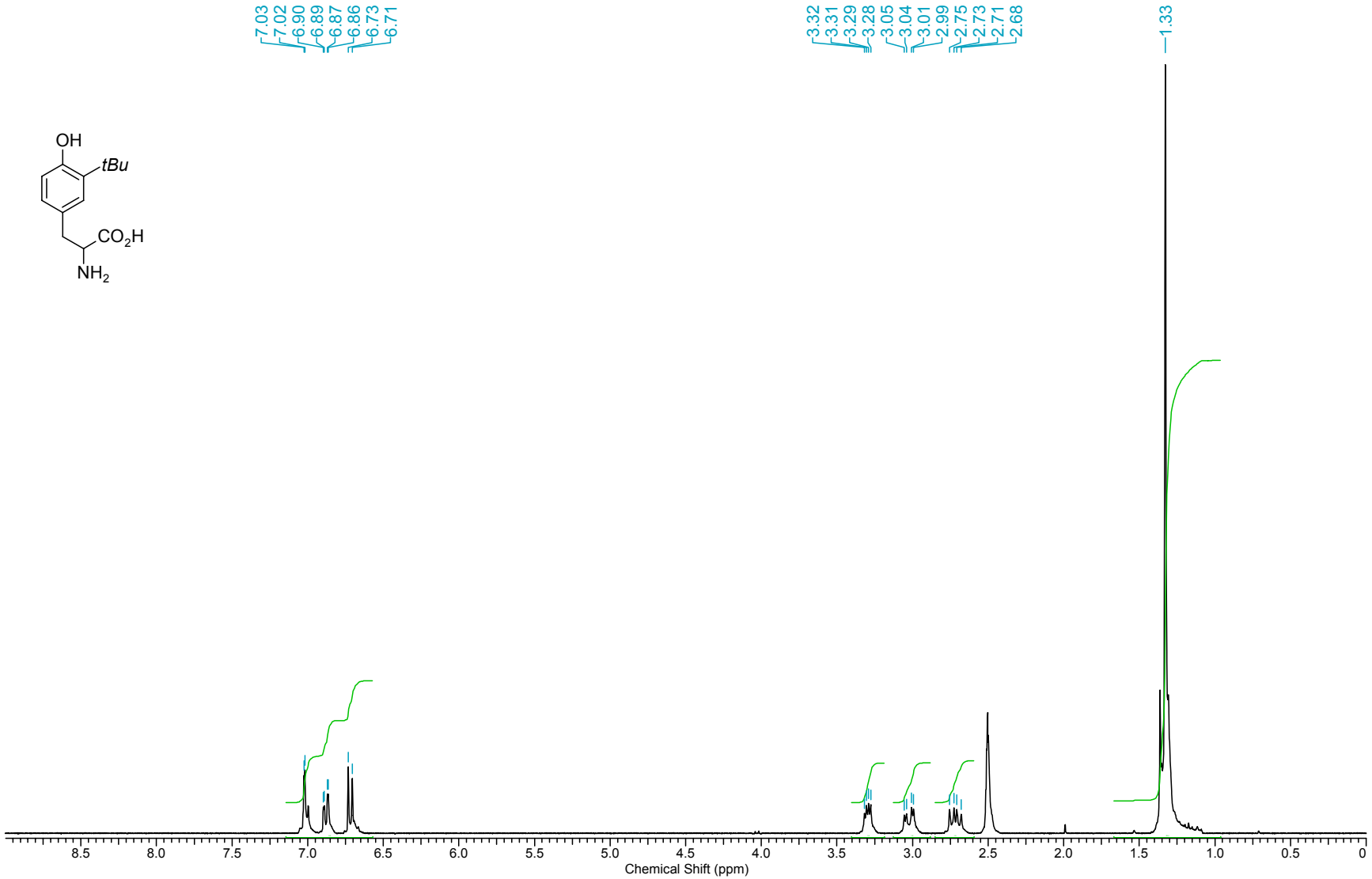
The Catalytic *Ortho*-Arylation of Tyrosine

Robin B. Bedford, Mairi F. Haddow, Ruth L. Webster and Charlotte J. Mitchell.

