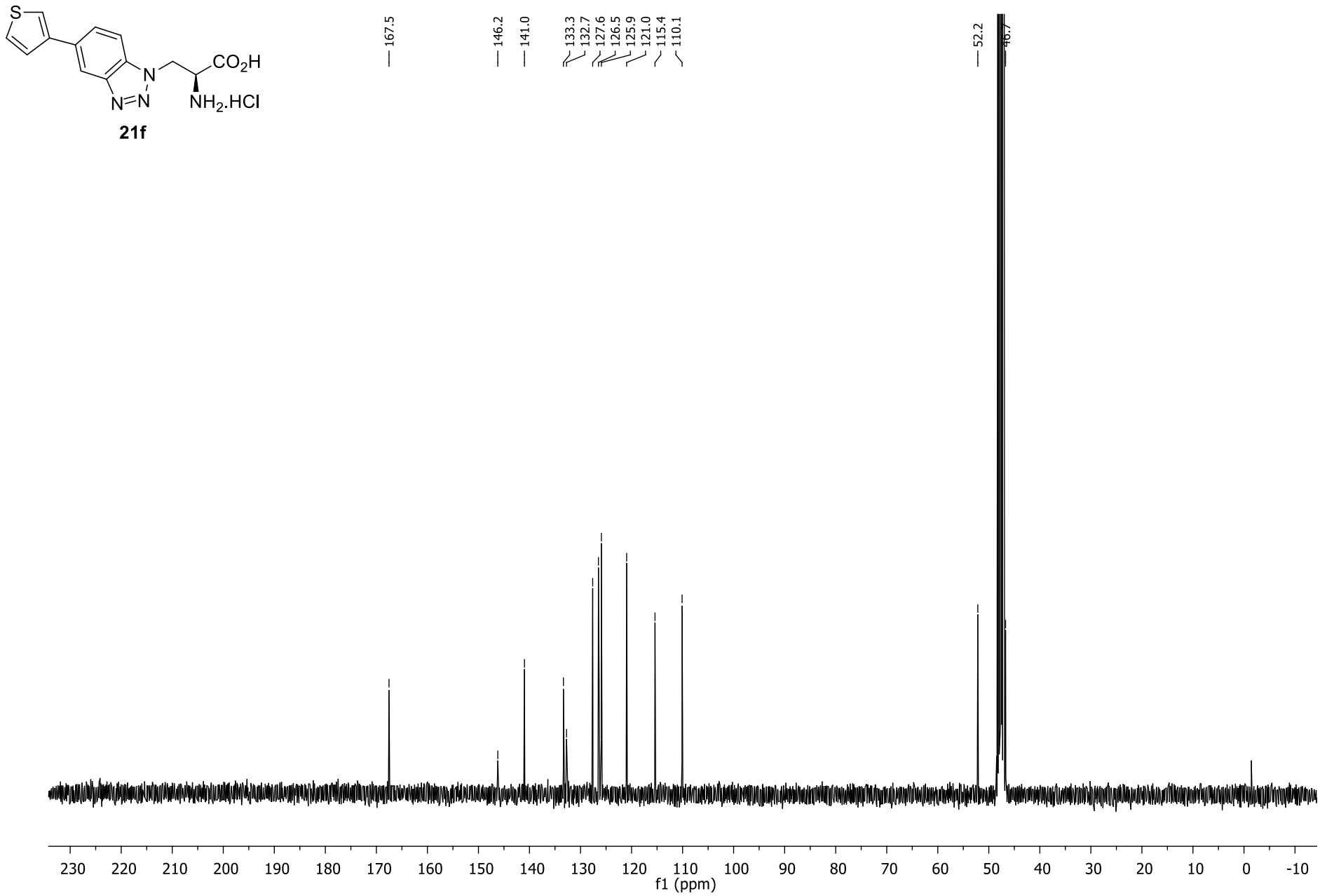

8.09
7.98
7.97
7.96
7.95
7.93
7.77
7.75
7.74
7.74
7.72
7.72
7.59
7.57
7.55
7.54
7.52
7.50
7.48
7.47
7.45
7.43
7.41
5.44
5.43
5.40
5.39
5.36
5.35
5.32
5.31
4.75
4.74
4.73
4.72
CO2H
NH2.HCl
21e
1.09
3.08
2.02
4.18
1.00
0.95
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

