Supporting Information

Palladium-catalyzed amidation of aryl halides using MOP-type ligand

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[‡]*School of Pharmacy, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, China*

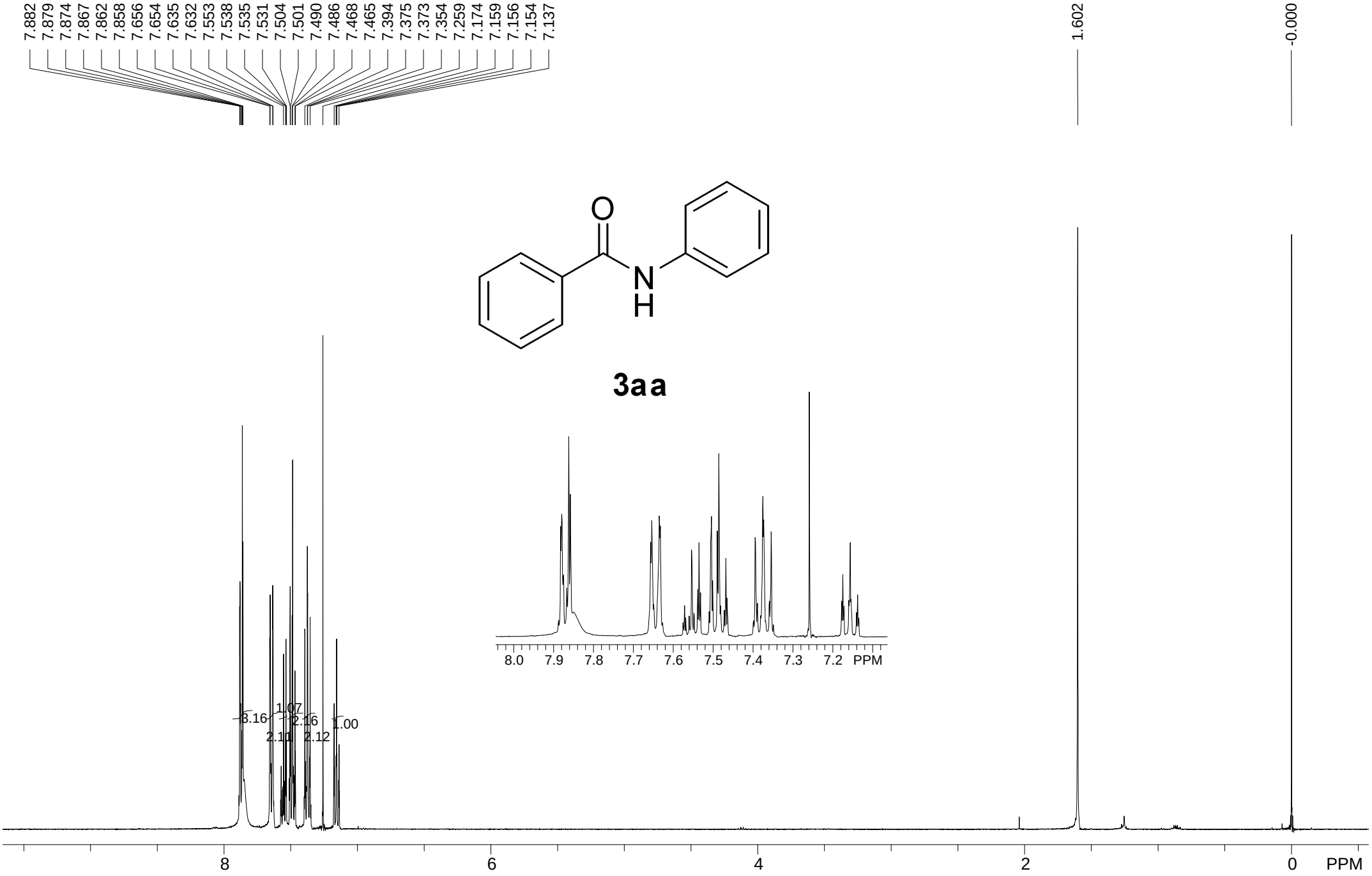
[§]*School of Chemistry, Chemical Engineering and Materials, Heilongjiang University, 74 Xuefu Road, Harbin, 150000*

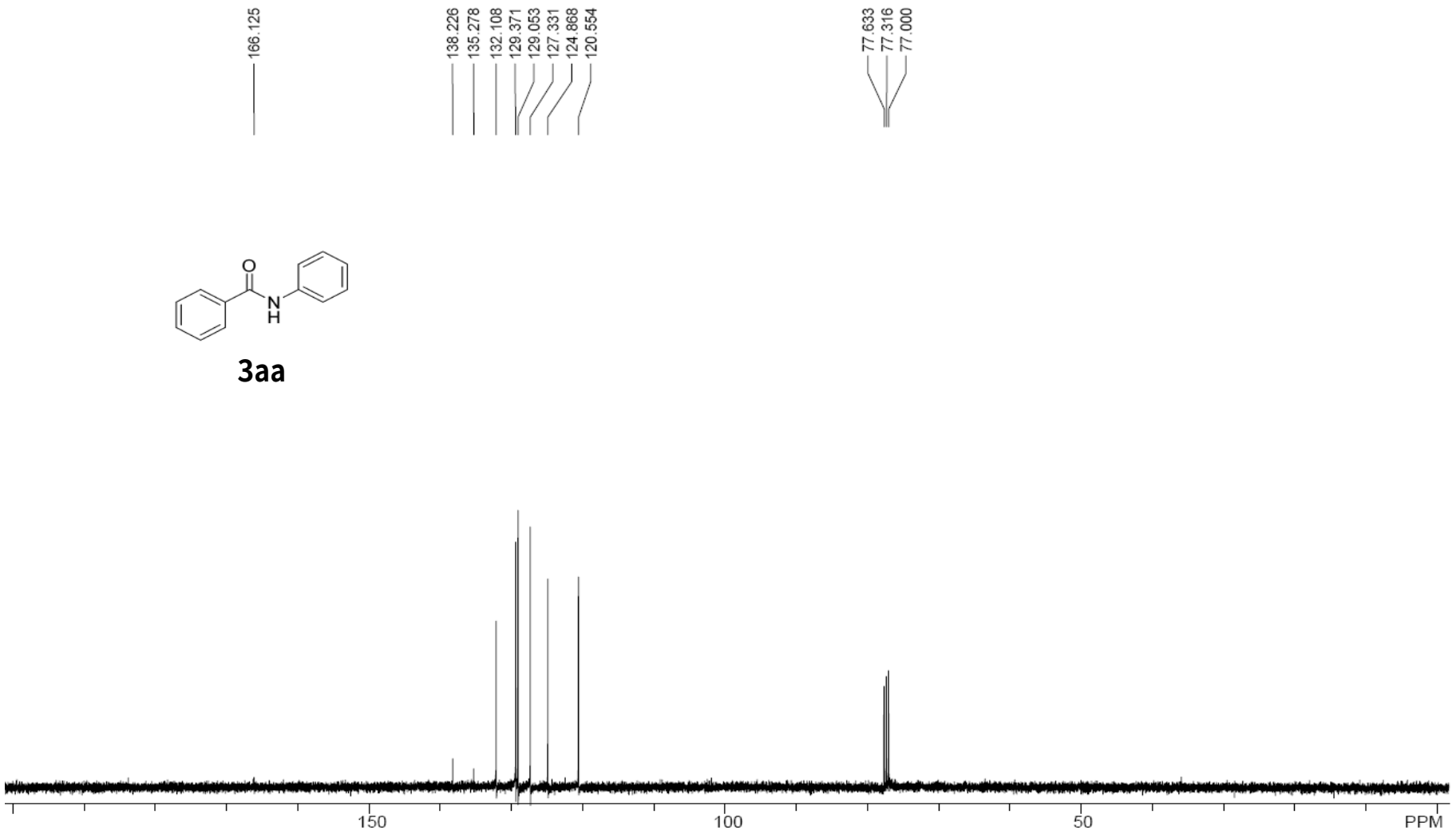
zhaoguo@sjtu.edu.cn

Phone: +86-2154748925, Fax: +86-21-5474-8925

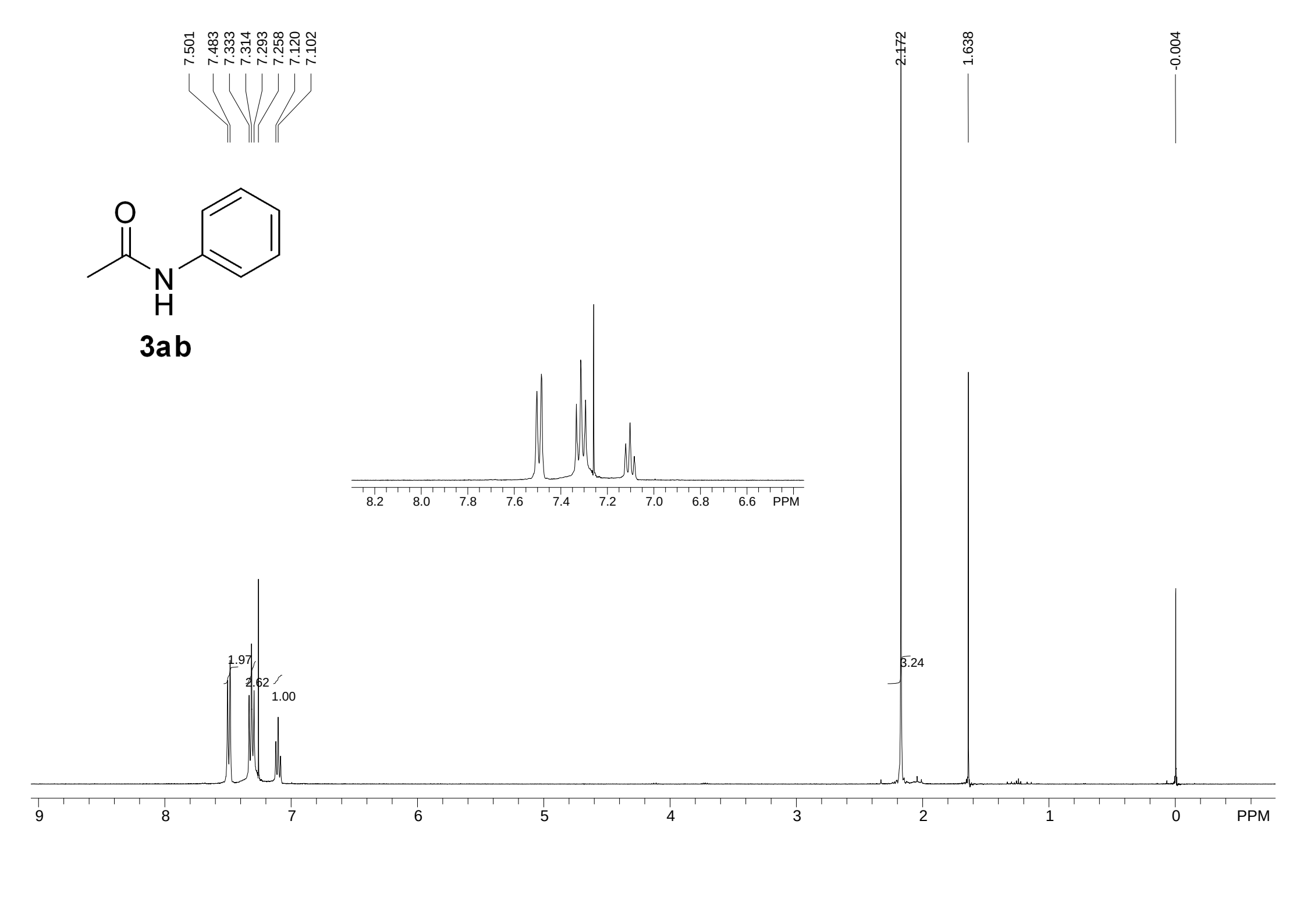
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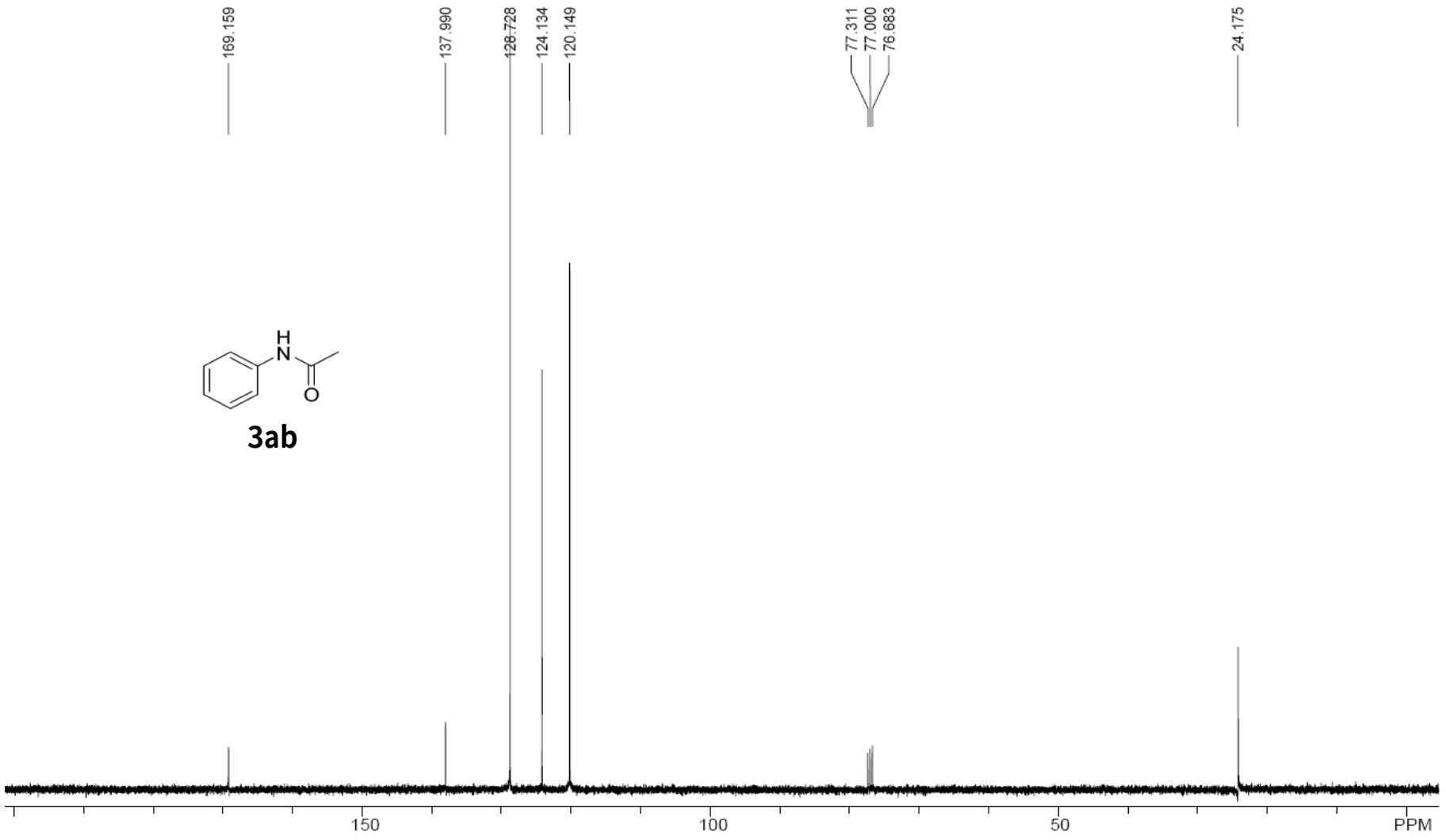
^{1}H and ^{13}C NMR spectra of the products S2-S57

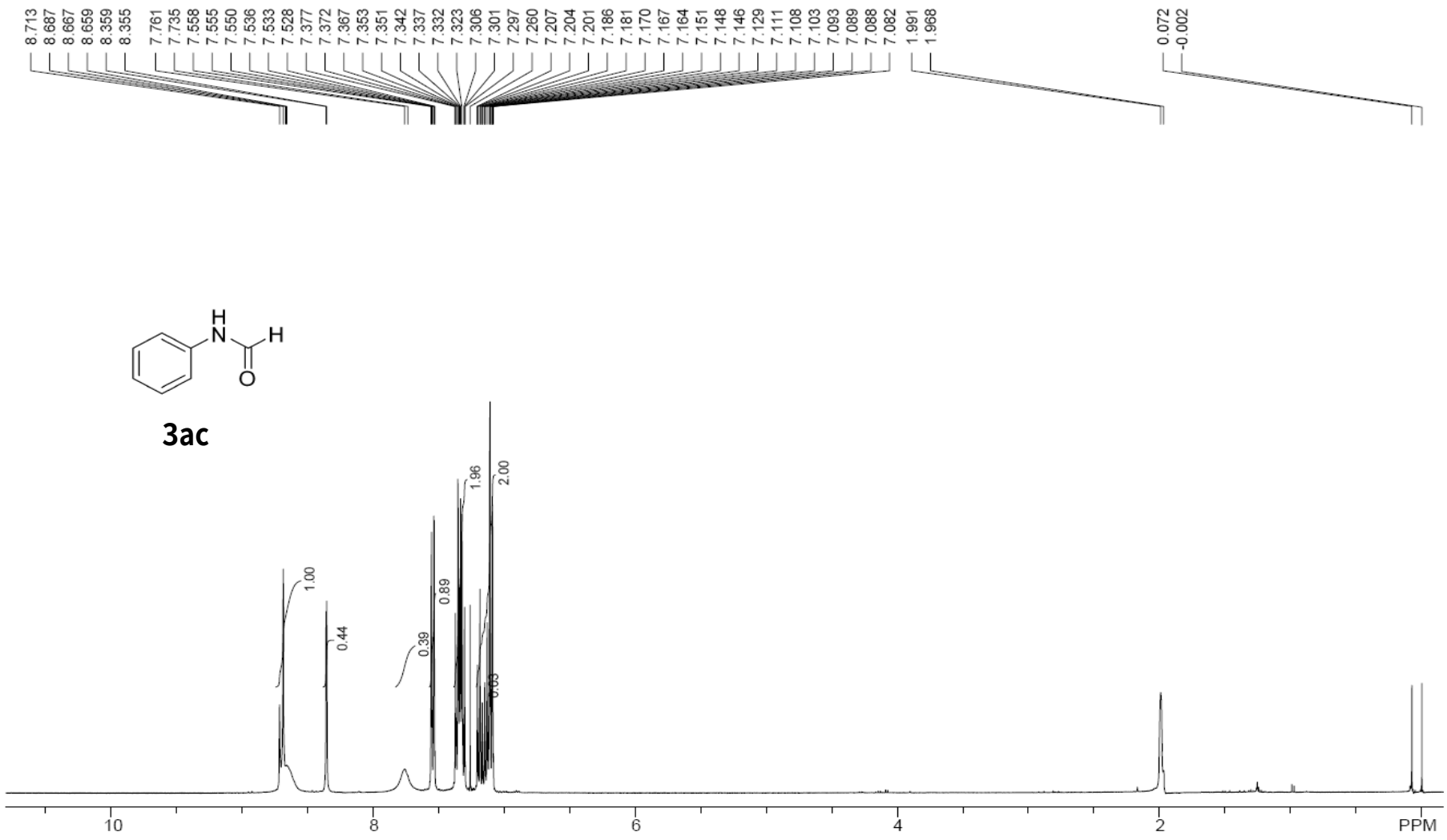

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7.531
7.504
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7.156
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H
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7.6
7.5
7.4
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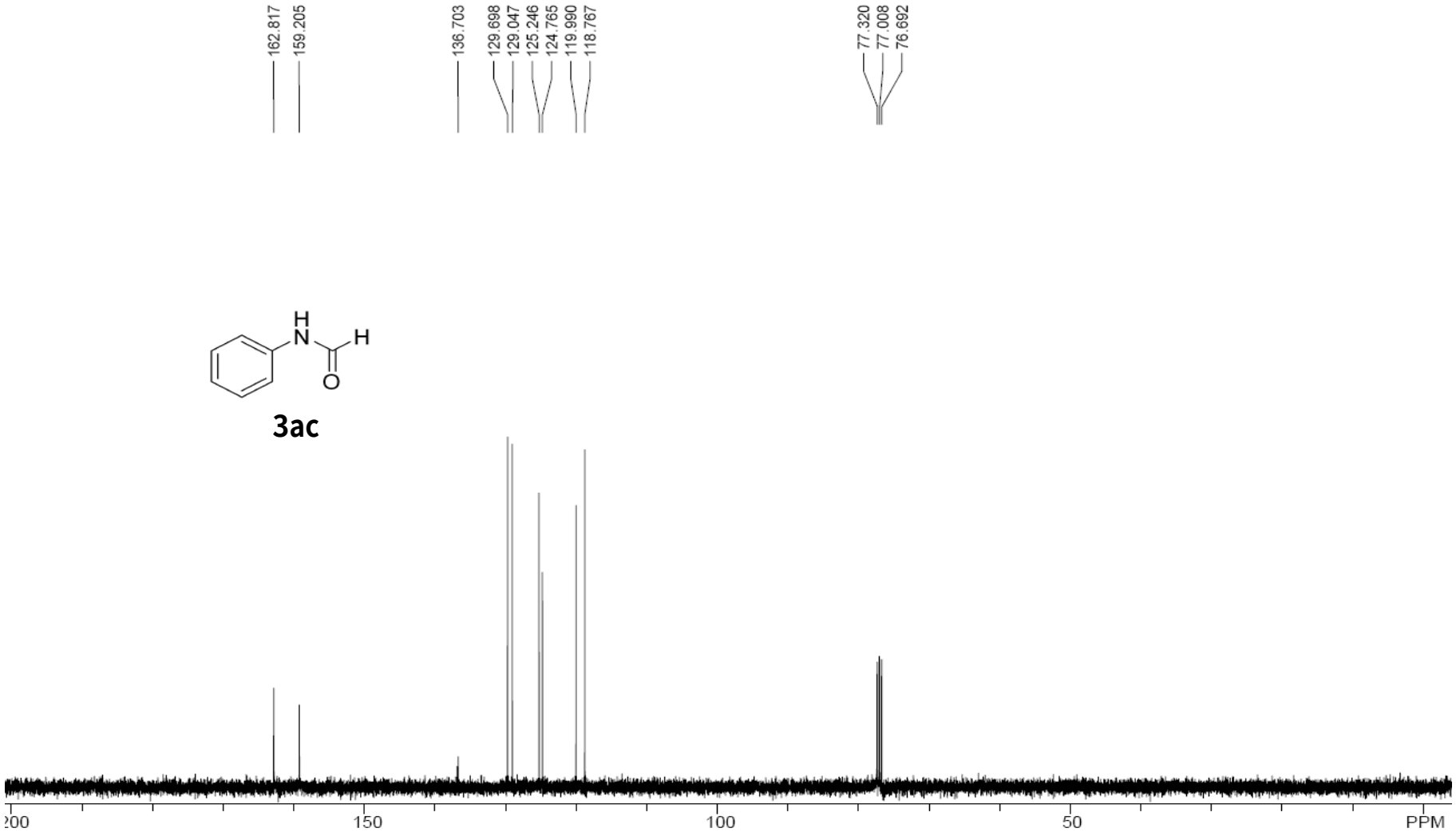