Supporting Information

General experimental conditions. Chemical reagents were used as supplied from commercial sources unless otherwise specified. All reactions used anhydrous solvents. All reactions were performed in oven dried glassware and flame dried prior to each reaction. Reactions were prepared in a glovebox or using standard schlenk line techniques. Compounds **1** and **4b** were dried by toluene azeotrope (x 3) prior to use. Melting points were uncorrected. The microwave reaction was carried out with an Emrys Optimiser Microwave (0-20 bar pressure range, 15-300 W power range from a magnetron operating at 2.45 GHz). The reaction was carried out in a 5 mL sealed microwave vial equipped with magnetic stirrer, heating to 150 °C at a rate of 2 to 5 °C/s, then held for 3 h. The temperature was monitored by an internal IR sensor.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3.04
3.01
2.99
2.75
2.73
2.71
2.68
1.33
OH
tBu
CO2H
NH2
8.5
8.0
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7.0
6.5
6.0
5.5
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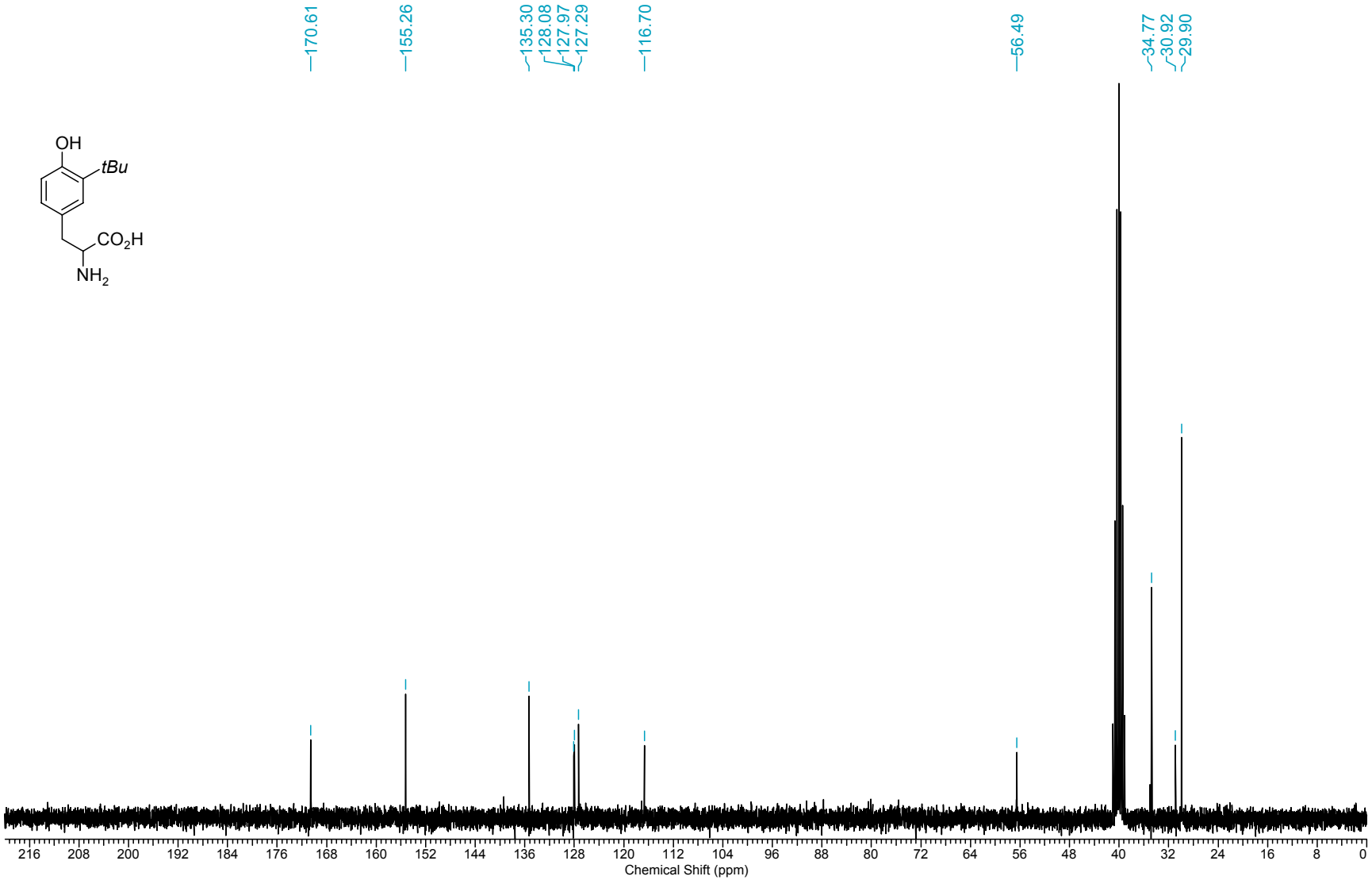
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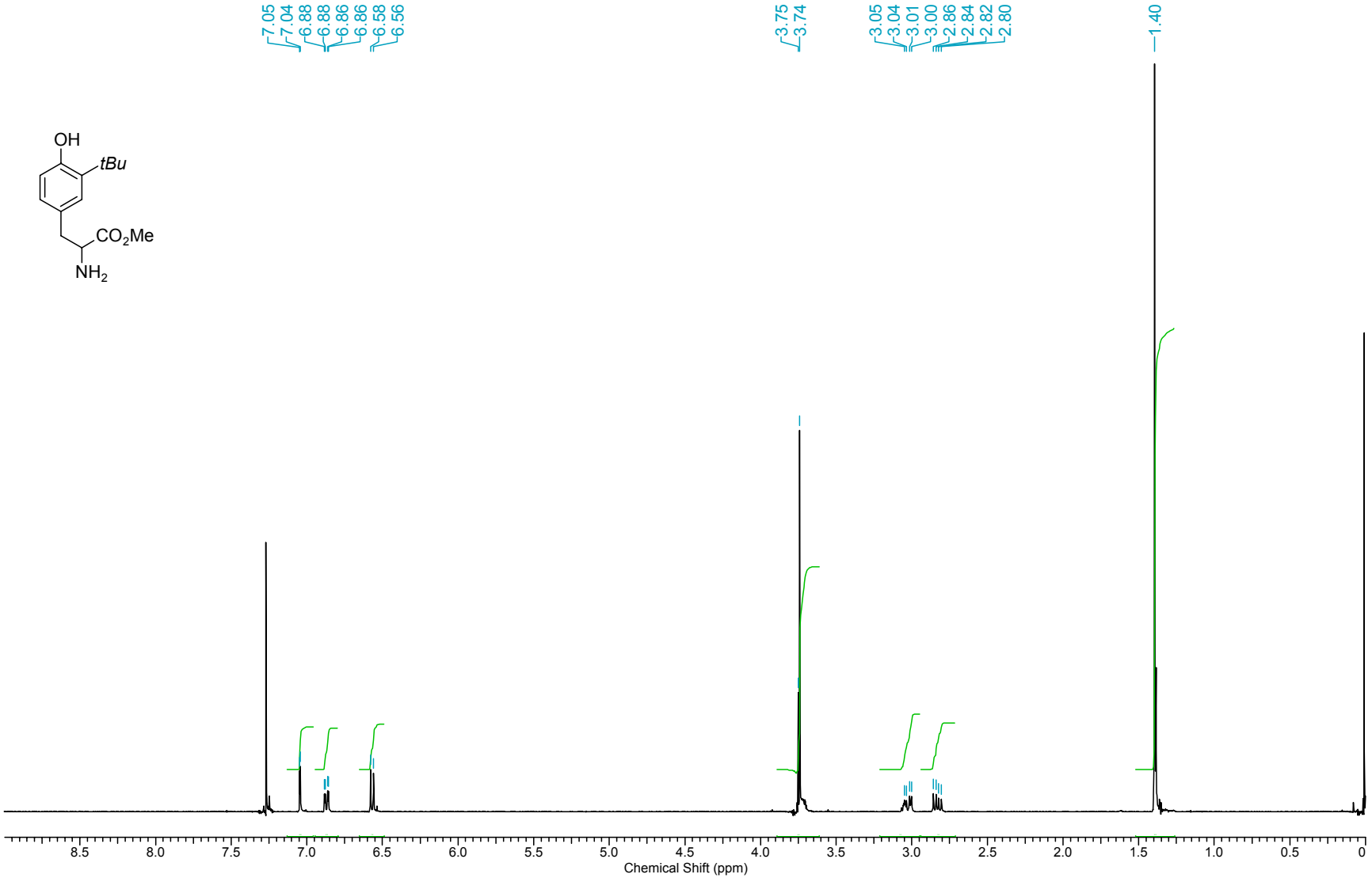
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3.00
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2.82
2.80
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tBu
CO2Me
NH2
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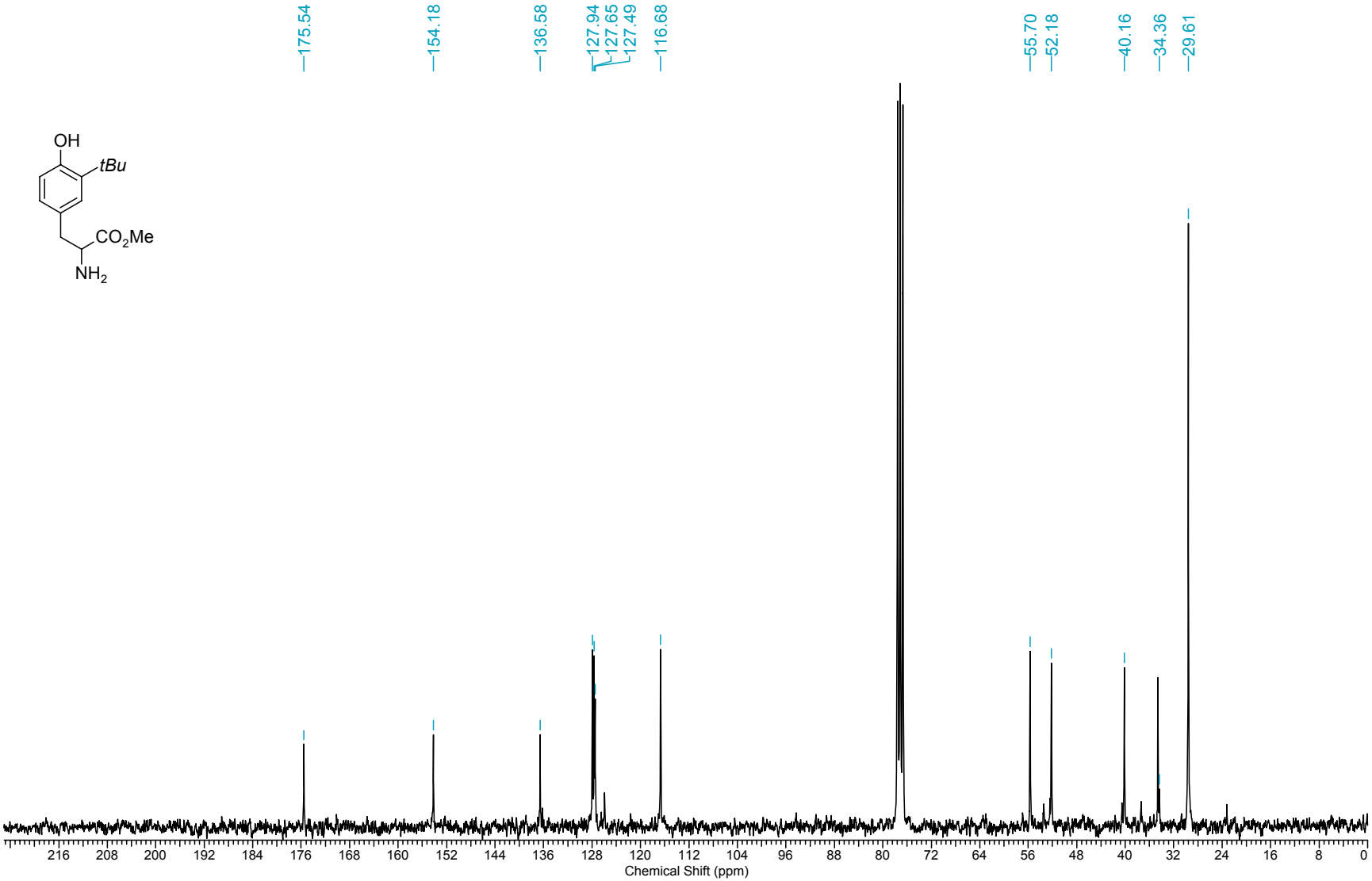
Chemical Shift (ppm)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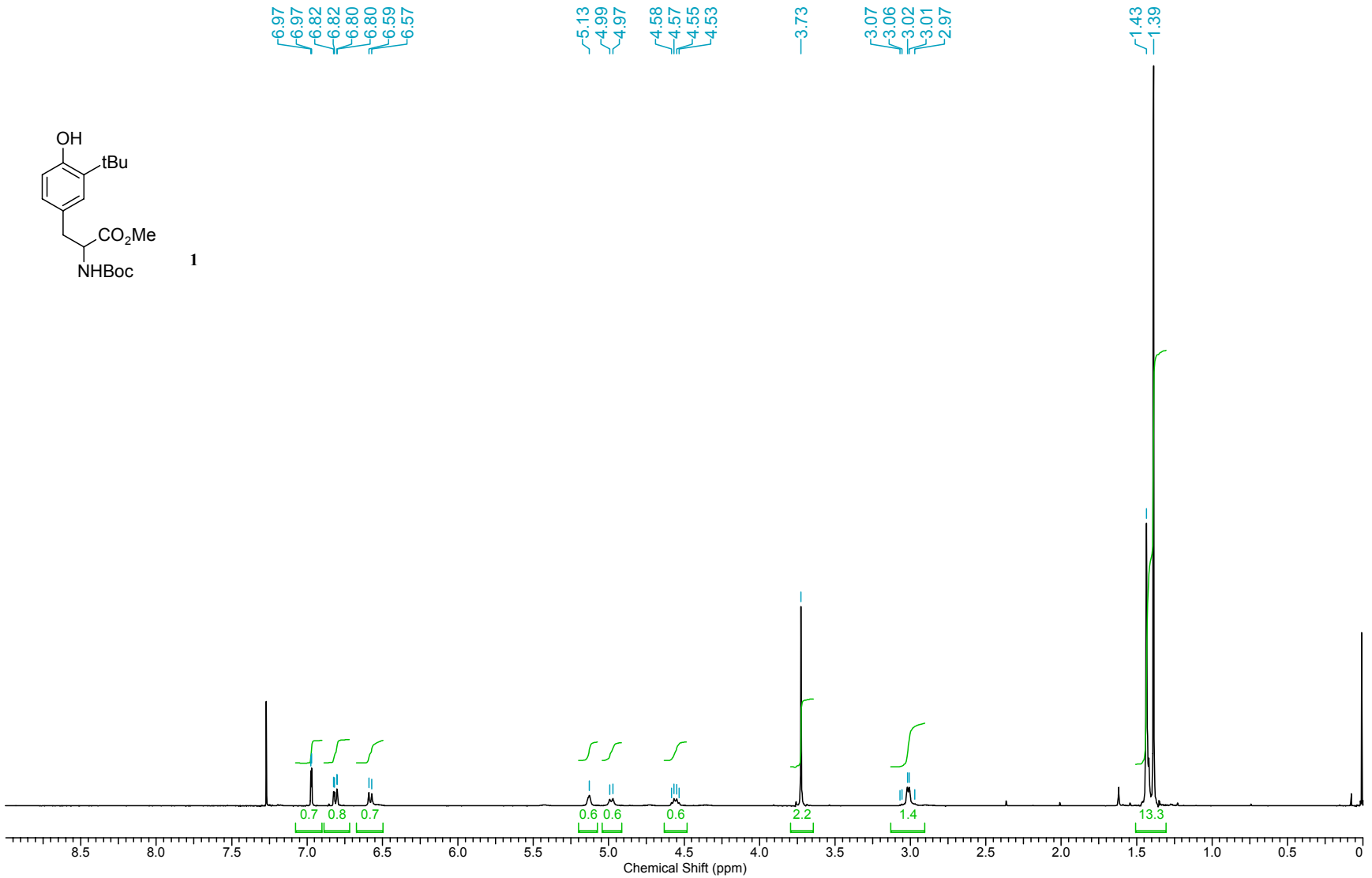
Chemical Shift (ppm)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3.06
3.02
3.01
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1.39
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CO2Me
NHBoc
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0.6
2.2
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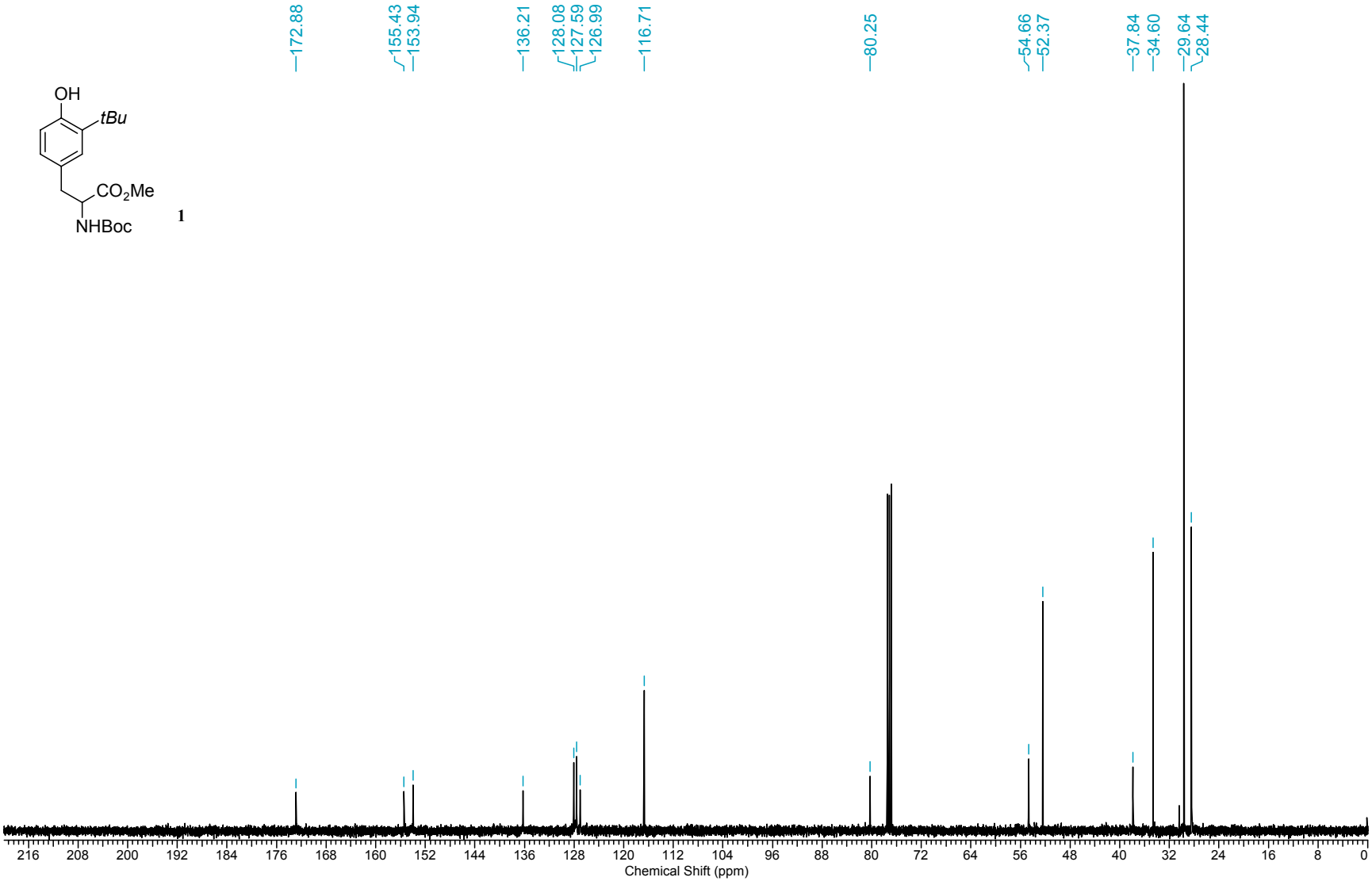
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29.64
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NHBoc
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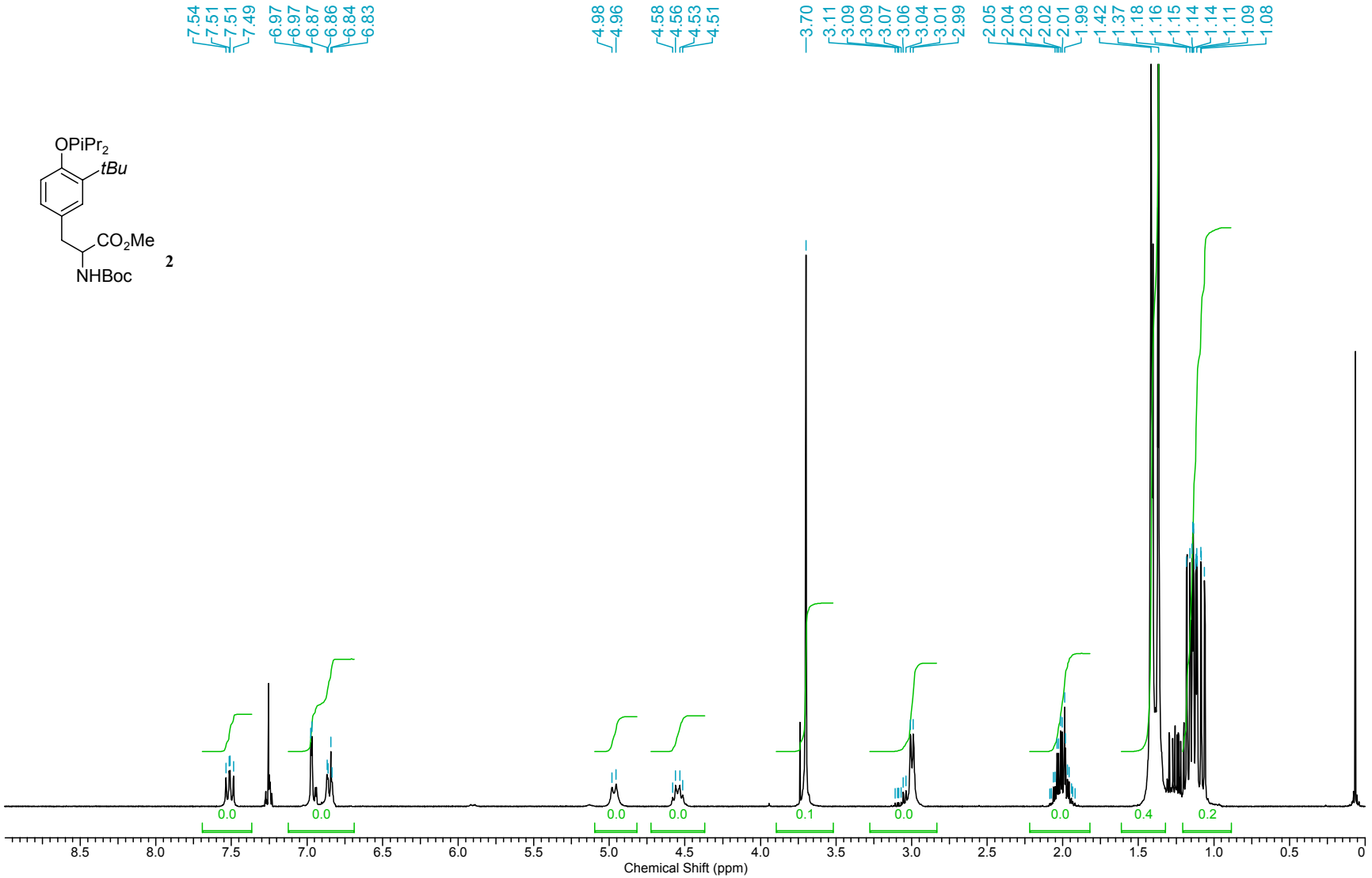
Chemical Shift (ppm)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2.05
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2.02
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1.15
1.14
1.14
1.11
1.09
1.08
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CO2Me
NHBoc
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0.2
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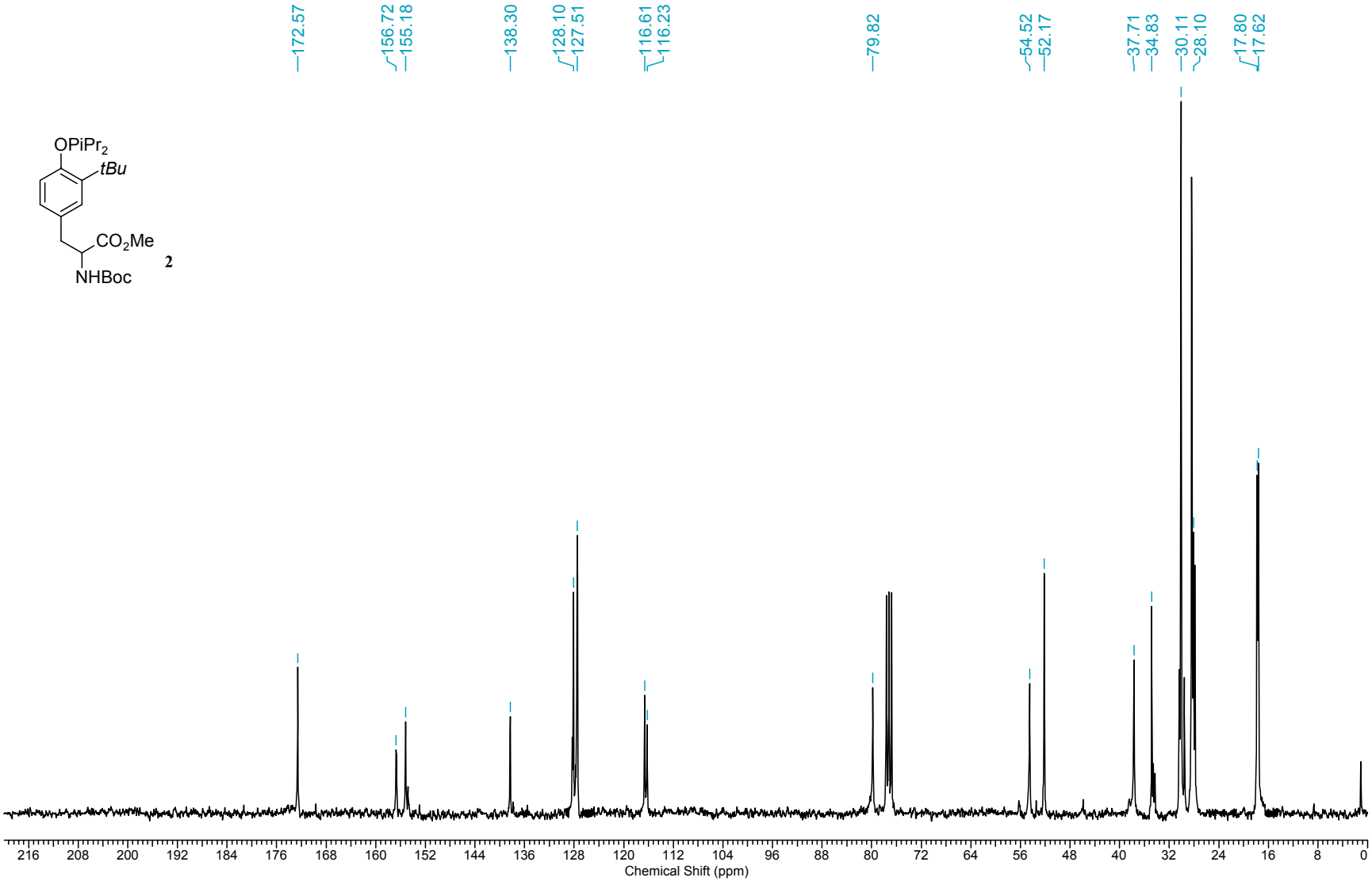
Chemical Shift (ppm)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28.10
17.80
17.62
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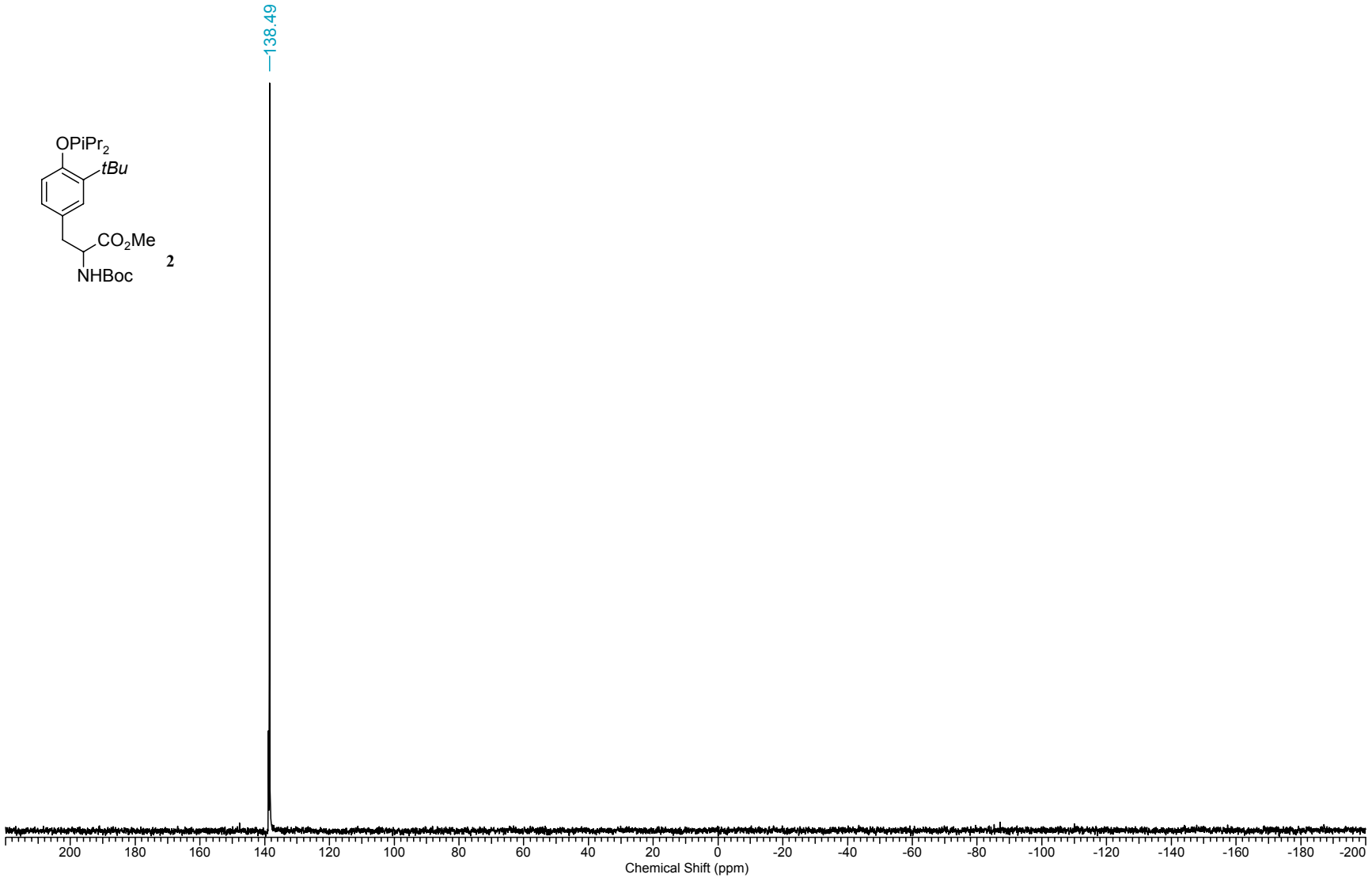
Chemical Shift (ppm)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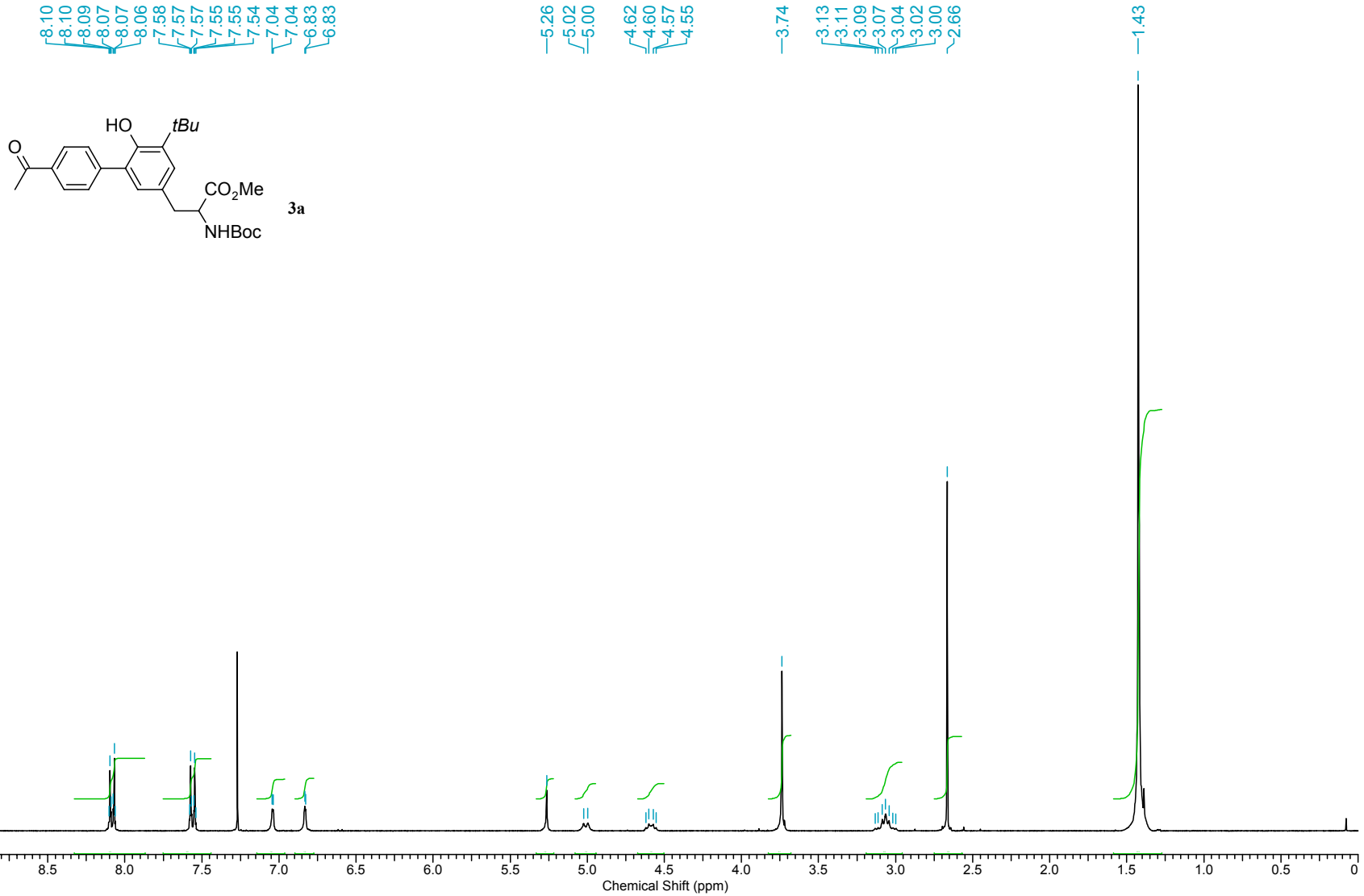
Chemical Shift (ppm)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3.74
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HO
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O
CO2Me
NHBoc
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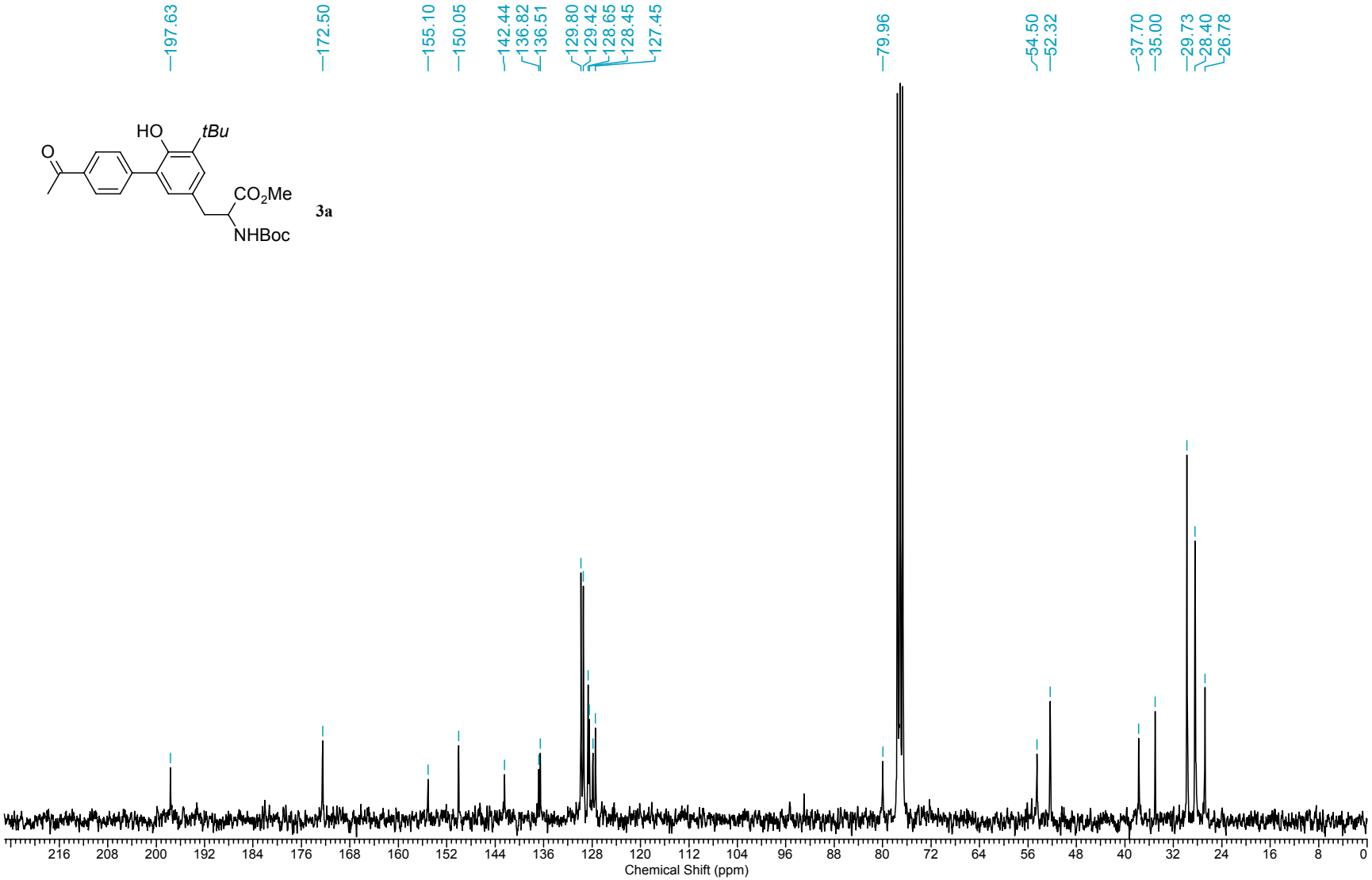
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52.32
37.70
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26.78
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NHBoc
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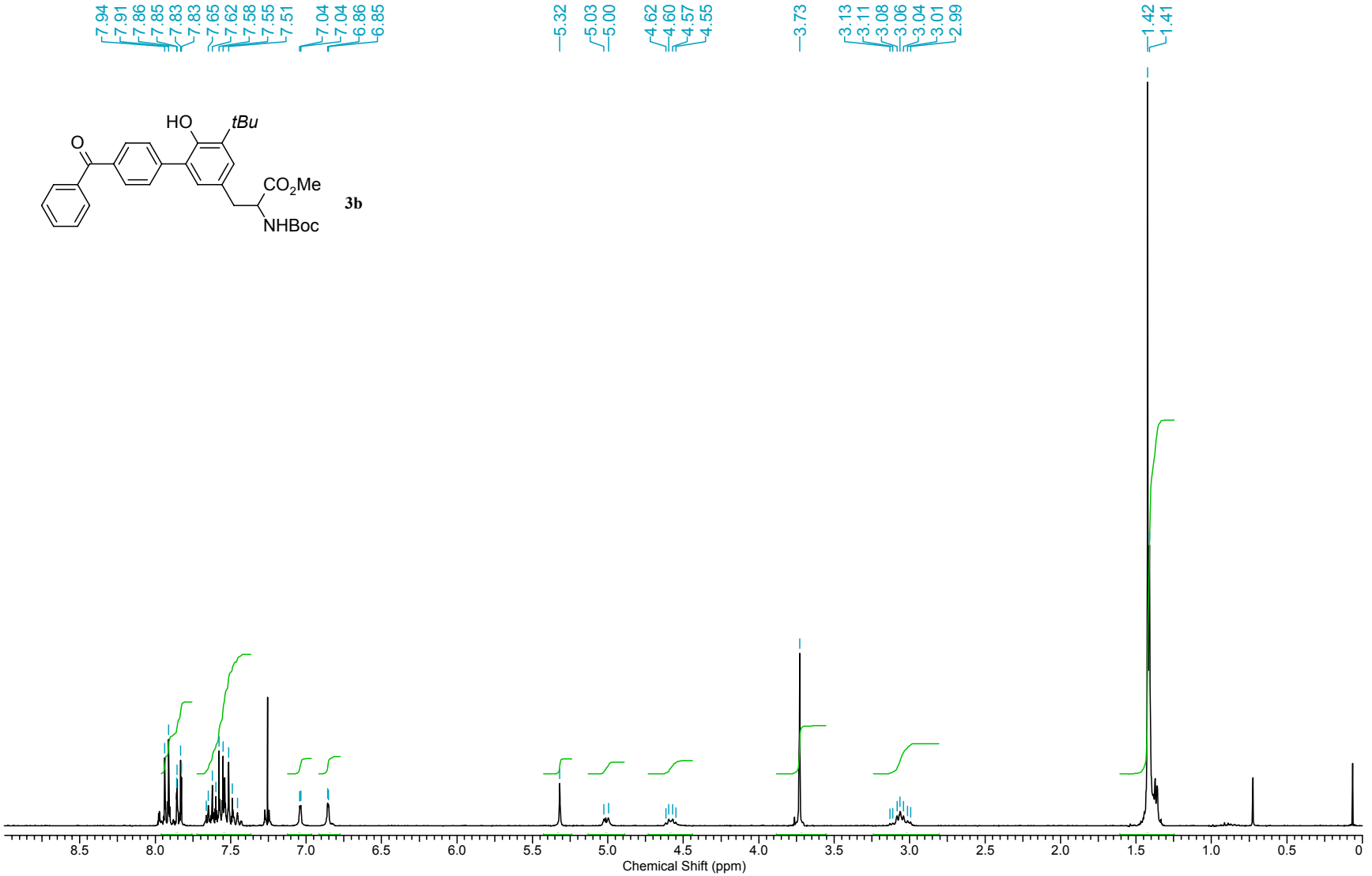