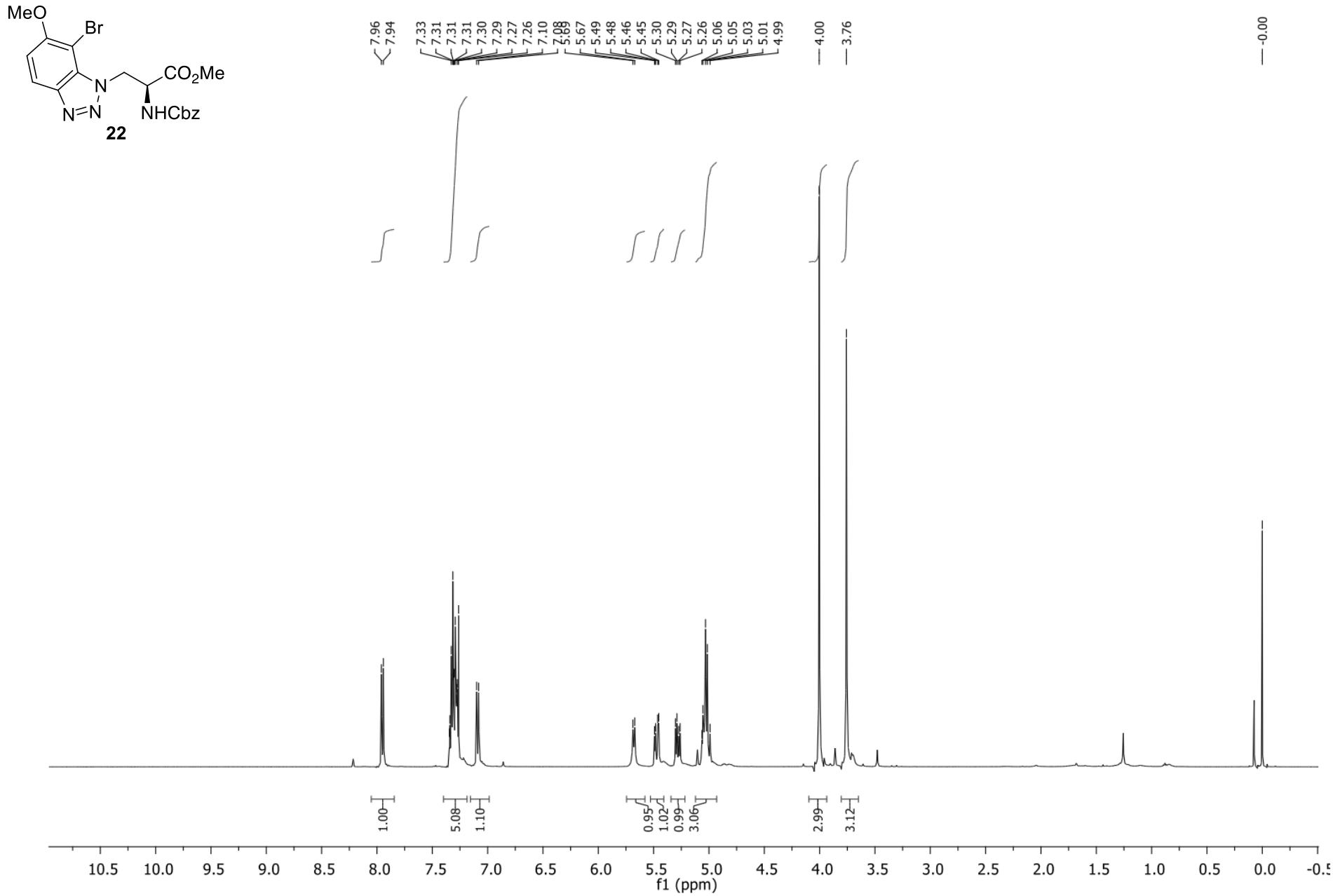

CO2H
N
N=N
NH2.HCl

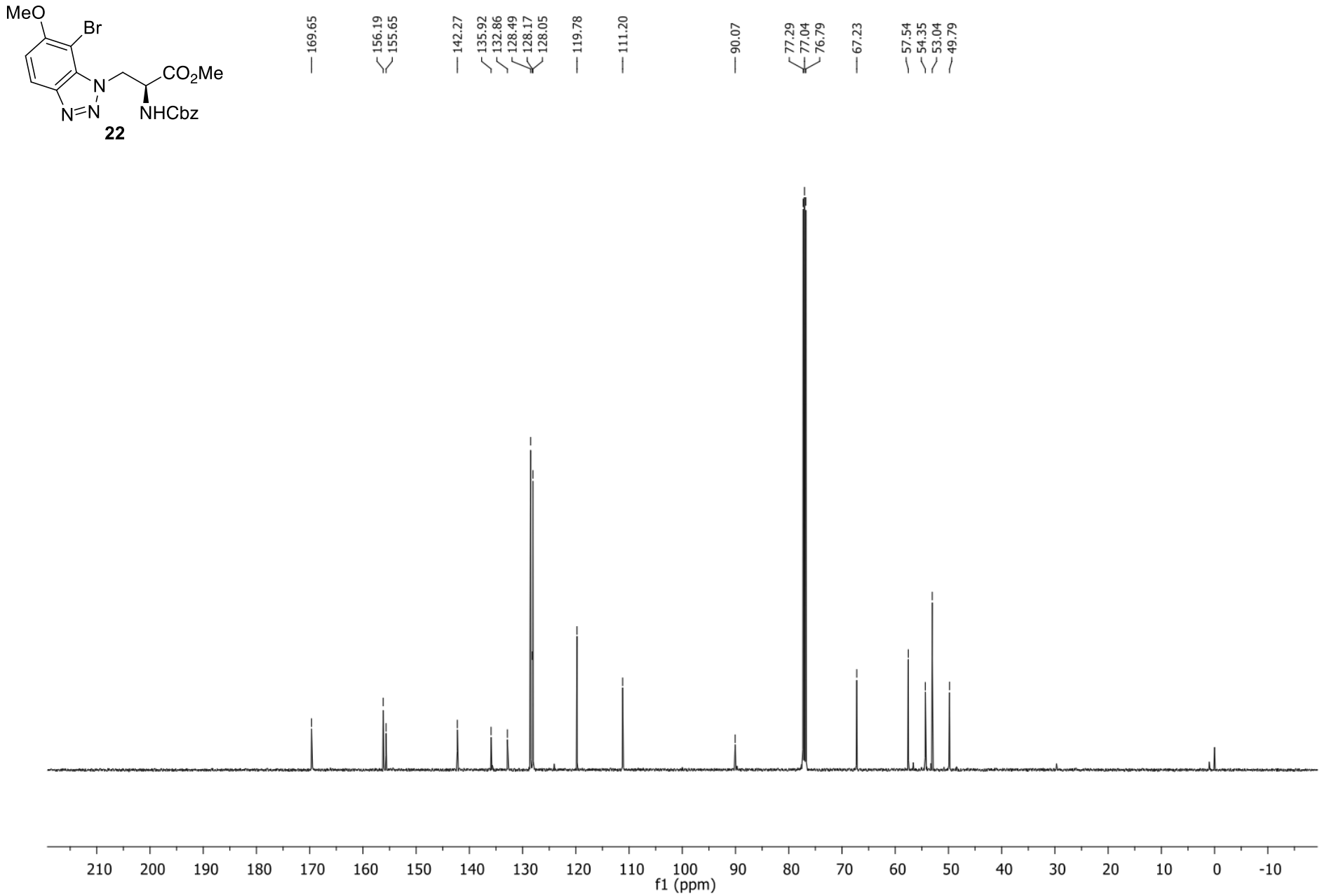