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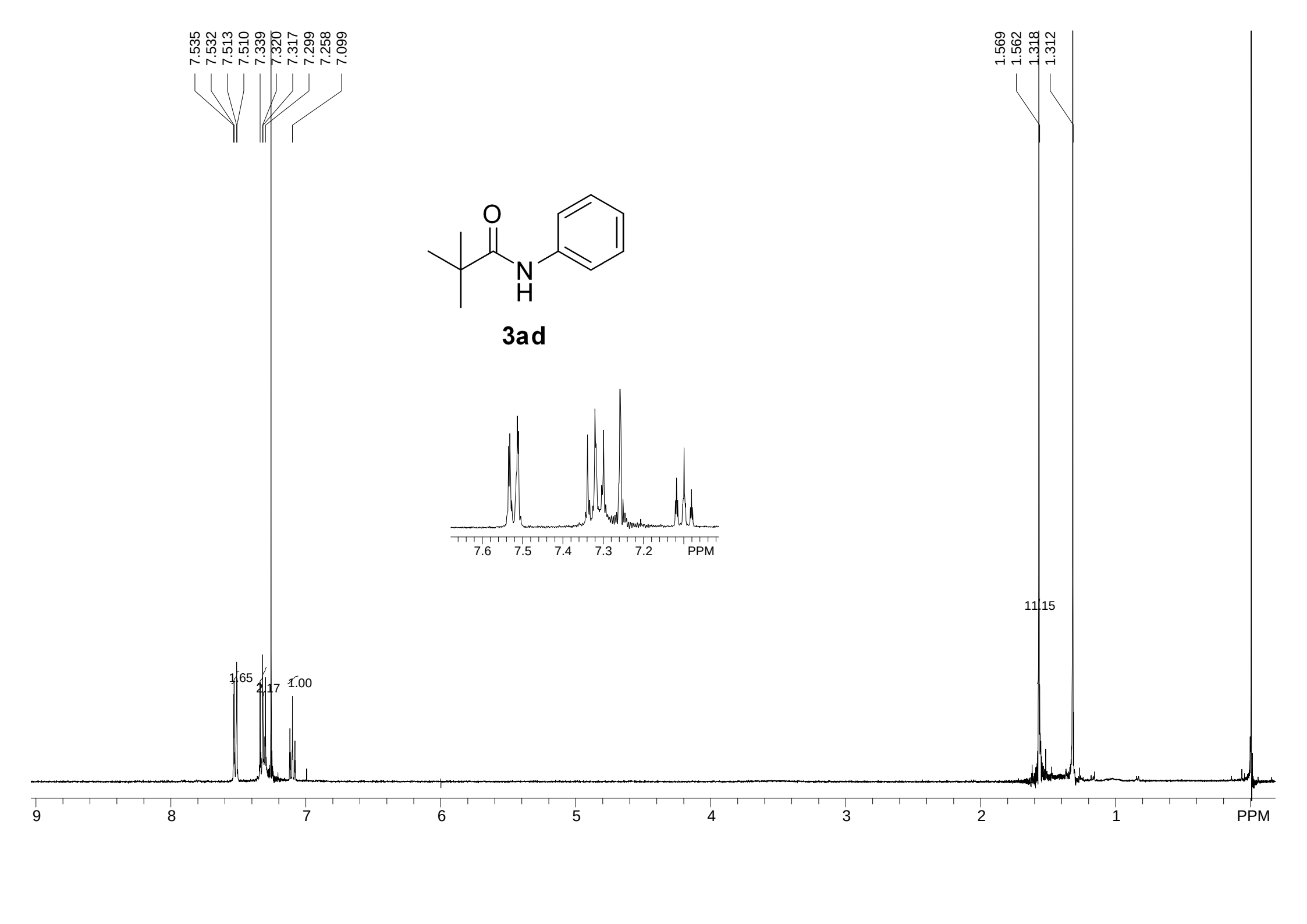
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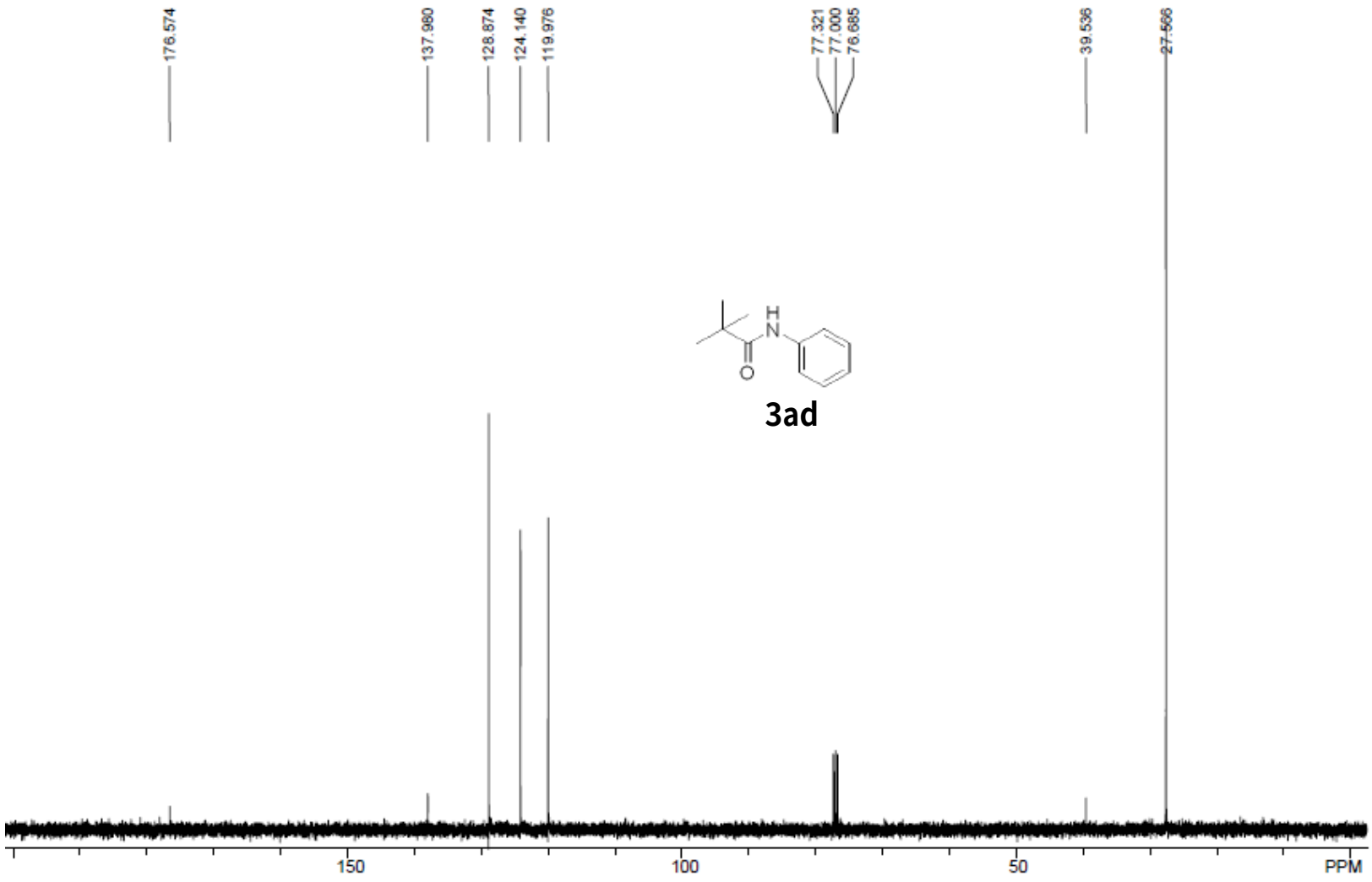

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7.120
7.102
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O
N
H
3ab
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
PPM
1.97
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1.00
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9
8
7
6
5
4
3
2
1
0
PPM


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PPM

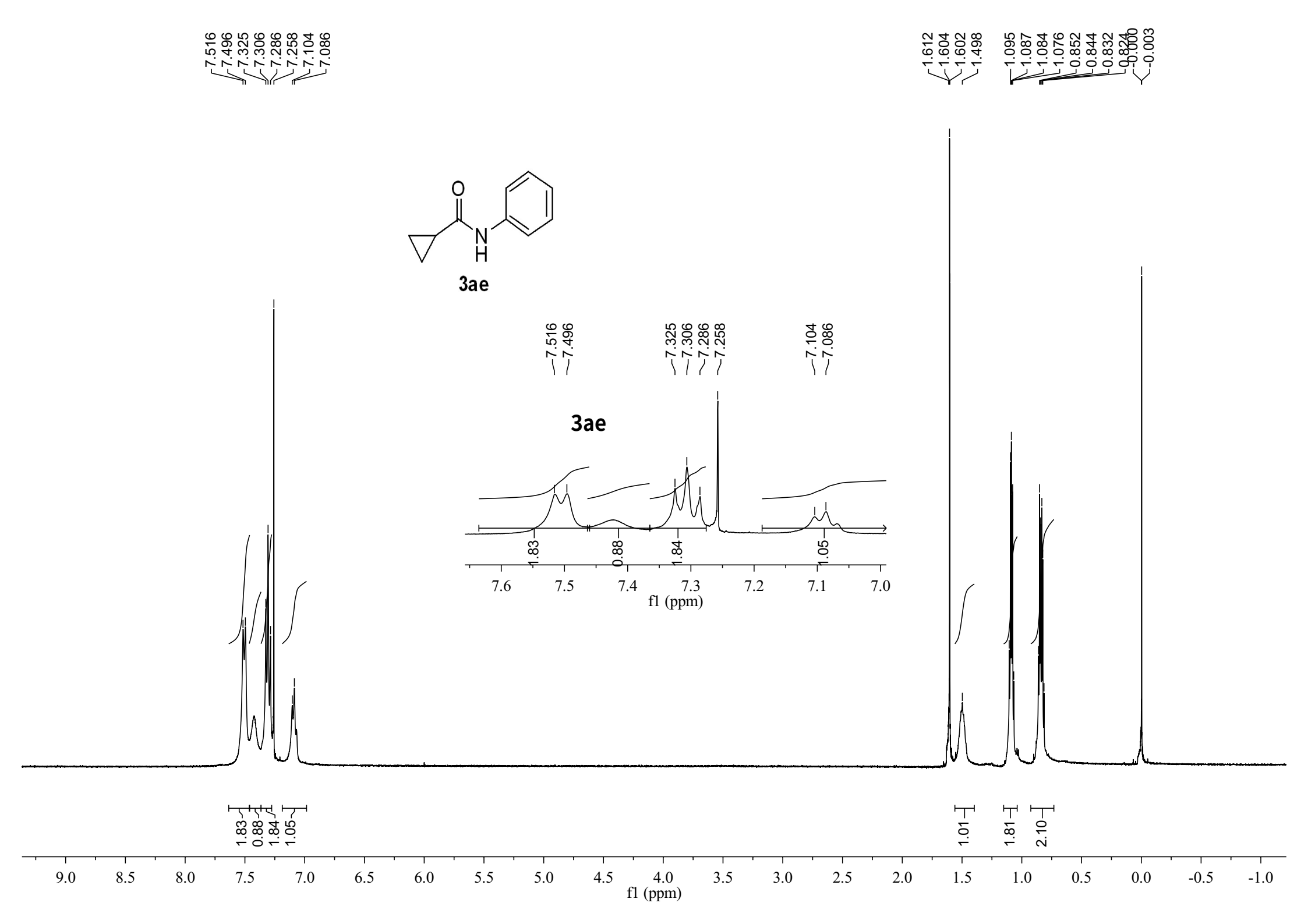

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7.528
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7.351
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7.337
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7.306
7.301
7.297
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7.204
7.201
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7.181
7.170
7.167
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7.148
7.146
7.129
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7.103
7.093
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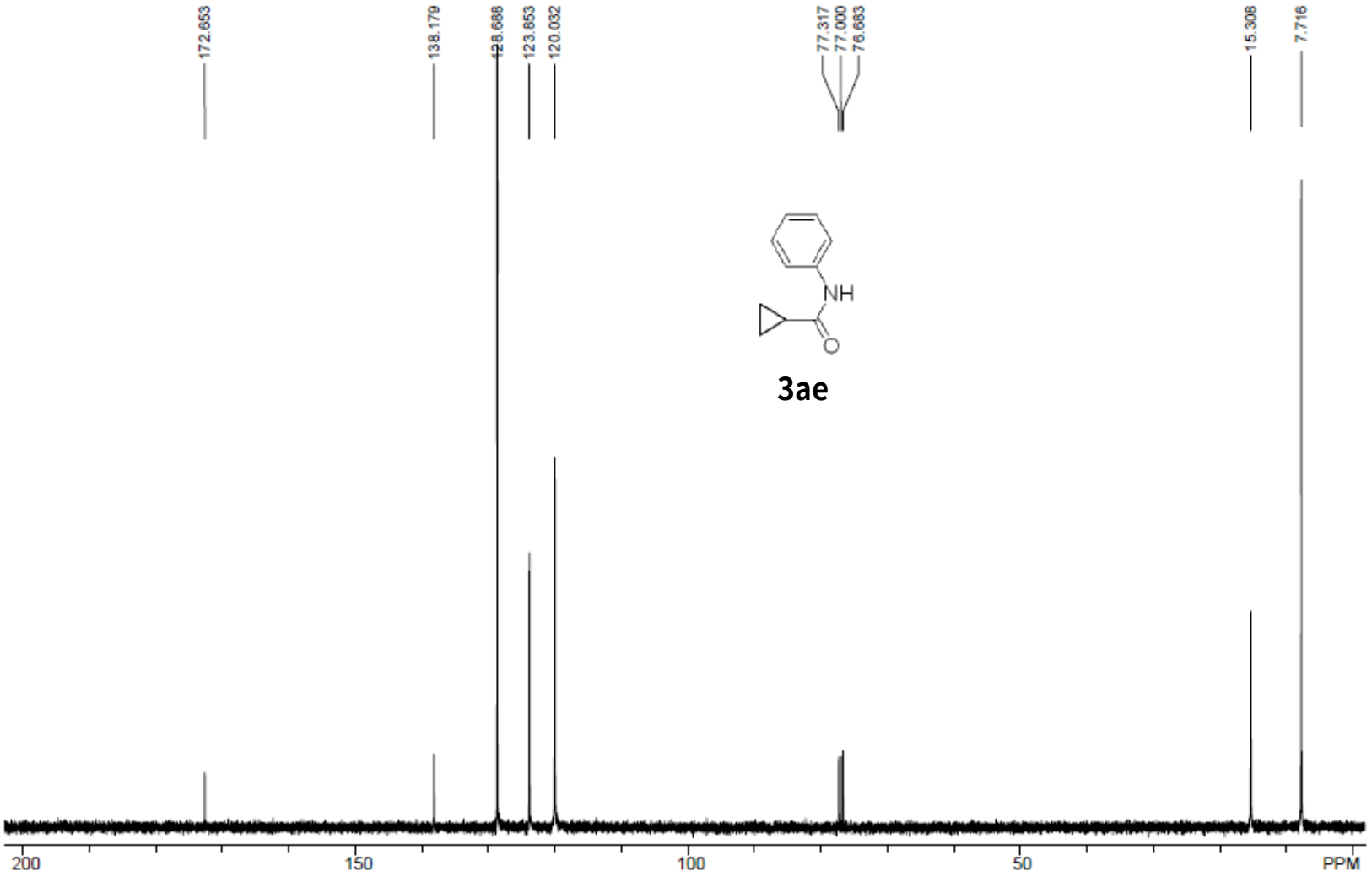

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H
O
3ac
200
150
100
50
PPM


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7.513
7.510
7.339
7.320
7.317
7.299
7.258
7.099
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1.562
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1.312
O
N
H
3ad
7.6
7.5
7.4
7.3
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2
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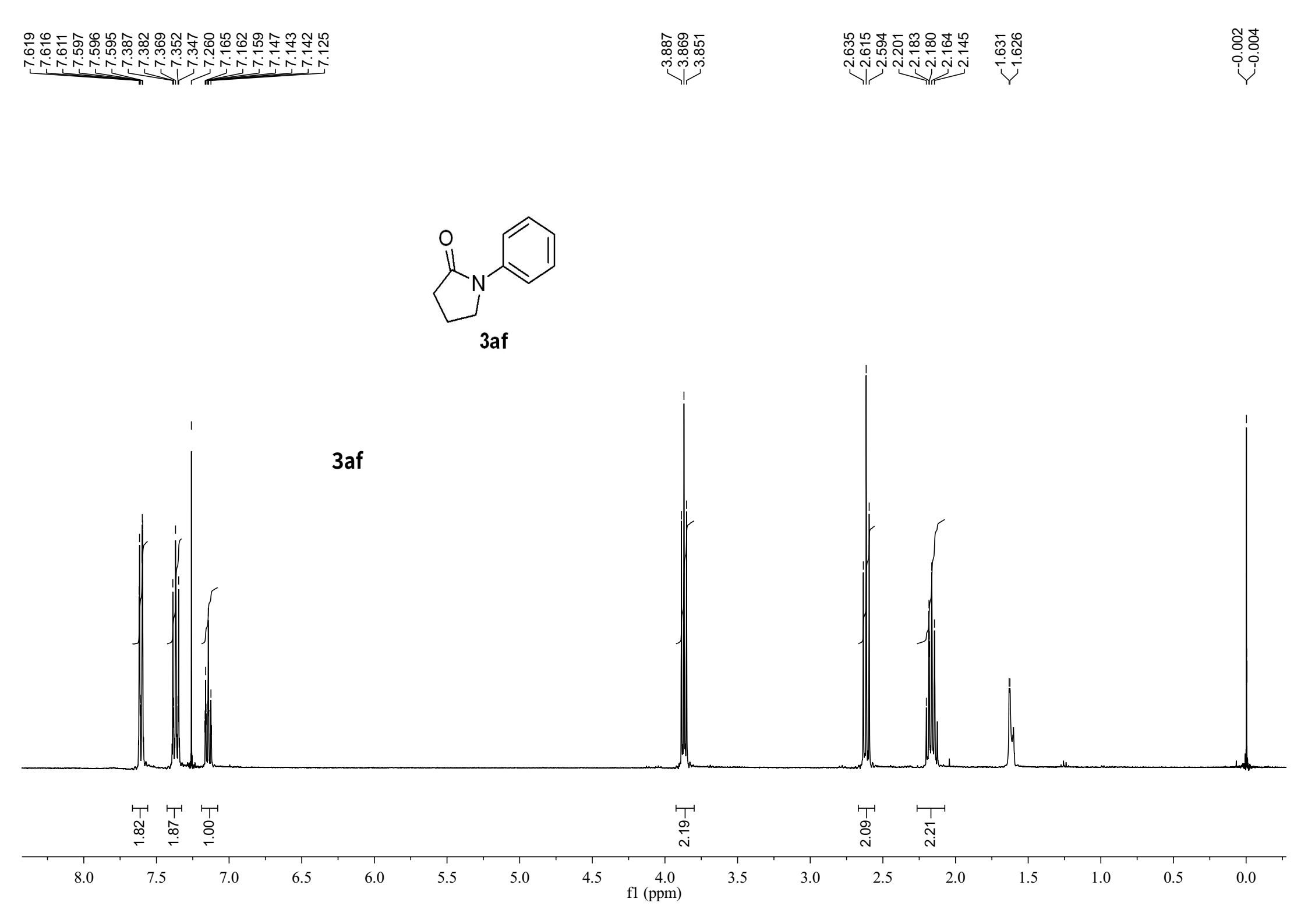