Chemical Shift (ppm)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4.55
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3.11
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3.01
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1.41
HO
tBu
O
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NHBoc
3b
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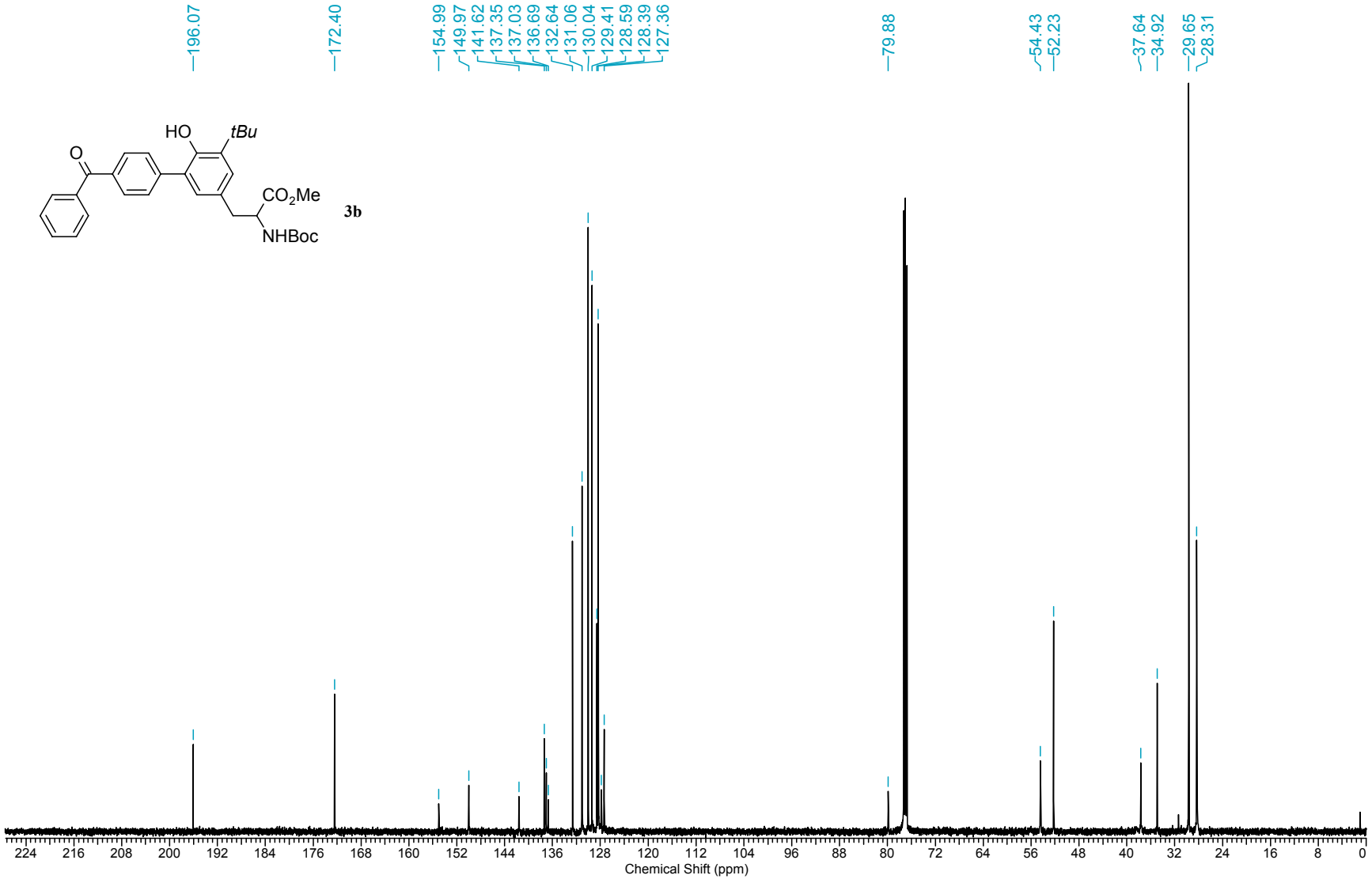
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28.31
HO
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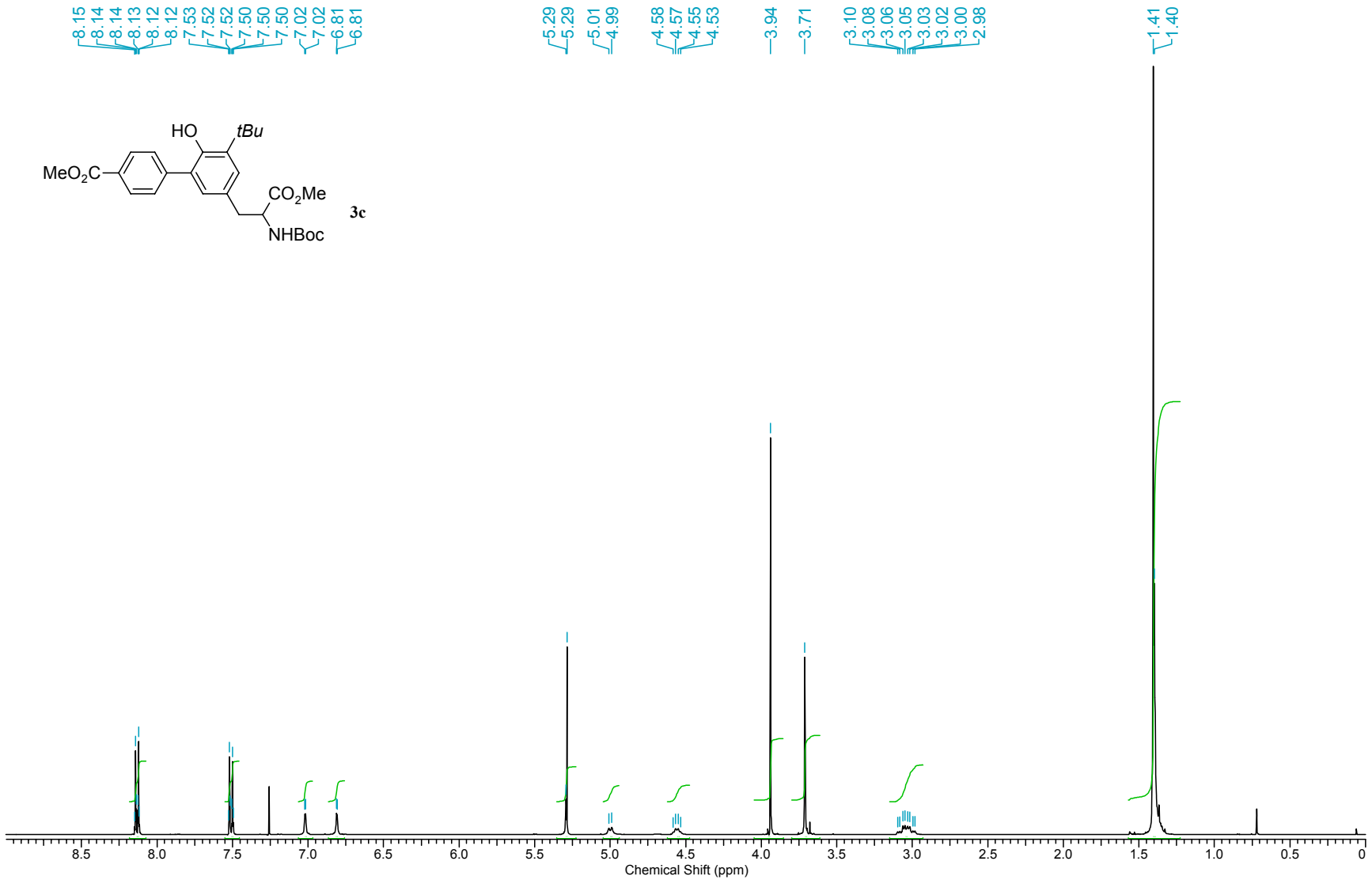
Chemical Shift (ppm)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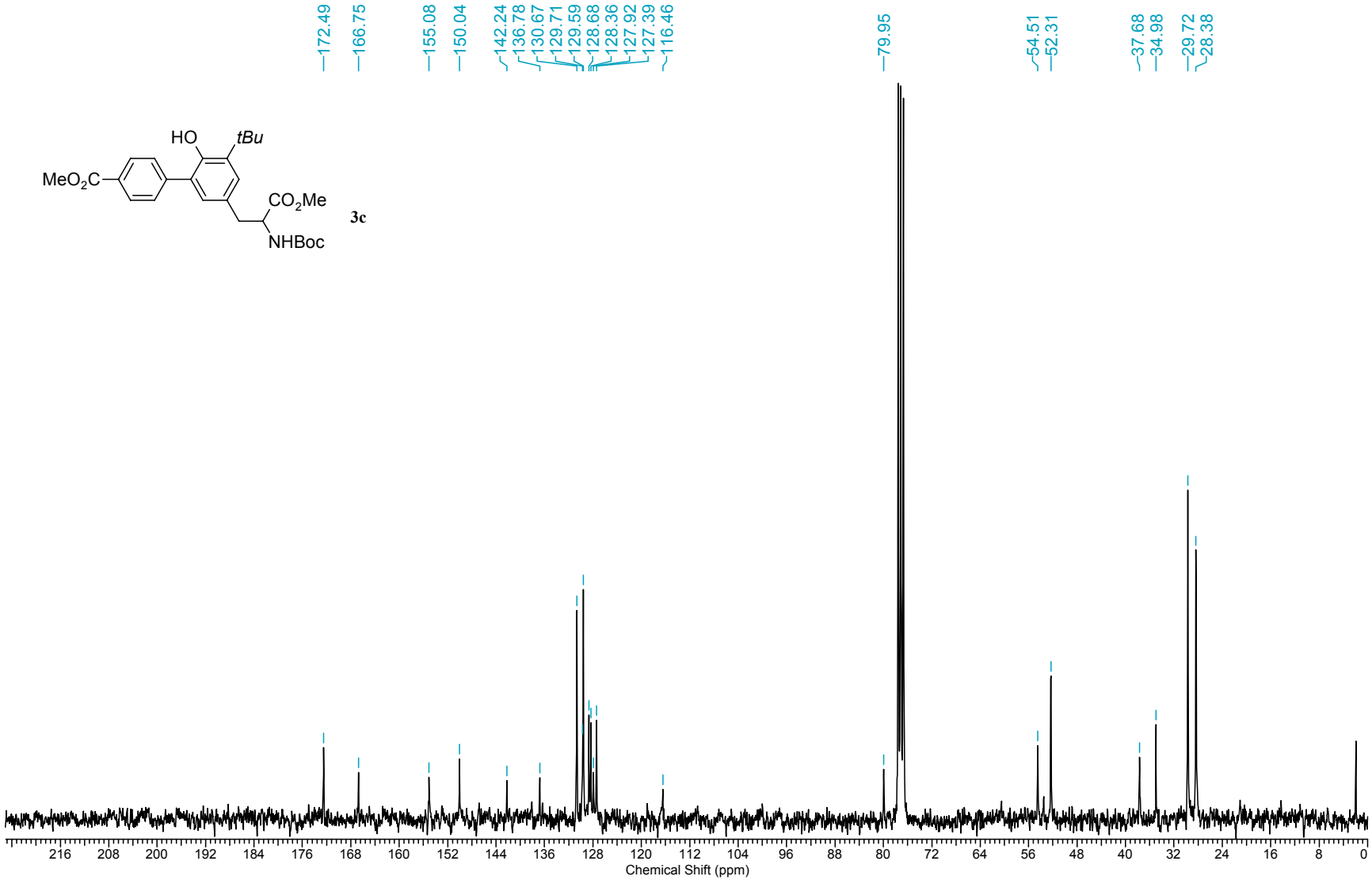
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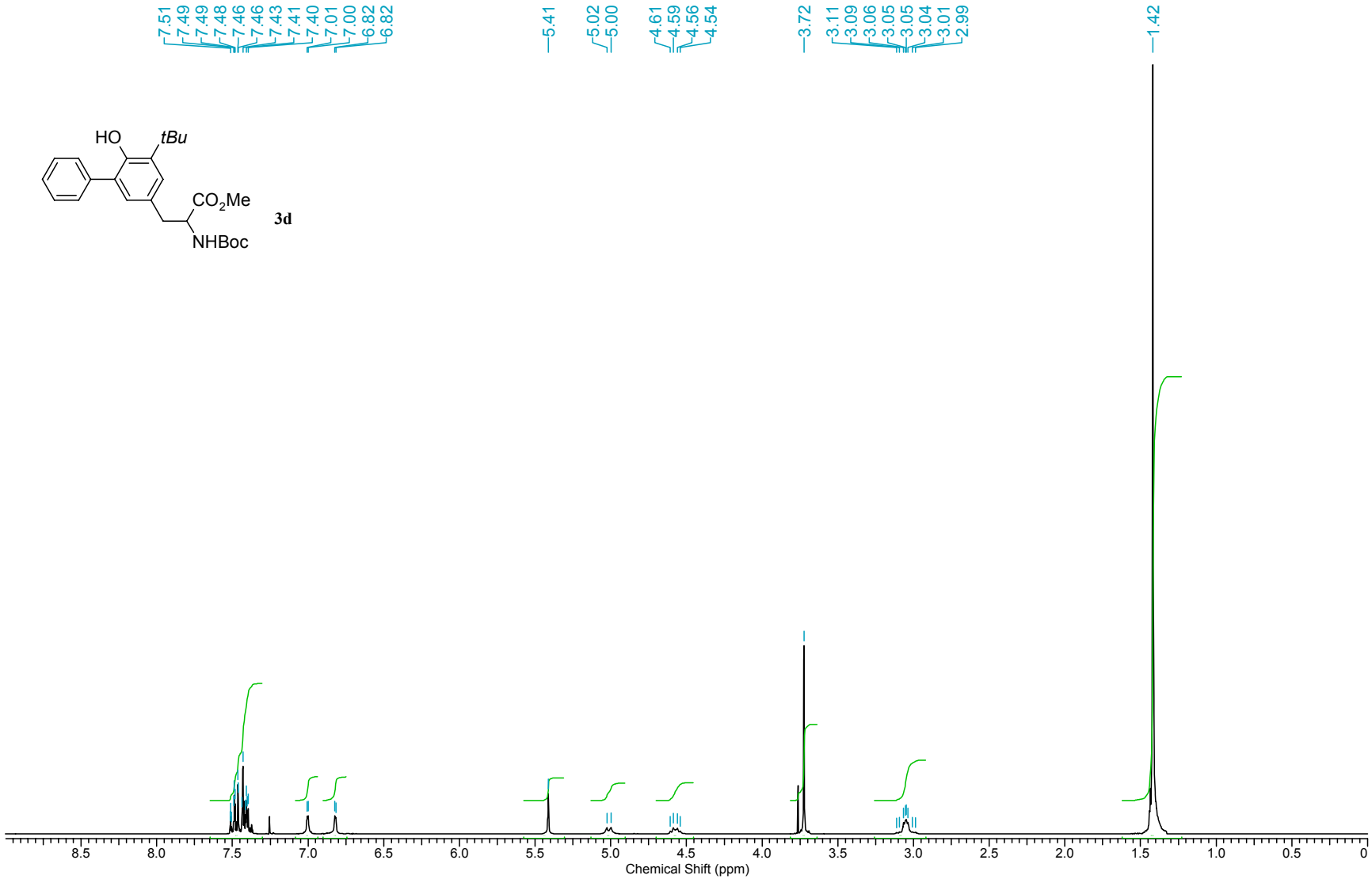
CO2Me
NHBoc
3c
Chemical Shift (ppm)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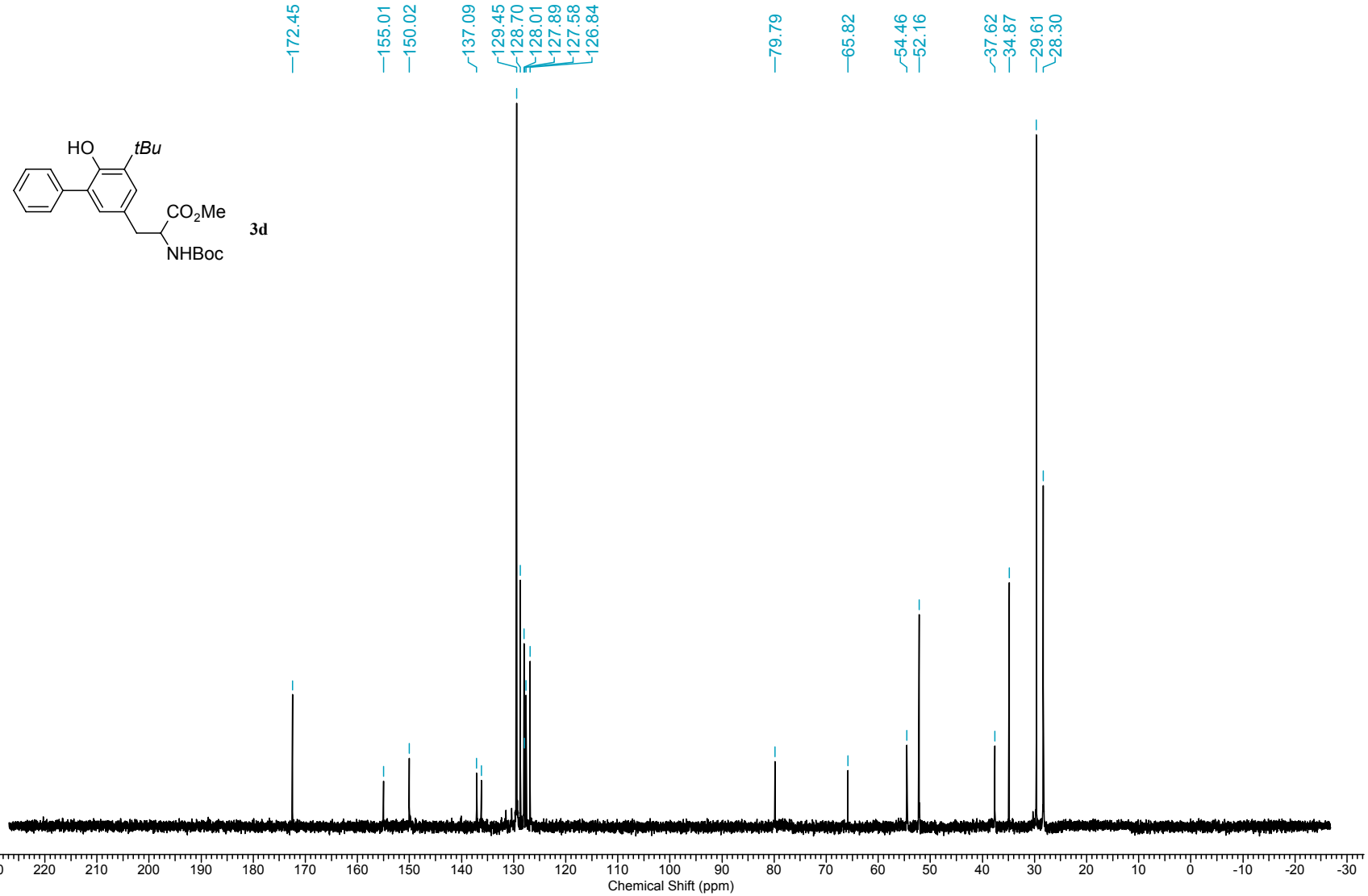
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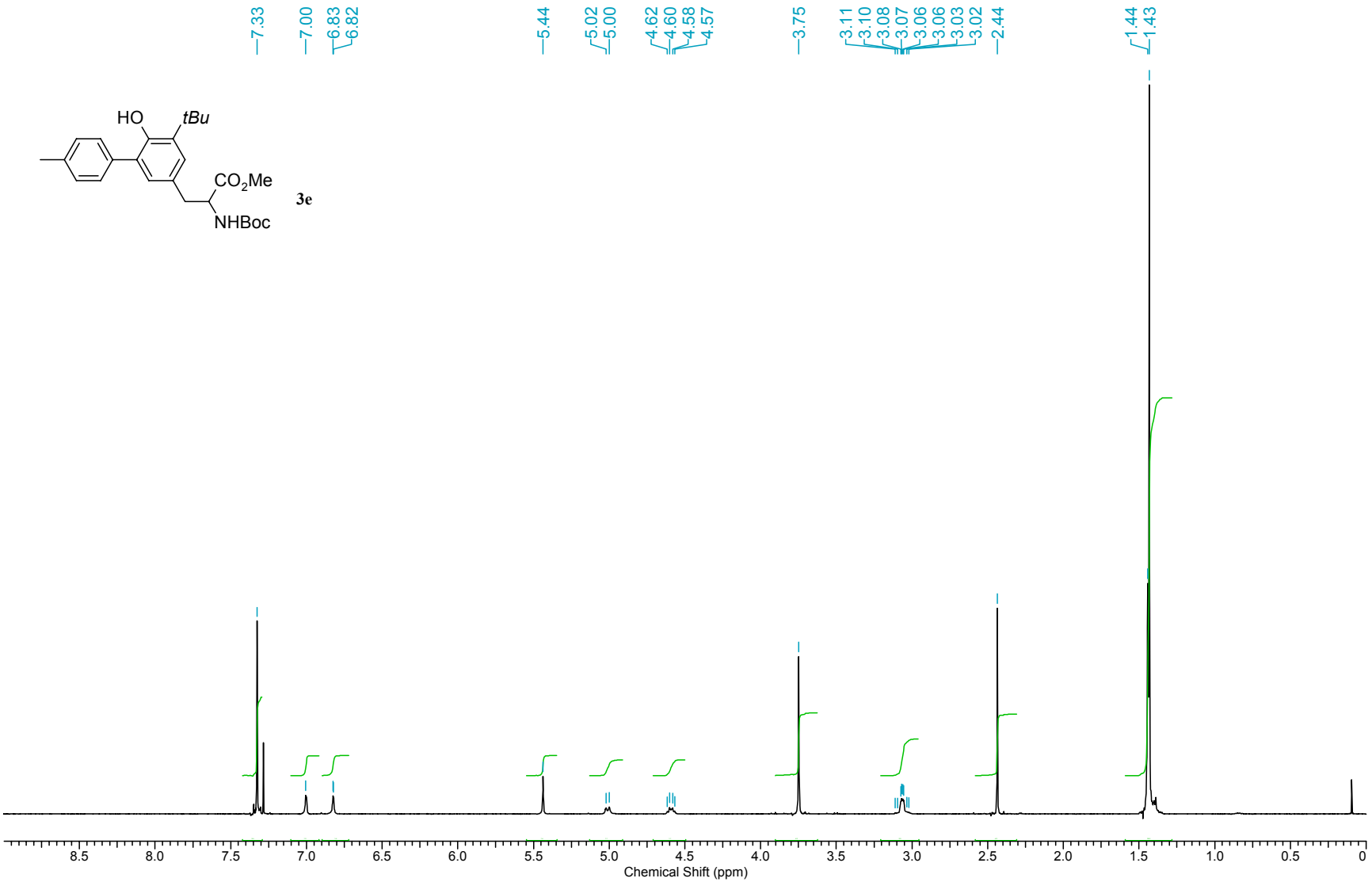
3d
Chemical Shift (ppm)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3.10
3.08
3.07
3.06
3.06
3.03
3.02
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1.44
1.43
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NHBoc
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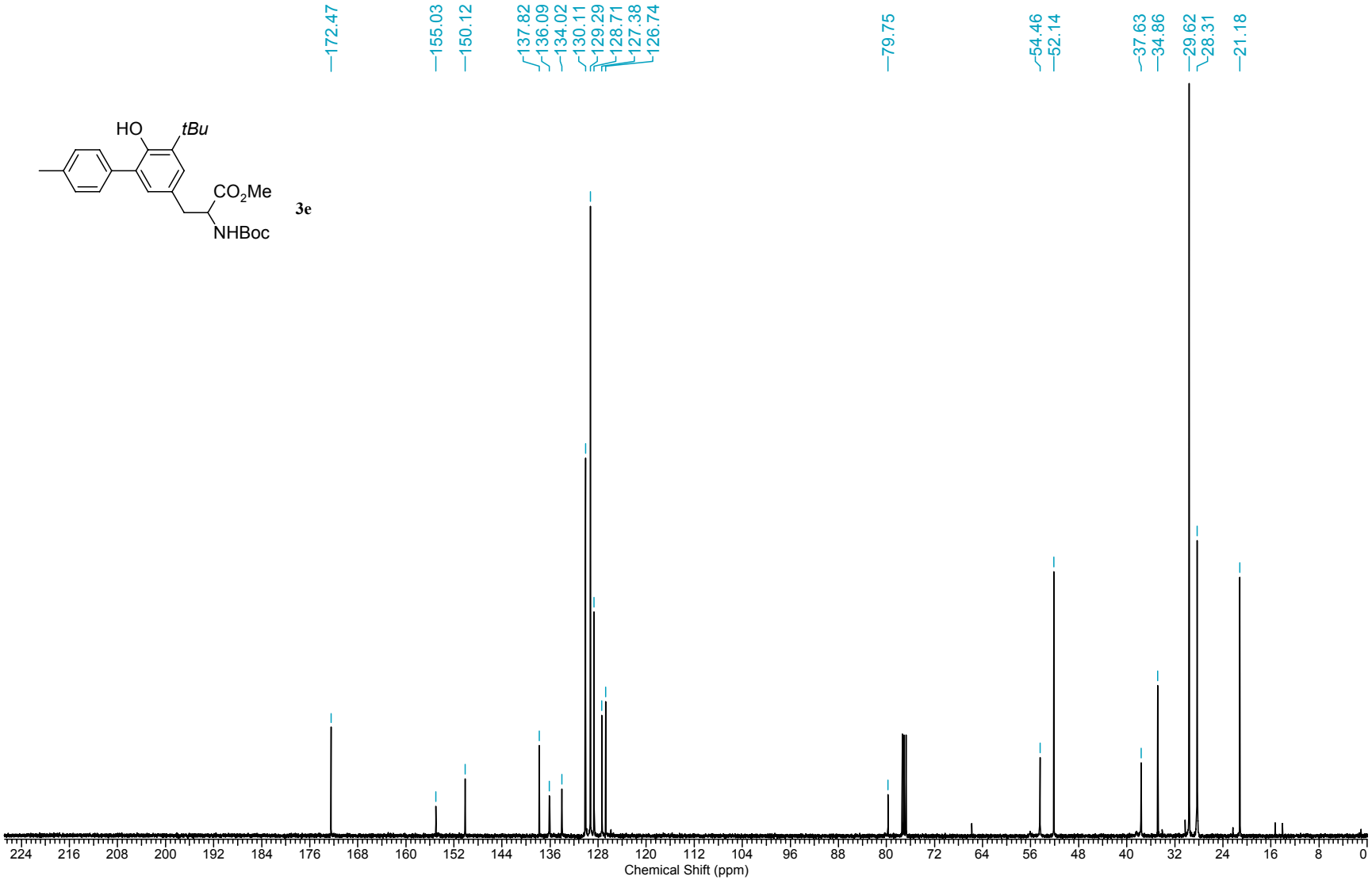
Chemical Shift (ppm)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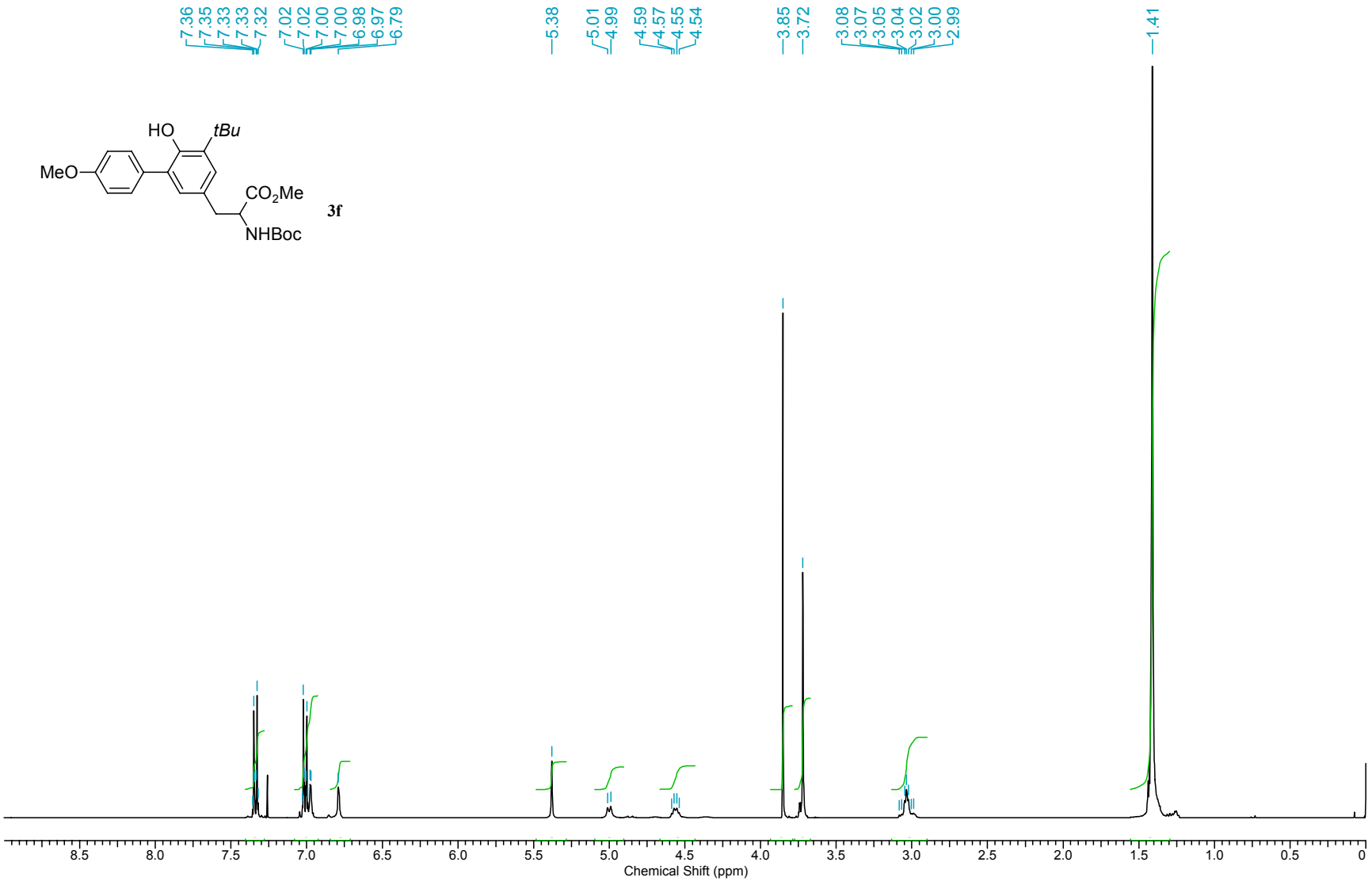
Chemical Shift (ppm)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4.55
4.54
3.85
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CO2Me
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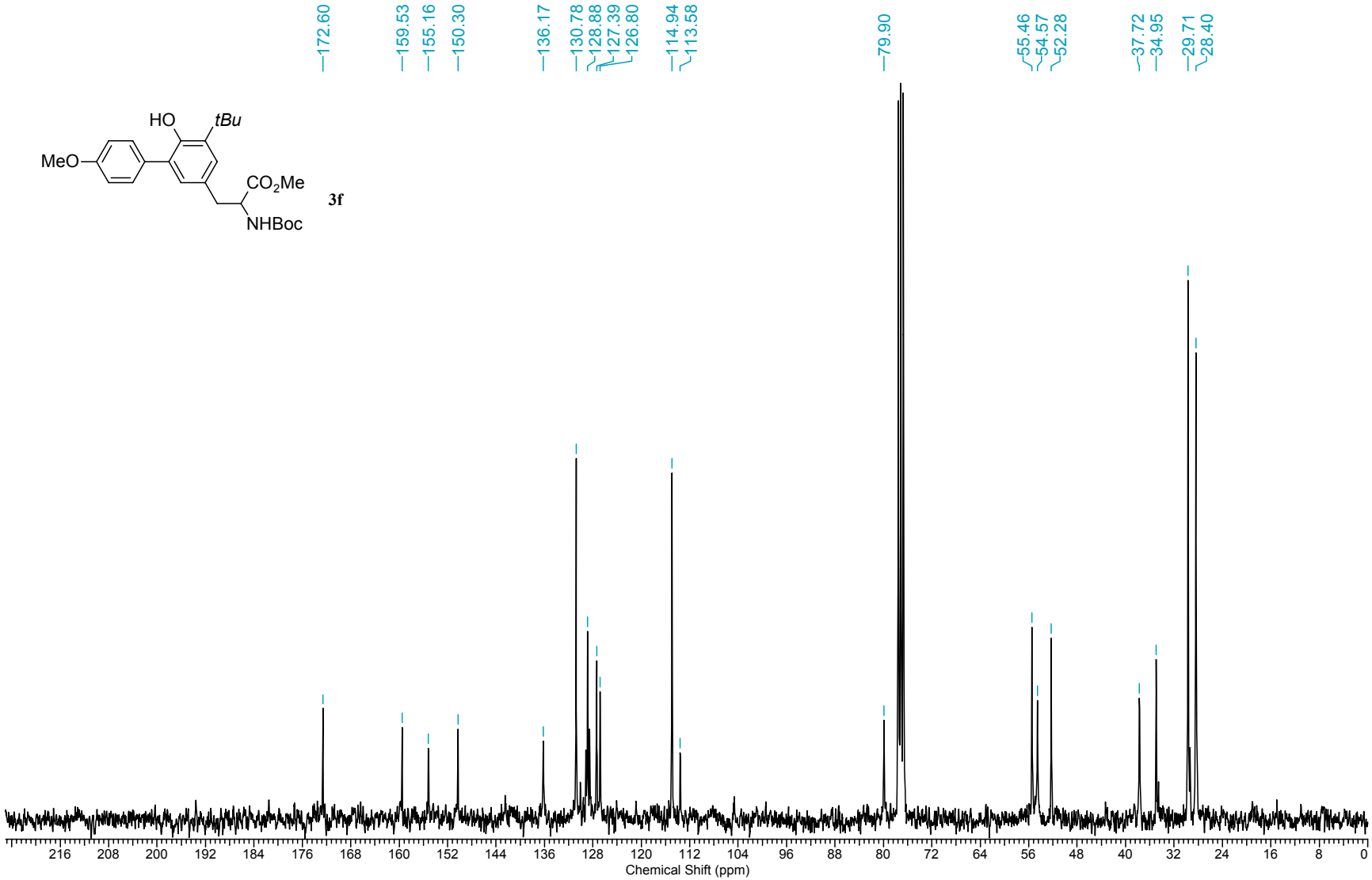
Chemical Shift (ppm)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54.57
52.28
37.72
34.95
29.71
28.40
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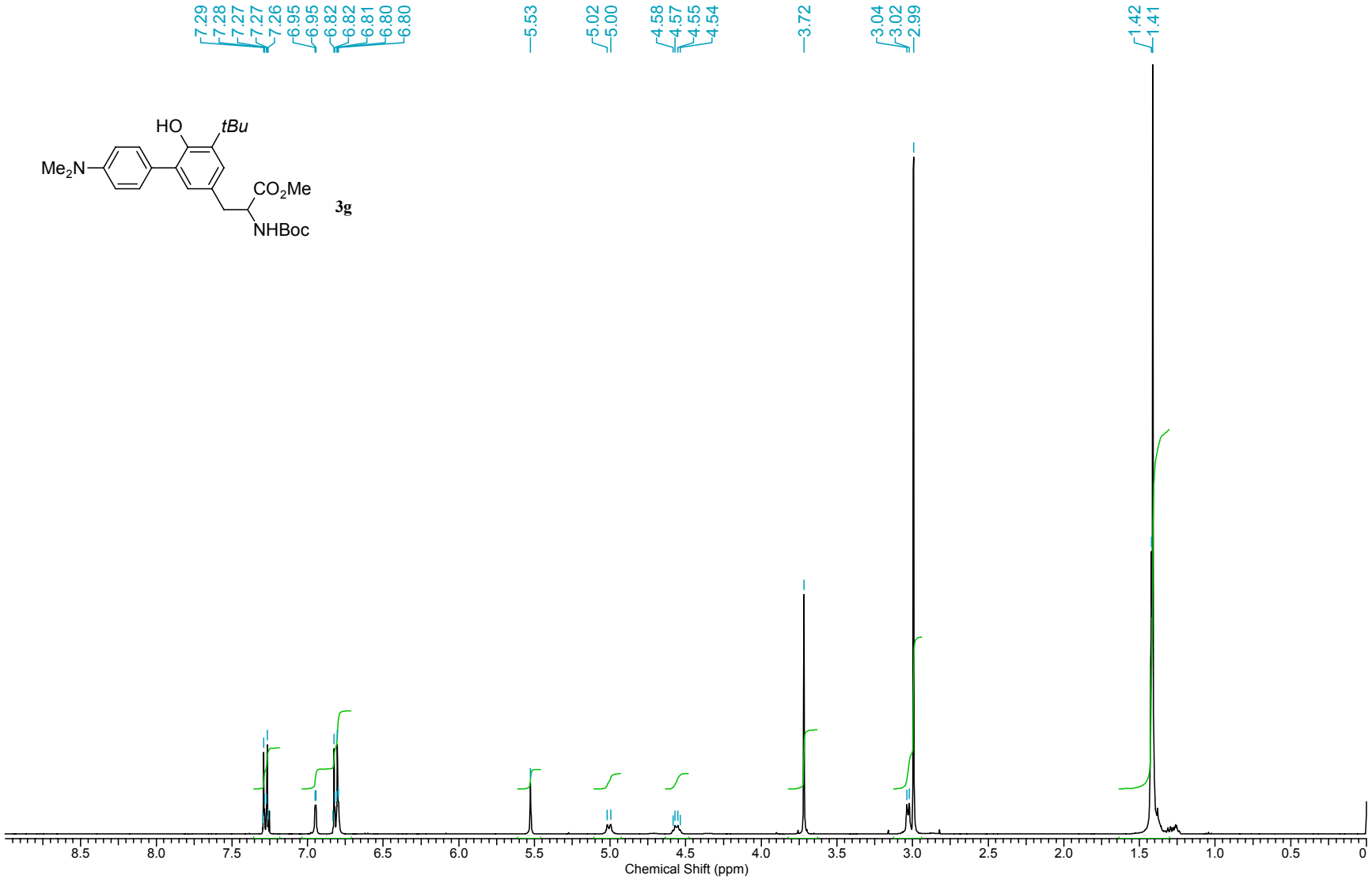
Chemical Shift (ppm)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5.00
4.58
4.57
4.55
4.54
3.72
3.04
3.02
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1.41
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tBu
Me2N
CO2Me
NHBoc
3g
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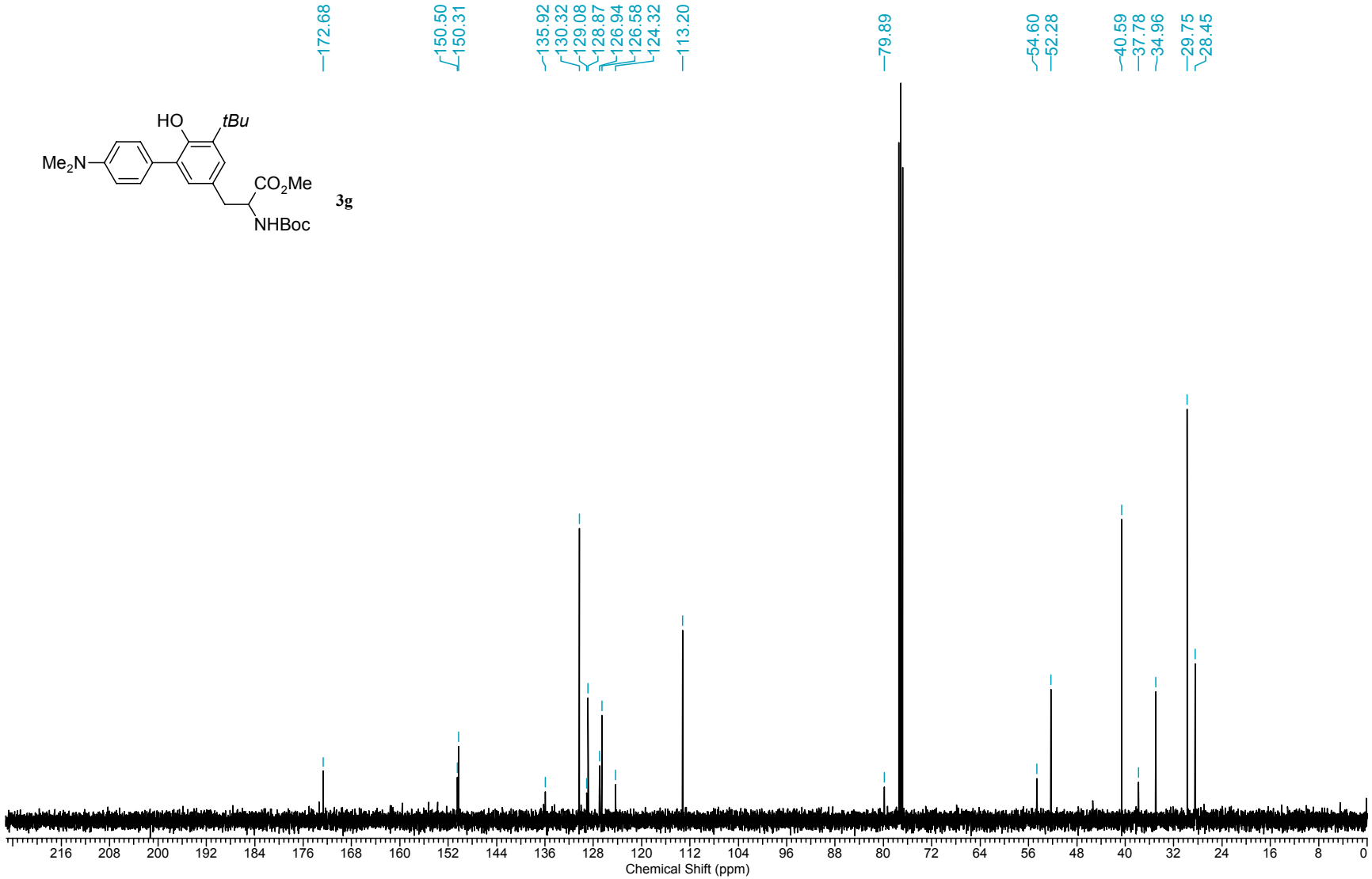
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28.45
HO
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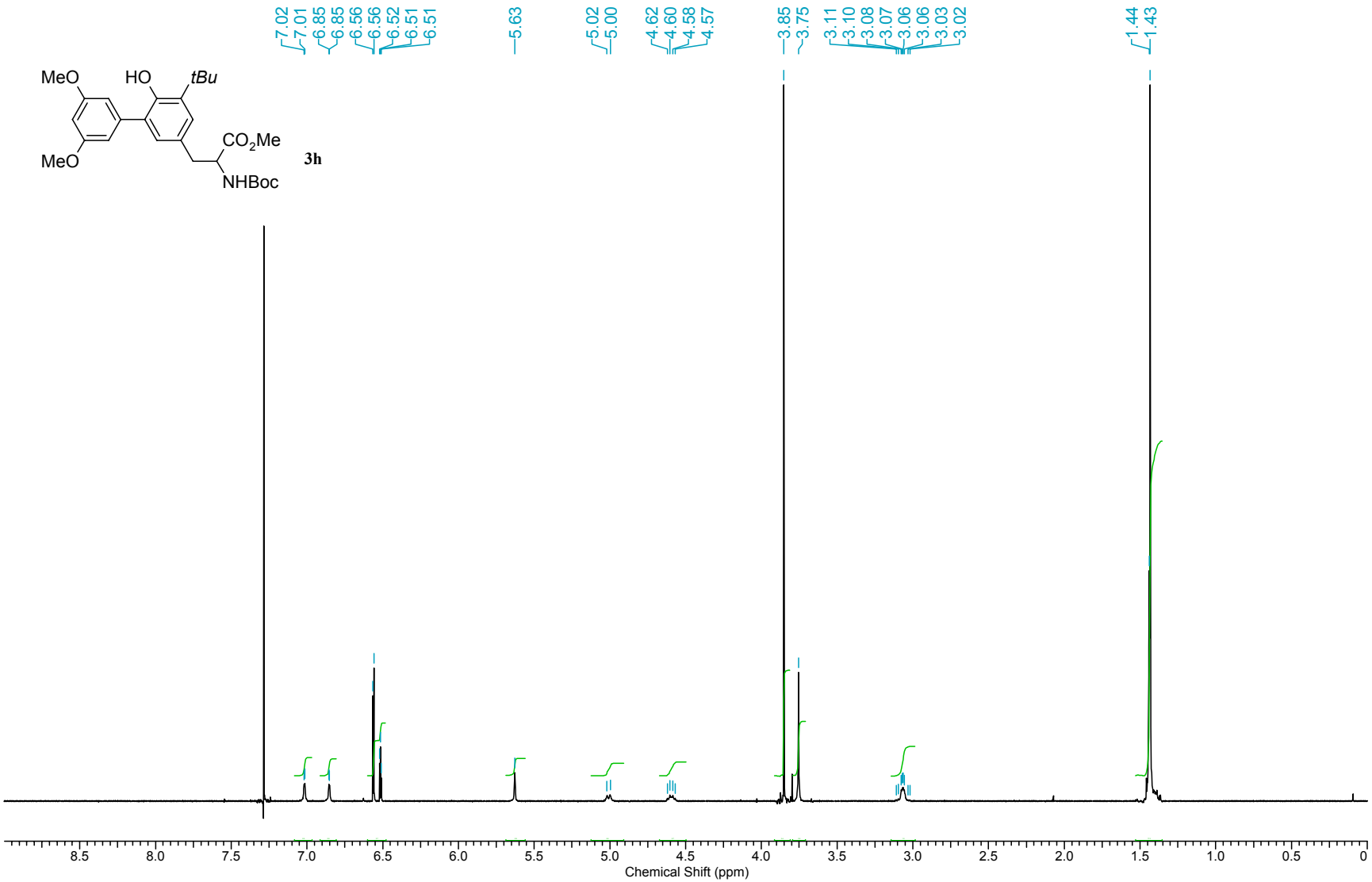
Chemical Shift (ppm)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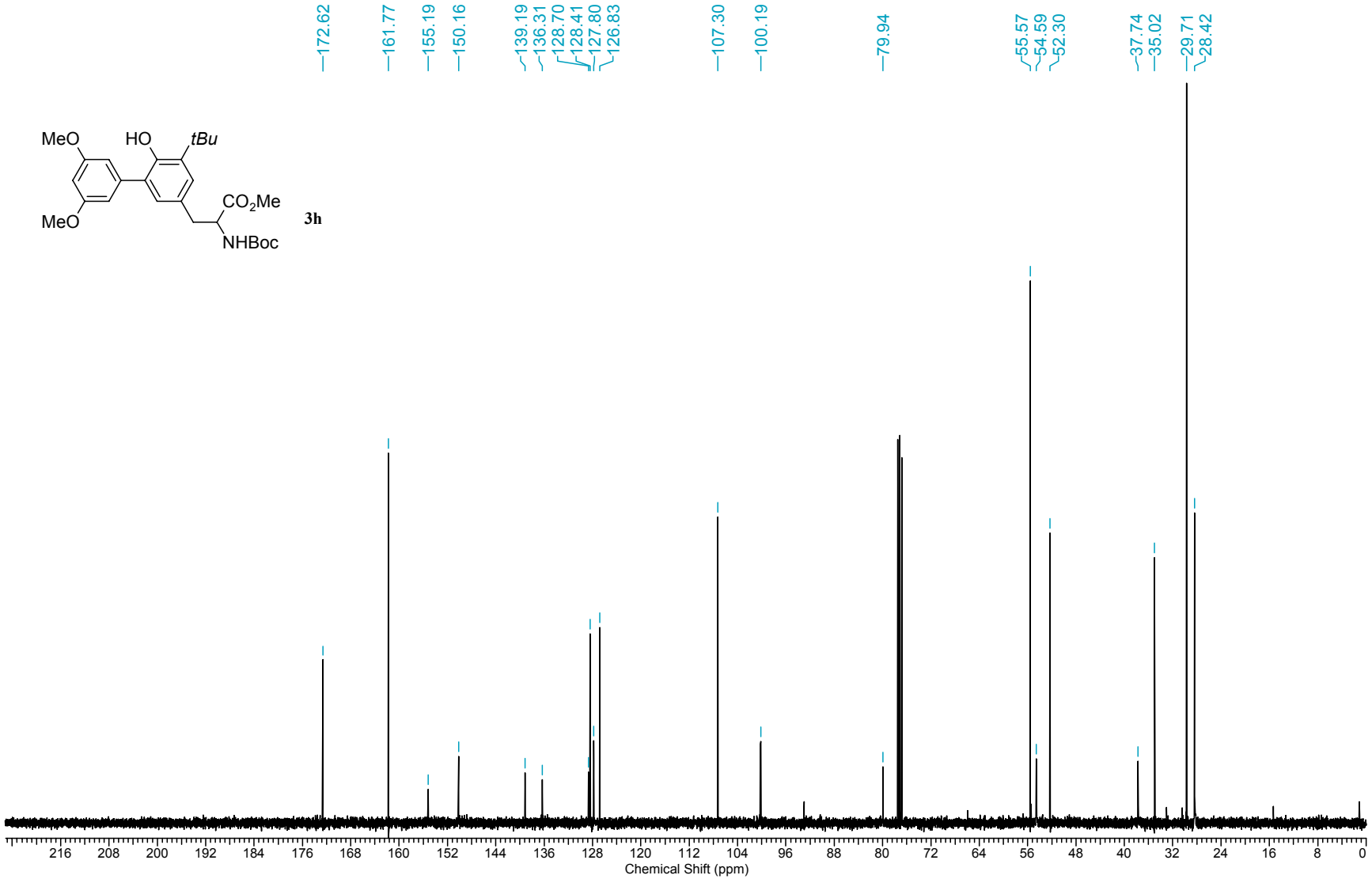
CO2Me
MeO
NHBoc
3h
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)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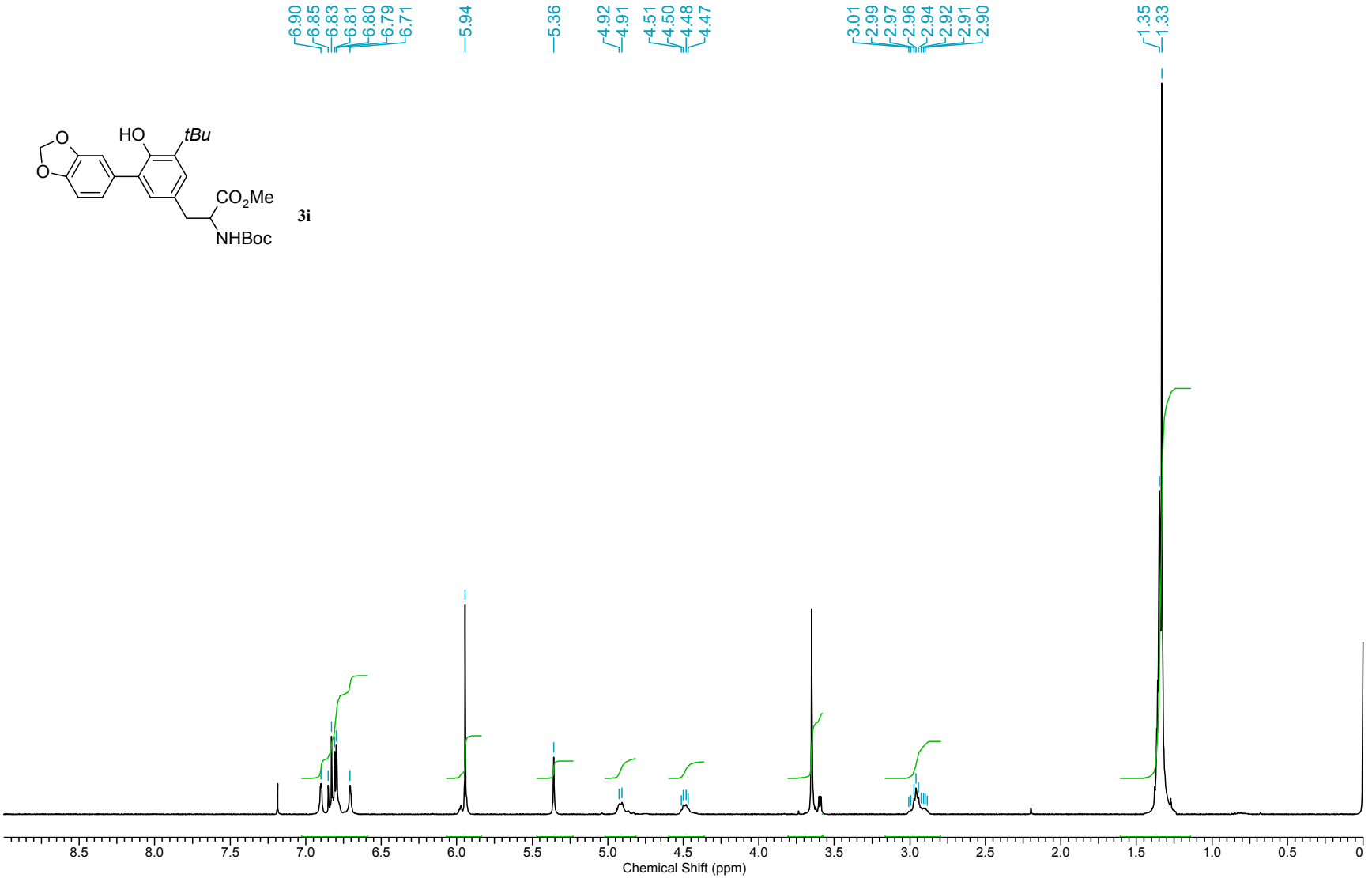
161.77
155.19
150.16
139.19
136.31
128.70
128.41
127.80
126.83
107.30
100.19
79.94
55.57
54.59
52.30
37.74
35.02
29.71
28.42
MeO
HO
tBu
CO2Me
MeO
NHBoc
3h
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)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6.85
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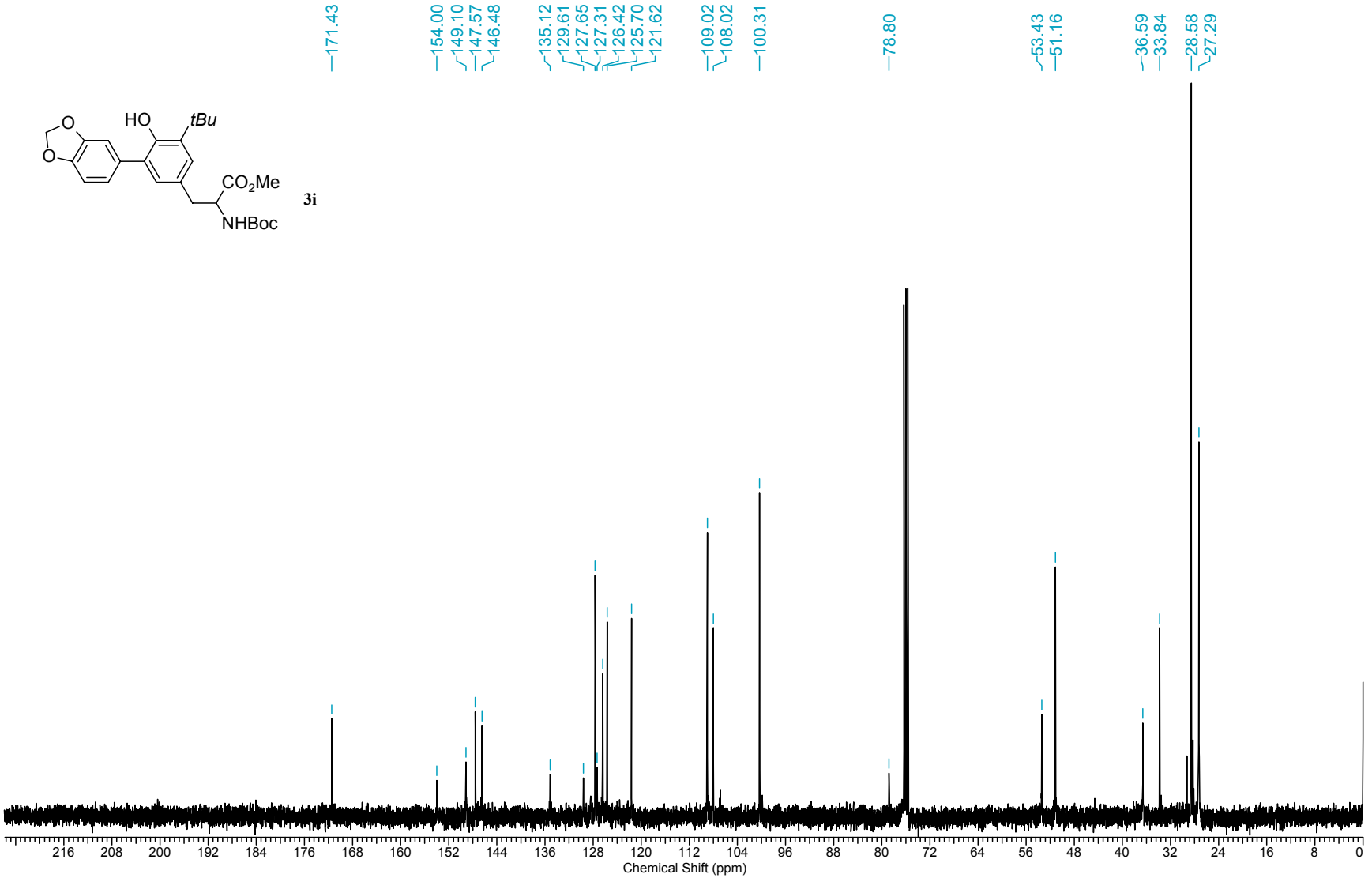
6.80
6.79
6.71
5.94
5.36
4.92
4.91
4.51
4.50
4.48
4.47
3.01
2.99
2.97
2.96
2.94
2.92
2.91
2.90
1.35
1.33
HO
tBu
O
O
CO2Me
NHBoc
3i
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)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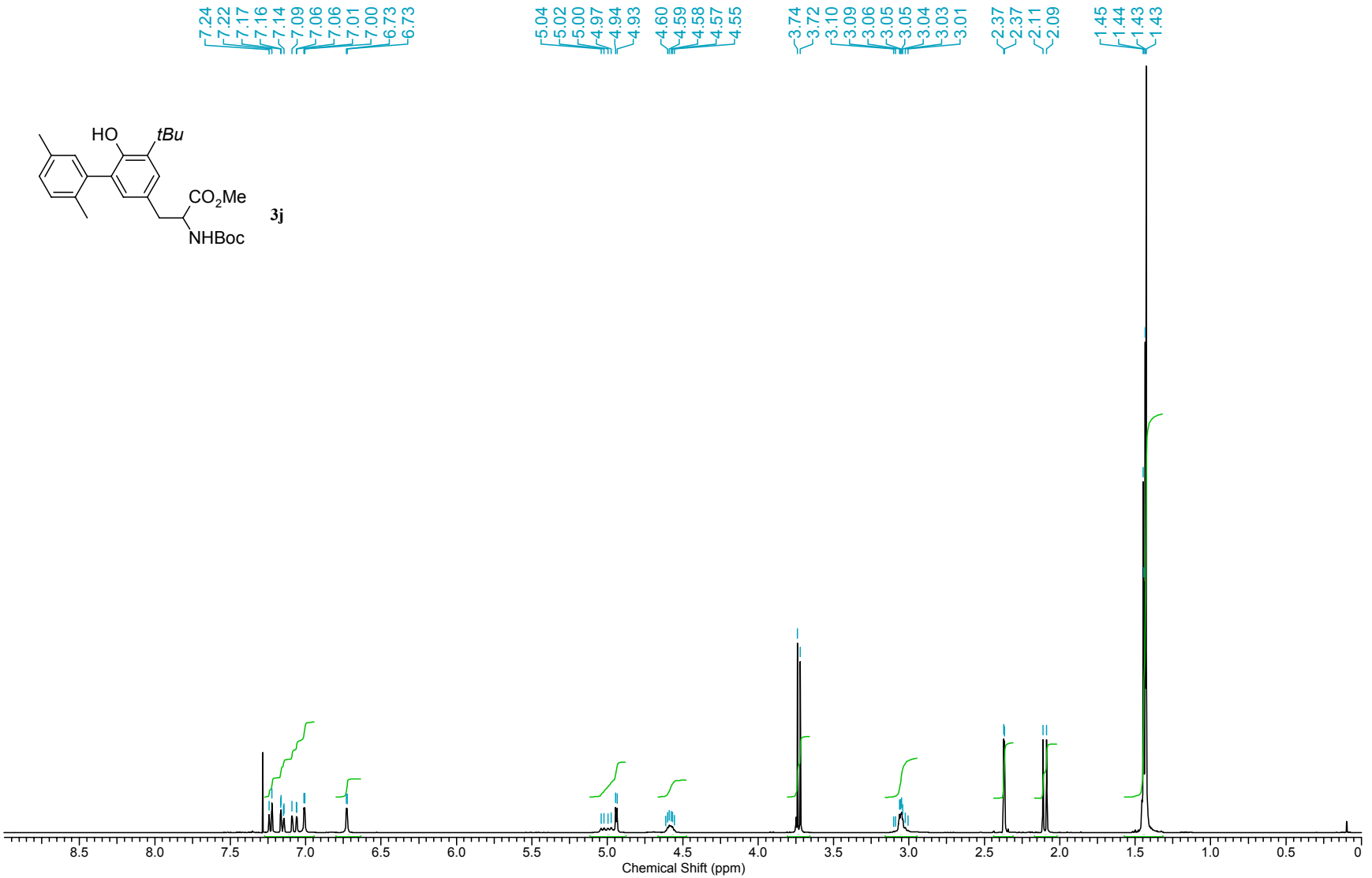
154.00
149.10
147.57
146.48
135.12
129.61
127.65
127.31
126.42
125.70
121.62
109.02
108.02
100.31
78.80
53.43
51.16
36.59
33.84
28.58
27.29
HO
tBu
O
O
CO2Me
NHBoc
3i
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)