21e

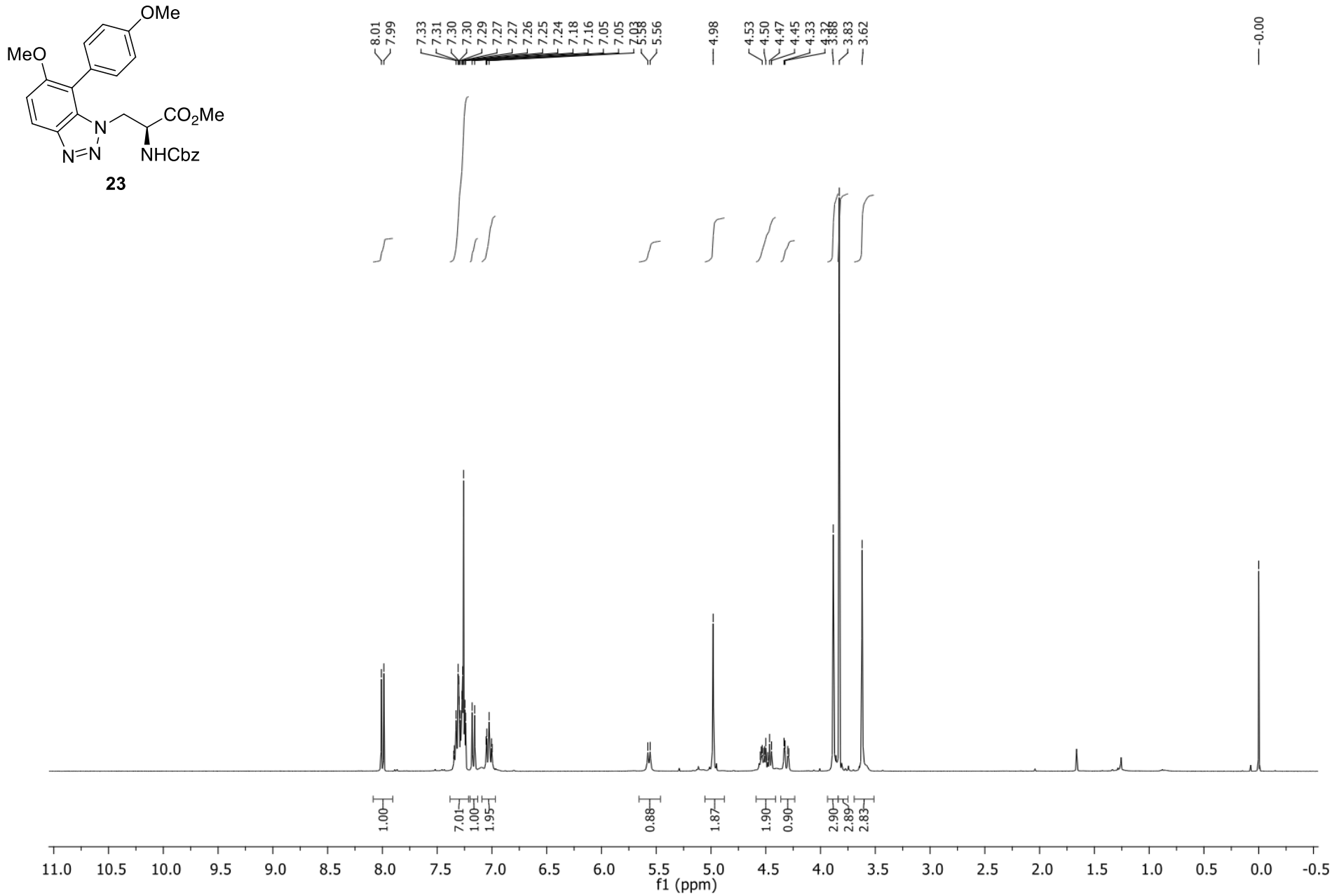
168.1
145.8
137.9
134.0
130.7
128.2
127.9
127.1
126.0
125.7
125.1
125.0
119.5
109.7
52.7
47.0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