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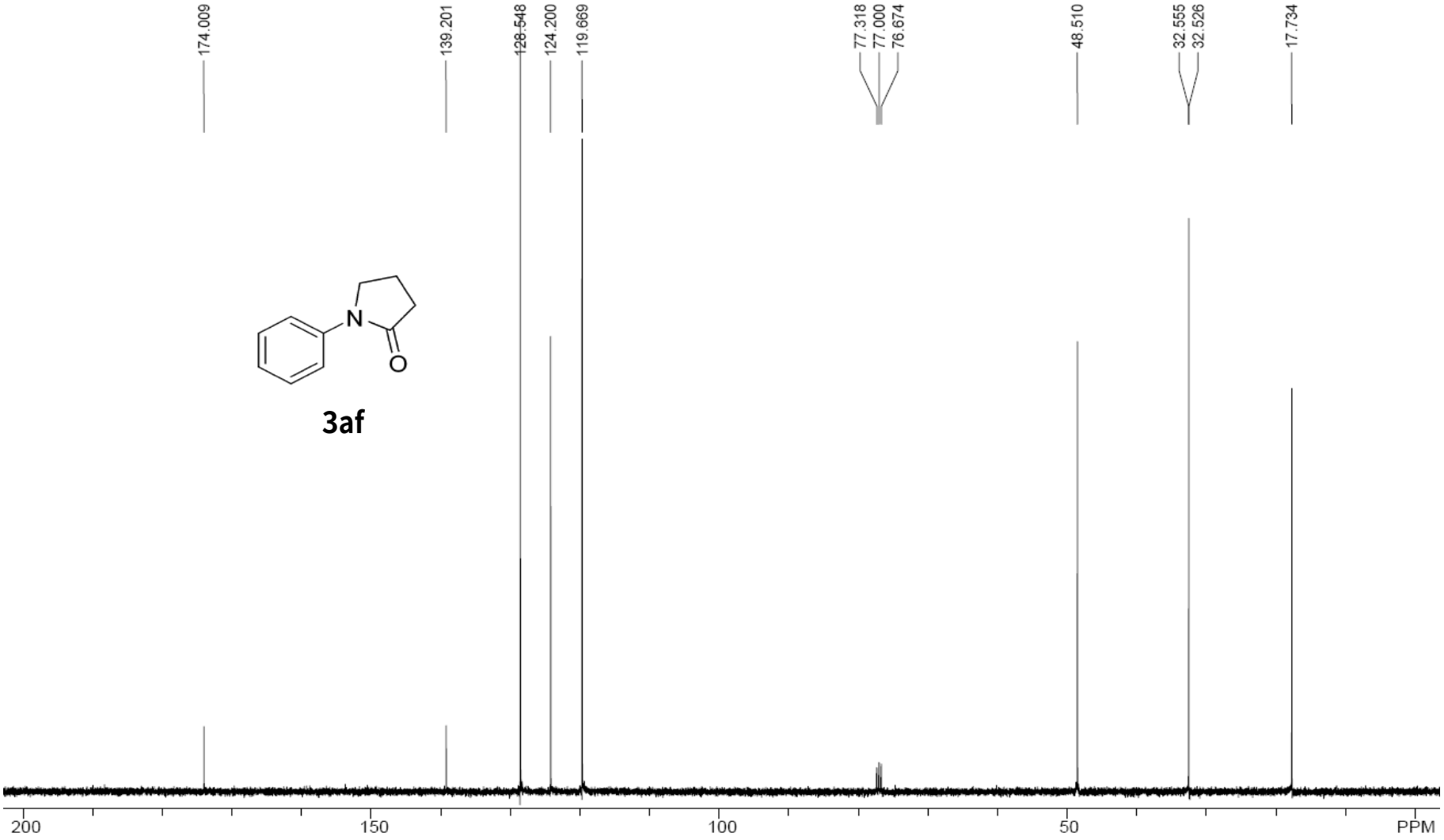
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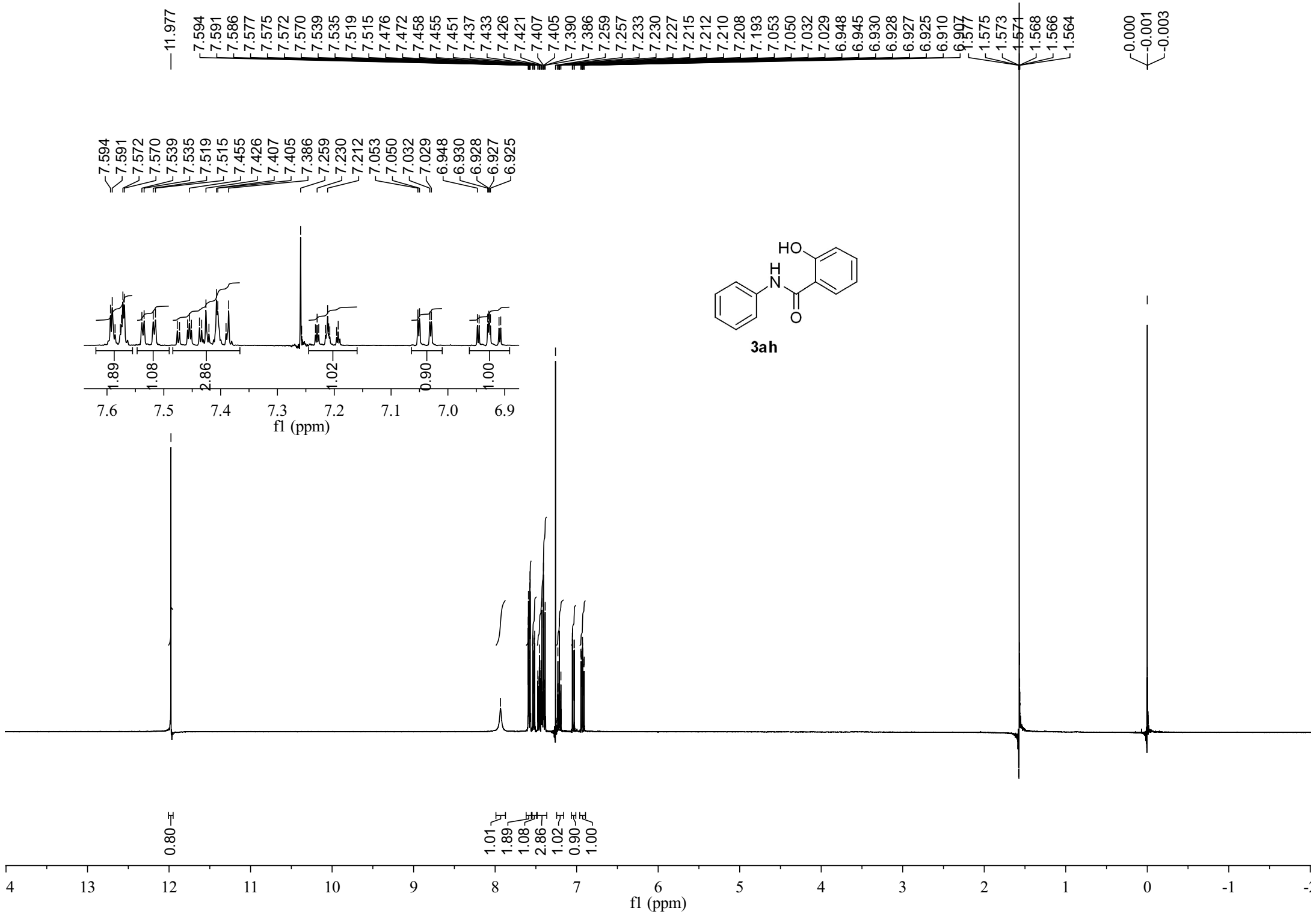

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1.087
1.084
1.076
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0.824
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N
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0.88
1.84
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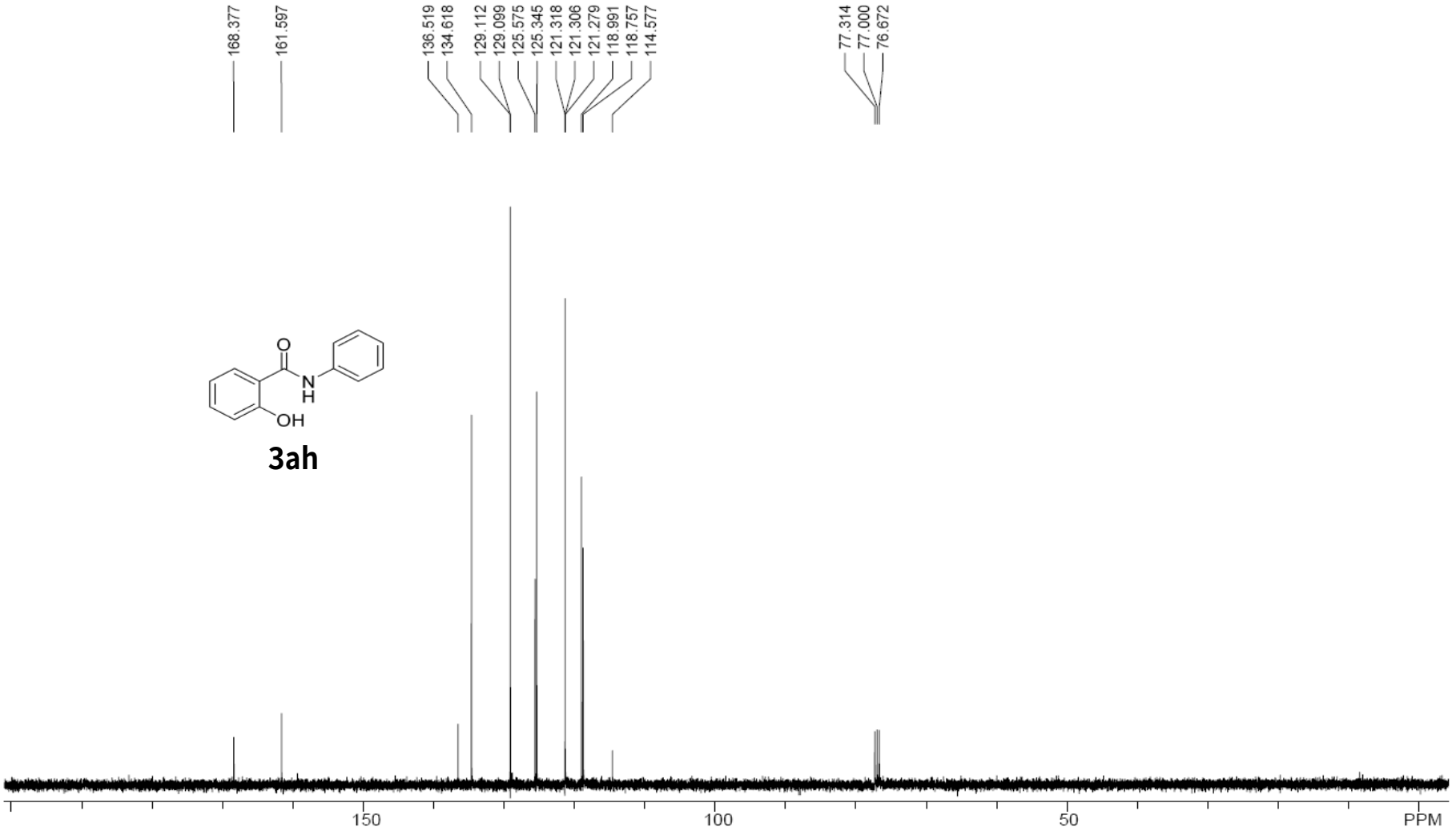

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PPM

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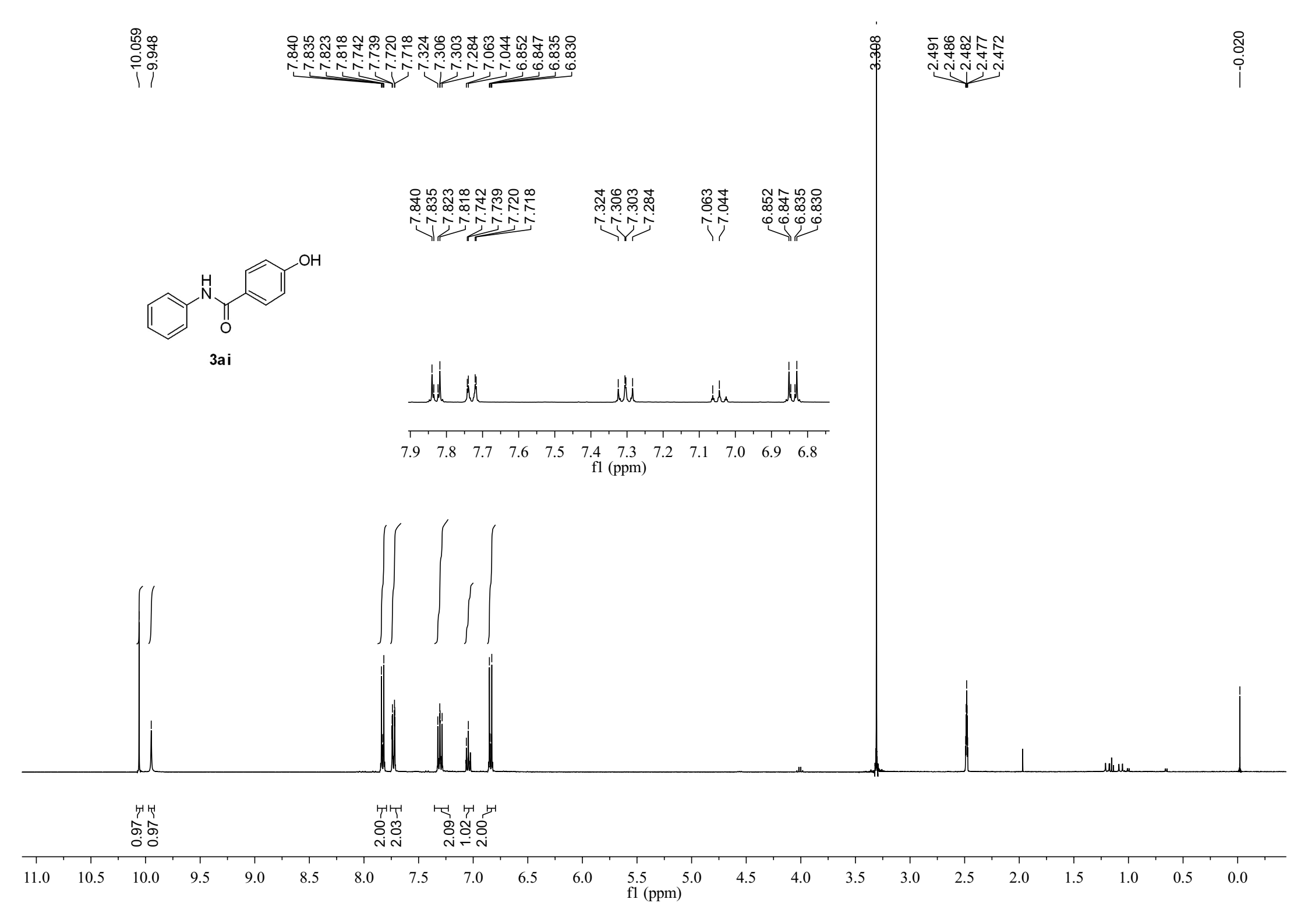

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7.159
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7.125
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2.615
2.594
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2.180
2.164
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1.87
1.00
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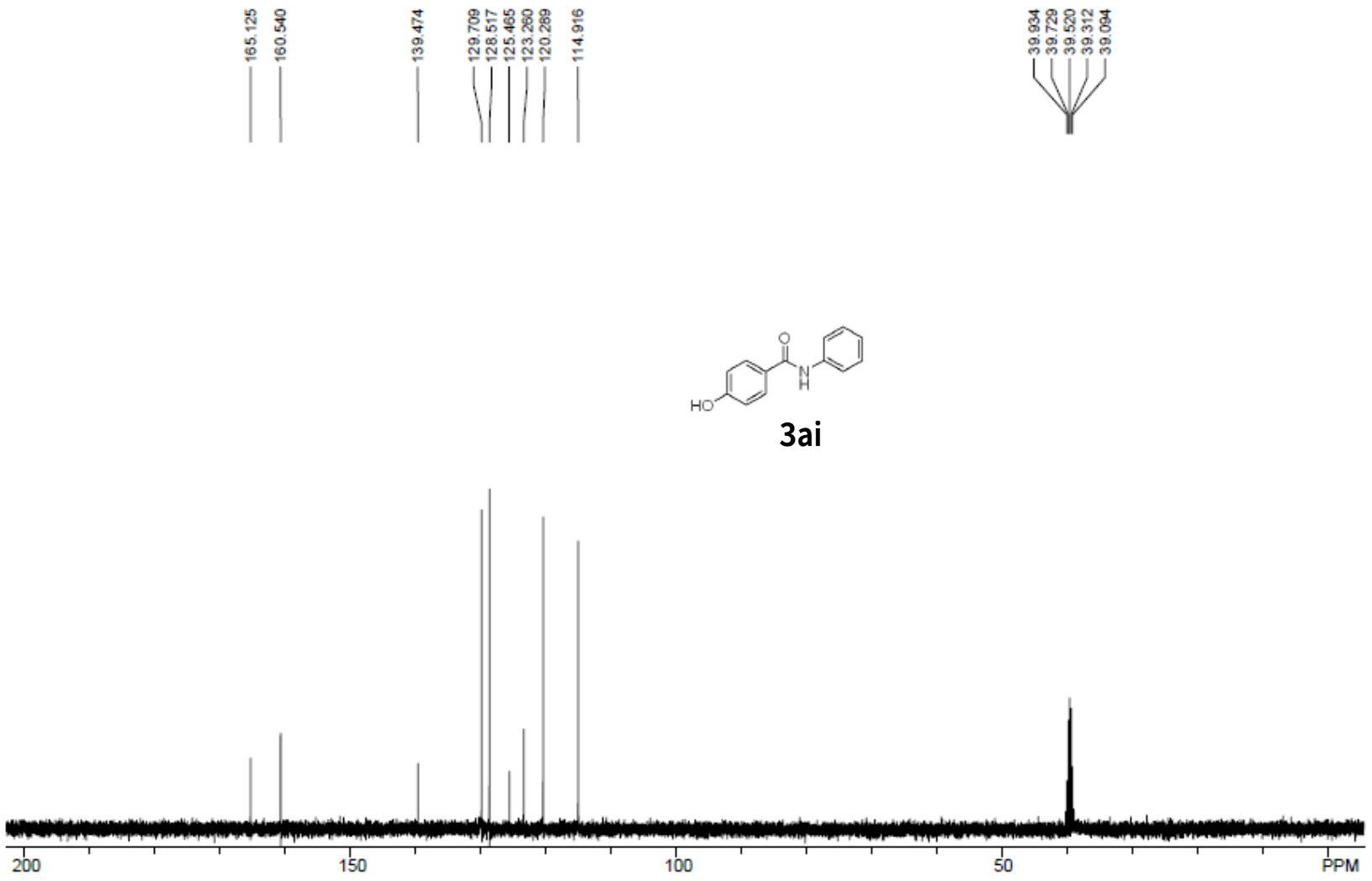

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150
100
50
PPM


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1.02
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7.3
7.2
7.1
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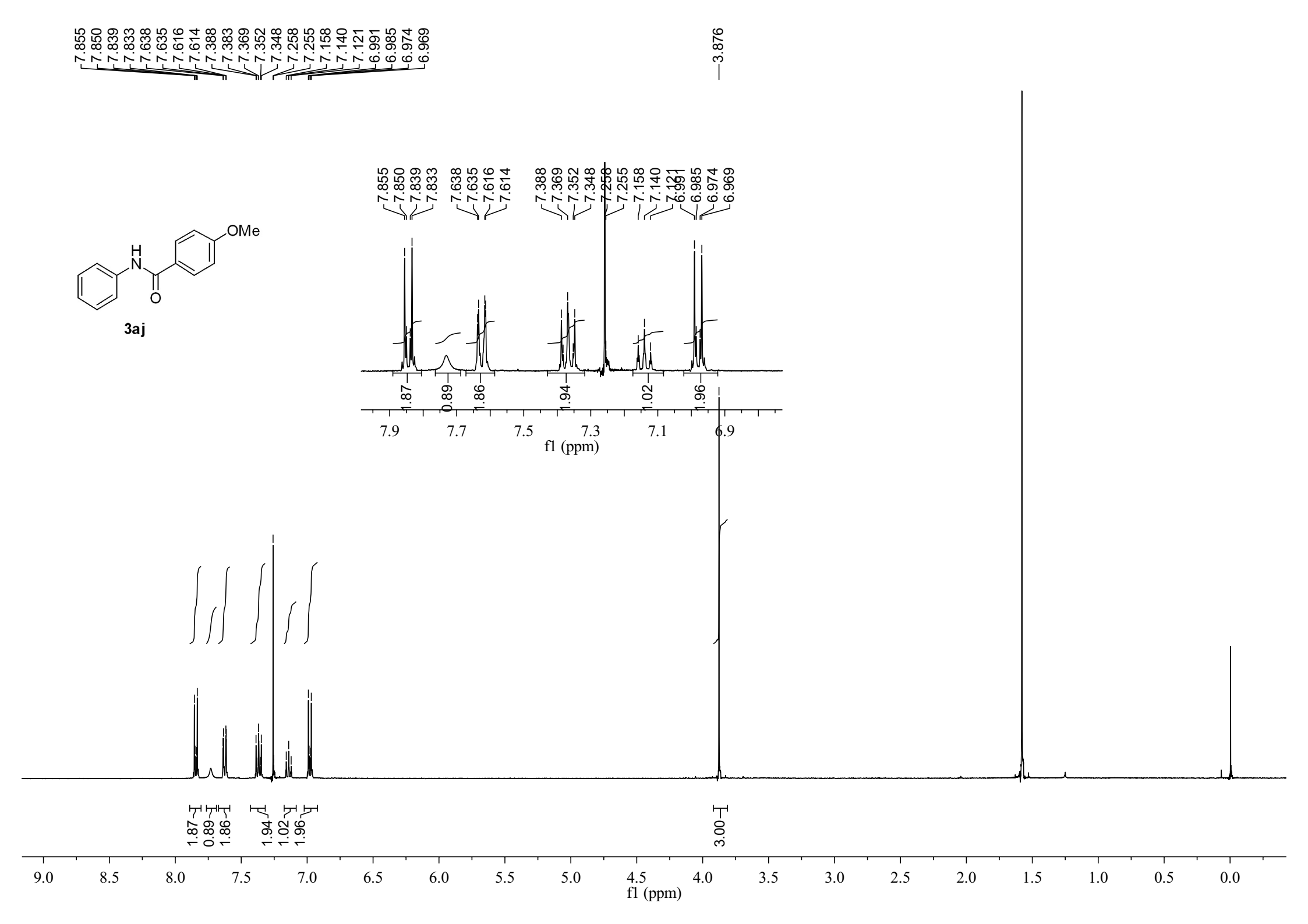