7.24
7.22
7.17
7.16
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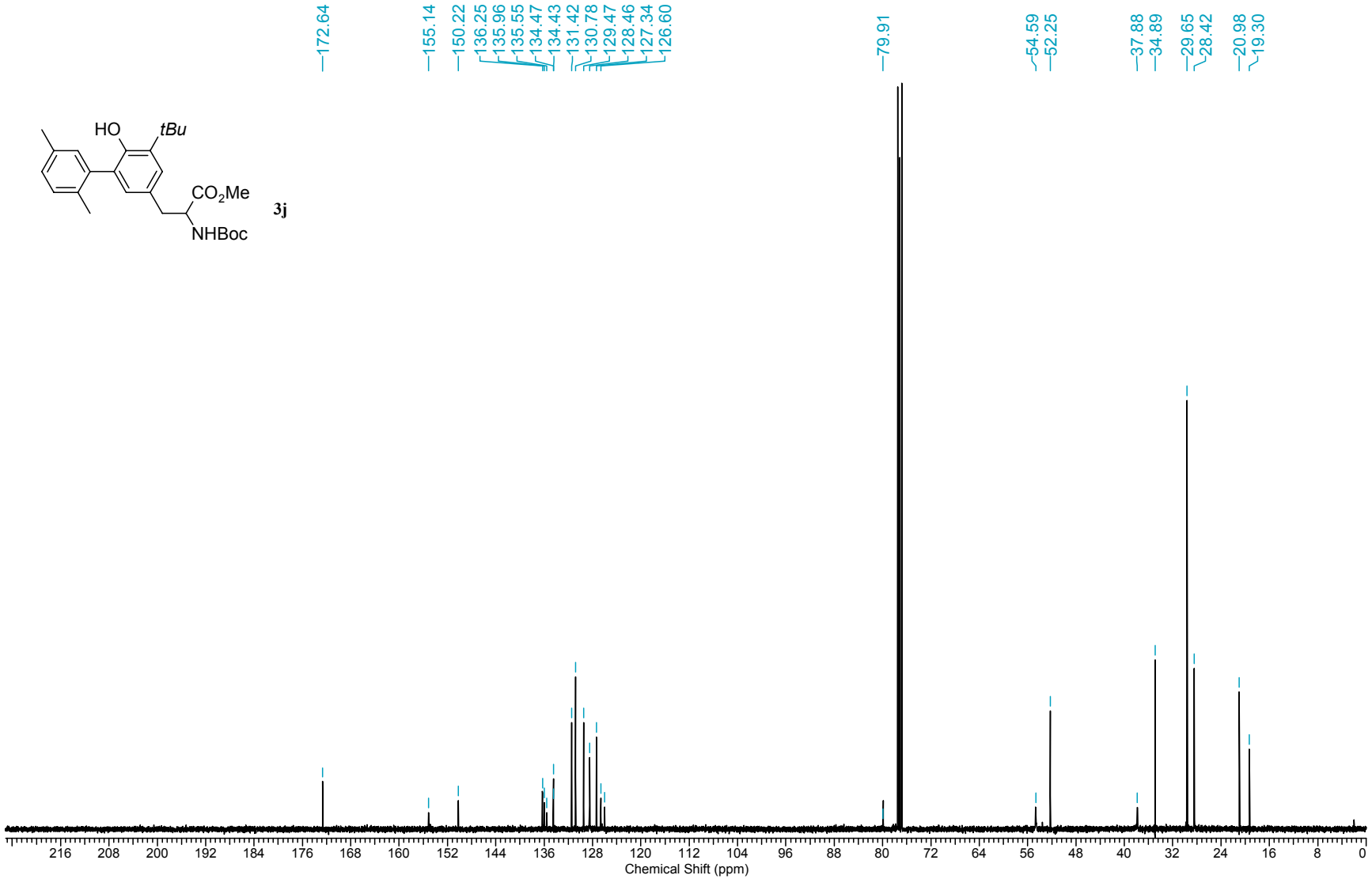
7.09
7.06
7.06
7.01
7.00
6.73
6.73
5.04
5.02
5.00
4.97
4.94
4.93
4.60
4.59
4.58
4.57
4.55
3.74
3.72
3.10
3.09
3.06
3.05
3.05
3.04
3.03
3.01
2.37
2.37
2.11
2.09
1.45
1.44
1.43
1.43
HO
tBu
CO2Me
NHBoc
3j
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)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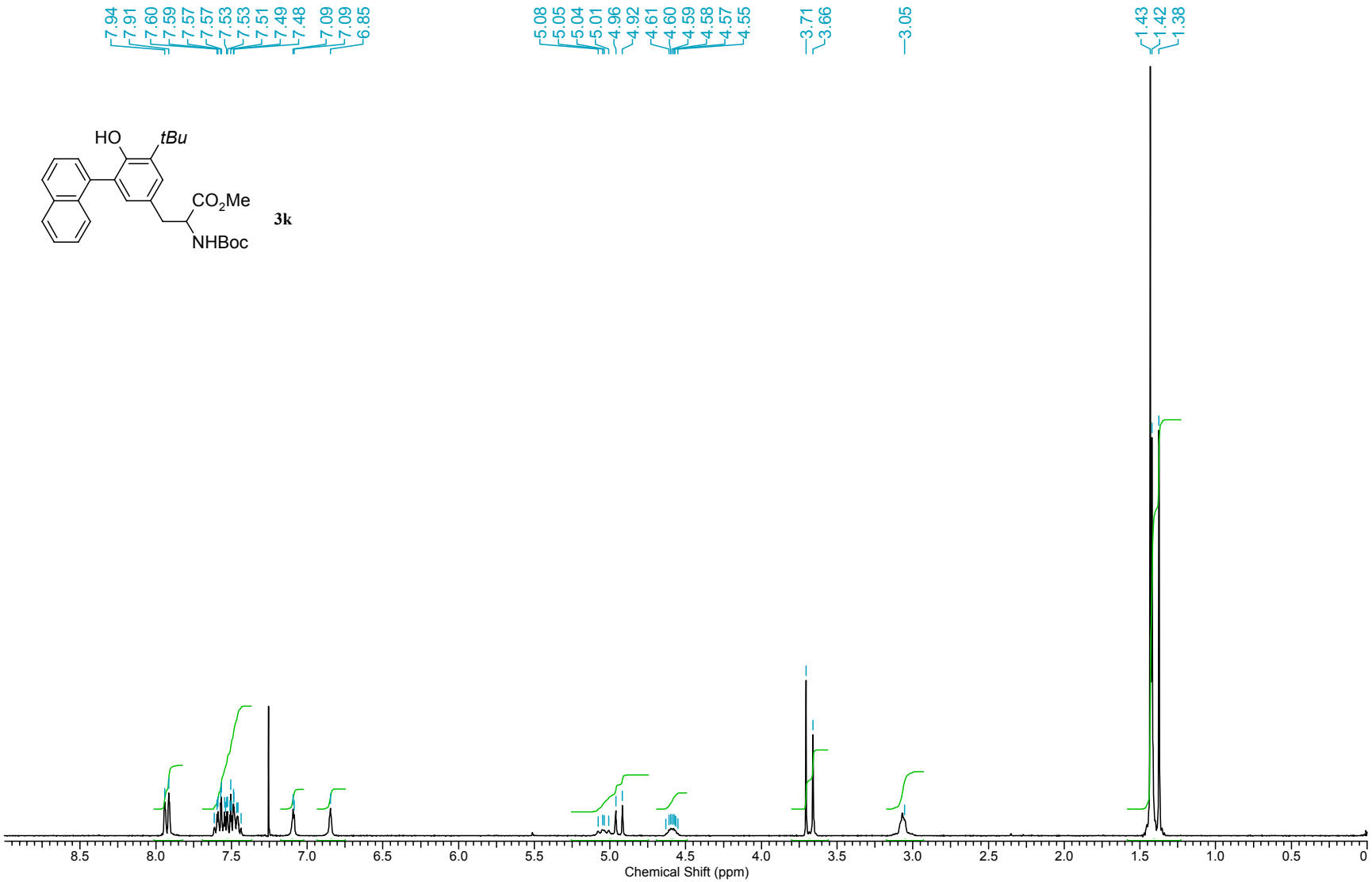
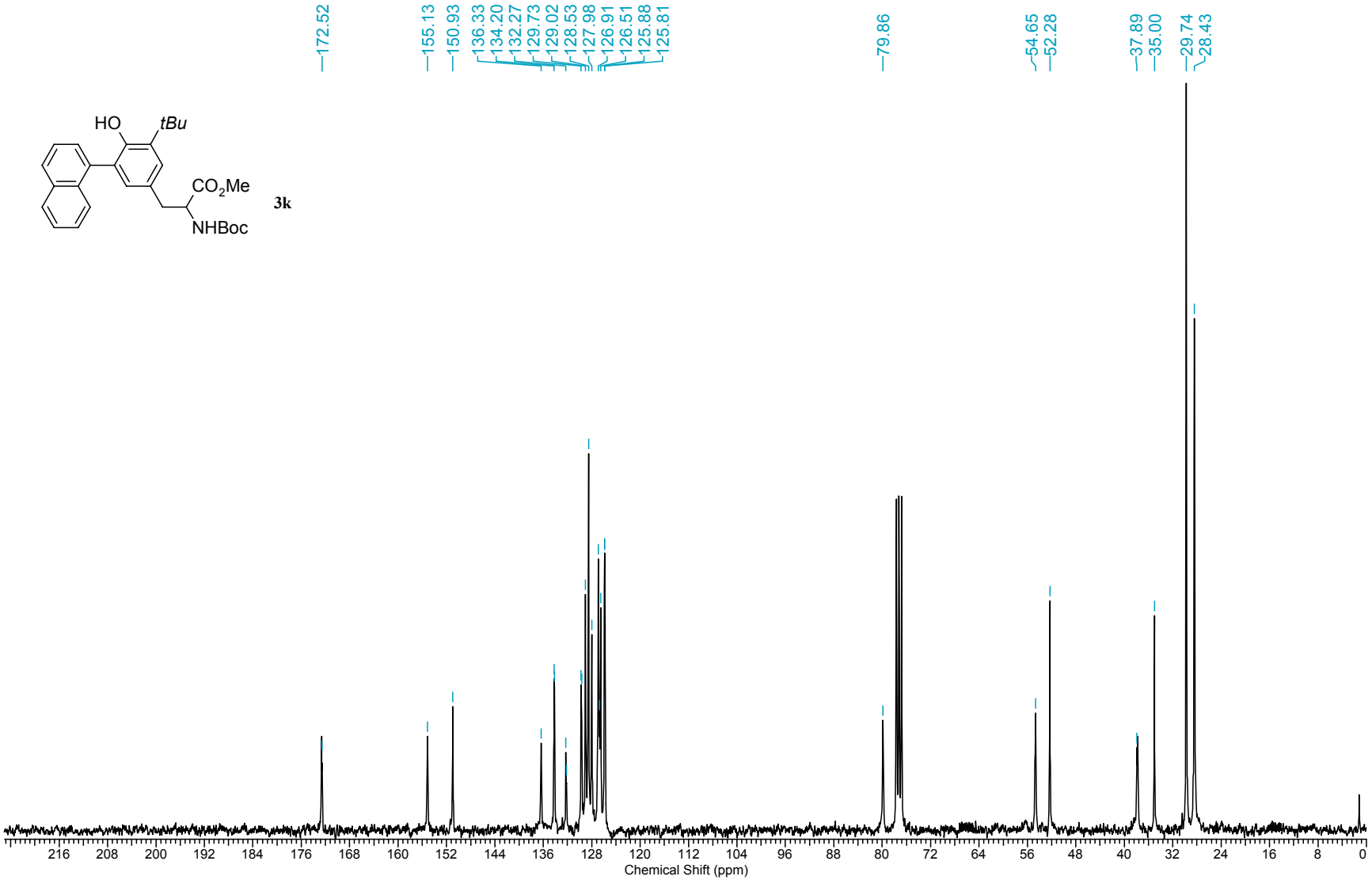
155.14
150.22
136.25
135.96
135.55
134.47
134.43
131.42
130.78
129.47
128.46
127.34
126.60
79.91
54.59
52.25
37.88
34.89
29.65
28.42
20.98
19.30
HO
tBu
CO2Me
NHBoc
3j
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)