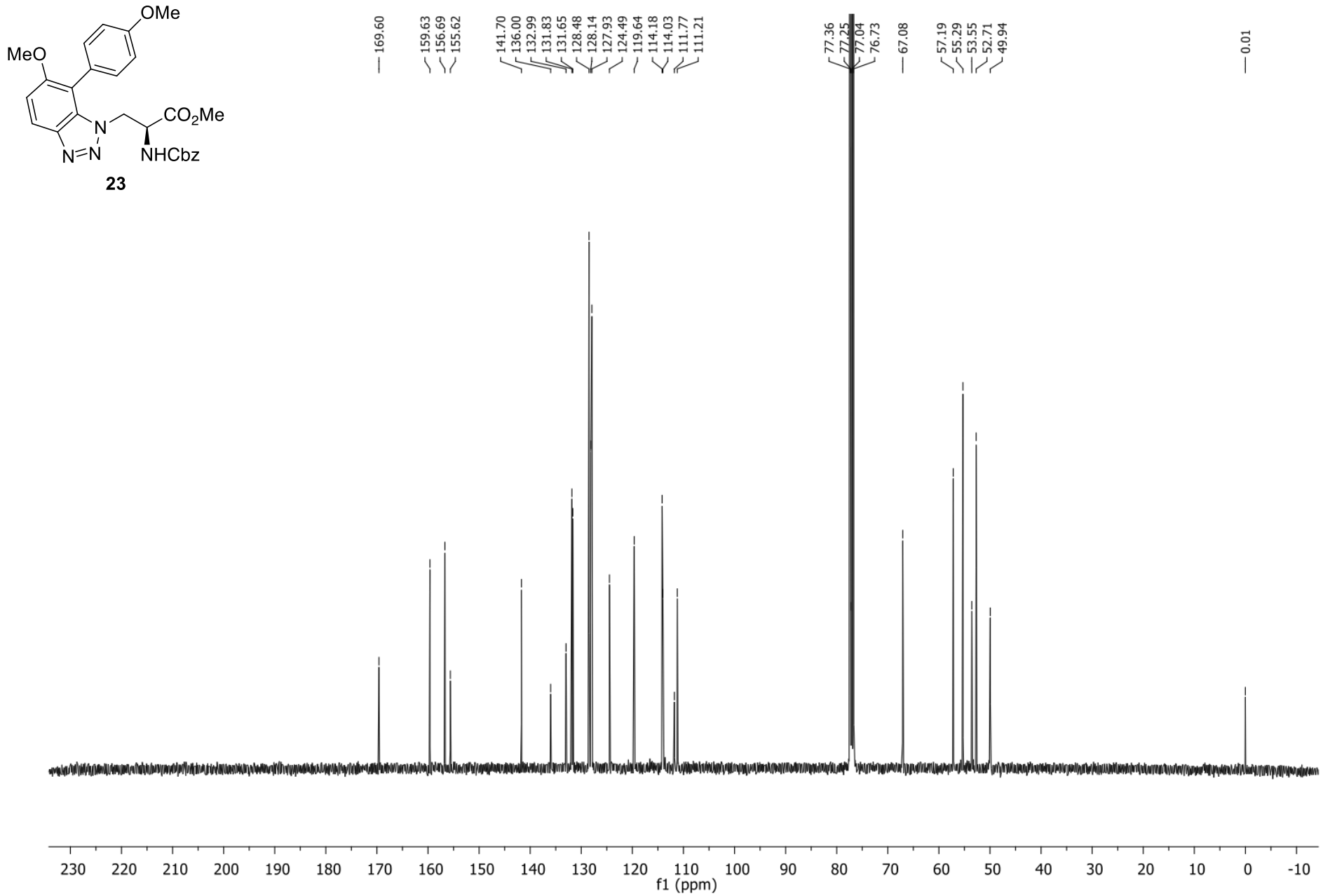

S
N
N
N
CO2H
NH2.HCl
21f
8.26
7.99
7.99
7.97
7.97
7.87
7.84
7.77
7.76
7.76
7.75
7.57
7.57
7.56
7.56
7.55
7.54
7.54
7.53
5.40
5.38
5.36
5.34
5.30
5.29
5.26
5.25
4.82
4.81
4.81
4.80
0.97
1.02
1.08
0.96
0.86
0.78
0.99
1.01
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