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PPM

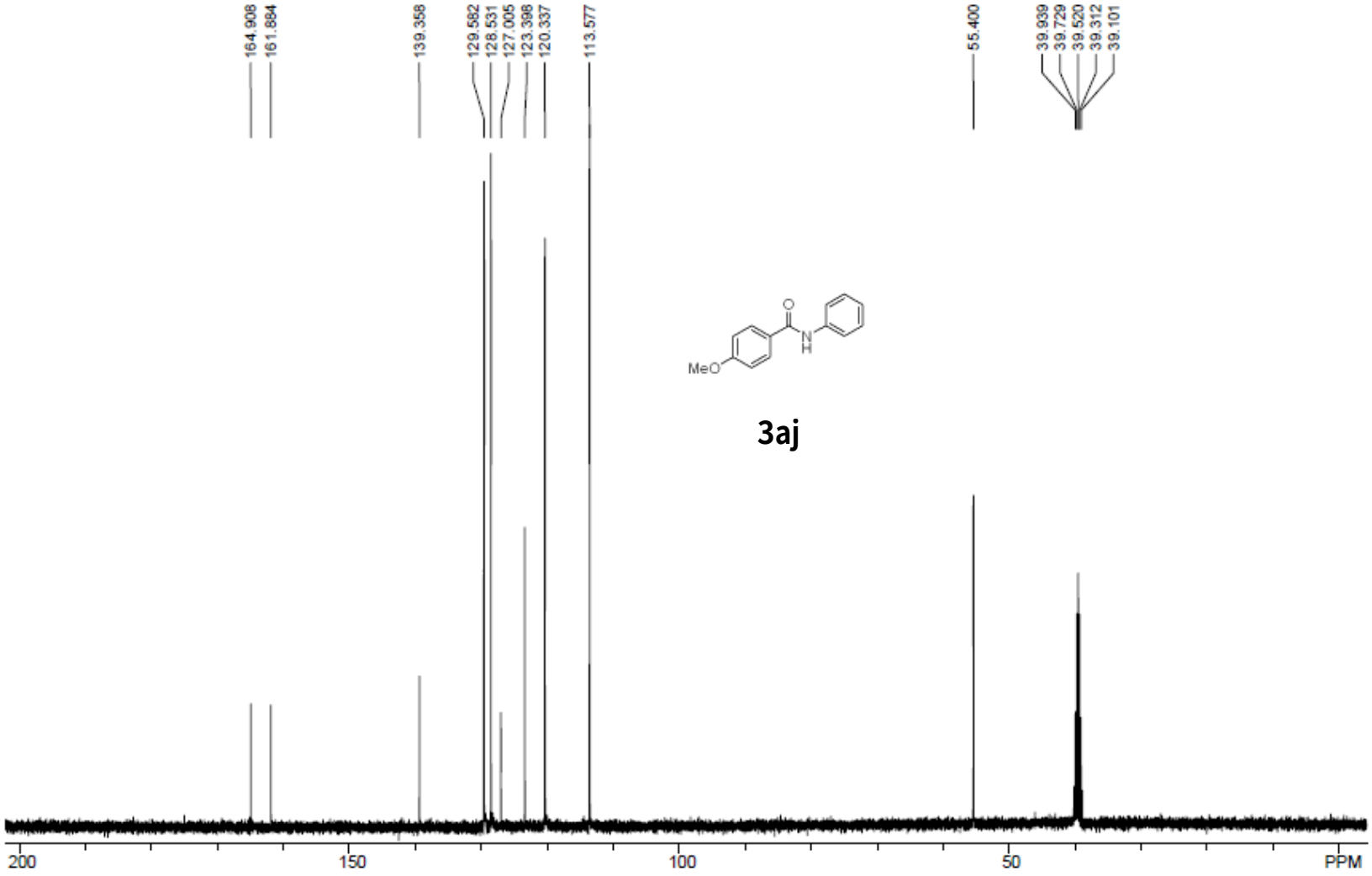
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7.284
7.063
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6.830
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2.03
2.09
1.02
2.00
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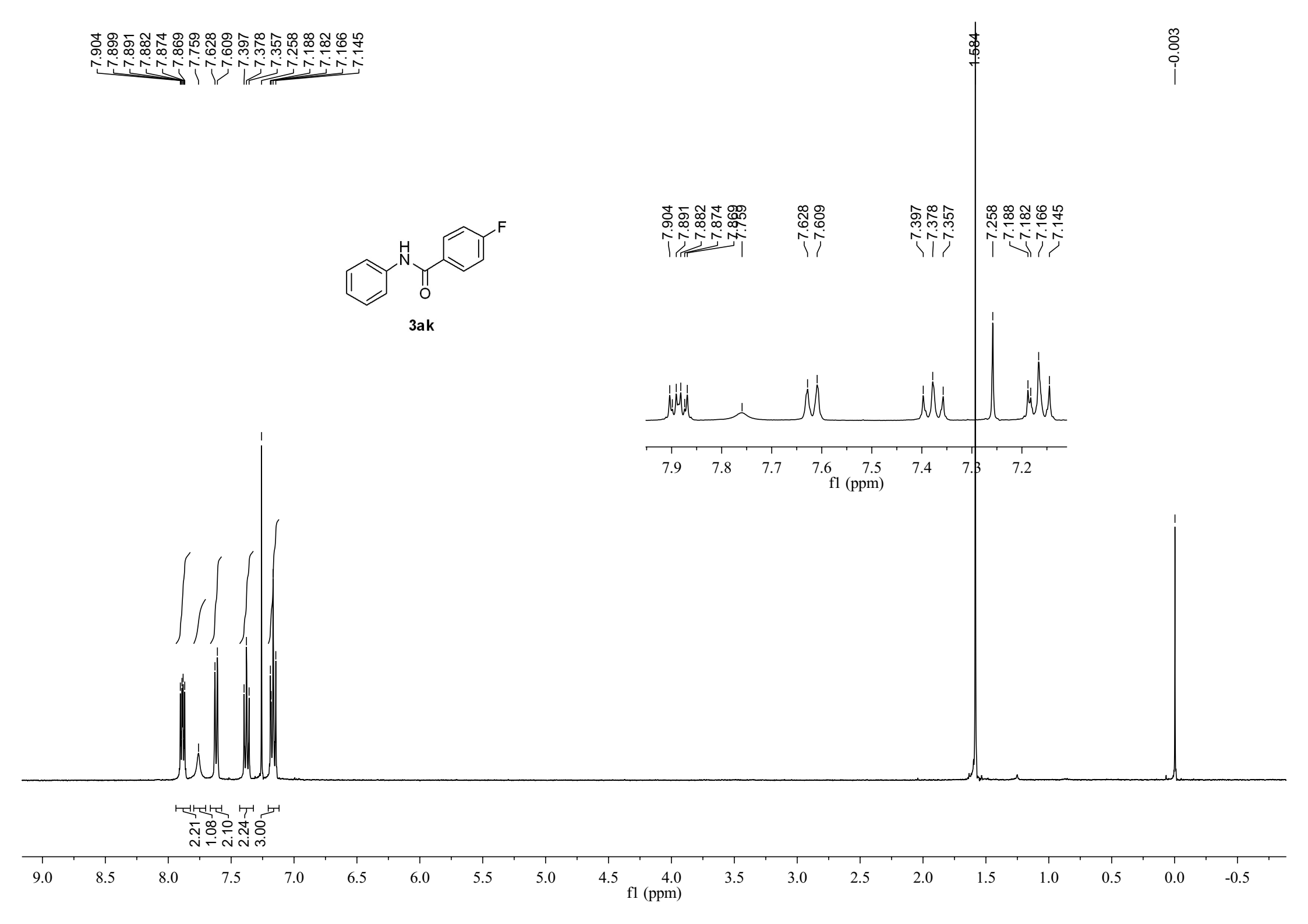

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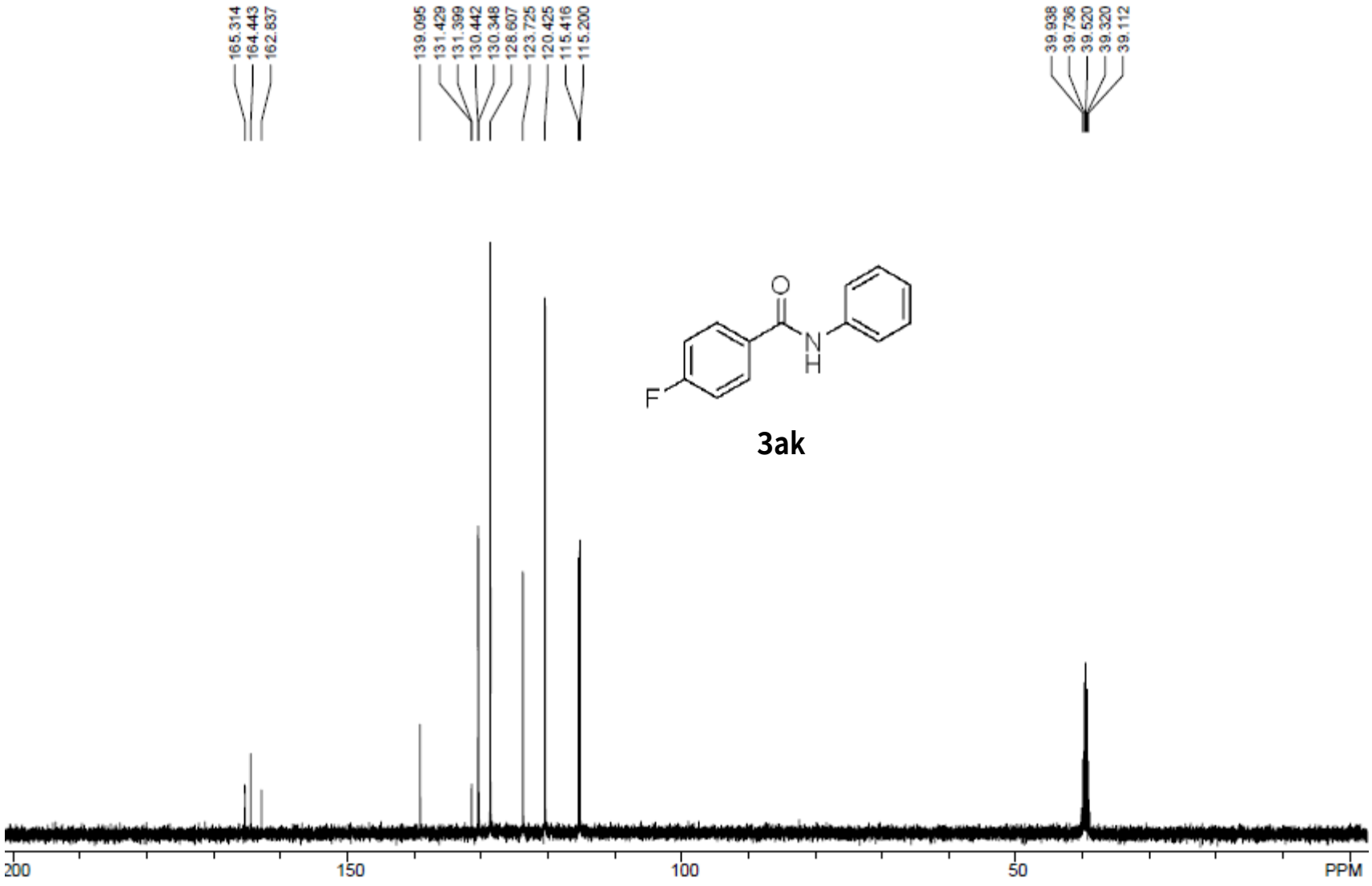
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7.255
7.158
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7.121
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6.974
6.969
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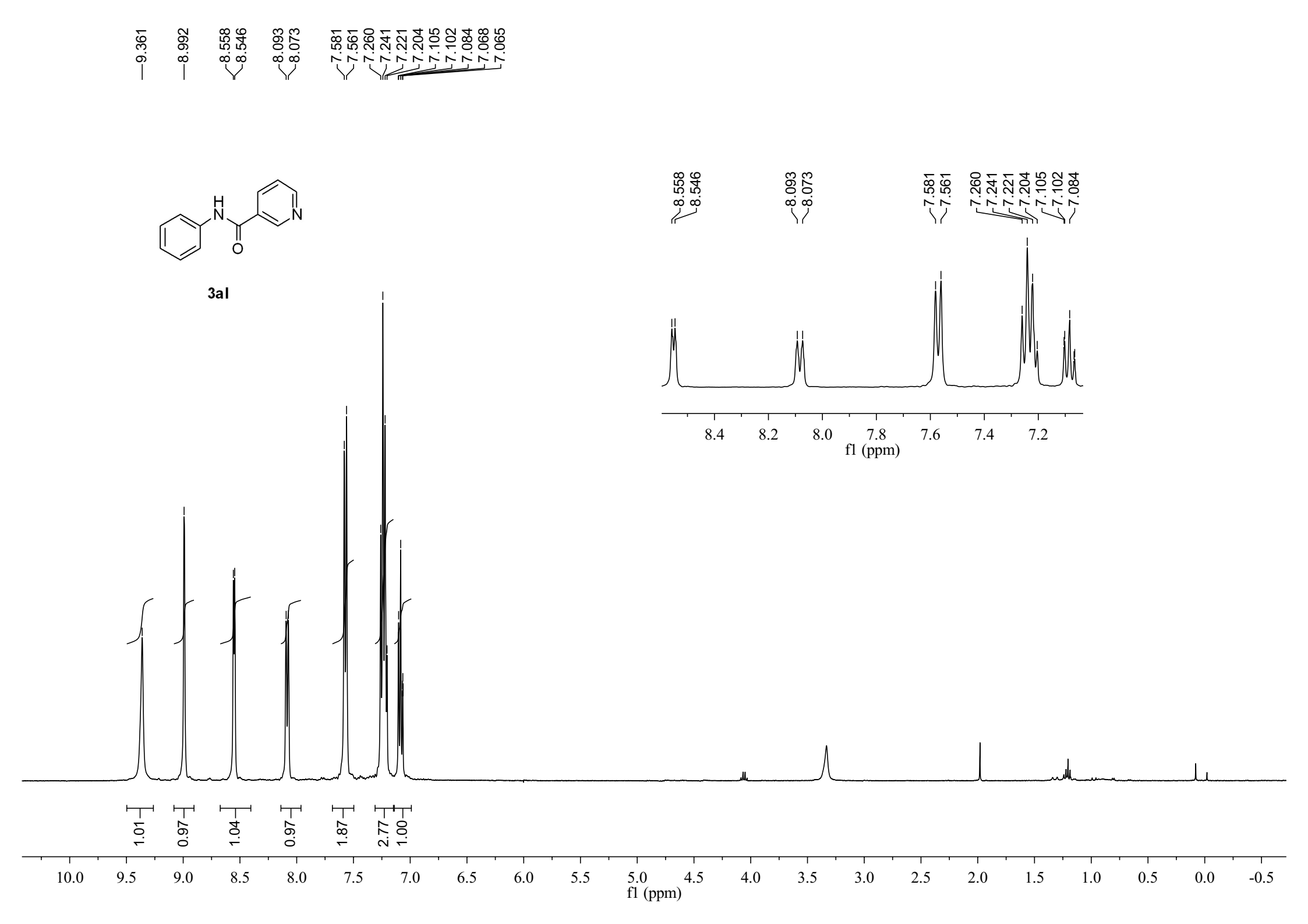

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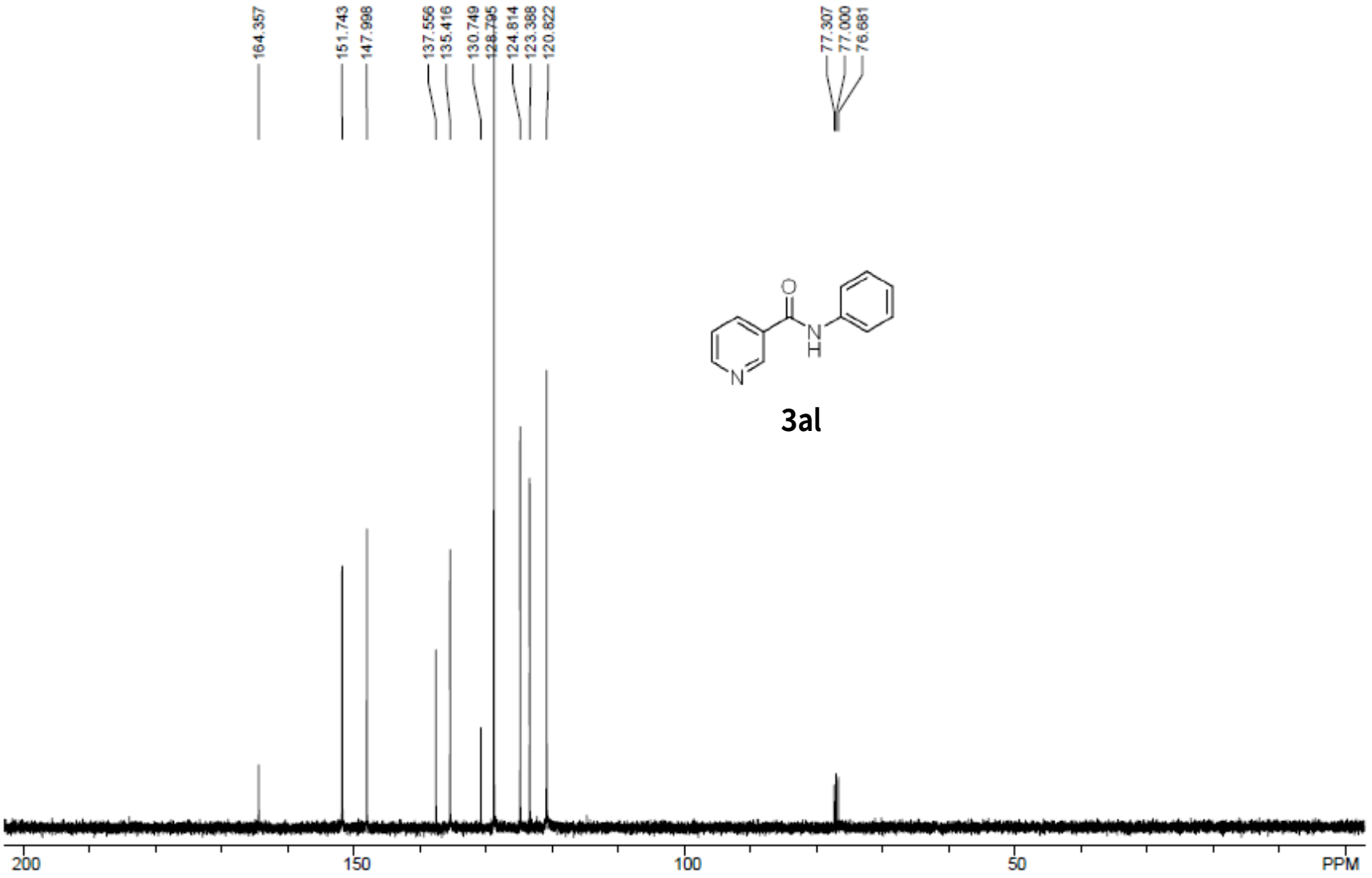
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7.2
f1 (ppm)