7.94
7.91
7.60
7.59
7.57
7.57
7.53
7.53
7.51
7.49
7.48
7.09
7.09
6.85
5.08
5.05
5.04
5.01
4.96
4.92
4.61
4.60
4.59
4.58
4.57
4.55
3.71
3.66
3.05
1.43
1.42
1.38
HO
tBu
CO2Me
NHBoc
3k
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
Chemical Shift (ppm)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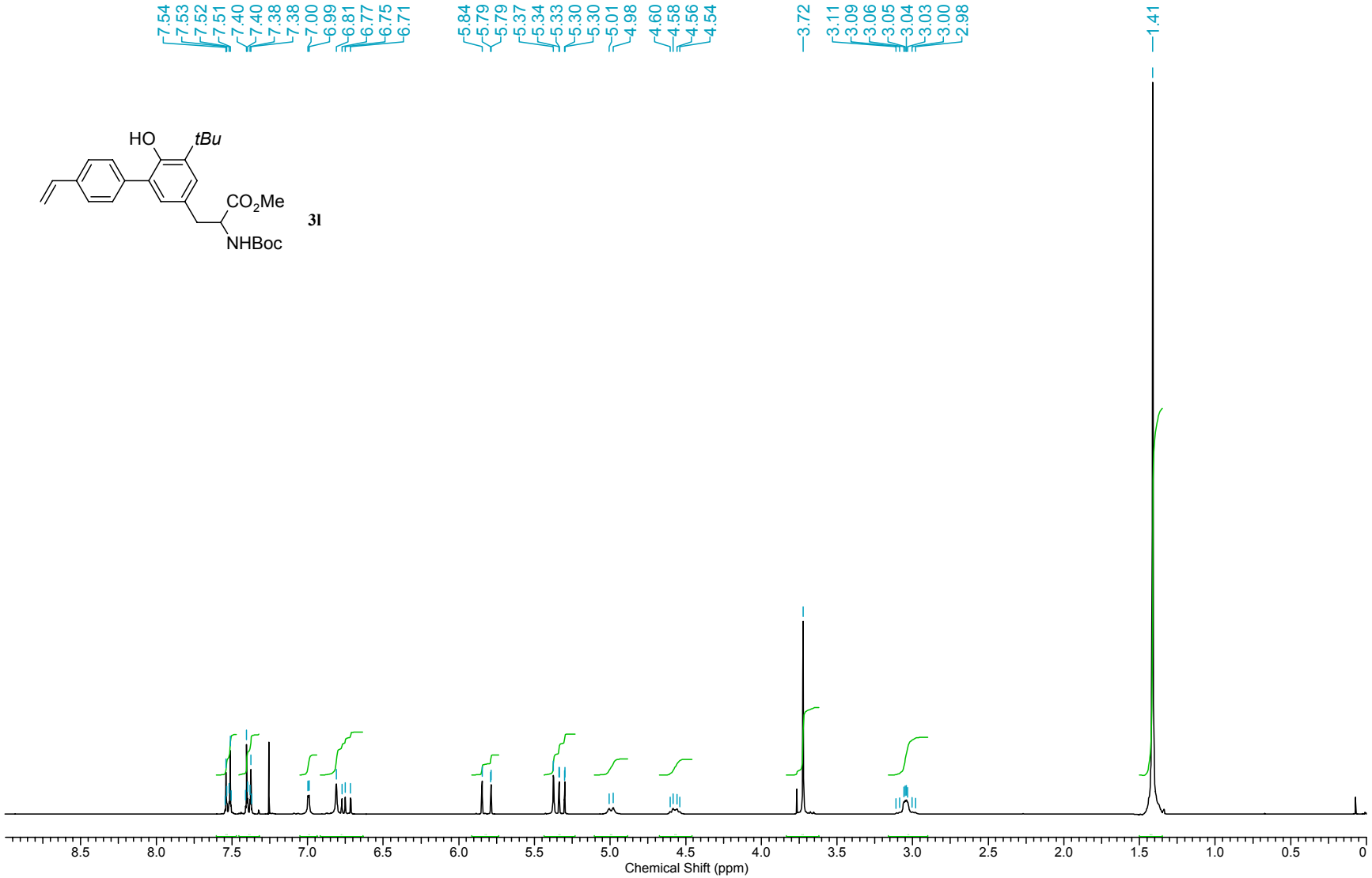
155.13
150.93
136.33
134.20
132.27
129.73
129.02
128.53
127.98
126.91
126.51
125.88
125.81
79.86
54.65
52.28
37.89
35.00
29.74
28.43
HO
tBu
CO2Me
NHBoc
3k
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)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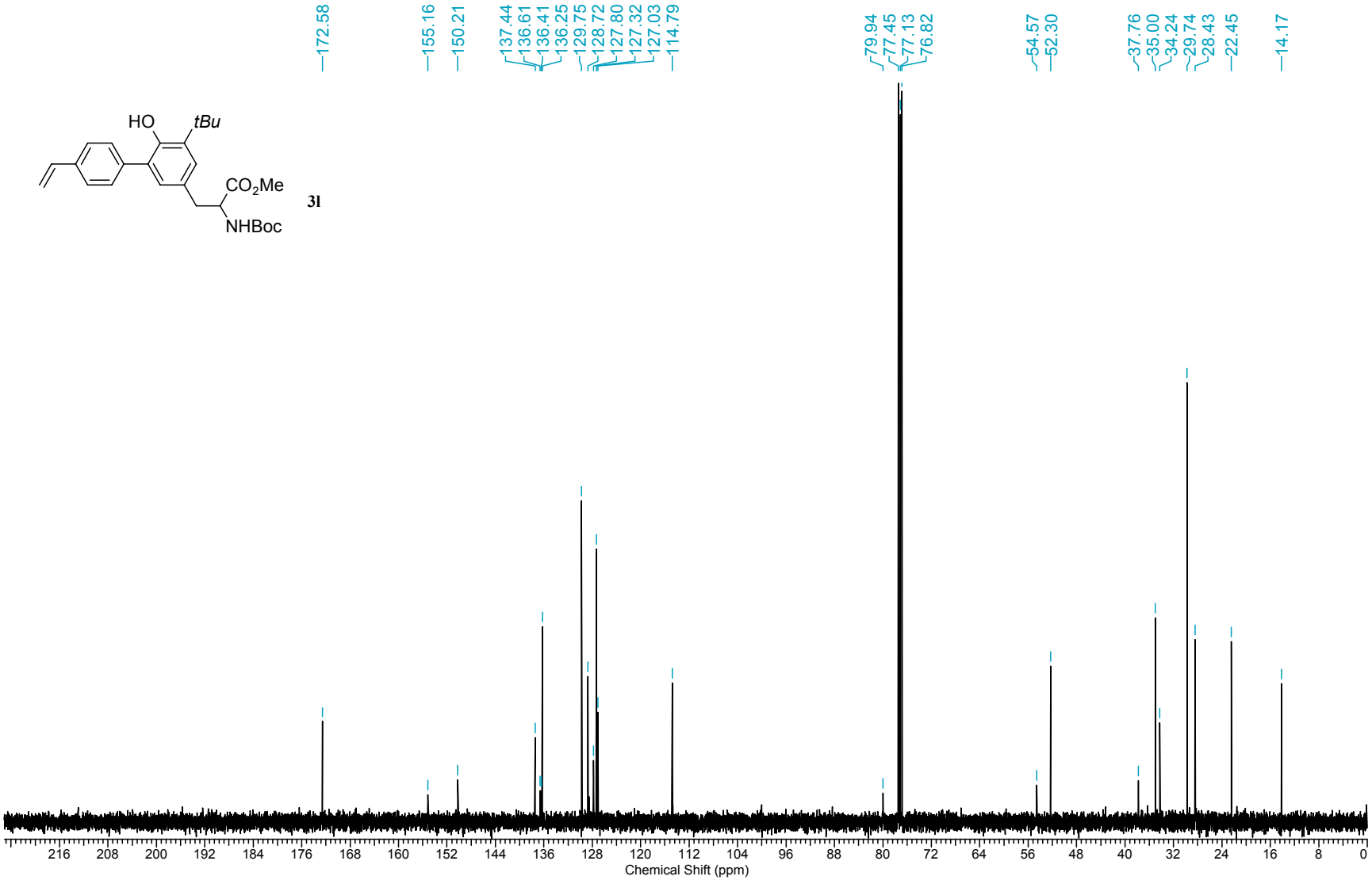
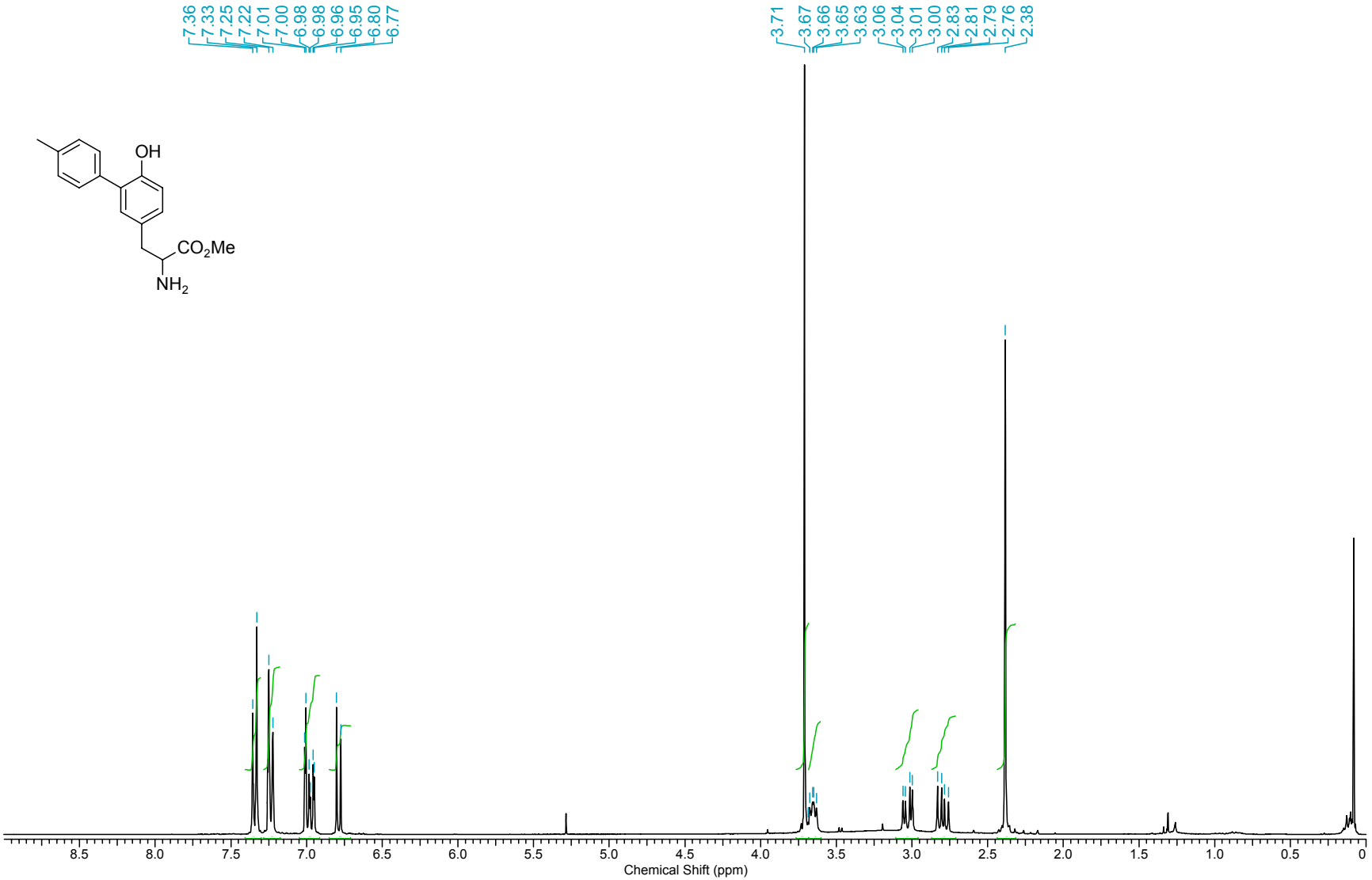
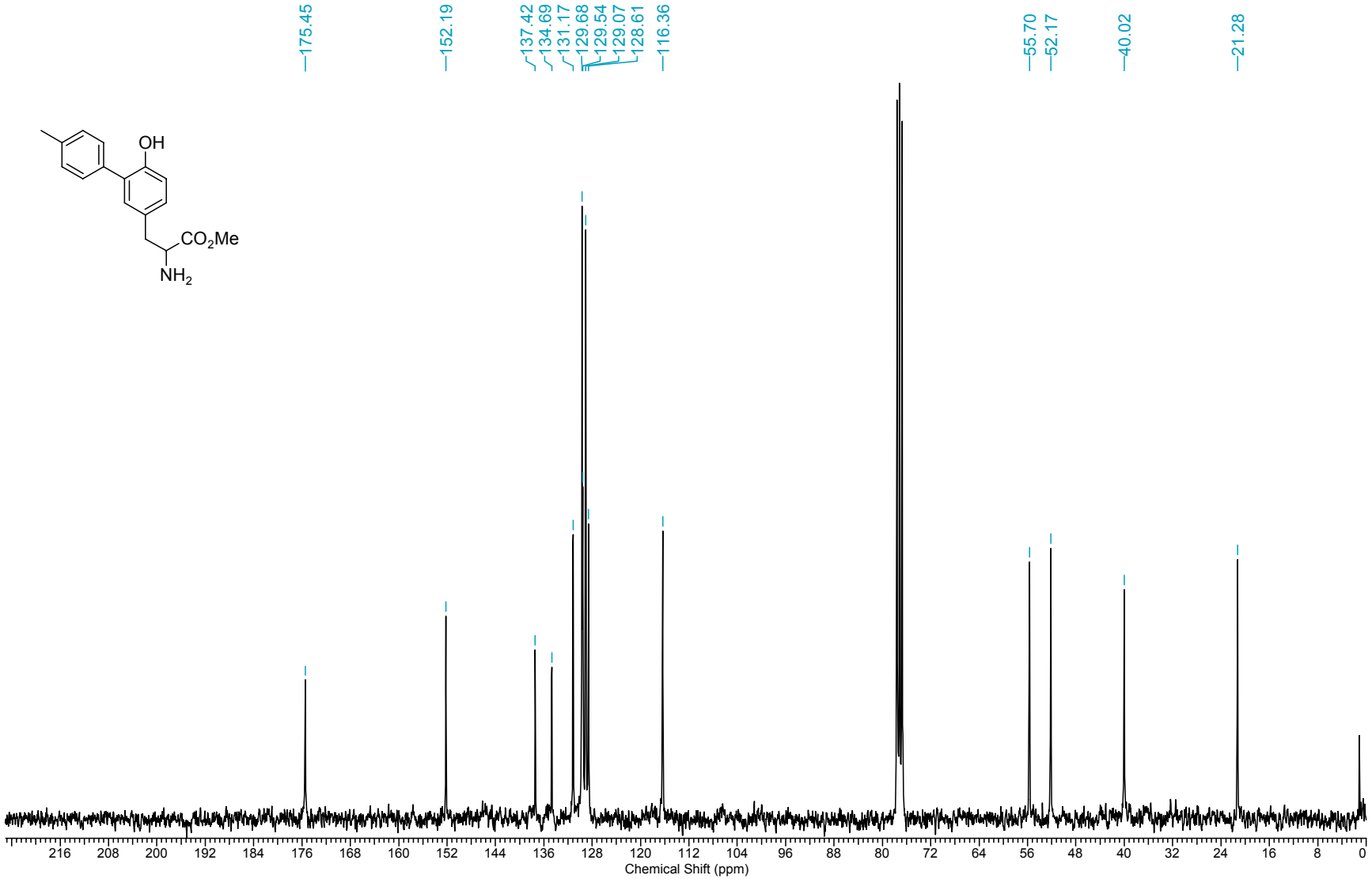
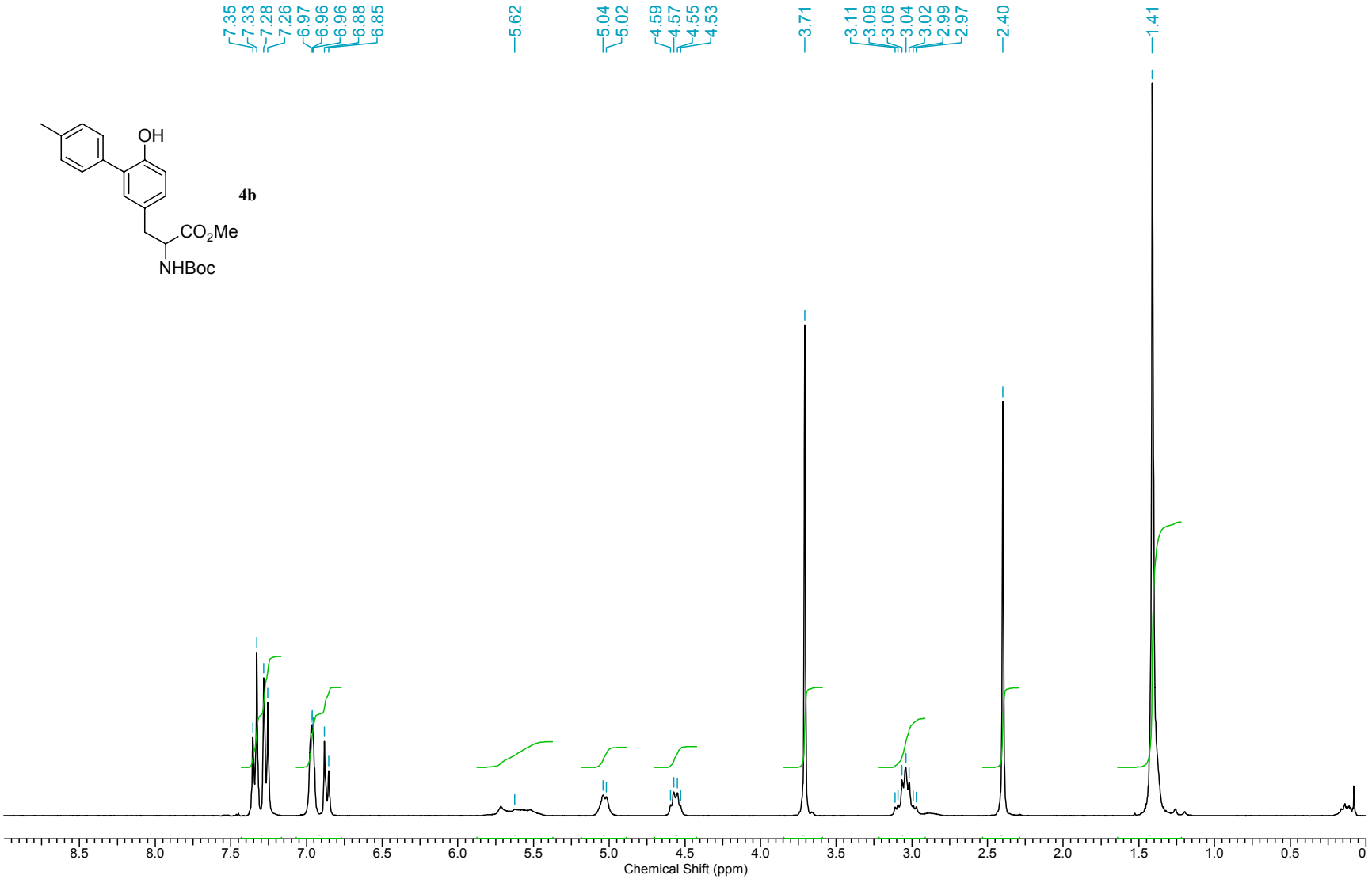
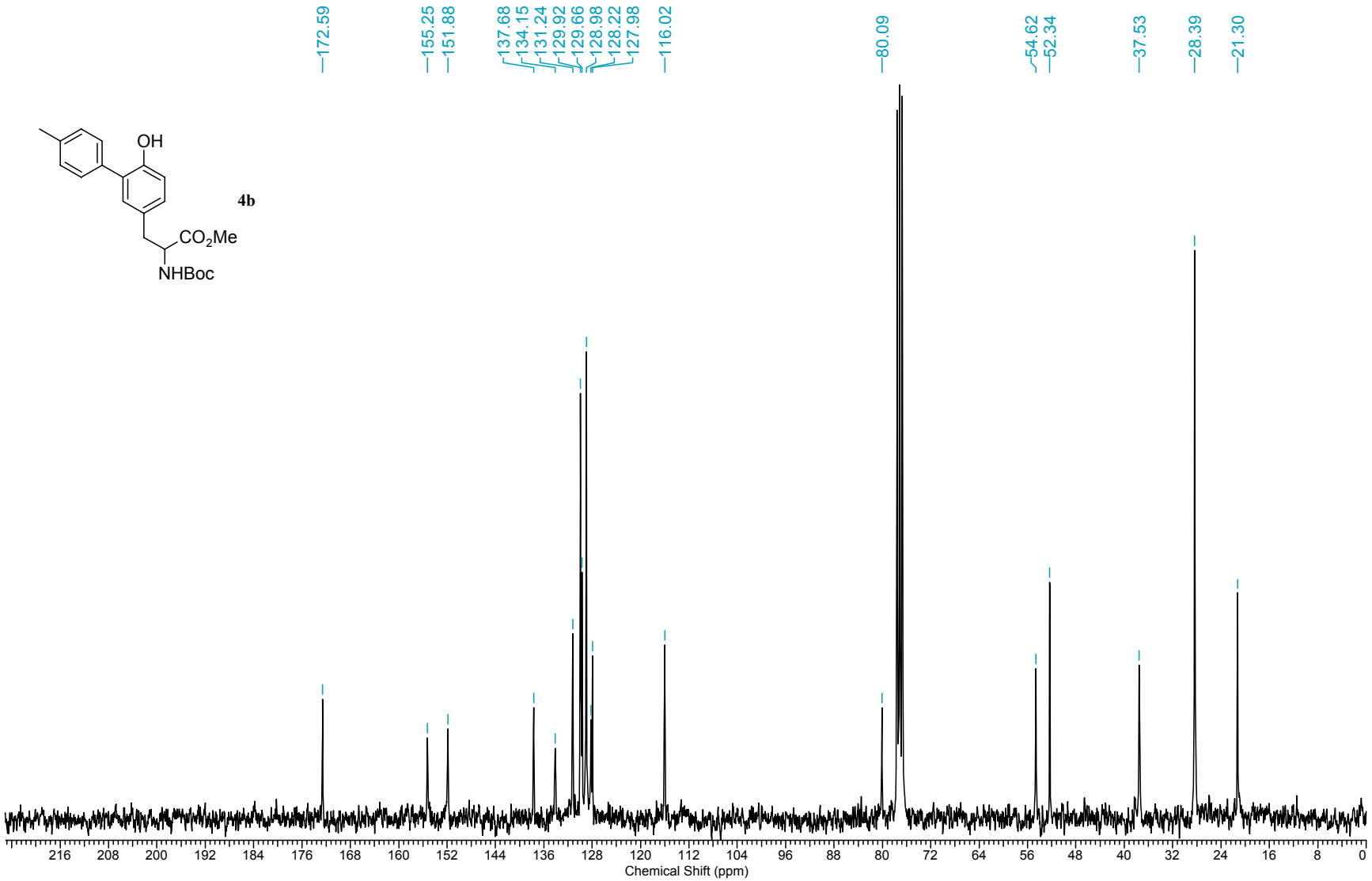
7.53
7.52
7.51
7.40
7.40
7.38
7.38
7.00
6.99
6.81
6.77
6.75
6.71
5.84
5.79
5.79
5.37
5.34
5.33
5.30
5.30
5.01
4.98
4.60
4.58
4.56
4.54
3.72
3.11
3.09
3.06
3.05
3.04
3.03
3.00
2.98
1.41
HO
tBu
CO2Me
NHBoc
31
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)