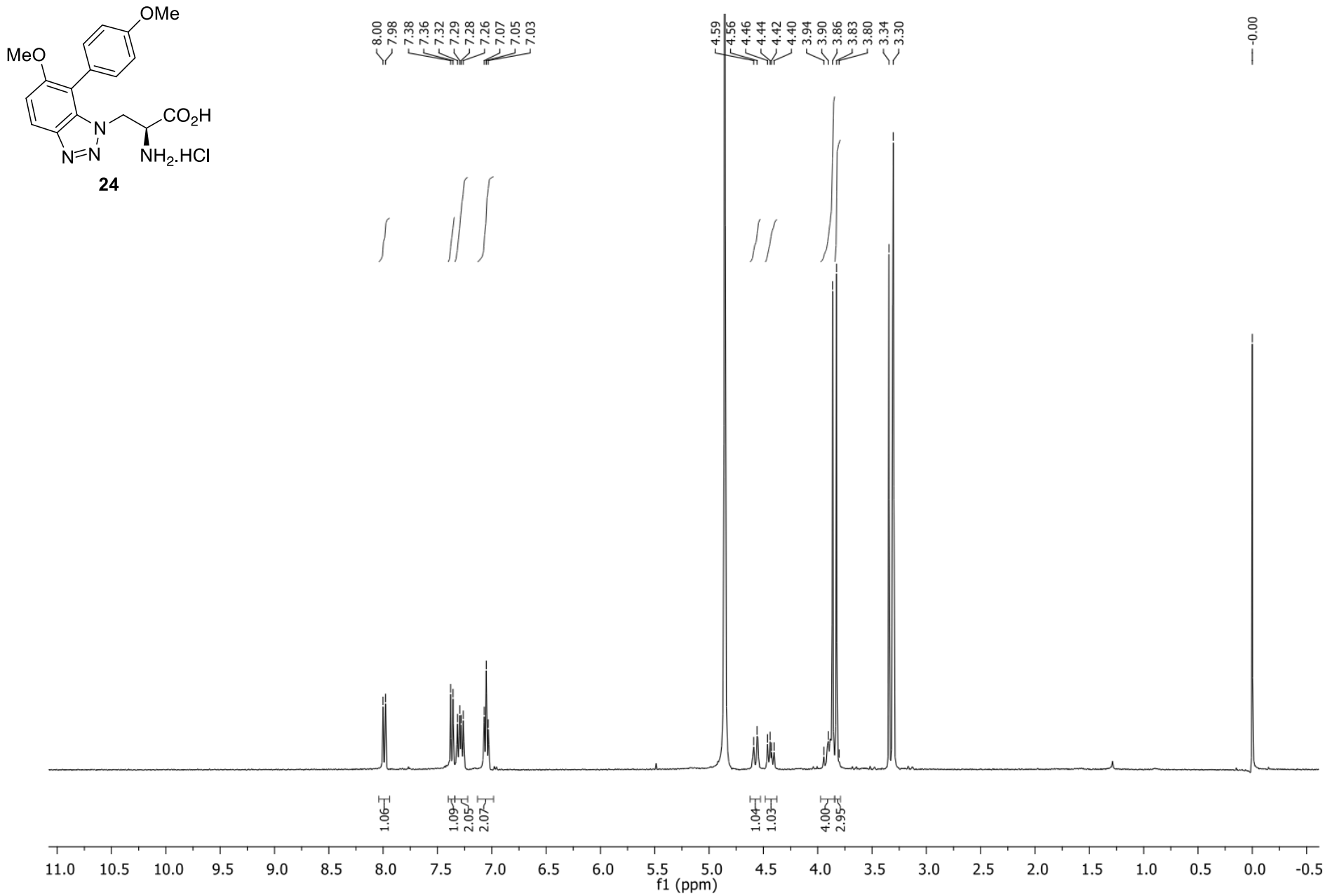

S
N
N
N
CO2H
NH2.HCl
21f
167.5
146.2
141.0
133.3
132.7
127.6
126.5
125.9
121.0
115.4
110.1
52.2
46.7
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