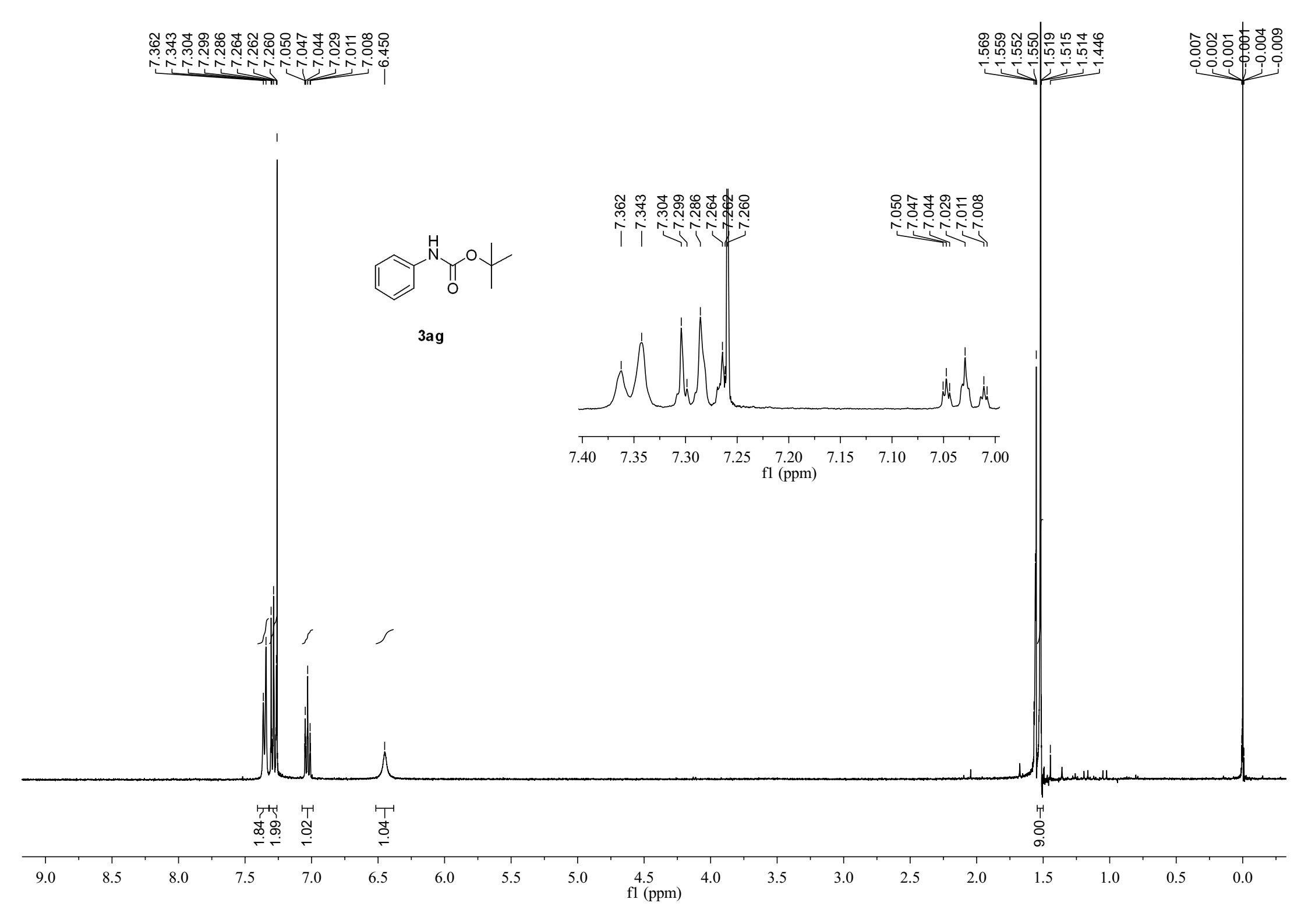

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PPM

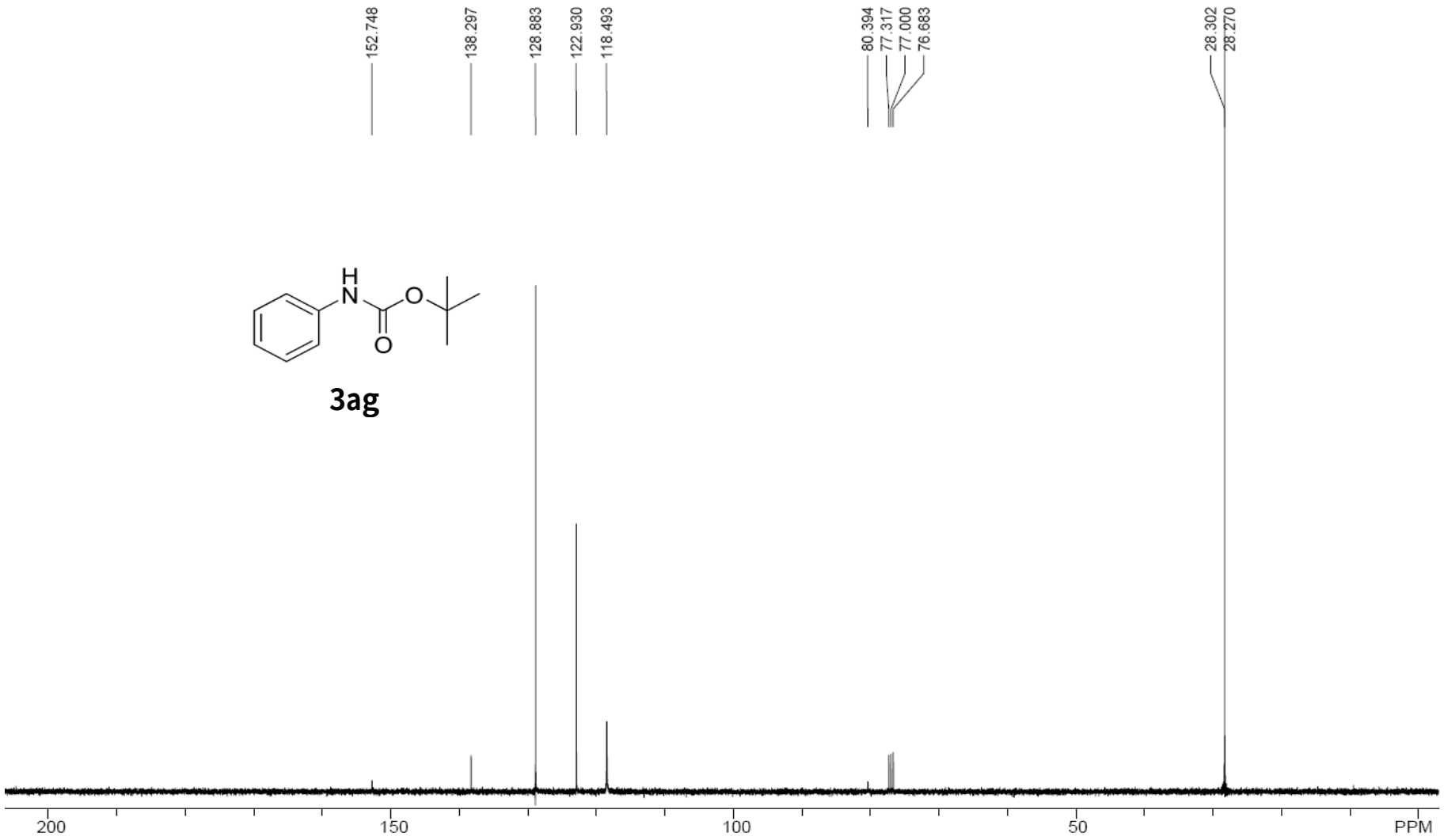
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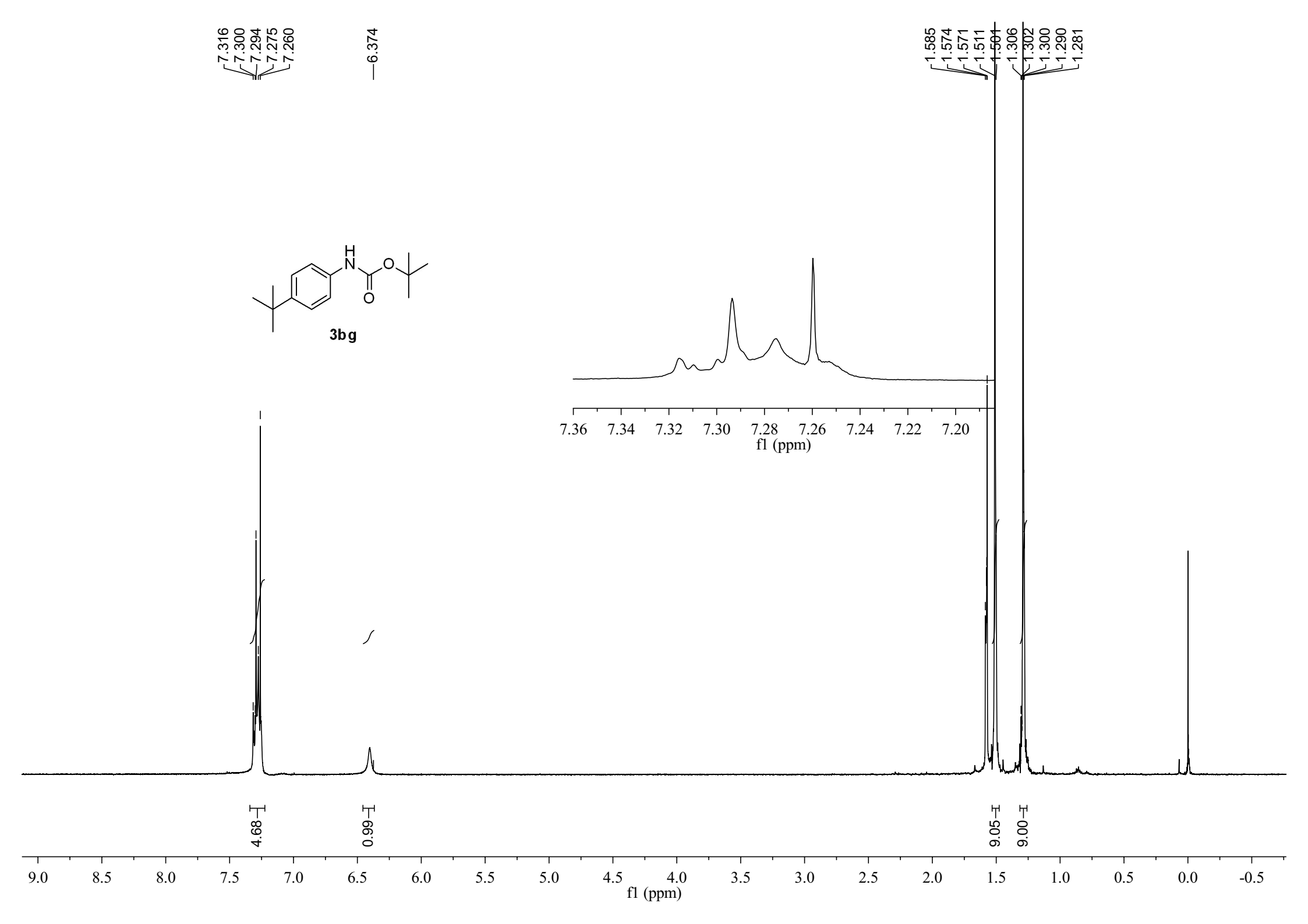

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130.749
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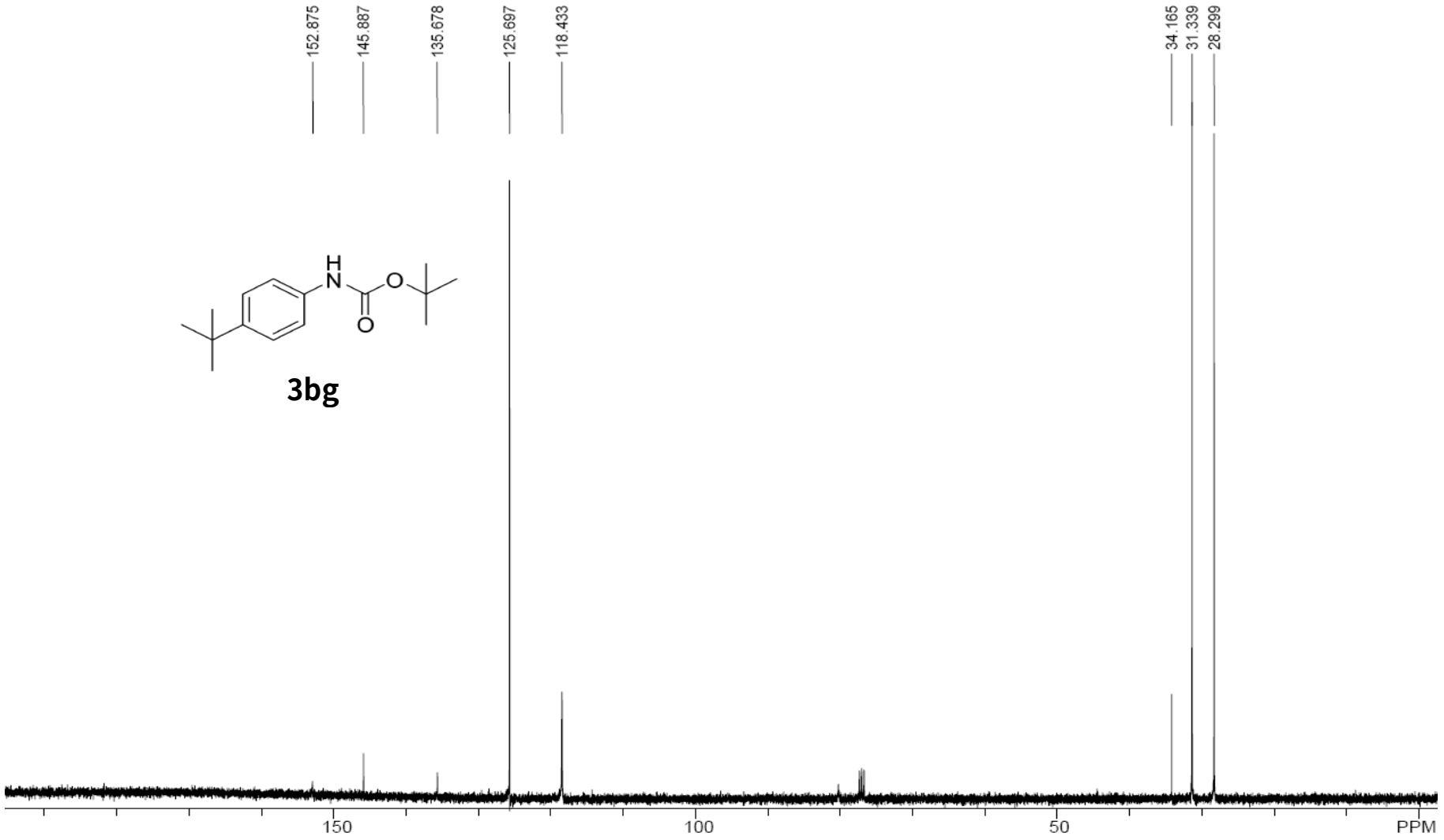
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f1 (ppm)
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1.99
1.02
1.04
9.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

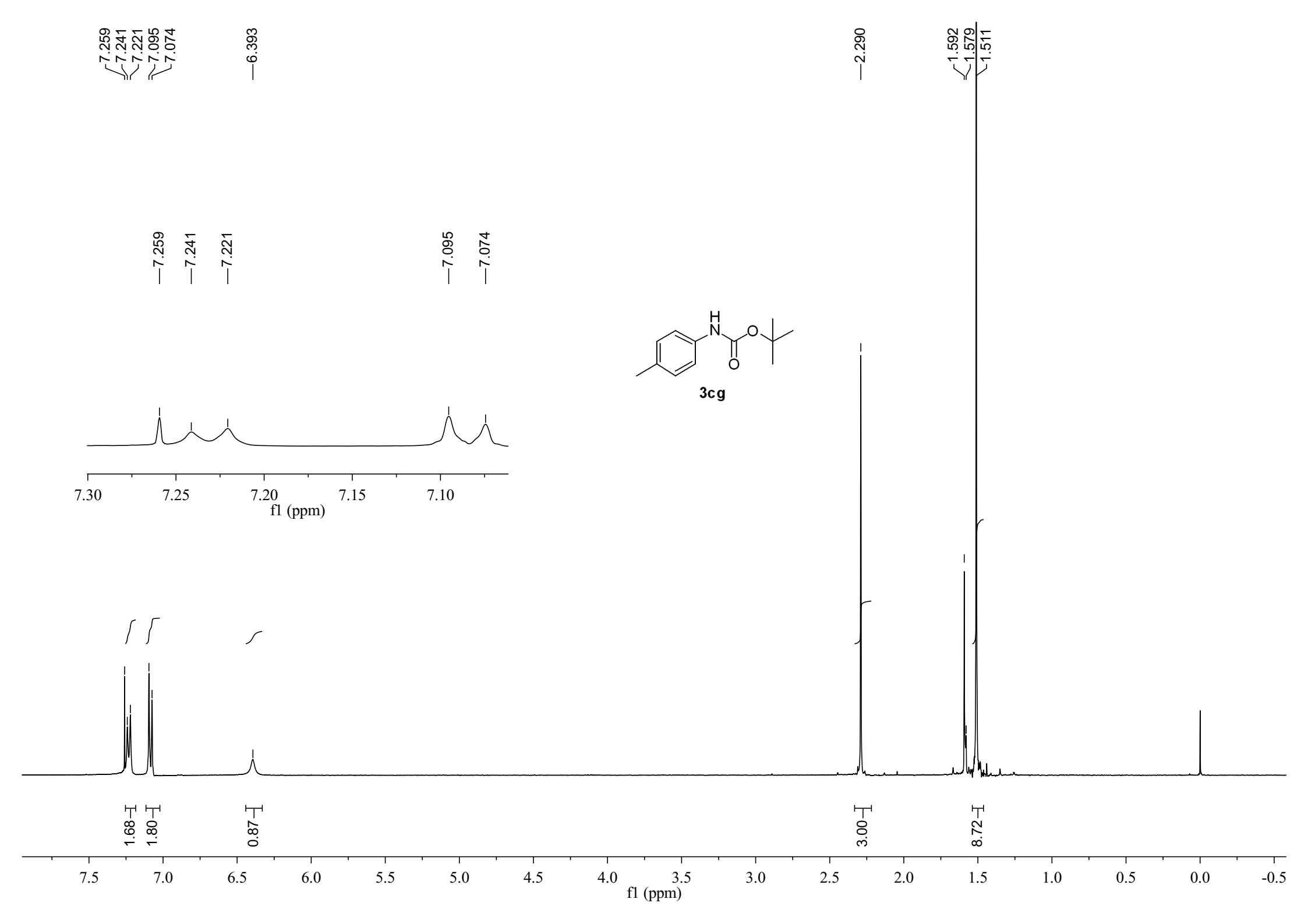

152.748
138.297
128.883
122.930
118.493
80.394
77.317
77.000
76.683
28.302
28.270
H
N
O
O
200
150
100
50
PPM

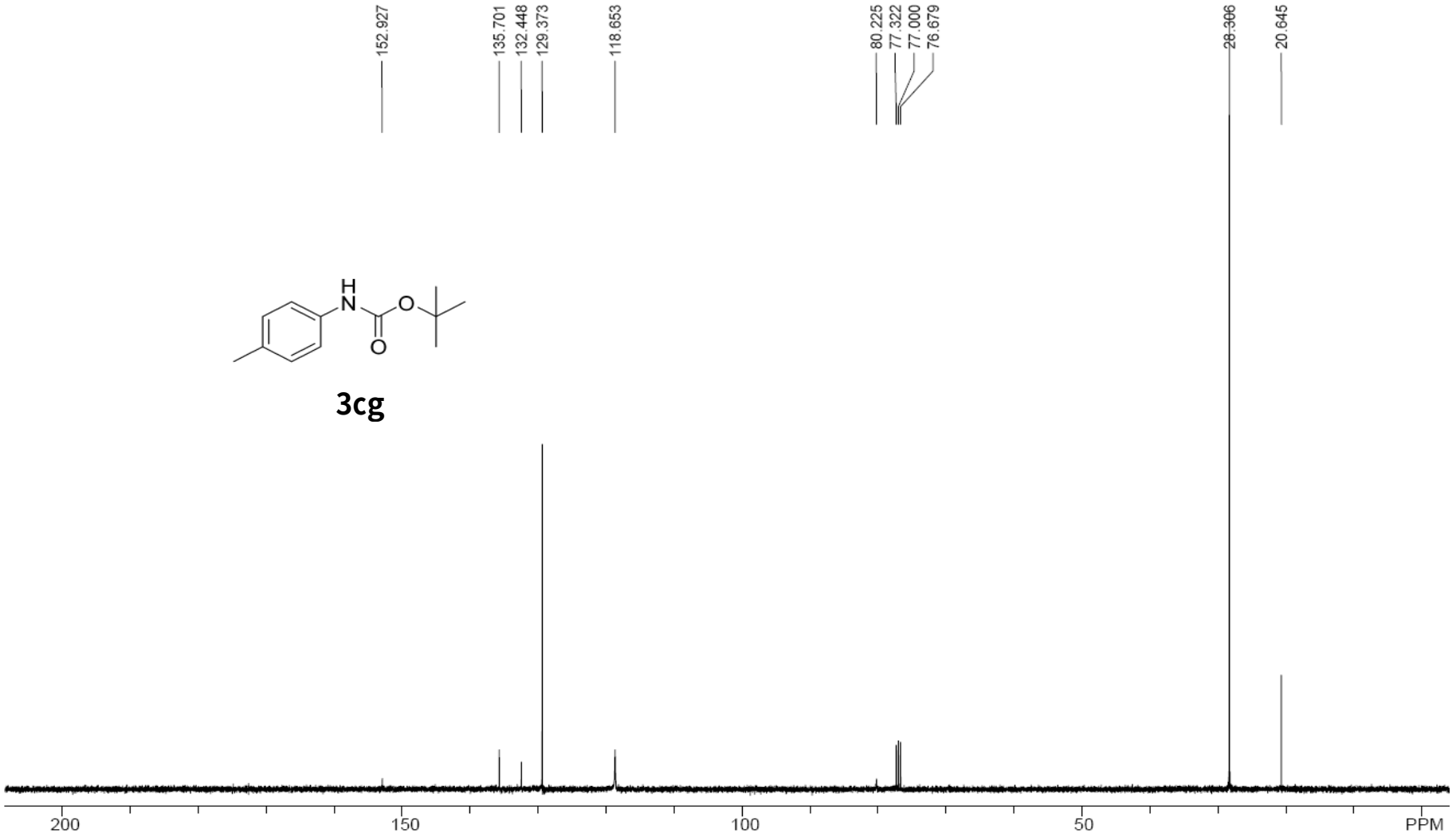
3ag


7.316
7.300
7.294
7.275
7.260
6.374
1.585
1.574
1.571
1.511
1.504
1.306
1.302
1.300
1.290
1.281
3bg
7.36 7.34 7.32 7.30 7.28 7.26 7.24 7.22 7.20
f1 (ppm)
4.68
0.99
9.05
9.00
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)