172.58
155.16
150.21
137.44
136.61
136.41
136.25
129.75
128.72
127.80
127.32
127.03
114.79
79.94
77.45
77.13
76.82
54.57
52.30
37.76
35.00
34.24
29.74
28.43
22.45
14.17
HO
tBu
CO2Me
NHBoc
3l
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)


7.36
7.33
7.25
7.22
7.01
7.00
6.98
6.98
6.96
6.95
6.80
6.77
3.71
3.67
3.66
3.65
3.63
3.06
3.04
3.01
3.00
2.83
2.81
2.79
2.76
2.38
OH
CO2Me
NH2
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
Chemical Shift (ppm)


175.45
152.19
137.42
134.69
131.17
129.68
129.54
129.07
128.61
116.36
55.70
52.17
40.02
21.28
OH
CO2Me
NH2
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)


7.35
7.33
7.28
7.26
6.97
6.96
6.96
6.88
6.85
5.62
5.04
5.02
4.59
4.57
4.55
4.53
3.71
3.11
3.09
3.06
3.04
3.02
2.99
2.97
2.40
1.41
OH
4b
CO2Me
NHBoc
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
Chemical Shift (ppm)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155.25
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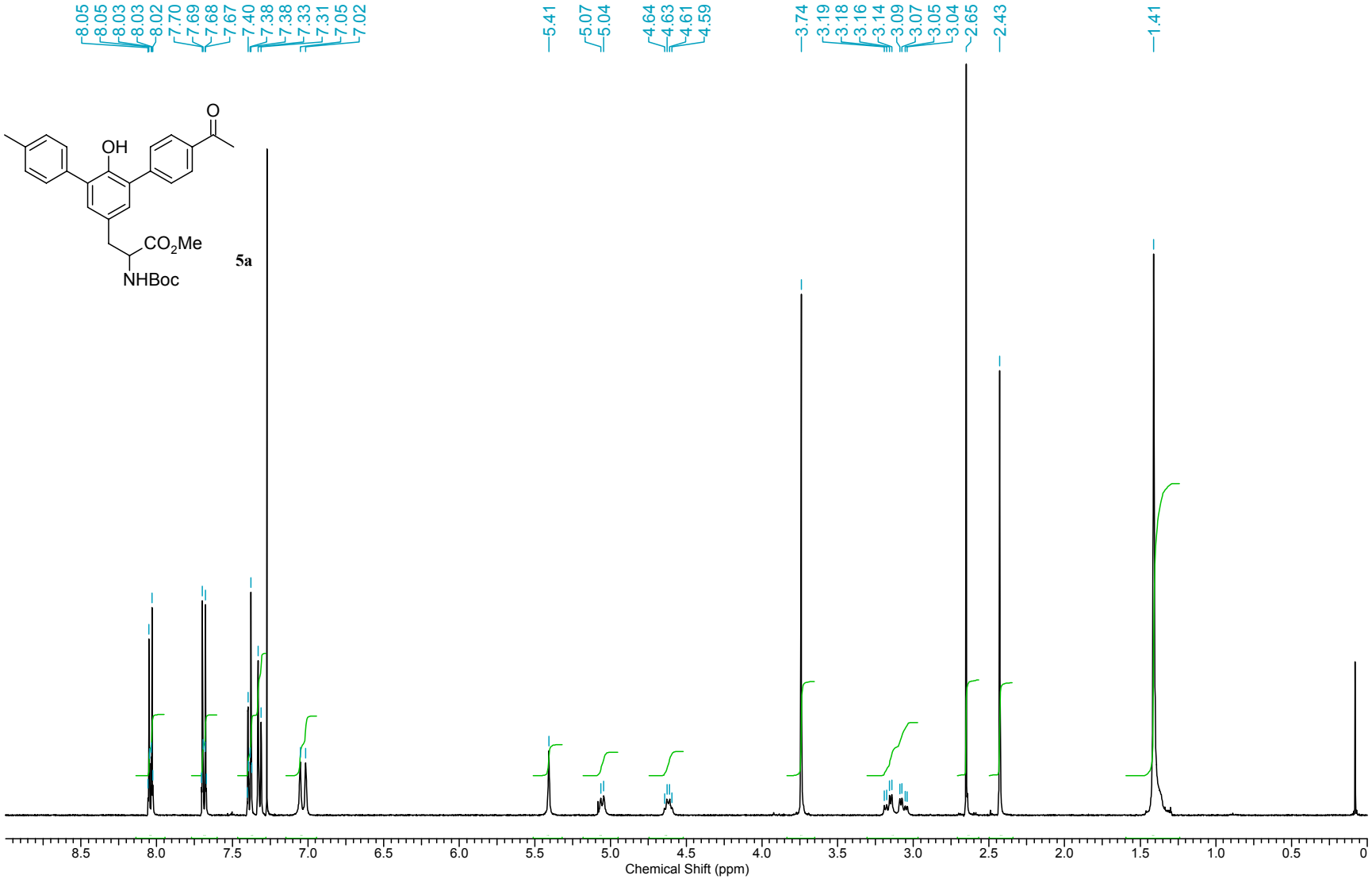
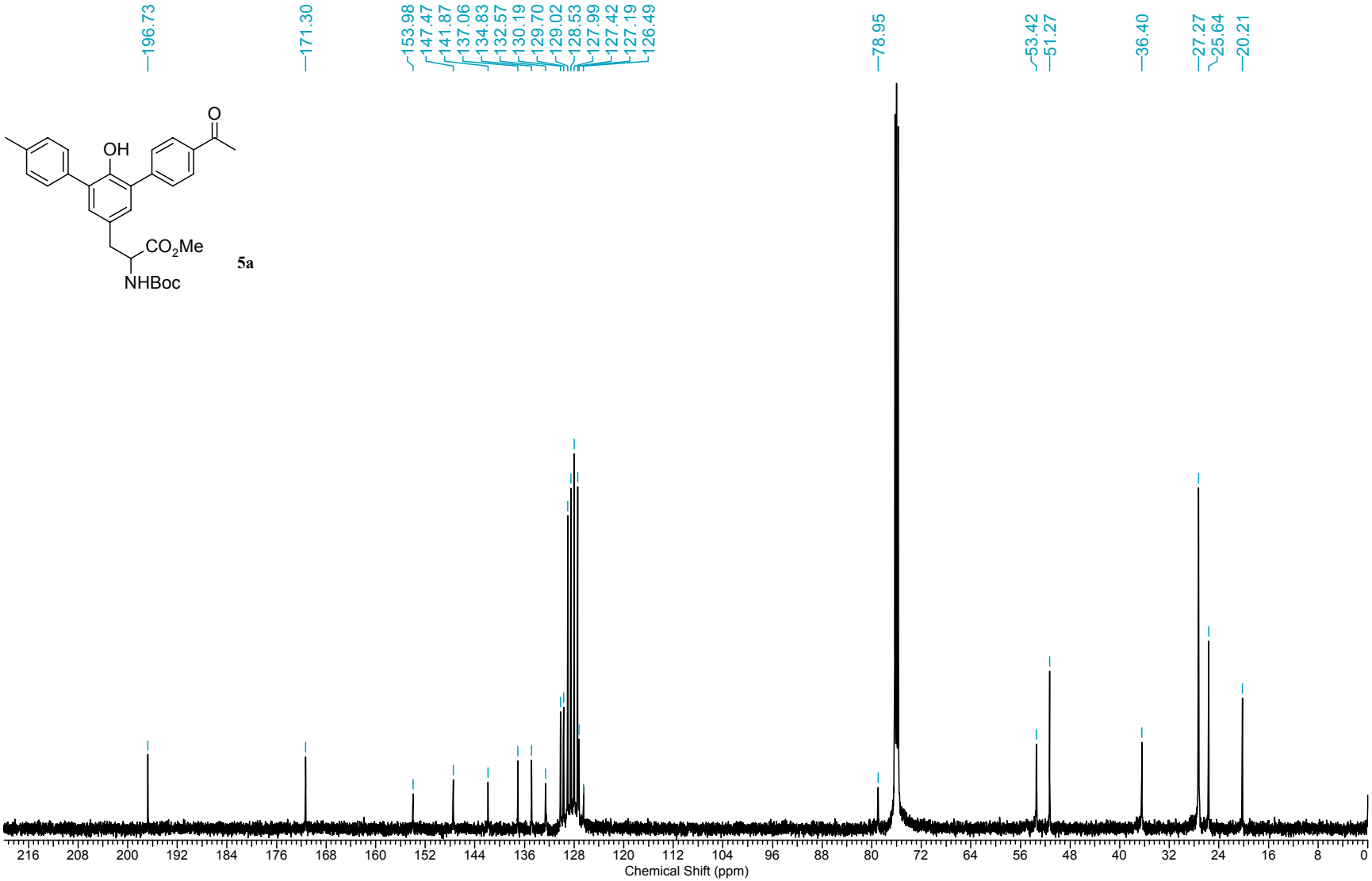
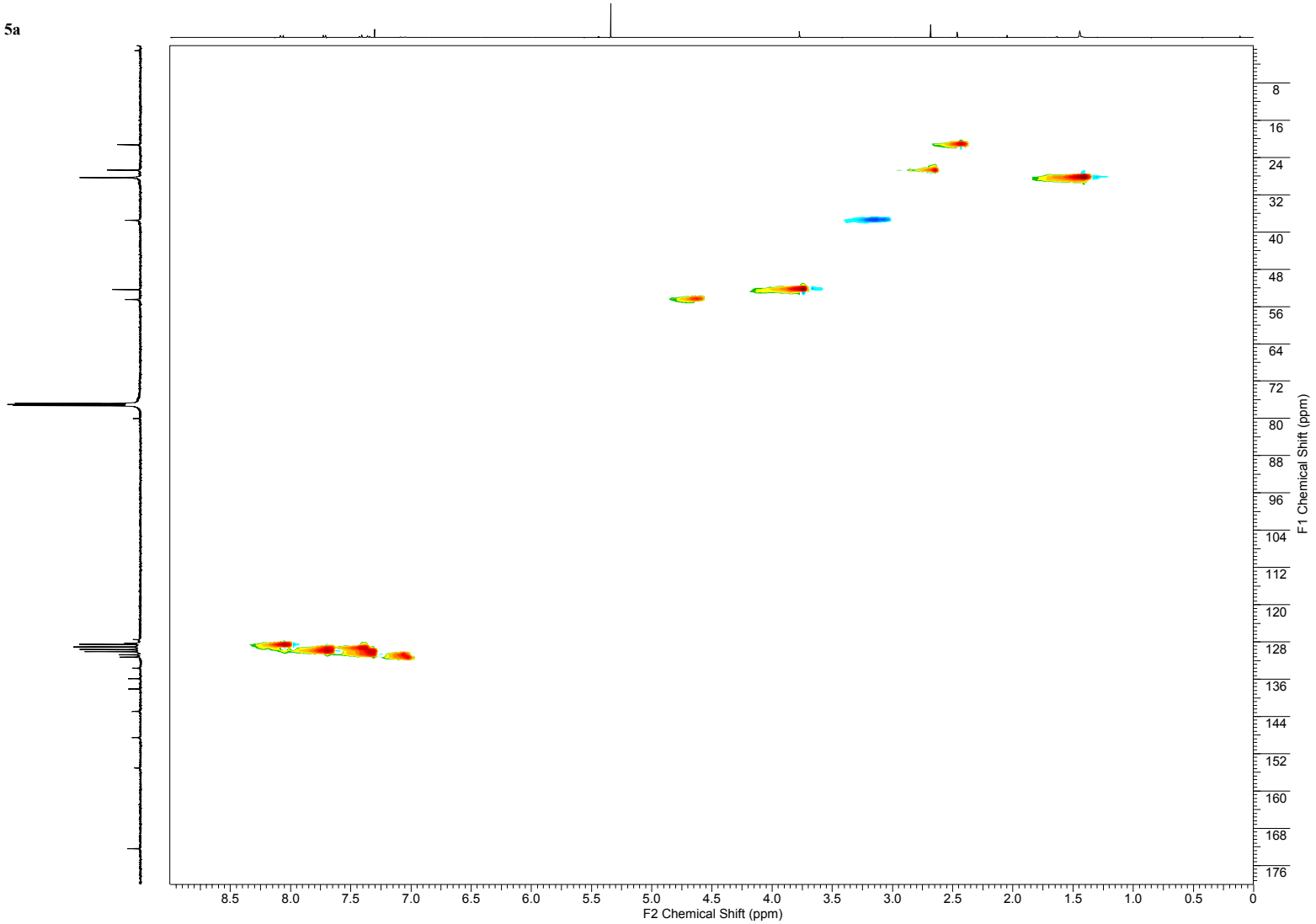
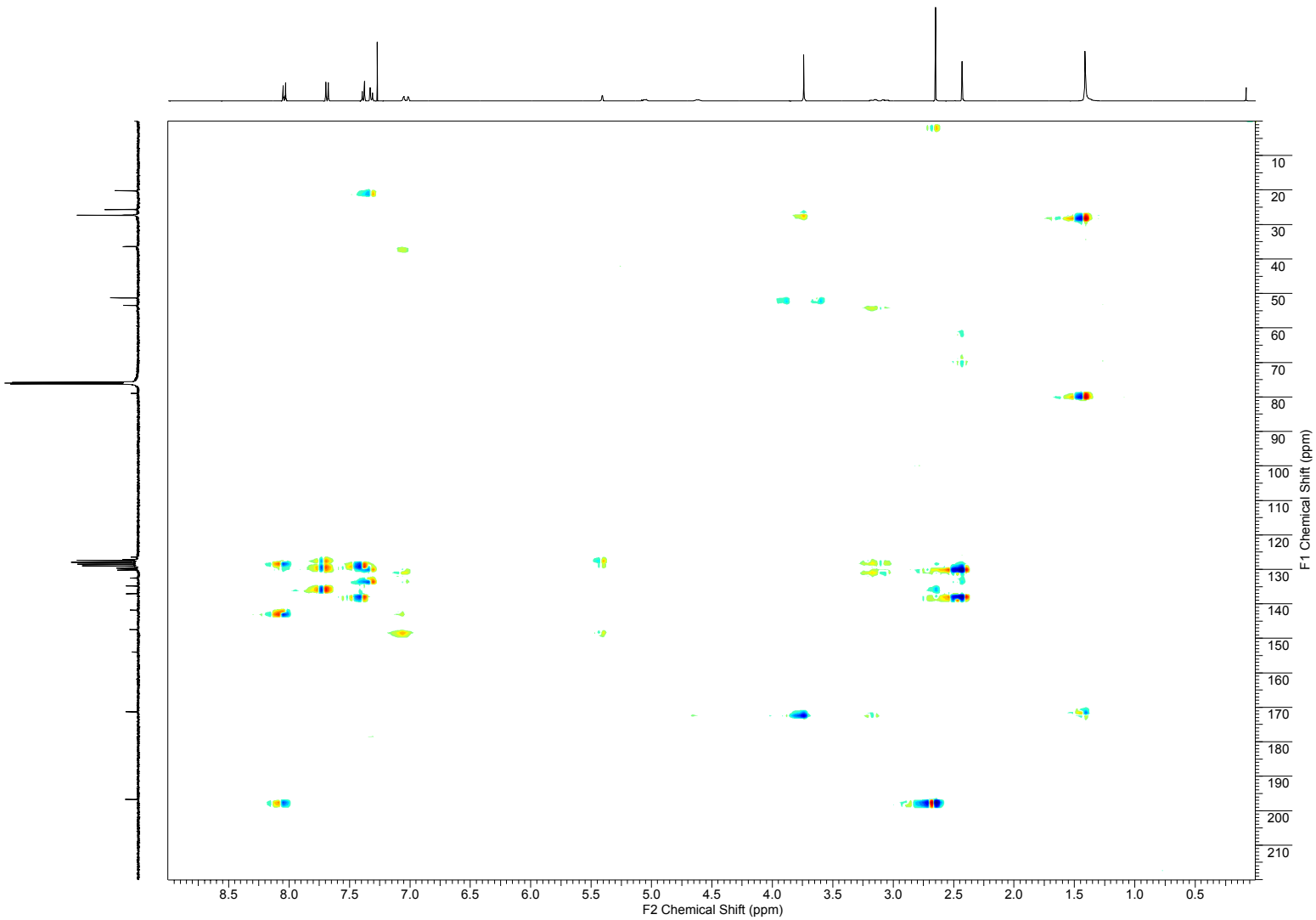
134.15
131.24
129.92
129.66
128.98
128.22
127.98
116.02
80.09
54.62
52.34
37.53
28.39
21.30
OH
CO2Me
NHBoc
4b
Chemical Shift (ppm)

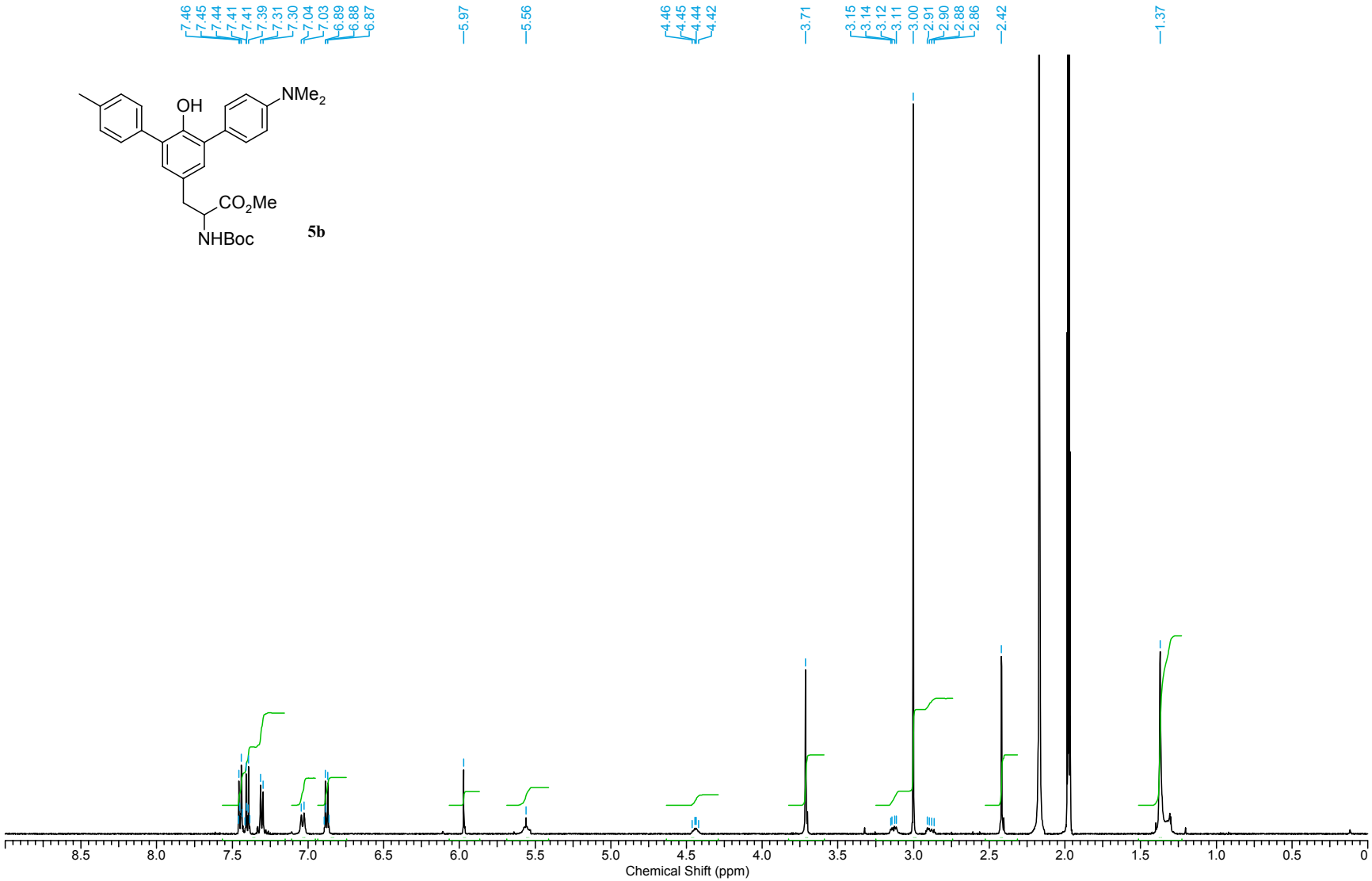

8.05
8.05
8.03
8.03
8.02
7.70
7.69
7.68
7.67
7.40
7.38
7.33
7.31
7.05
7.02
5.41
5.07
5.04
4.64
4.63
4.61
4.59
3.74
3.19
3.18
3.16
3.14
3.09
3.07
3.05
3.04
2.65
2.43
1.41
O
OH
CO2Me
NHBoc
5a
Chemical Shift (ppm)

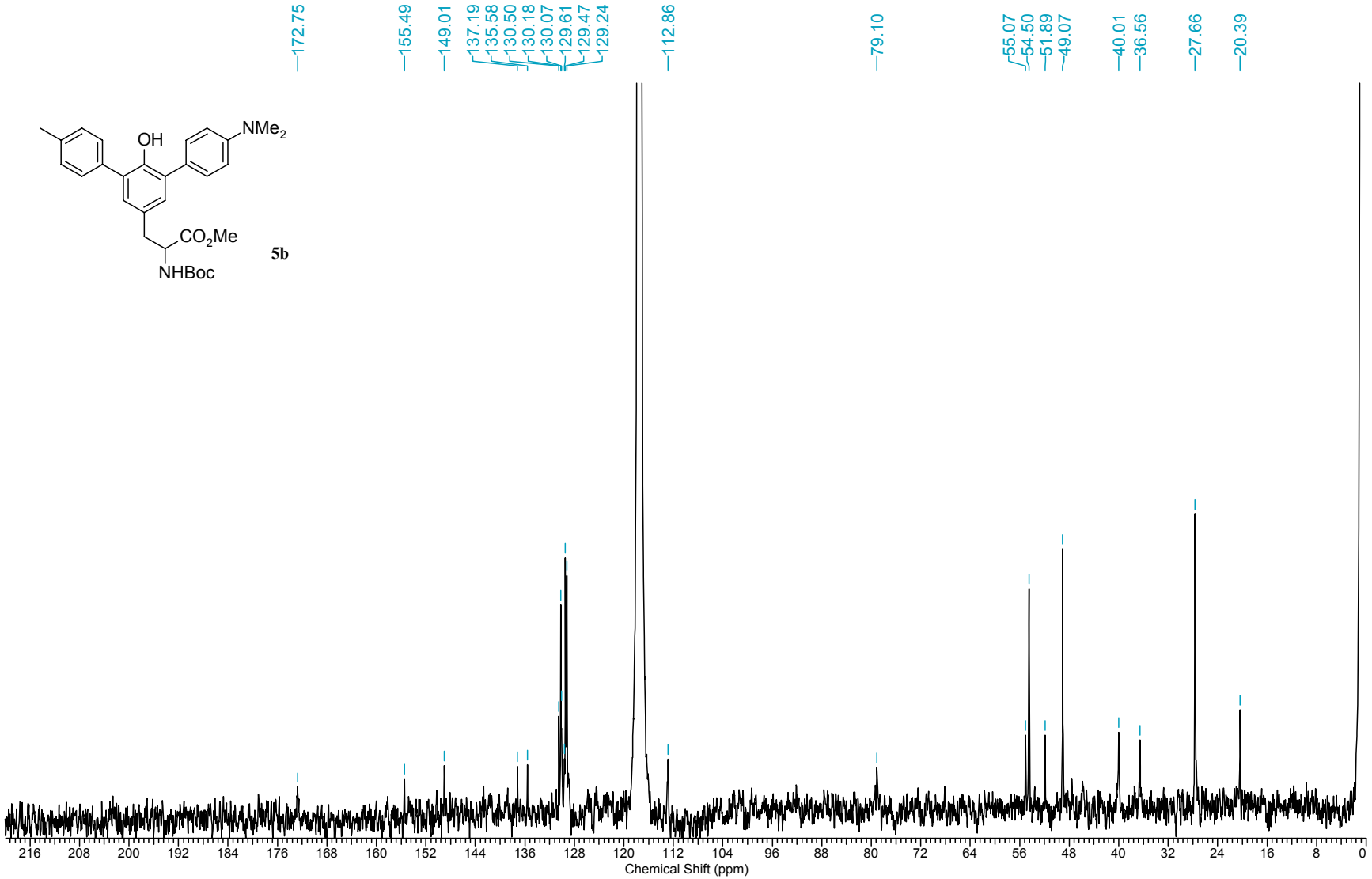

196.73
171.30
153.98
147.47
141.87
137.06
134.83
132.57
130.19
129.70
129.02
128.53
127.99
127.42
127.19
126.49
78.95
53.42
51.27
36.40
27.27
25.64
20.21
O
OH
CO2Me
NHBoc
5a
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)


5a
F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)

5a




7.46
7.45
7.44
7.41
7.41
7.39
7.31
7.30
7.04
7.03
6.89
6.88
6.87
5.97
5.56
4.46
4.45
4.44
4.42
3.71
3.15
3.14
3.12
3.11
3.00
2.91
2.90
2.88
2.86
2.42
1.37
OH
NMe2
CO2Me
NHBoc
5b
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
Chemical Shift (ppm)