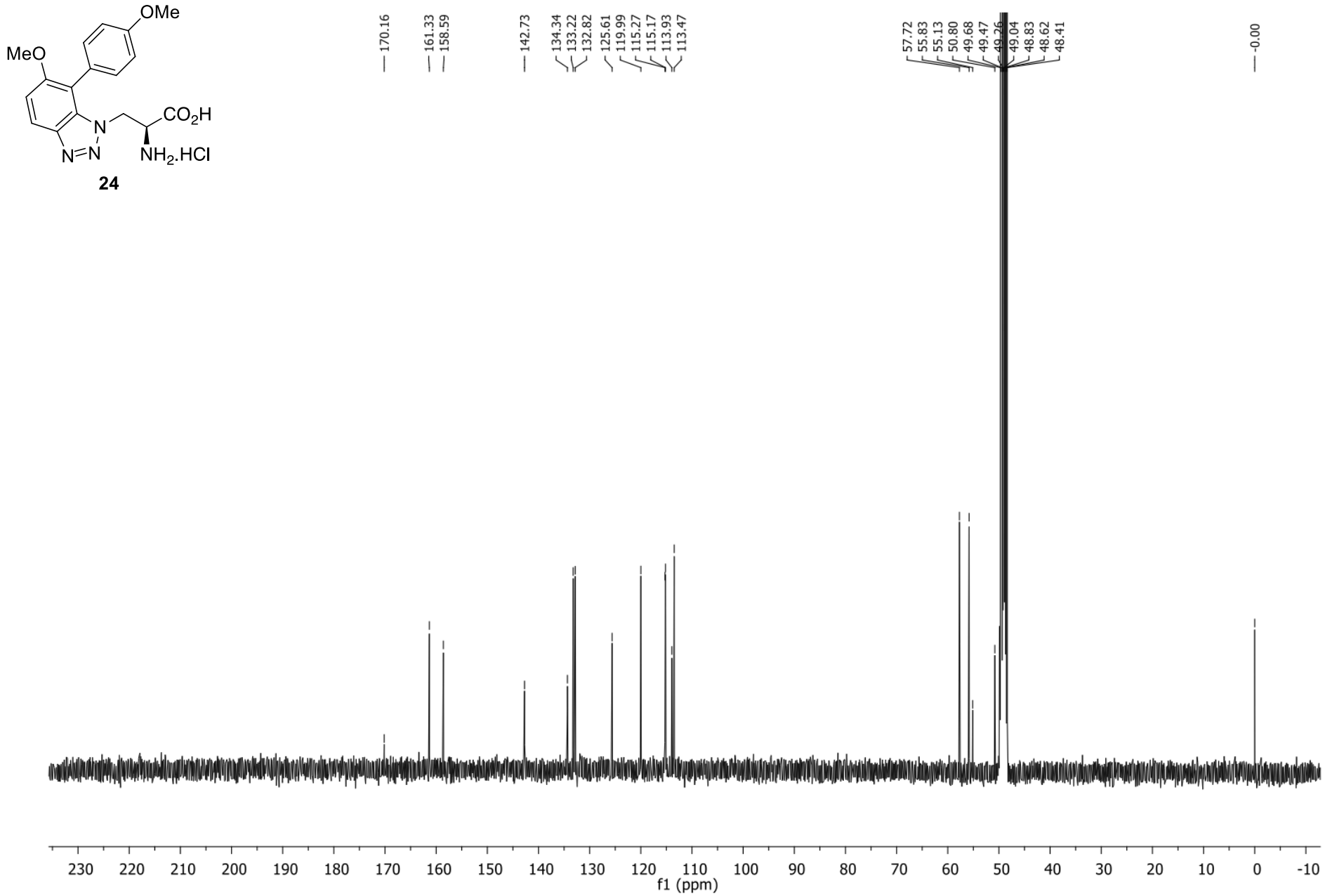

MeO
Br
N
N=N
CO2Me
NHCbz
22
7.96
7.94
7.33
7.31
7.31
7.31
7.30
7.29
7.27
7.26
7.10
5.67
5.49
5.48
5.46
5.45
5.30
5.29
5.27
5.26
5.06
5.05
5.03
5.01
4.99
4.00
3.76
-0.00
1.00
5.08
1.10
0.95
1.02
0.99
3.06
2.99
3.12
f1 (ppm)


MeO
Br
N
N=N
CO2Me
NHCbz
22
169.65
156.19
155.65
142.27
135.92
132.86
128.49
128.17
128.05
119.78
111.20
90.07
77.29
77.04
76.79
67.23
57.54
54.35
53.04
49.79
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OMe
MeO
CO2Me
N
N=N
NHCbz
23
8.01
7.99
7.33
7.31
7.30
7.30
7.29
7.27
7.27
7.26
7.25
7.24
7.18
7.16
7.05
7.05
7.03
5.58
5.56
4.98
4.53
4.50
4.47
4.45
4.33
3.88
3.83
3.62
-0.00
1.00
7.01
1.00
1.95
0.88
1.87
1.90
0.90
2.90
2.89
2.83
11.0
10.5
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
0.0
-0.5
f1 (ppm)


OMe
MeO
CO2Me
N
N=N
NHCbz
23
169.60
159.63
156.69
155.62
141.70
136.00
132.99
131.83
131.65
128.48
128.14
127.93
124.49
119.64
114.18
114.03
111.77
111.21
77.36
77.25
77.04
76.73
67.08
57.19
55.29
53.55
52.71
49.94
0.01
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OMe
MeO
CO2H
N
N=N
NH2.HCl
24
8.00
7.98
7.38
7.36
7.32
7.29
7.28
7.26
7.07
7.05
7.03
4.59
4.56
4.46
4.44
4.42
4.40
3.94
3.90
3.86
3.83
3.80
3.34
3.30
-0.00
1.06
1.09
2.05
2.07
1.04
1.03
4.00
2.95
11.0
10.5
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
0.0
-0.5
f1 (ppm)


OMe
MeO
CO2H
N
N=N
NH2.HCl
24
170.16
161.33
158.59
142.73
134.34
133.22
132.82
125.61
119.99
115.27
115.17
113.93
113.47
57.72
55.83
55.13
50.80
49.68
49.47
49.26
49.04
48.83
48.62
48.41
-0.00
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)