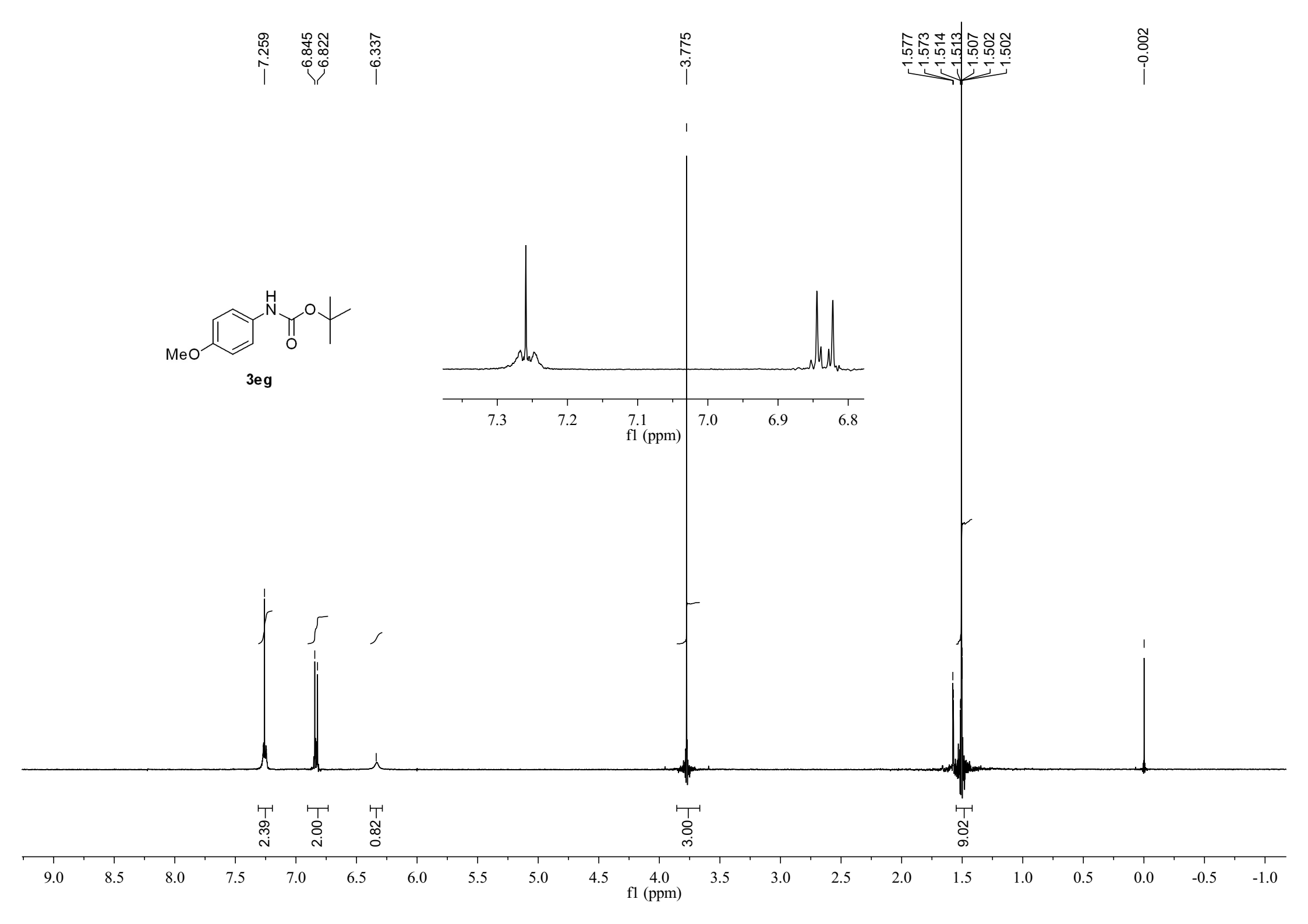

152.875
145.887
135.678
125.697
118.433
34.165
31.339
28.299
H
N
O
O
150
100
50
PPM

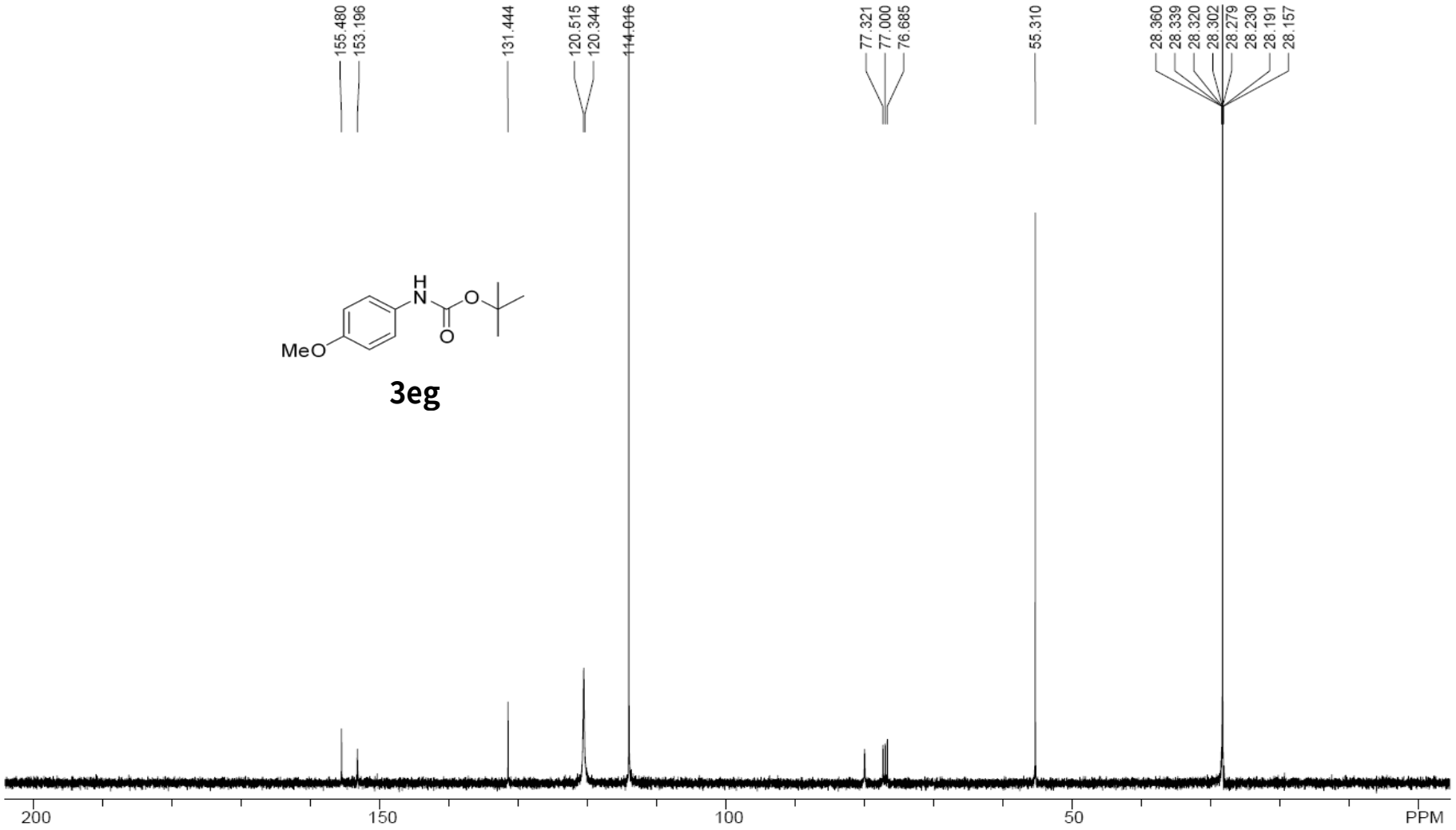
3bg


7.259
7.241
7.221
7.095
7.074
6.393
2.290
1.592
1.579
1.511
3cg
f1 (ppm)
1.68
1.80
0.87
3.00
8.72

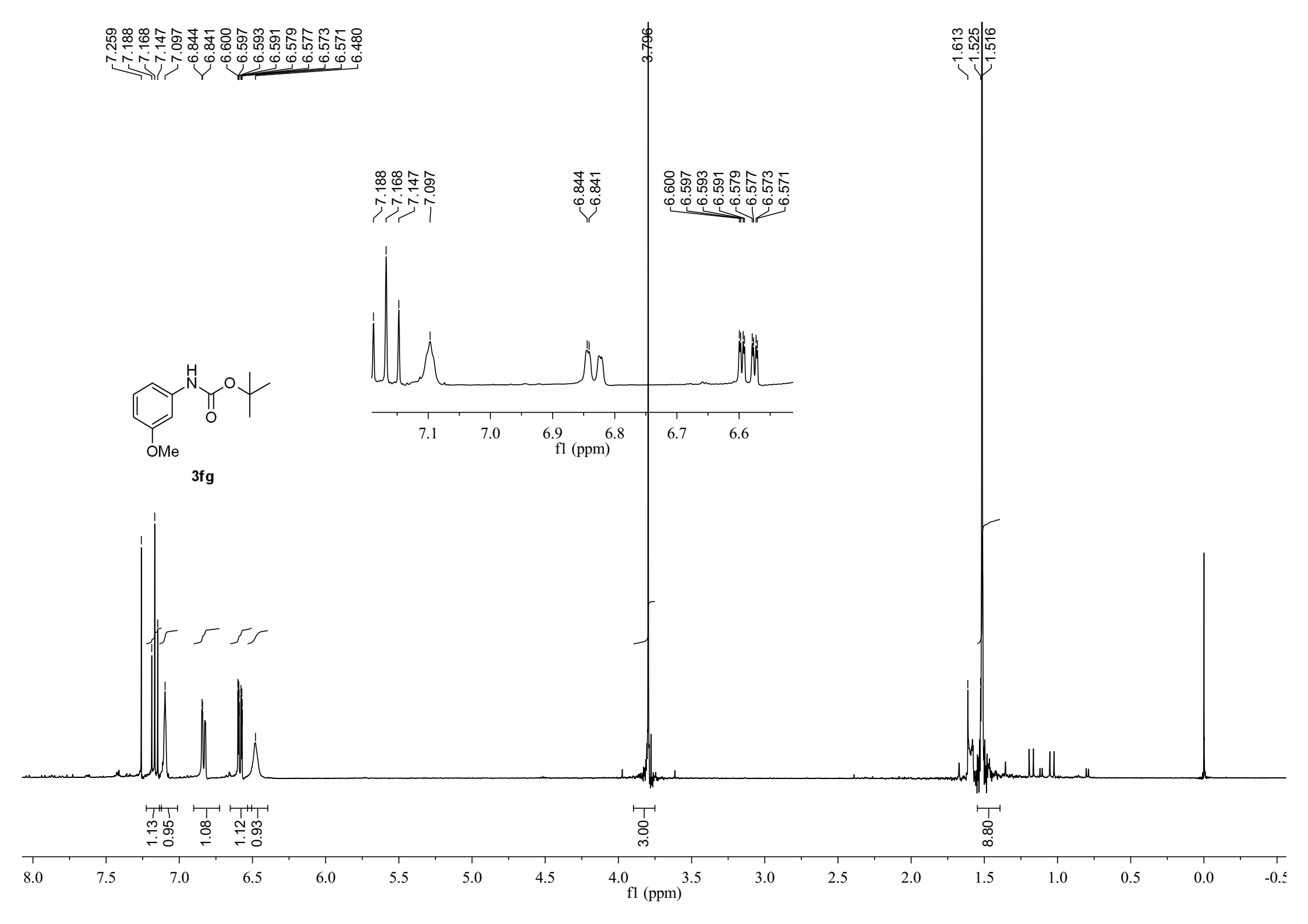

152.927
135.701
132.448
129.373
118.653
80.225
77.322
77.000
76.679
28.306
20.645
H
N
O
O
200
150
100
50
PPM

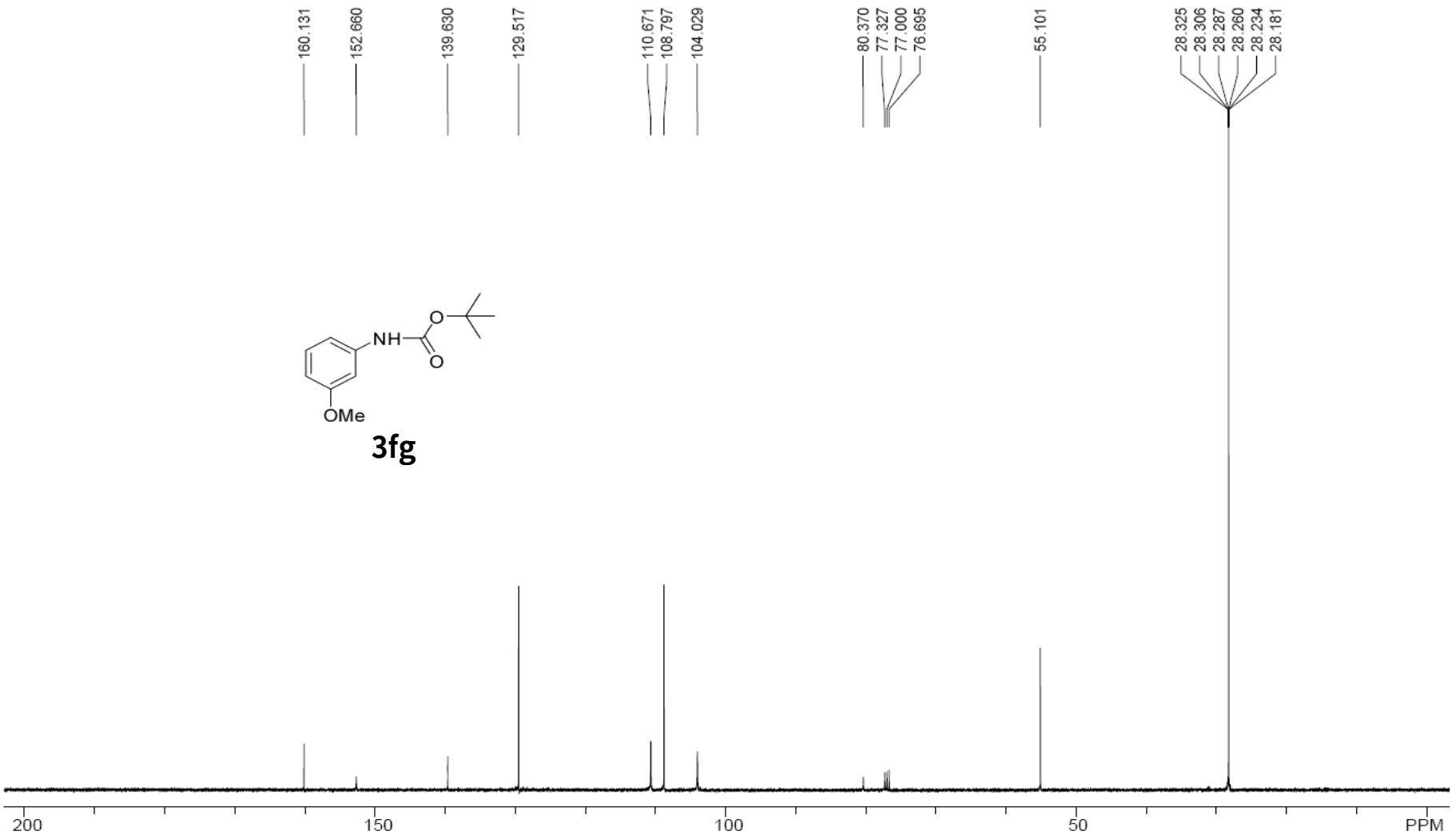
3cg


7.259
6.845
6.822
6.337
3.775
1.577
1.573
1.514
1.513
1.507
1.502
1.502
-0.002
MeO
H
N
O
O
3eg
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)
2.39
2.00
0.82
3.00
9.02
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)

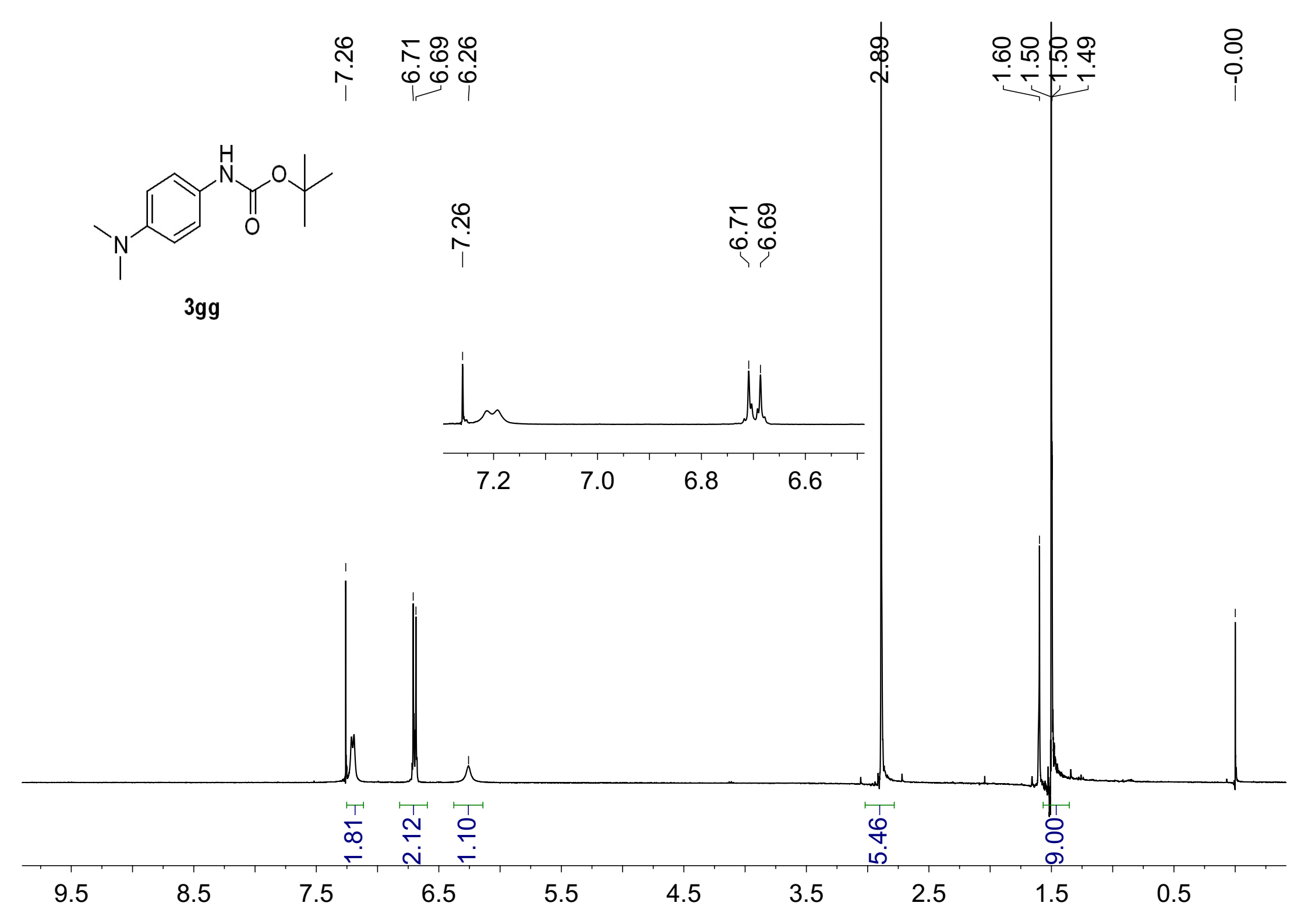

155.480
153.196
131.444
120.515
120.344
114.016
77.321
77.000
76.685
55.310
28.360
28.339
28.320
28.302
28.279
28.230
28.191
28.157
H
N
O
O
MeO
200
150
100
50
PPM

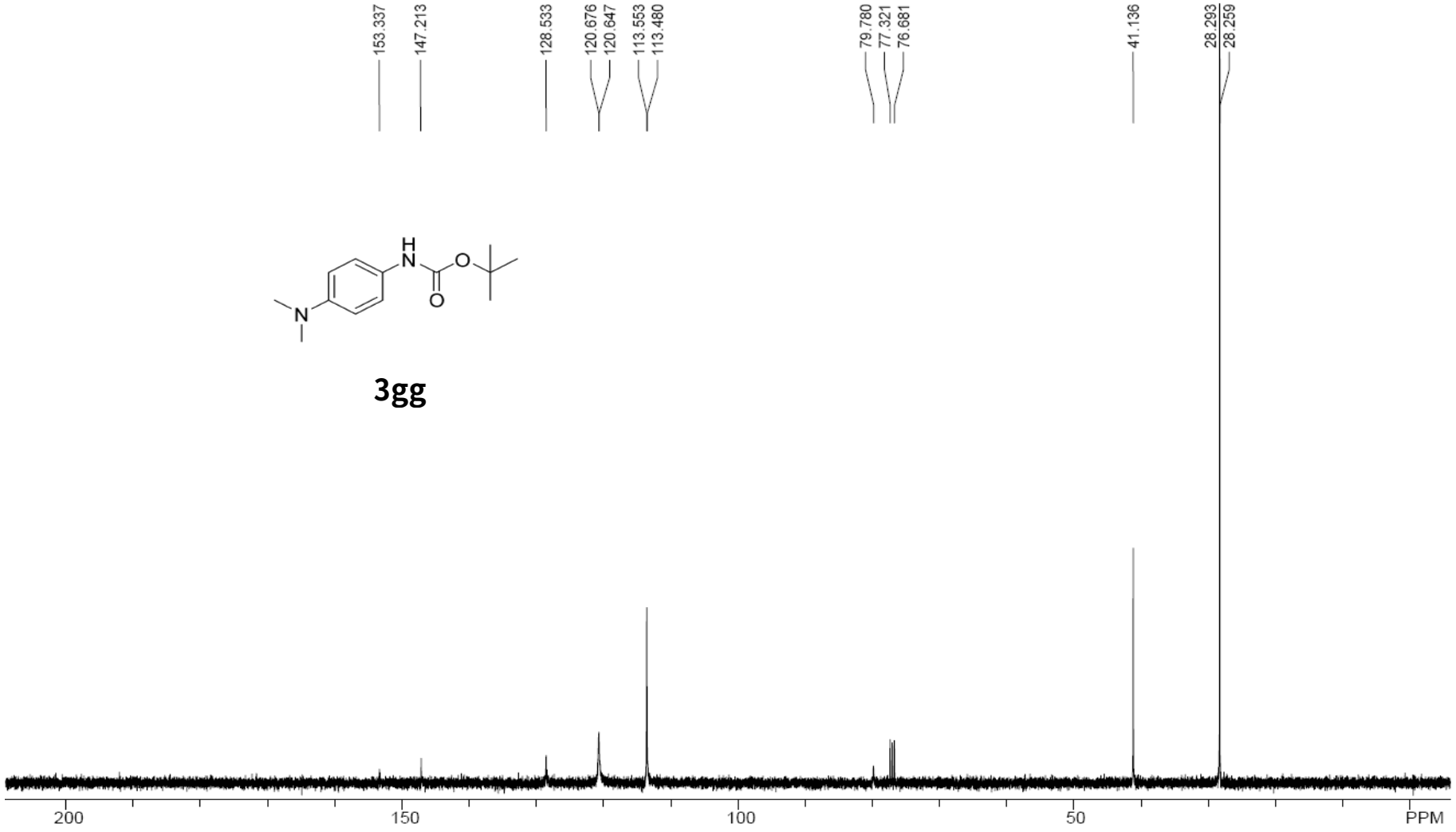
3eg


7.259
7.188
7.168
7.147
7.097
6.844
6.841
6.600
6.597
6.593
6.591
6.579
6.577
6.573
6.571
6.480
3.796
1.613
1.525
1.516
OMe
3fg
7.1
7.0
6.9
6.8
6.7
6.6
f1 (ppm)
1.13
0.95
1.08
1.12
0.93
3.00
8.80
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)