172.75
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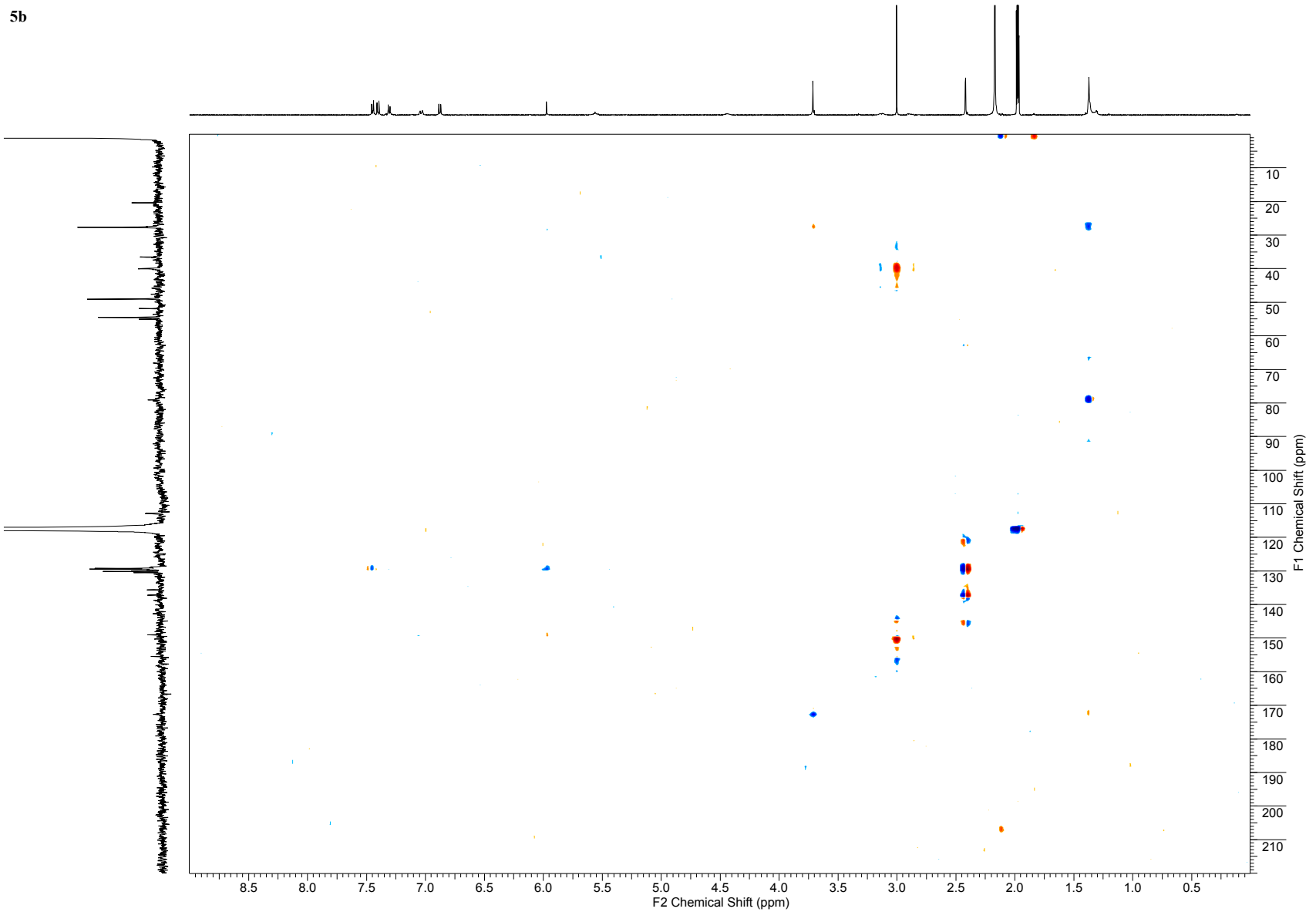
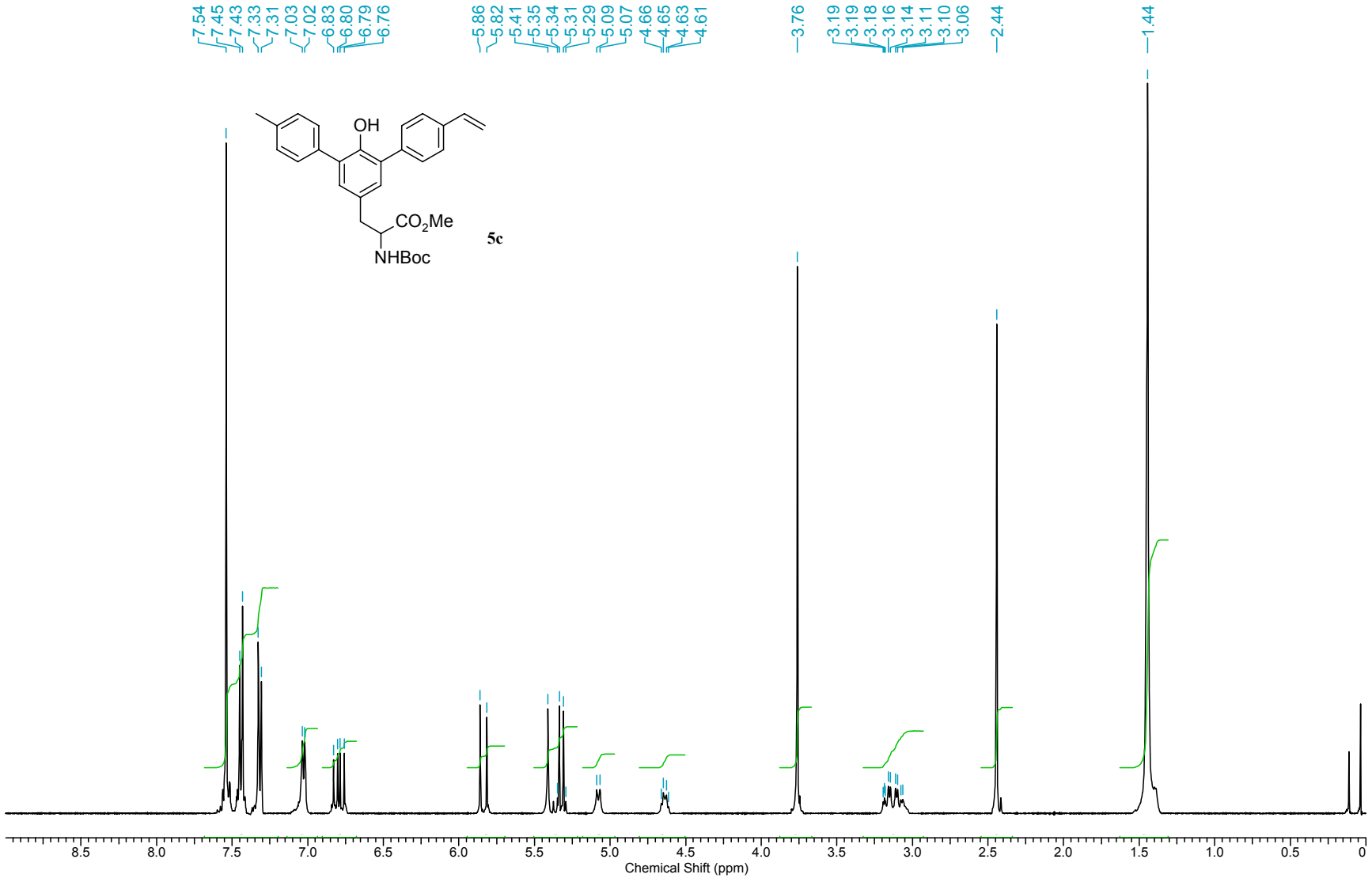
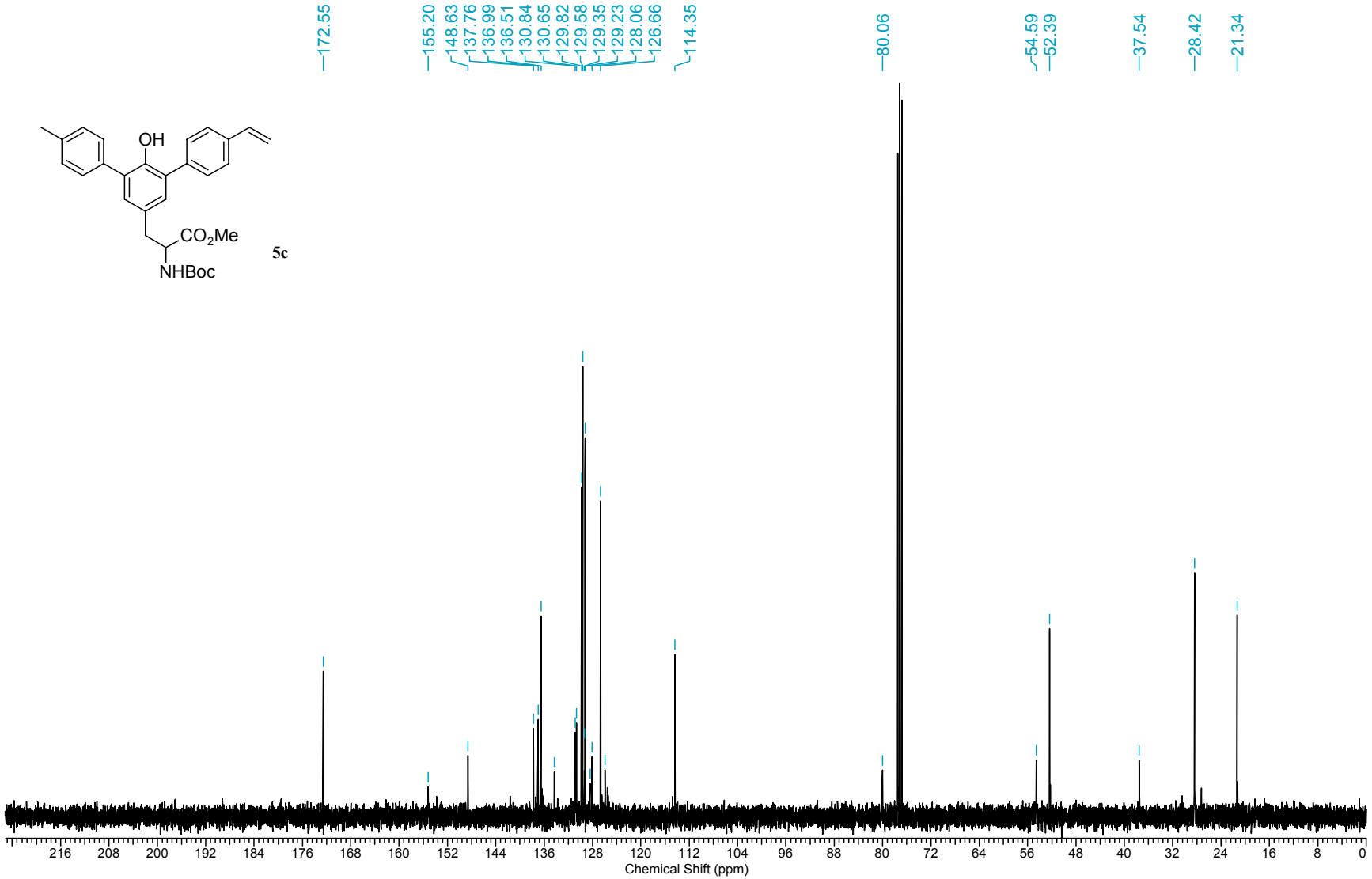
149.01
137.19
135.58
130.50
130.18
130.07
129.61
129.47
129.24
112.86
79.10
55.07
54.50
51.89
49.07
40.01
36.56
27.66
20.39
OH
NMe2
CO2Me
NHBoc
5b
216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)

5b




7.54
7.45
7.43
7.33
7.31
7.03
7.02
6.83
6.80
6.79
6.76
5.86
5.82
5.41
5.35
5.34
5.31
5.29
5.09
5.07
4.66
4.65
4.63
4.61
3.76
3.19
3.19
3.18
3.16
3.14
3.11
3.10
3.06
2.44
1.44
OH
CO2Me
NHBoc
5c
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
Chemical Shift (ppm)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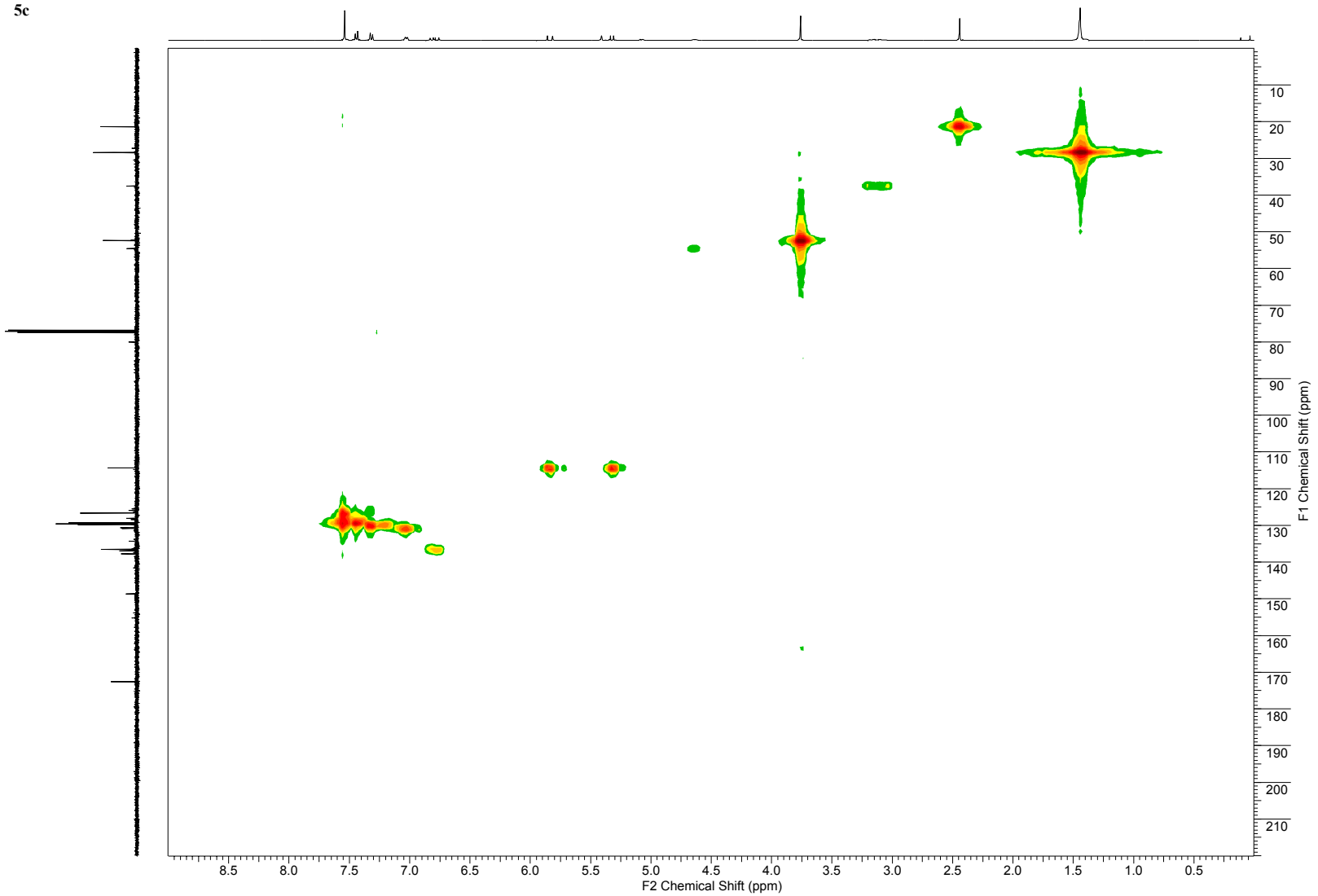
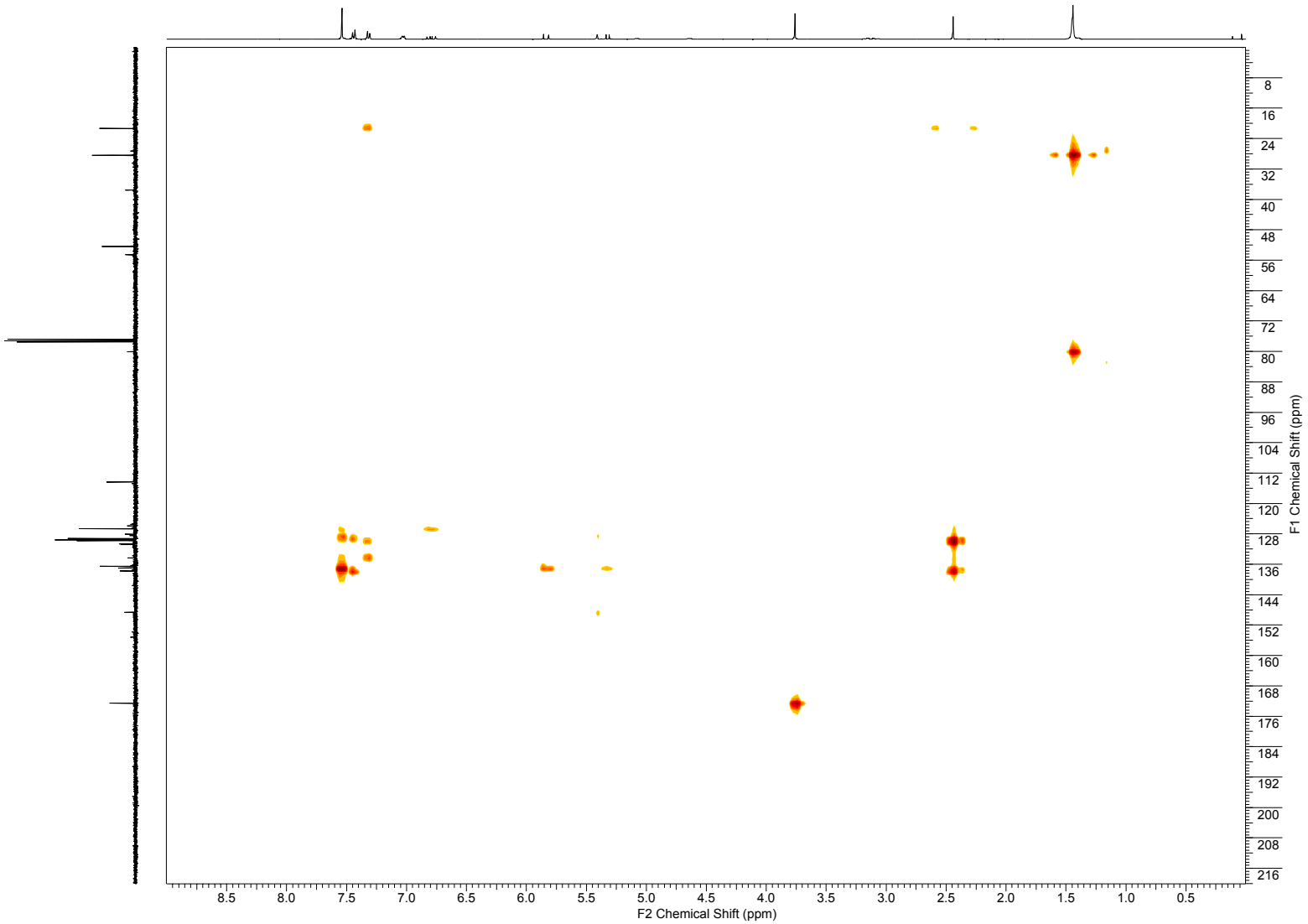
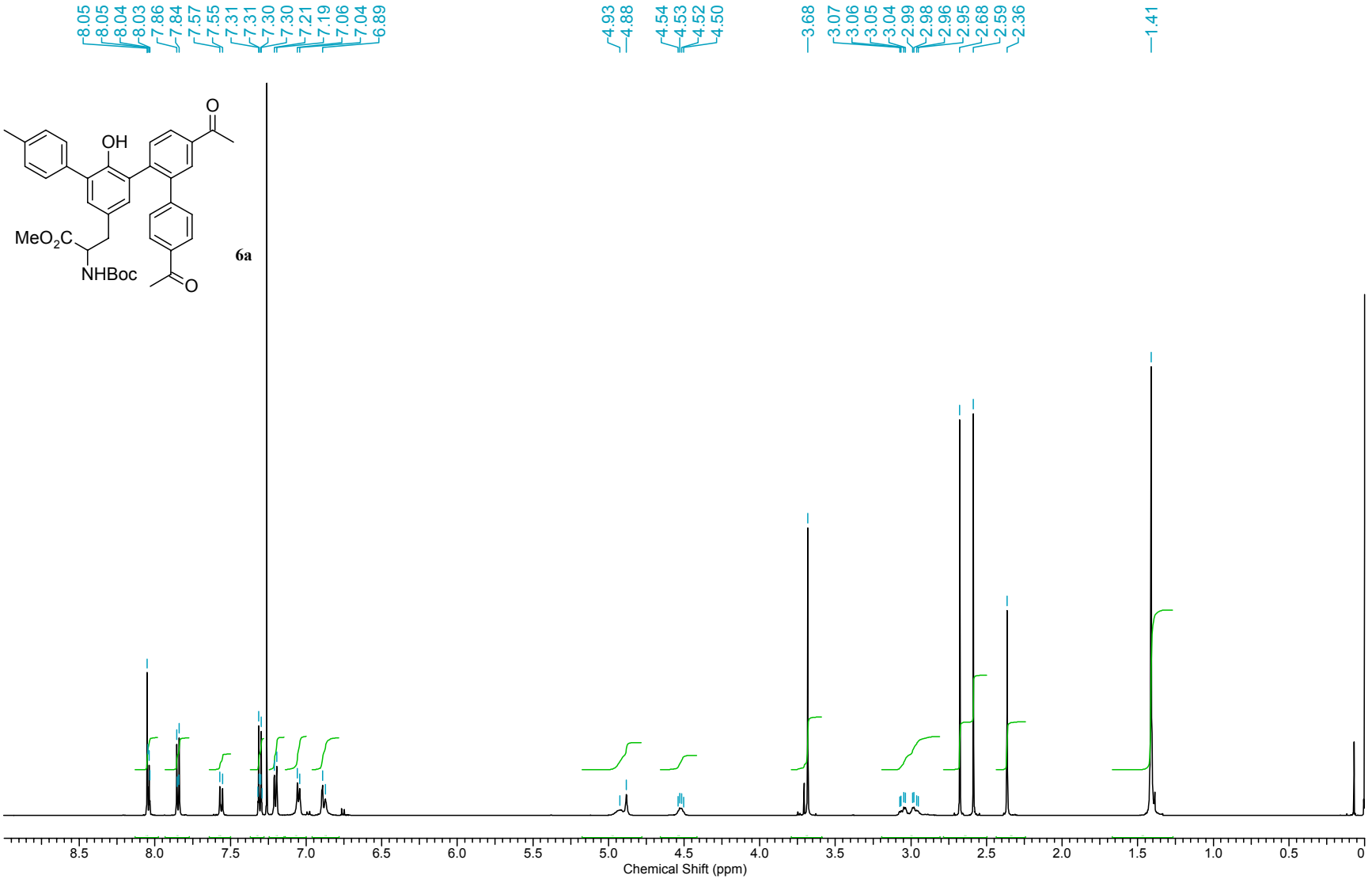
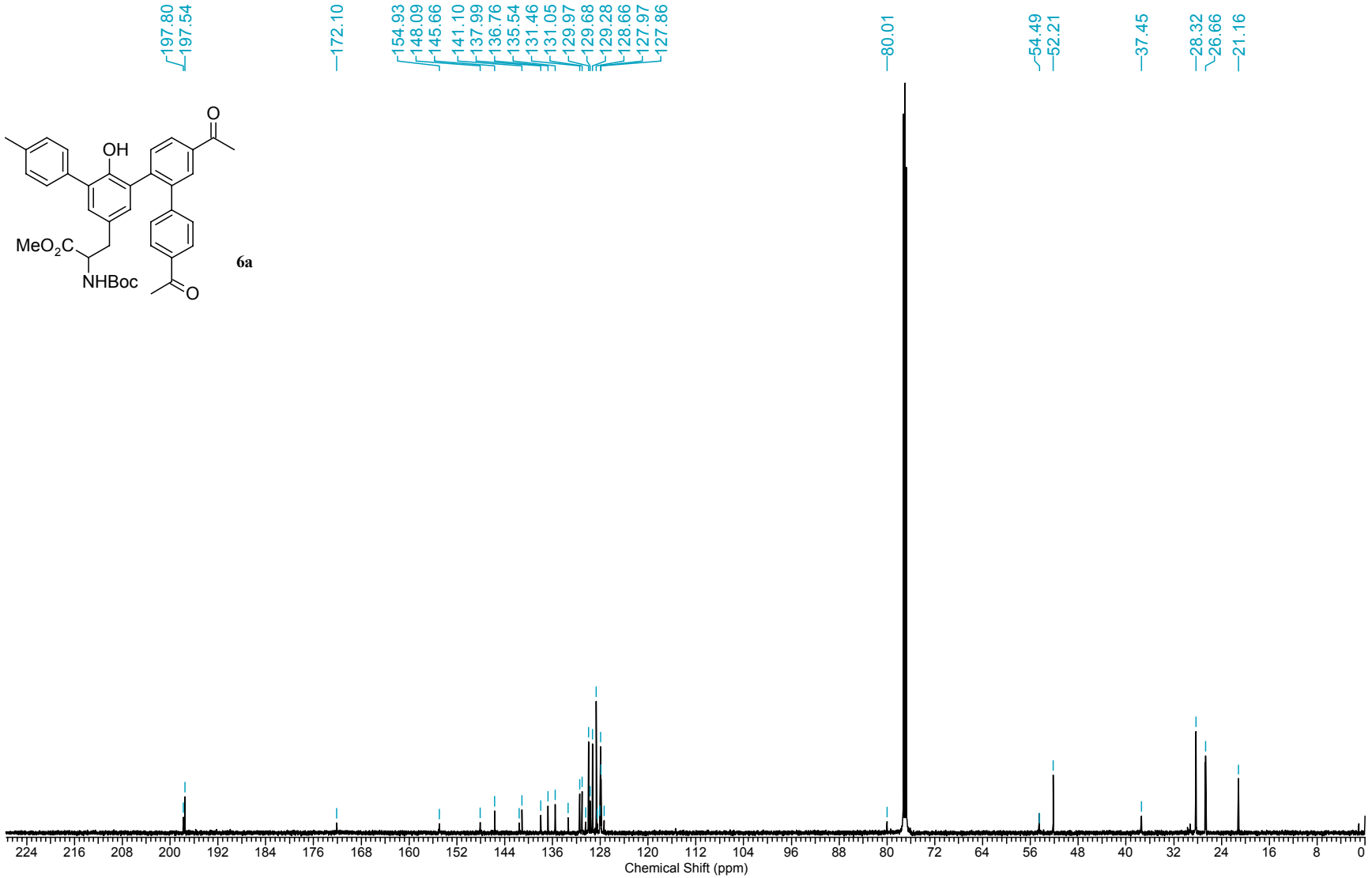
148.63
137.76
136.99
136.51
130.84
130.65
129.82
129.58
129.35
129.23
128.06
126.66
114.35
80.06
54.59
52.39
37.54
28.42
21.34
OH
CO2Me
NHBoc
5c
Chemical Shift (ppm)


5c
F2 Chemical Shift (ppm)
F1 Chemical Shift (ppm)

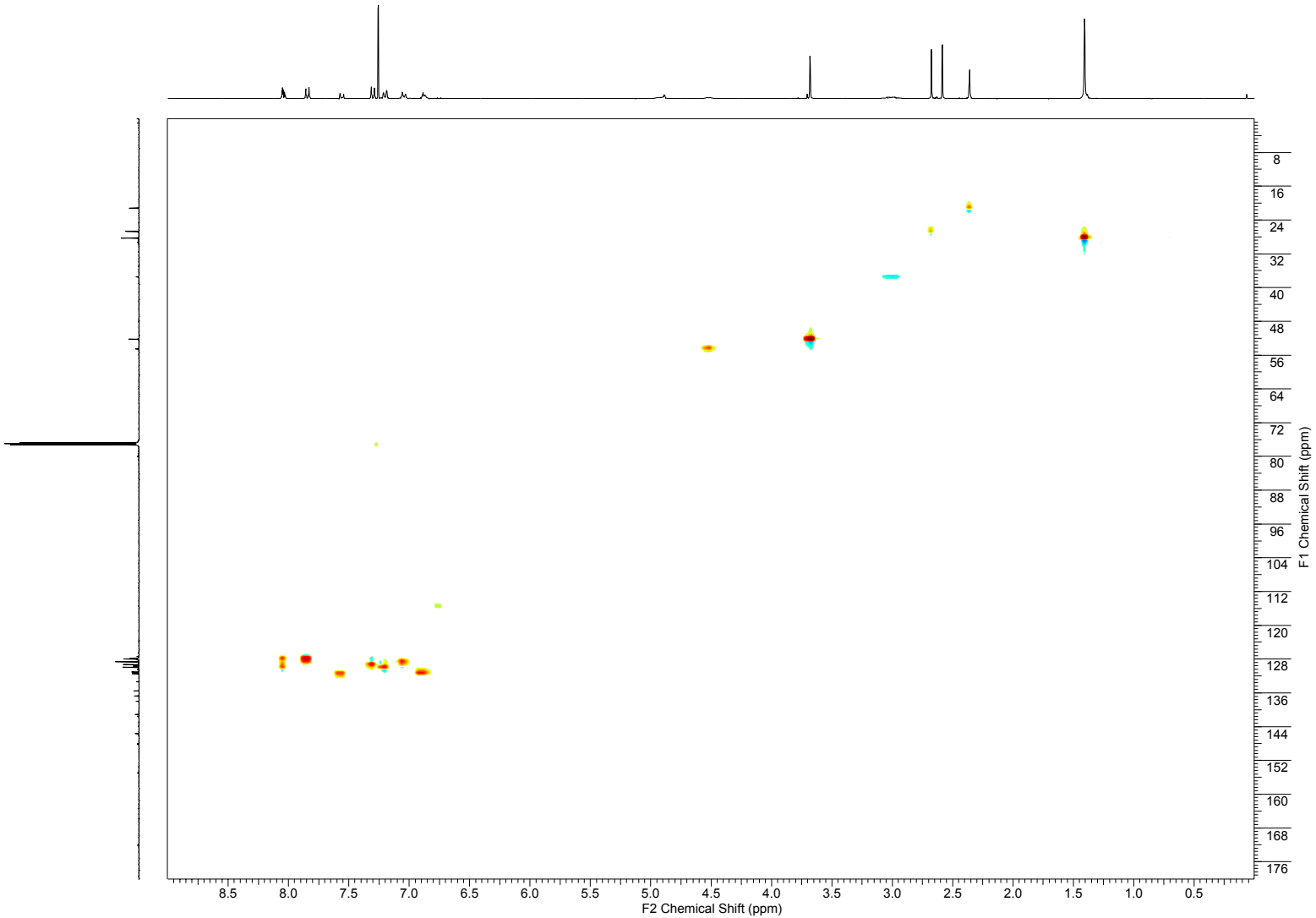
5c


8
16
24
32
40
48
56
64
72
80
88
96
104
112
120
128
136
144
152
160
168
176
184
192
200
208
216
F1 Chemical Shift (ppm)
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
F2 Chemical Shift (ppm)