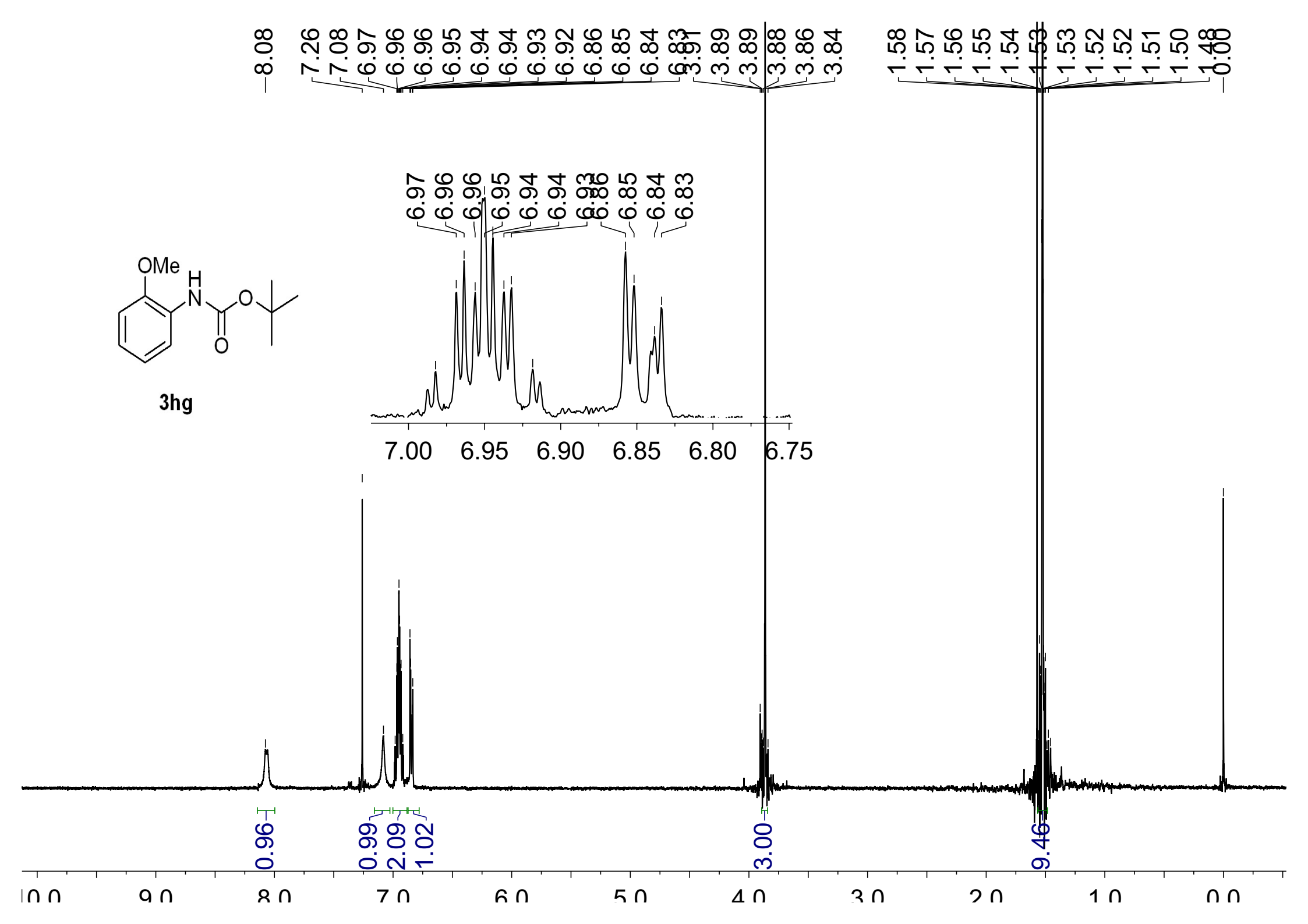

160.131
152.660
139.630
129.517
110.671
108.797
104.029
80.370
77.327
77.000
76.695
55.101
28.325
28.306
28.287
28.260
28.234
28.181
NH
O
O
OMe
200
150
100
50
PPM

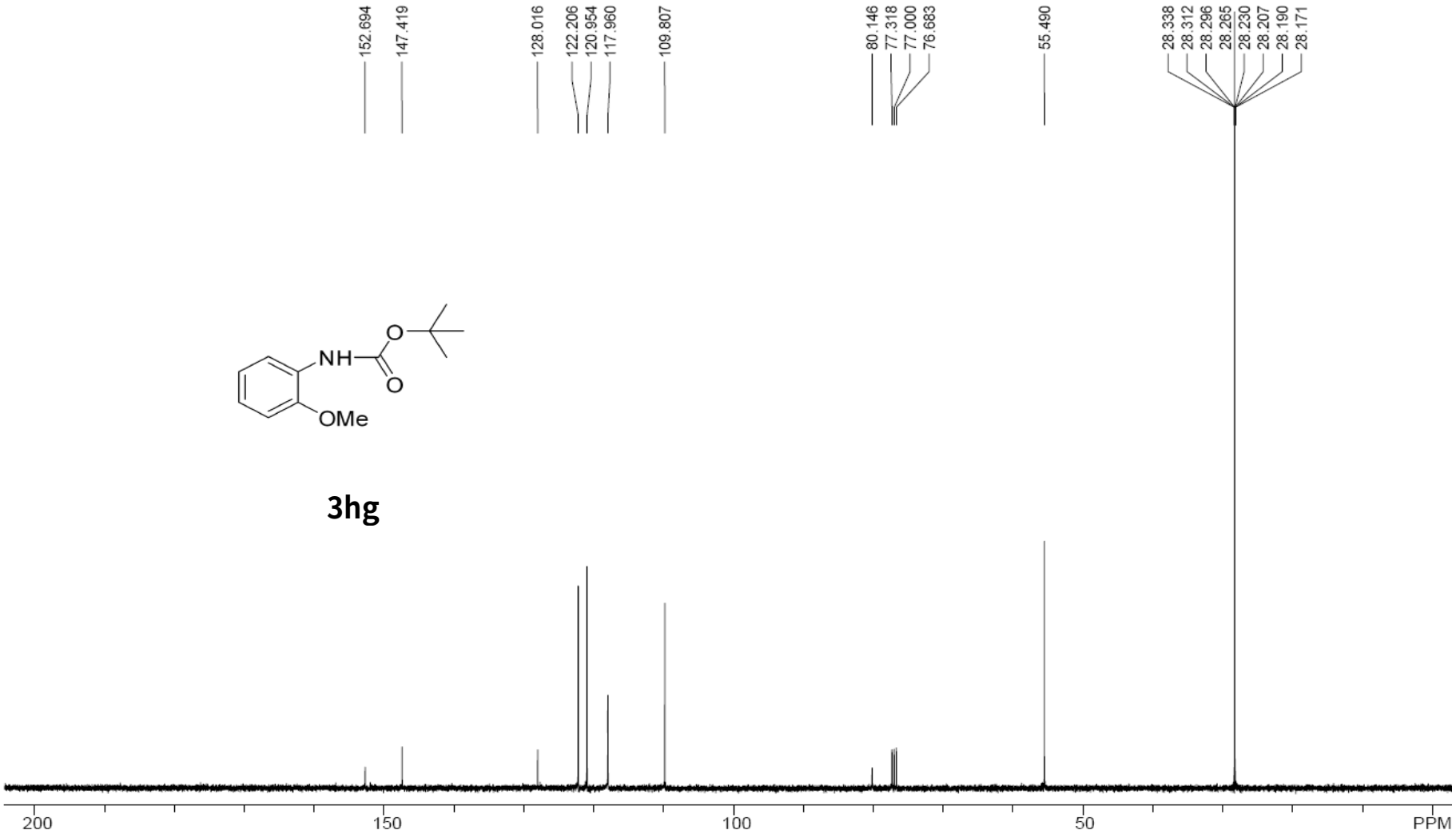
3fg


7.26
6.71
6.69
6.26
2.89
1.60
1.50
1.50
1.49
0.00
3gg
7.26
6.71
6.69
7.2
7.0
6.8
6.6
1.81
2.12
1.10
5.46
9.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

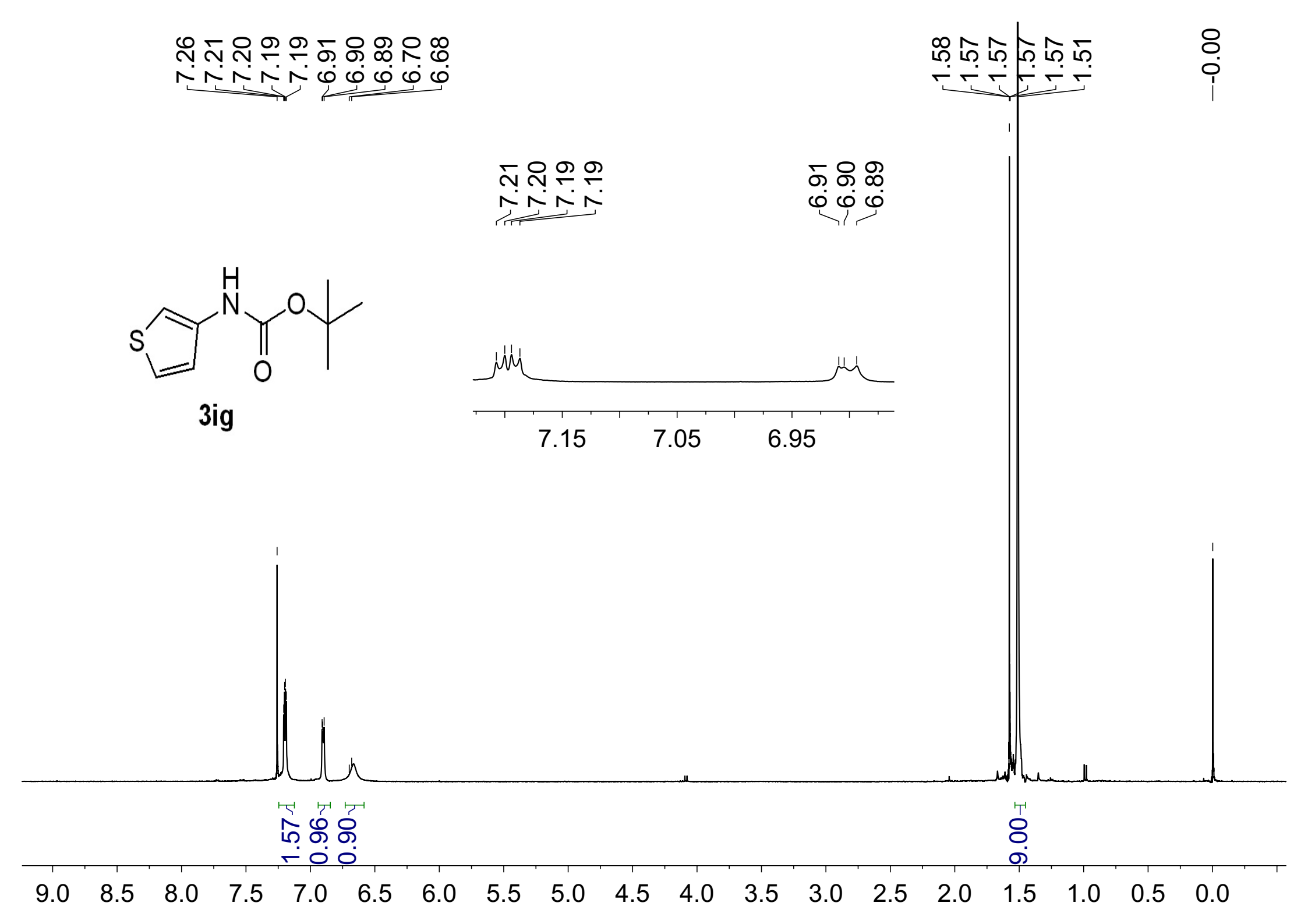

153.337
147.213
128.533
120.676
120.647
113.553
113.480
79.780
77.321
76.681
41.136
28.293
28.259
H
N
O
O
N
200
150
100
50
PPM

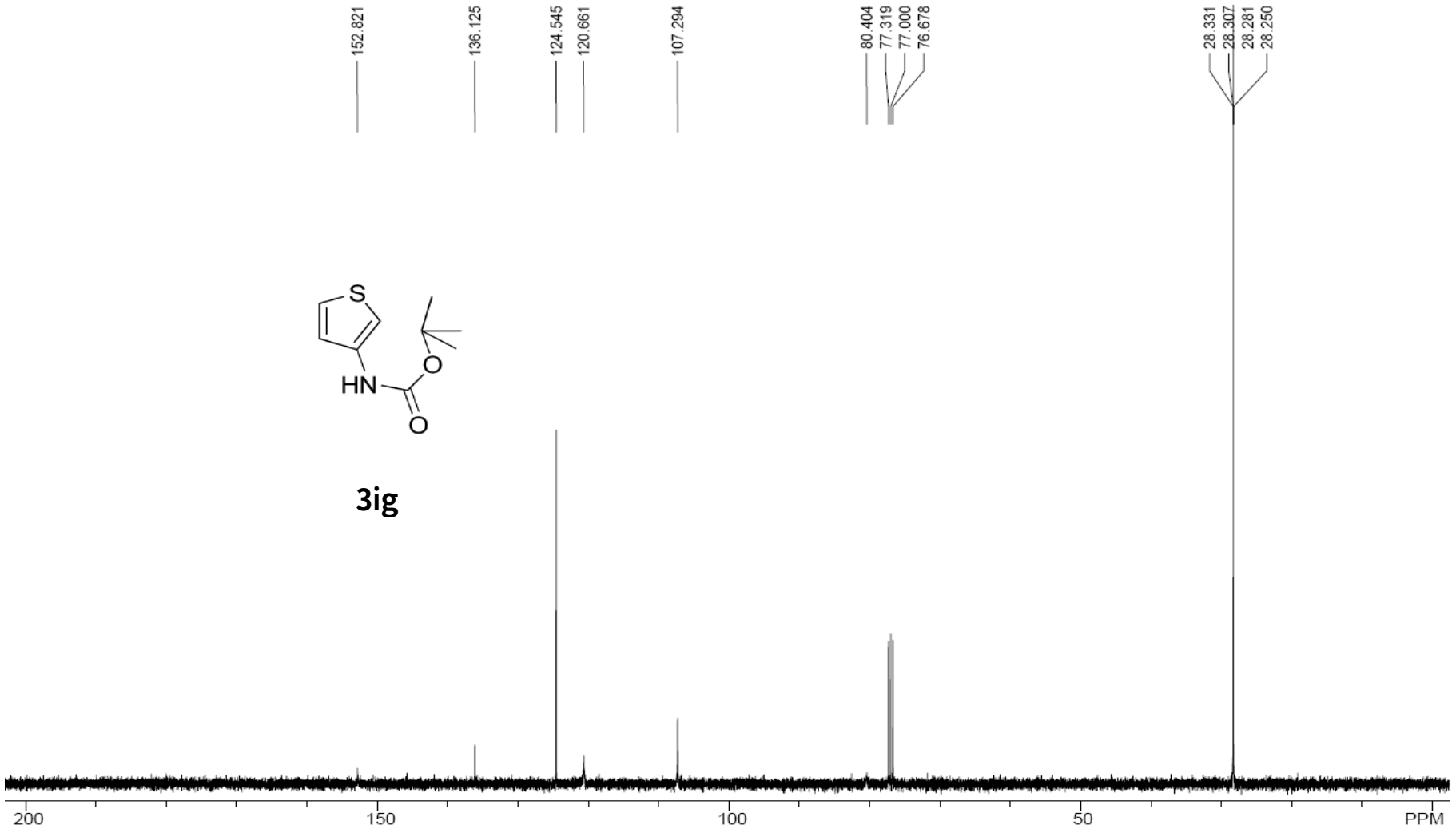
3gg


8.08
7.26
7.08
6.97
6.96
6.96
6.95
6.94
6.94
6.93
6.92
6.86
6.85
6.84
6.83
3.91
3.89
3.89
3.88
3.86
3.84
1.58
1.57
1.56
1.55
1.54
1.53
1.53
1.52
1.52
1.51
1.50
1.48
0.00
6.97
6.96
6.96
6.95
6.94
6.94
6.85
6.84
6.83
7.00
6.95
6.90
6.85
6.80
6.75
OMe
H
N
O
O
3hg
0.96
0.99
2.09
1.02
3.00
9.46
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

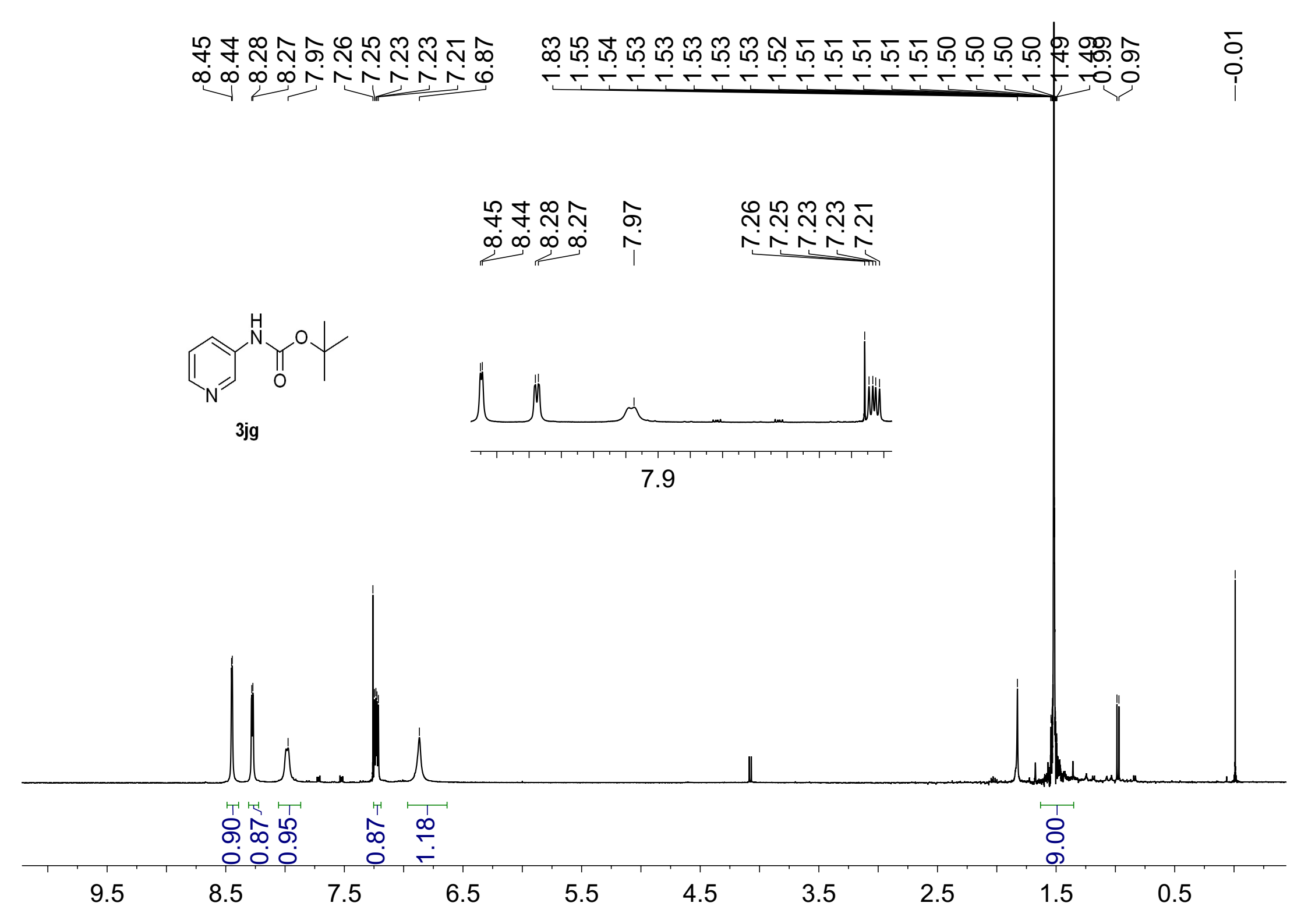

152.694
147.419
128.016
122.206
120.954
117.960
109.807
80.146
77.318
77.000
76.683
55.490
28.338
28.312
28.296
28.265
28.230
28.207
28.190
28.171
NH
O
O
OMe
200
150
100
50
PPM

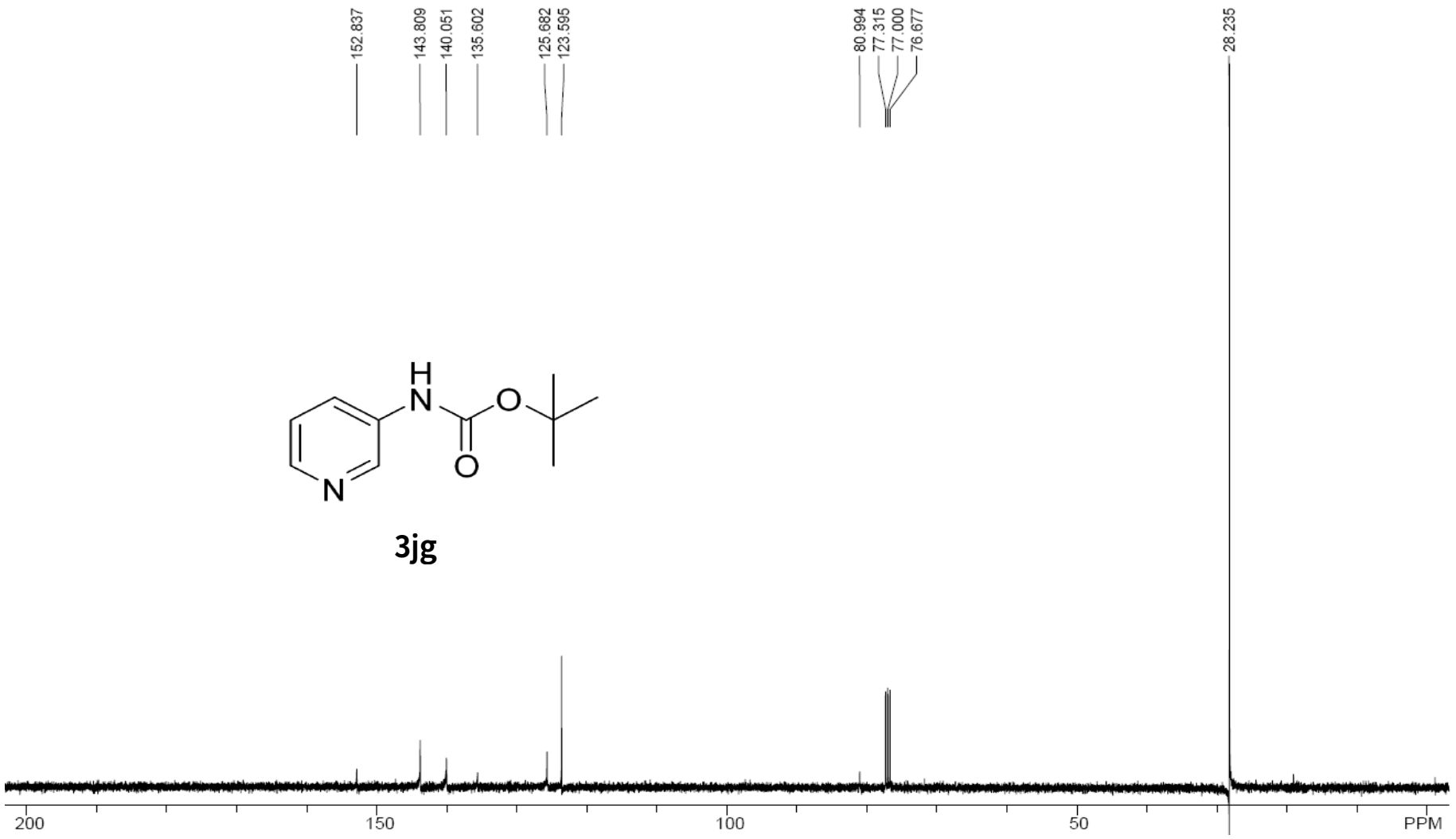
3hg


7.26
7.21
7.20
7.19
7.19
6.91
6.90
6.89
6.70
6.68
1.58
1.57
1.57
1.57
1.57
1.51
0.00
7.21
7.20
7.19
7.19
6.91
6.90
6.89
S
NH
O
O
3ig
7.15
7.05
6.95
1.57
0.96
0.90
9.00
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