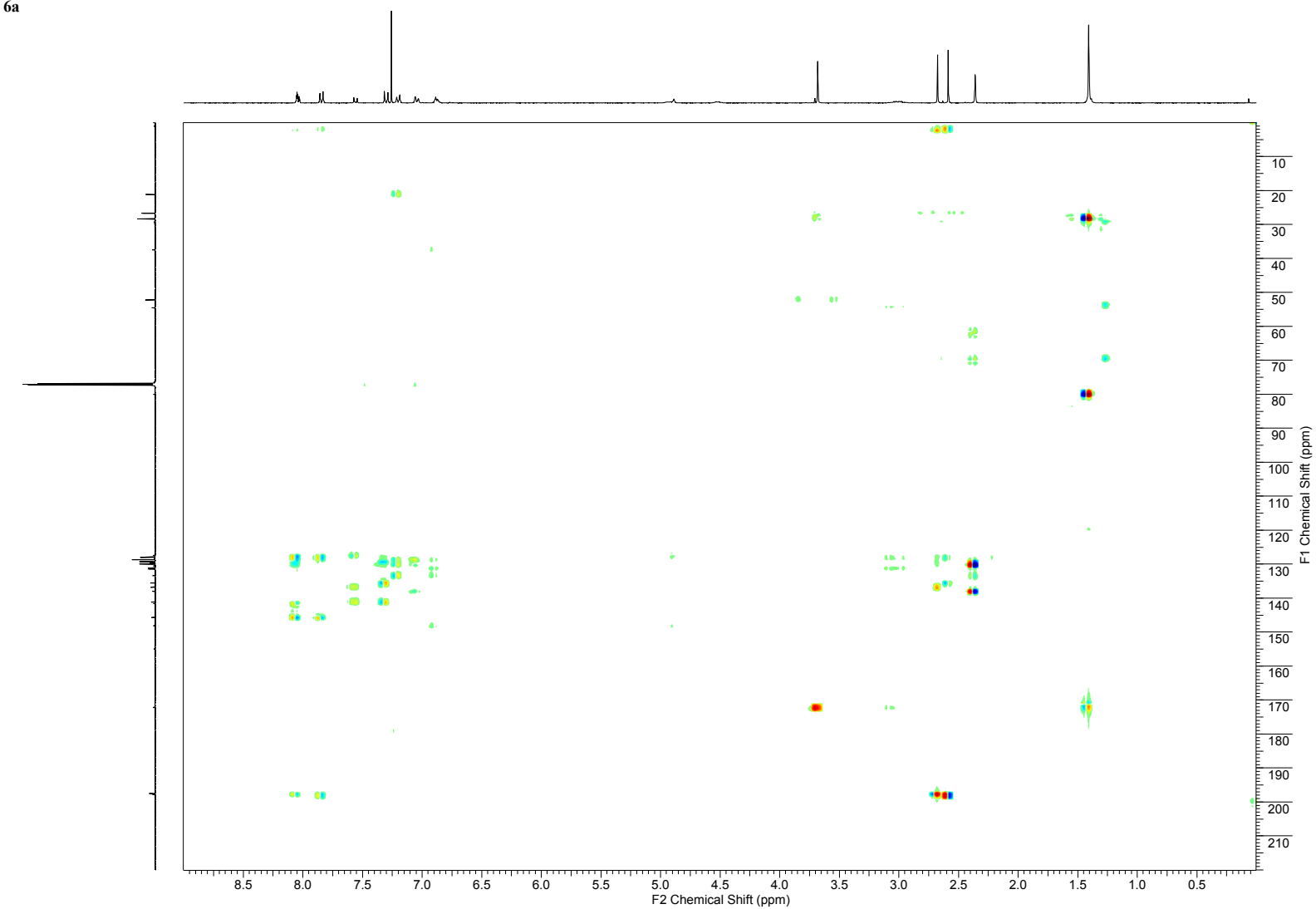

8.05
8.05
8.04
8.03
7.86
7.84
7.57
7.55
7.31
7.31
7.30
7.30
7.21
7.19
7.06
7.04
6.89
4.93
4.88
4.54
4.53
4.52
4.50
3.68
3.07
3.06
3.05
3.04
2.99
2.98
2.96
2.95
2.68
2.59
2.36
1.41
OH
O
MeO2C
NHBoc
O
6a
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

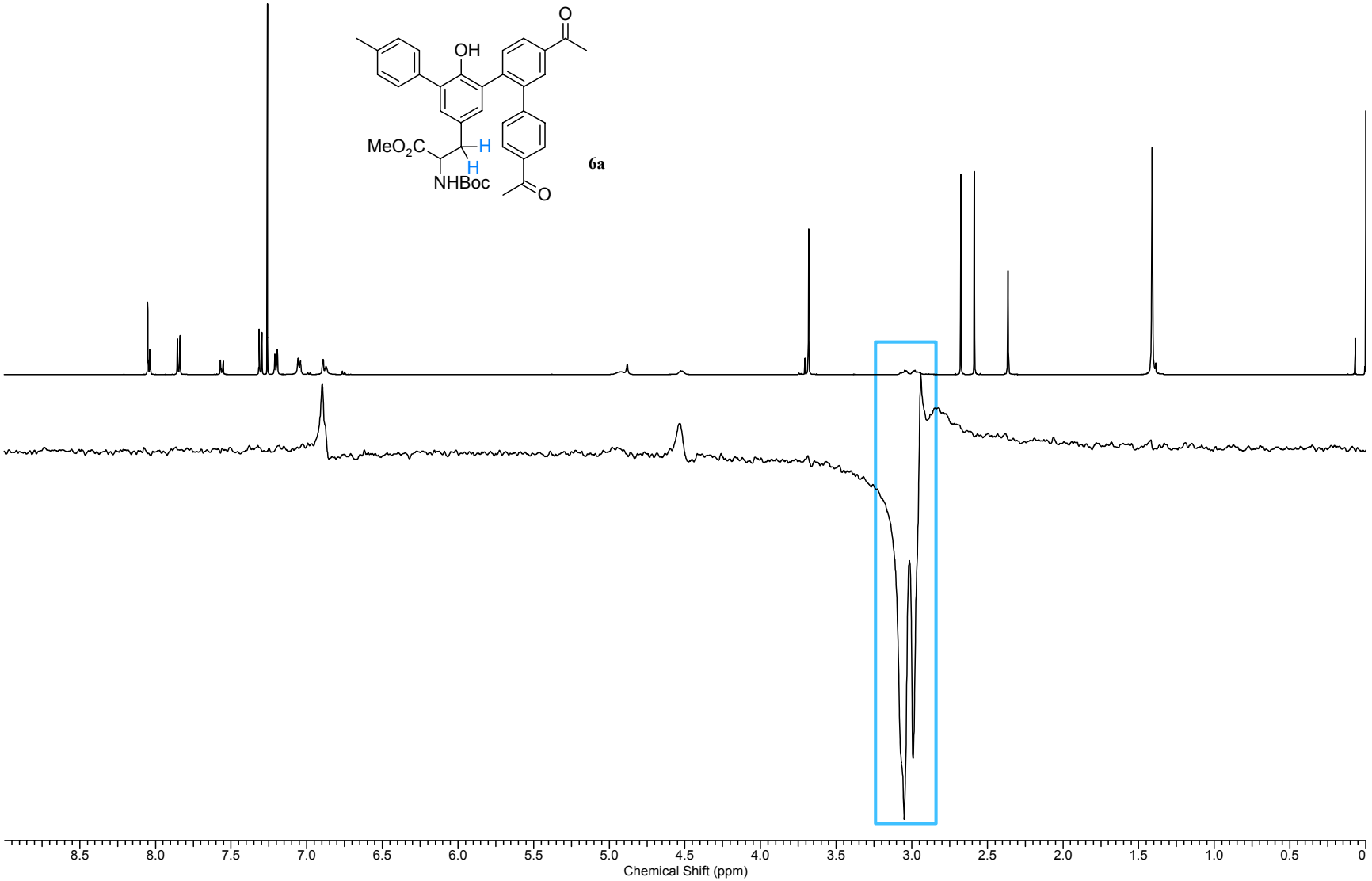

197.80
197.54
172.10
154.93
148.09
145.66
141.10
137.99
136.76
135.54
131.46
131.05
129.97
129.68
129.28
128.66
127.97
127.86
80.01
54.49
52.21
37.45
28.32
26.66
21.16
OH
O
MeO2C
NHBoc
O
6a
224 216 208 200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0
Chemical Shift (ppm)

6a

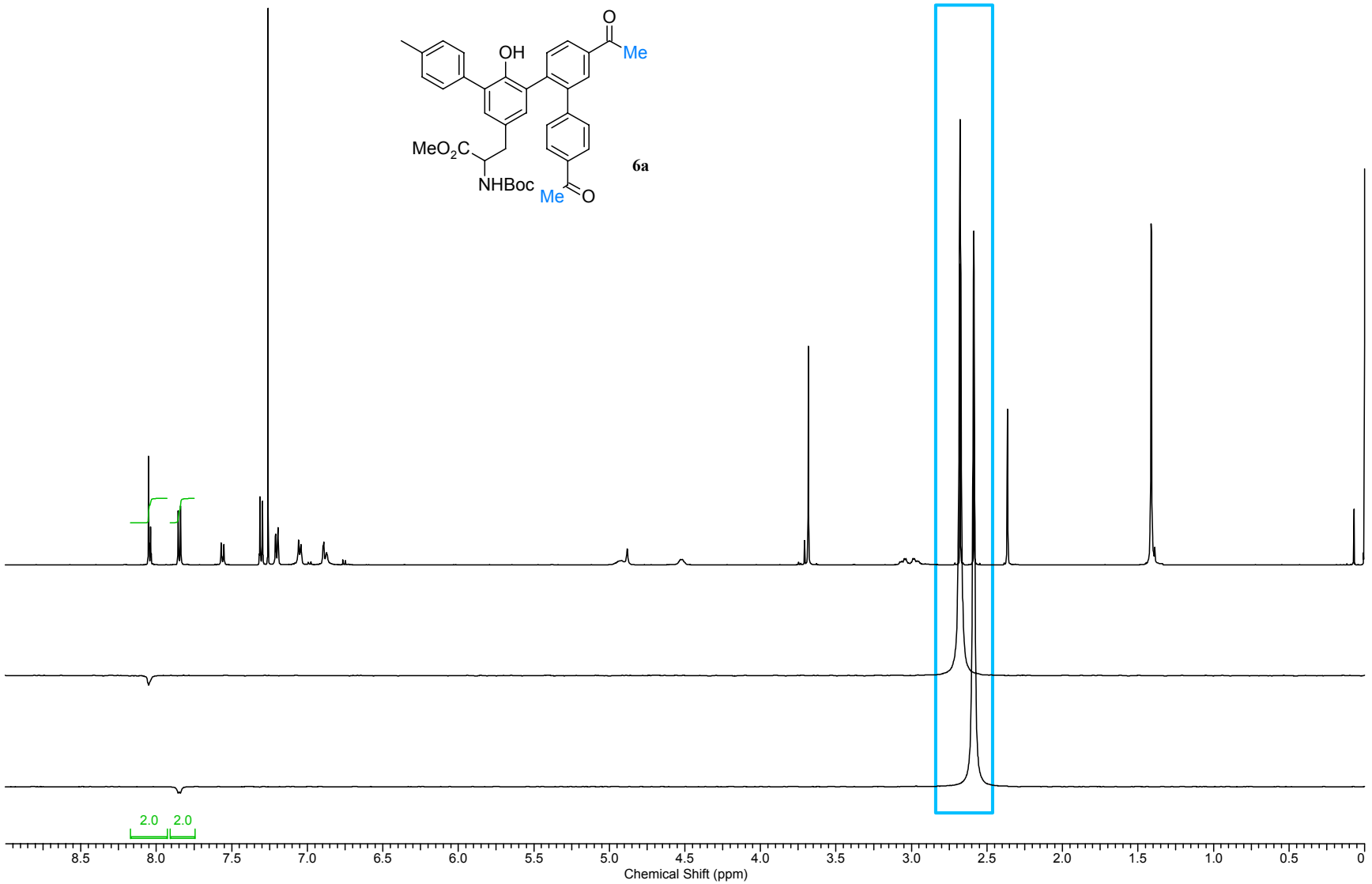

8
16
24
32
40
48
56
64
72
80
88
96
104
112
120
128
136
144
152
160
168
176
F1 Chemical Shift (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
F2 Chemical Shift (ppm)

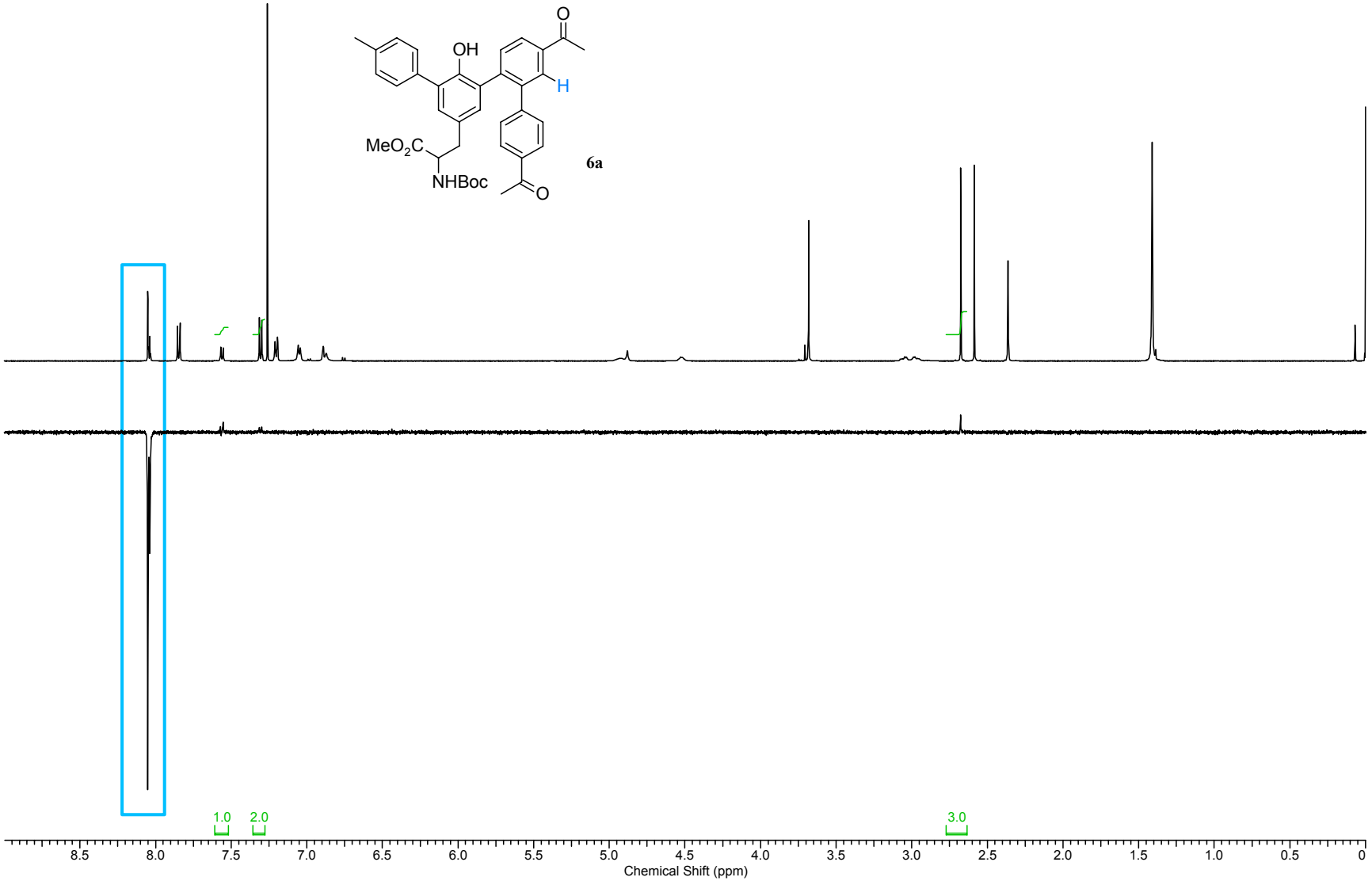
6a

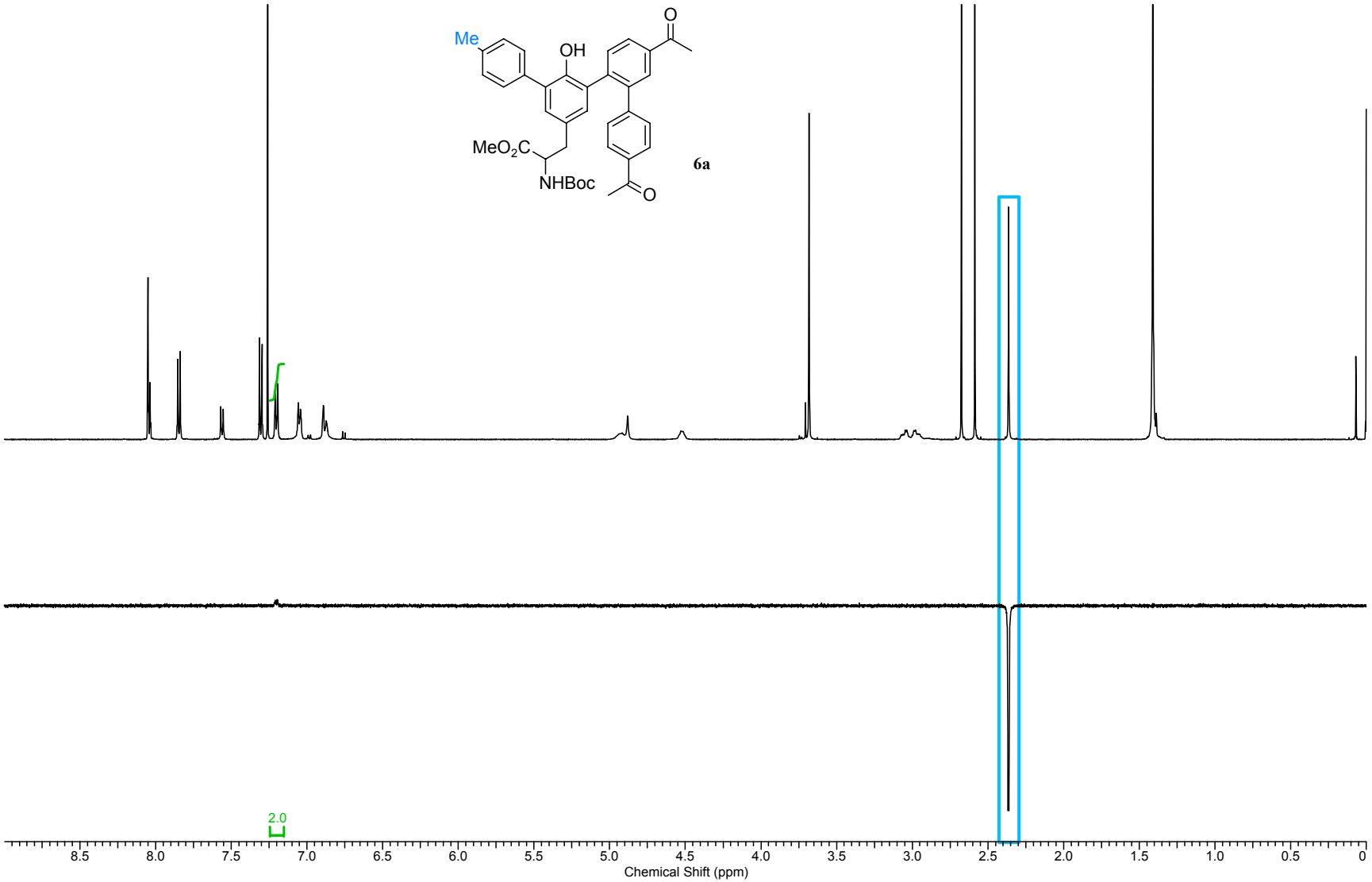



OH
O
MeO2C
H
H
NHBoc
O
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

6a


OH
O
Me
MeO2C
NHBoc
Me
O
6a
2.0
2.0
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
Chemical Shift (ppm)


O
OH
H
MeO2C
NHBoc
O
6a
1.0
2.0
3.0
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
Chemical Shift (ppm)

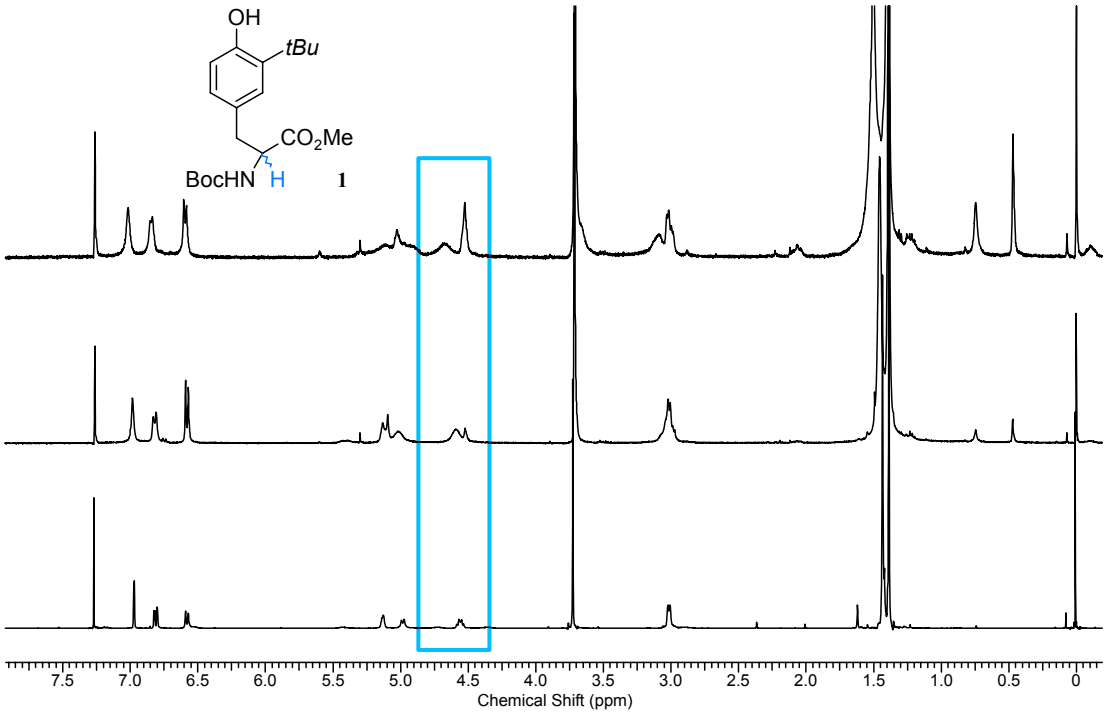

Me
OH
O
MeO2C
NHBoc
O
6a
2.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

NMR Lanthanide Shift Result

1 + 2 mg E\u(hfc)$_3$

1 +1 mg Eu(hfc)$_3$

1



Polarimetry: 1 $[\alpha]_D$ = 0.0 (1g per 100 mL MeOH, 22 °C)

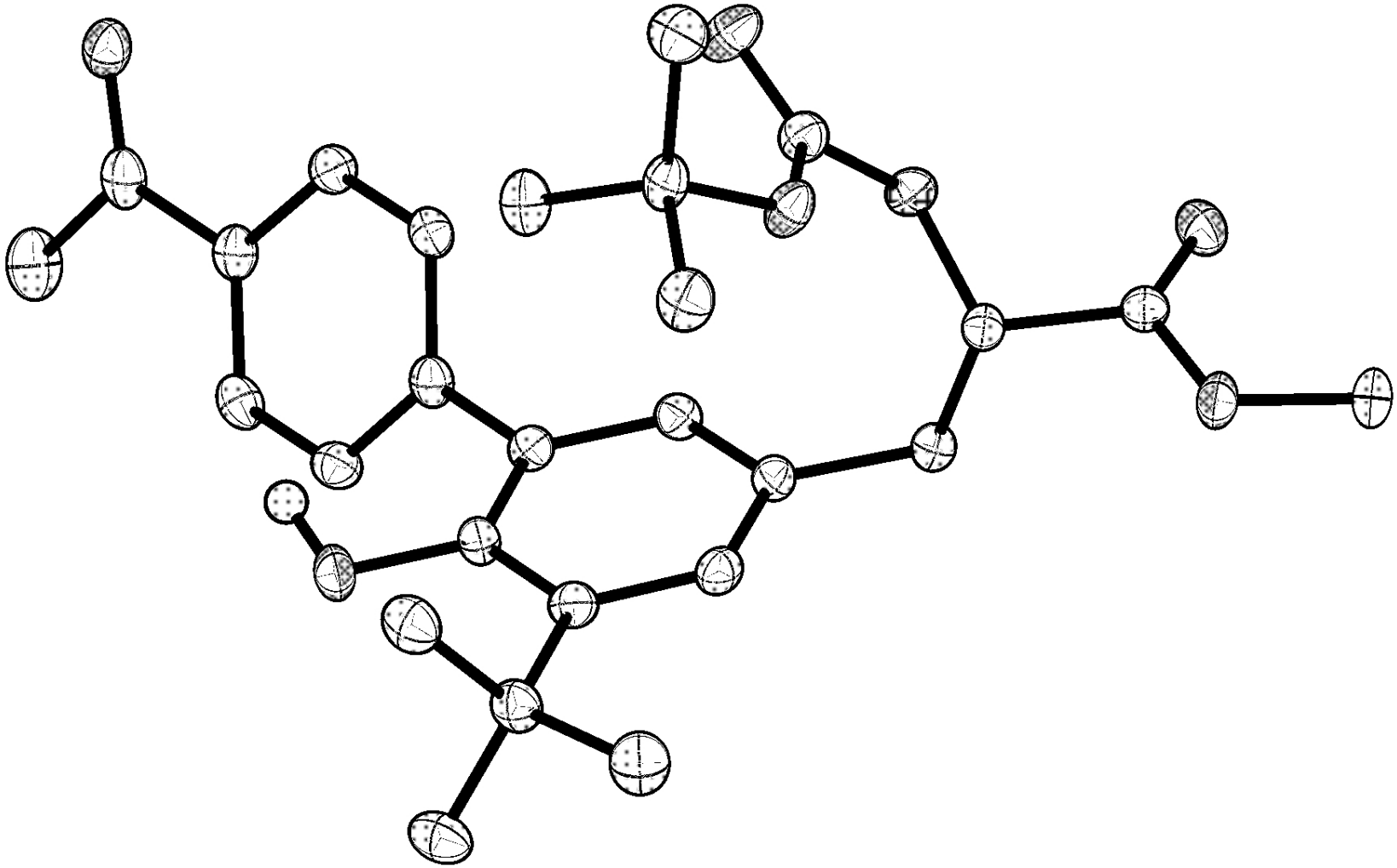


Figure S1. X-ray structure of **3a**, thermal ellipsoids set at 50%.

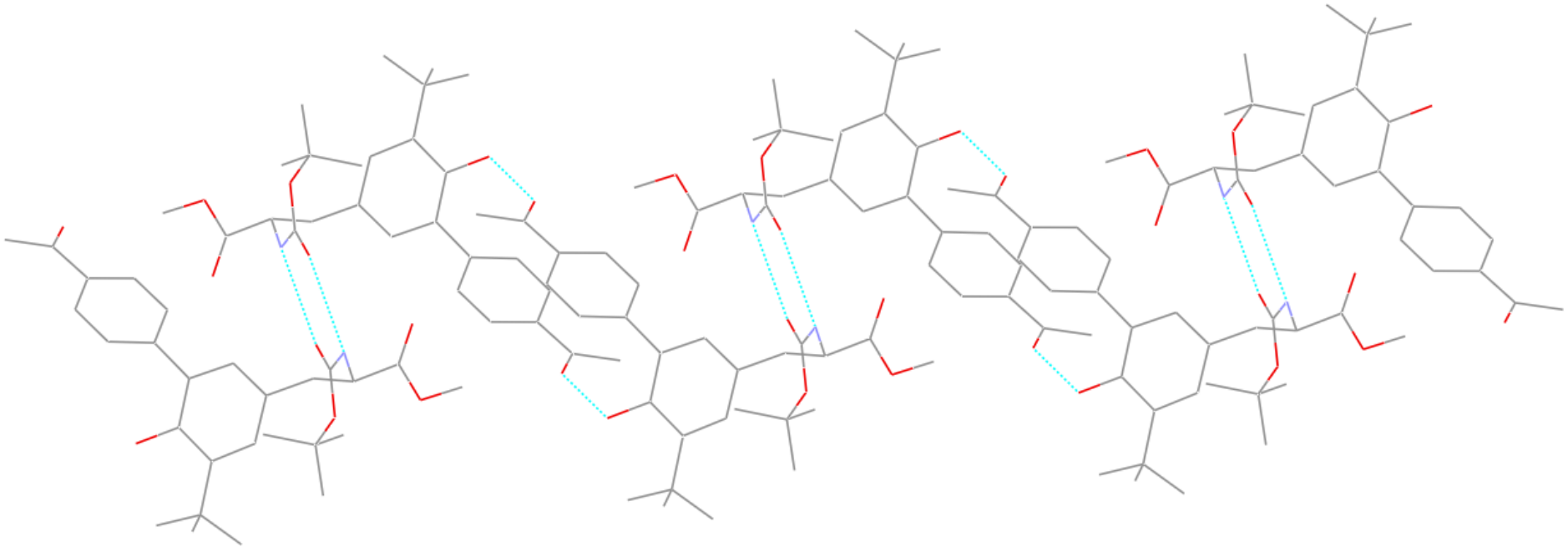


Figure S2. Packing diagram for **3a**.