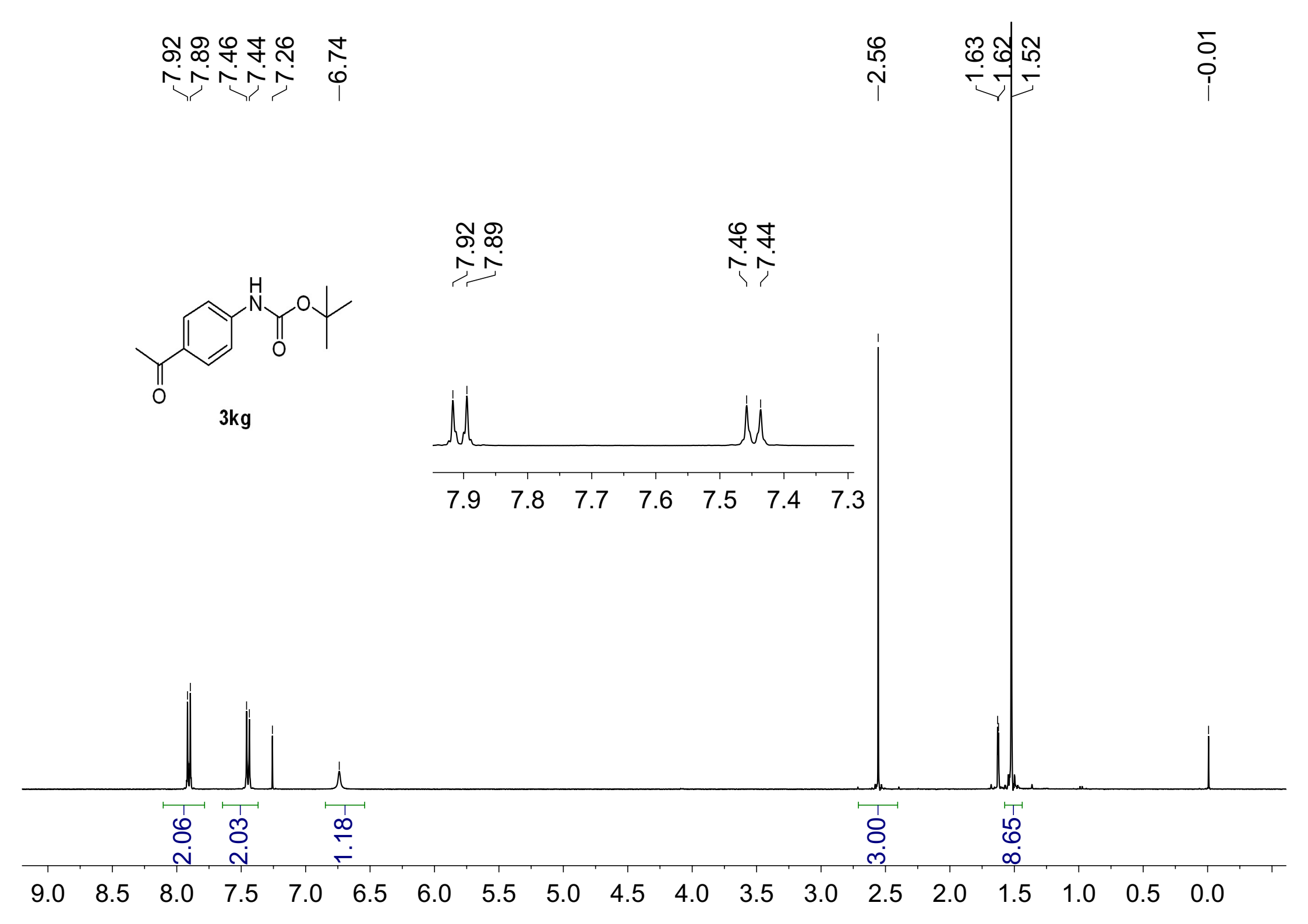

152.821
136.125
124.545
120.661
107.294
80.404
77.319
77.000
76.678
28.331
28.307
28.281
28.250
S
HN
O
O
200
150
100
50
PPM

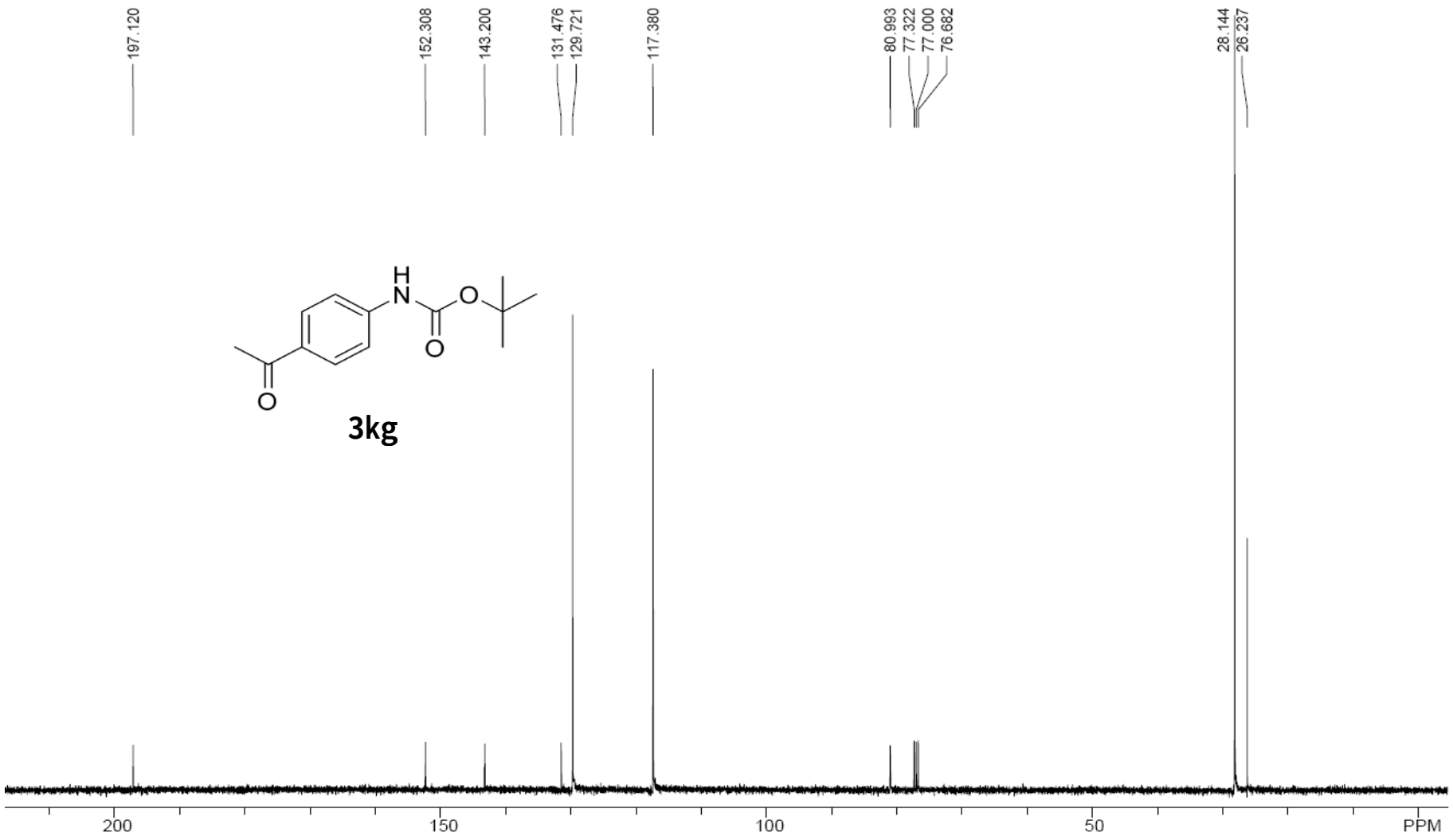
3ig


8.45
8.44
8.28
8.27
7.97
7.26
7.25
7.23
7.23
7.21
6.87
1.83
1.55
1.54
1.53
1.53
1.53
1.53
1.53
1.52
1.51
1.51
1.51
1.51
1.51
1.50
1.50
1.50
1.50
1.49
1.49
0.99
0.97
-0.01
3jg
7.9
0.90
0.87
0.95
0.87
1.18
9.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

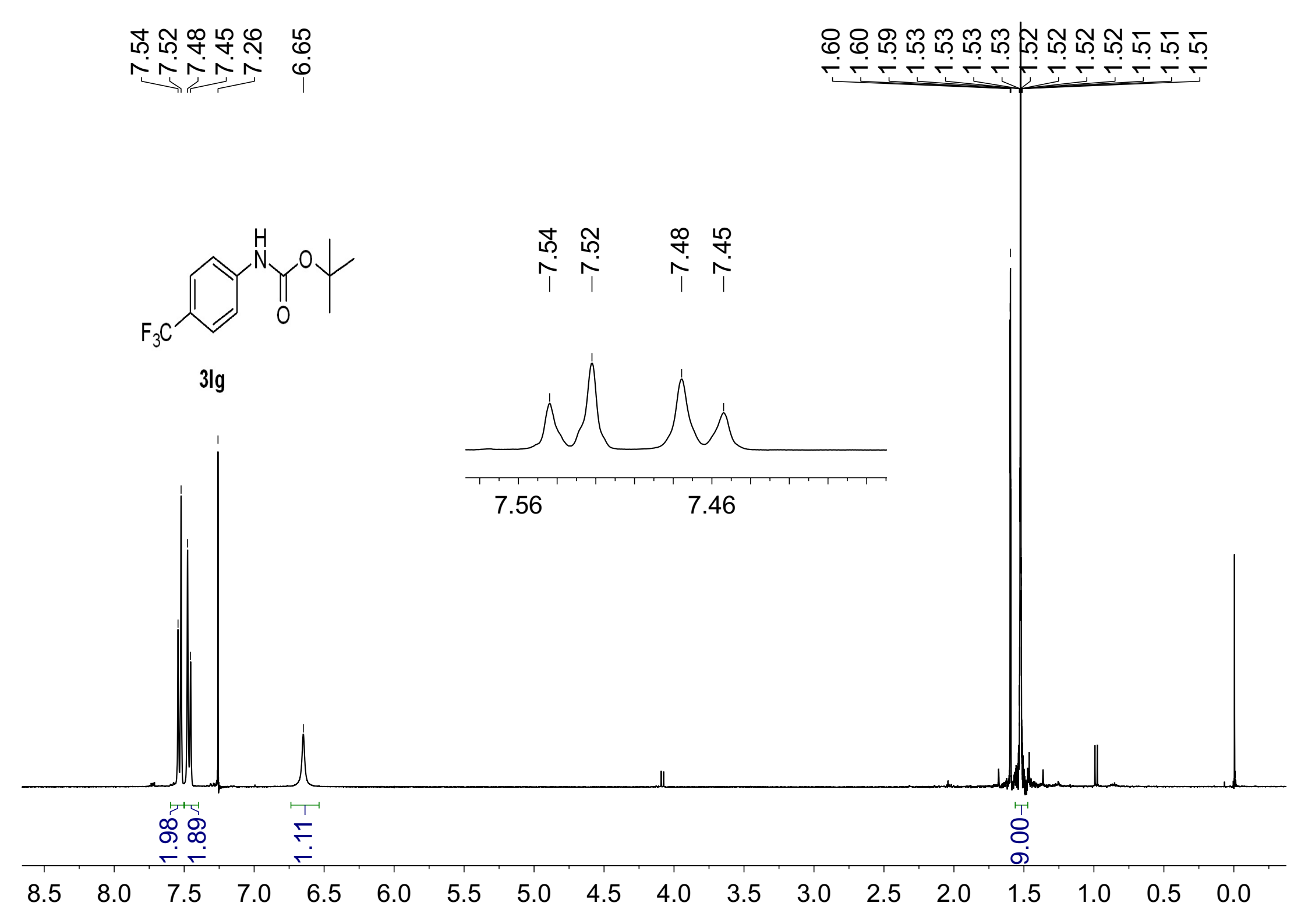

152.837
143.809
140.051
135.602
125.682
123.595
80.994
77.315
77.000
76.677
28.235
H
N
O
O
N
200
150
100
50
PPM

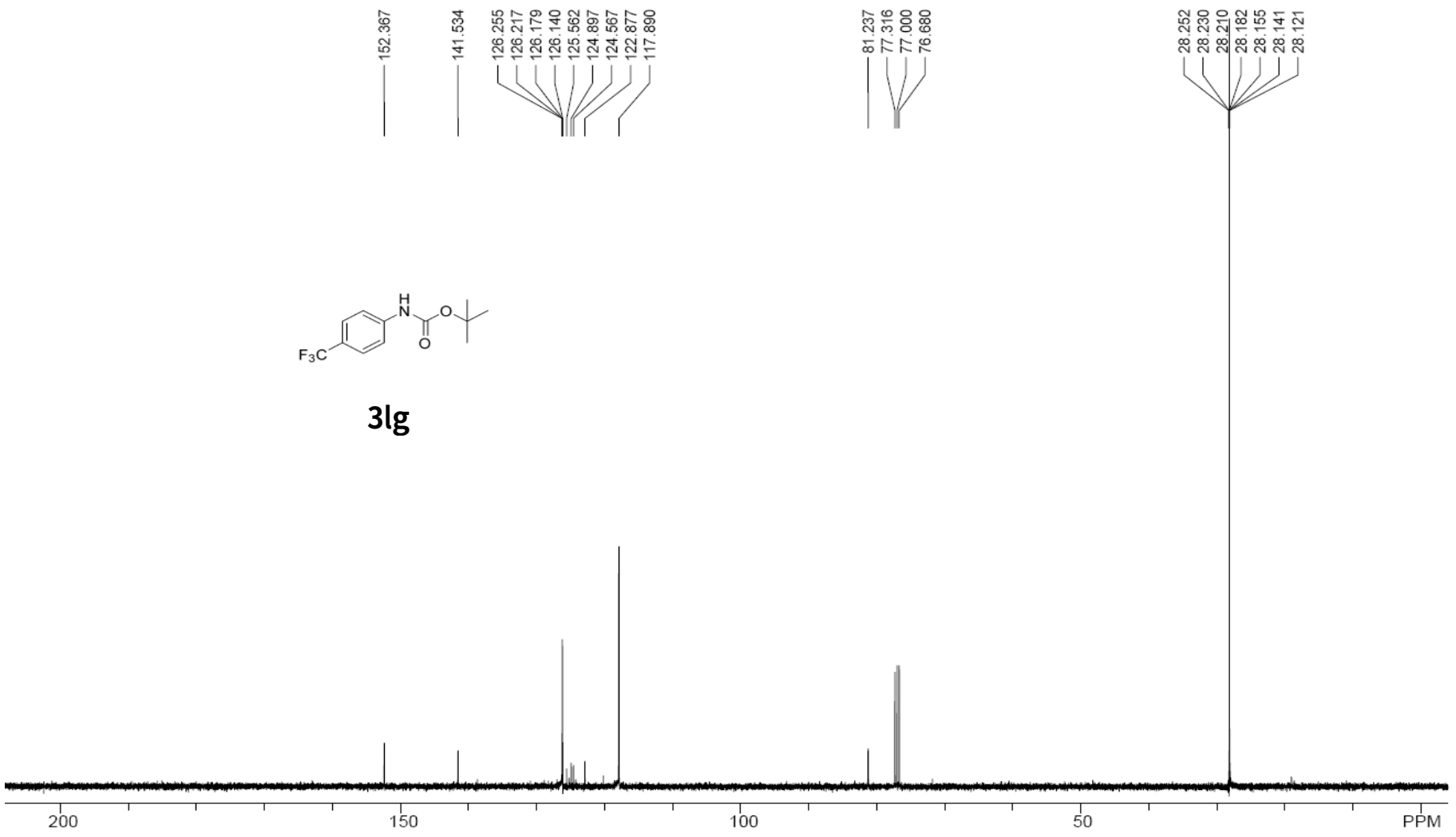
3jg


7.92
7.89
7.46
7.44
7.26
6.74
2.56
1.63
1.62
1.52
0.01
3kg
7.9
7.8
7.7
7.6
7.5
7.4
7.3
2.06
2.03
1.18
3.00
8.65
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

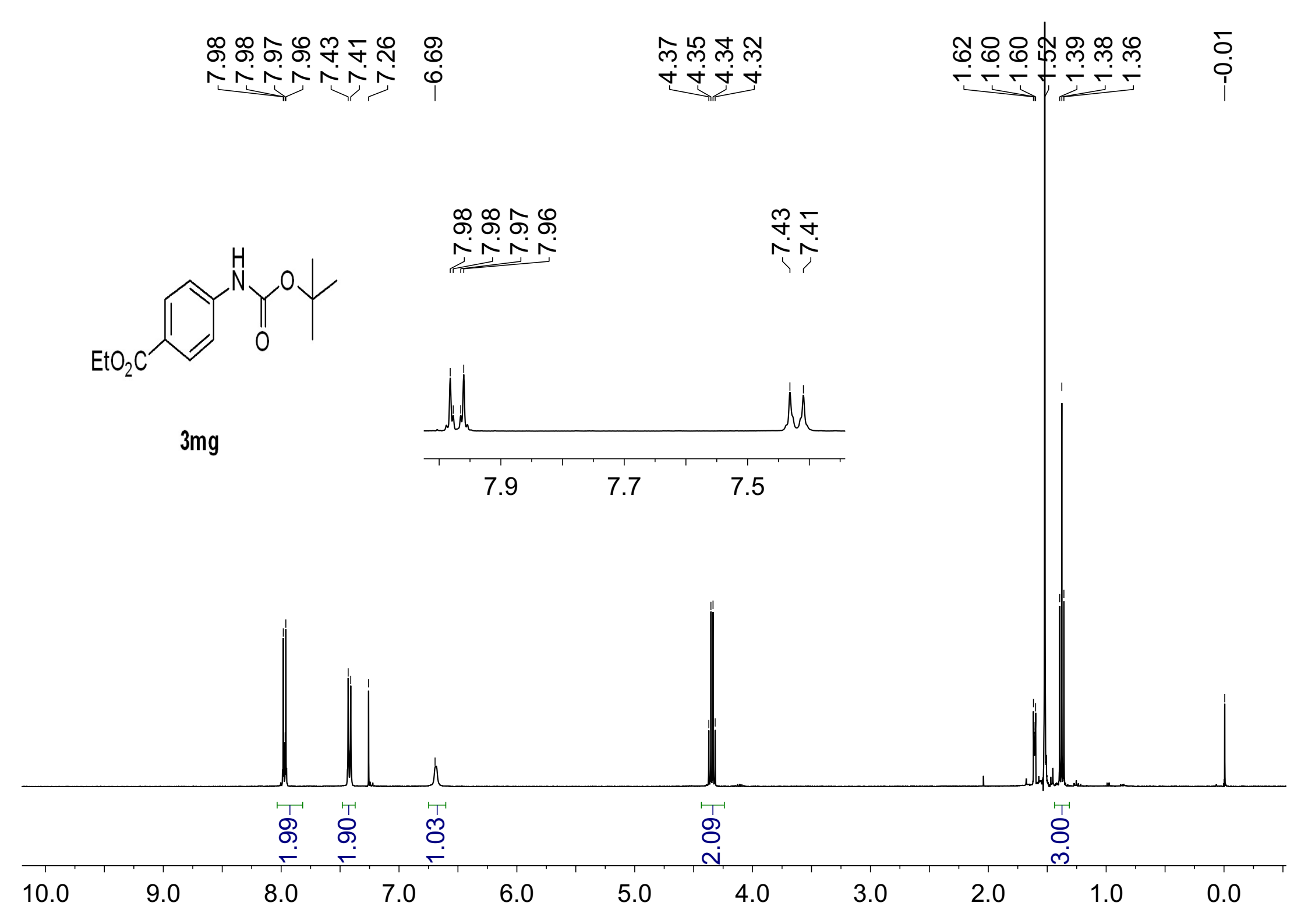

197.120
152.308
143.200
131.476
129.721
117.380
80.993
77.322
77.000
76.682
28.144
26.237
H
N
O
O
O
200
150
100
50
PPM

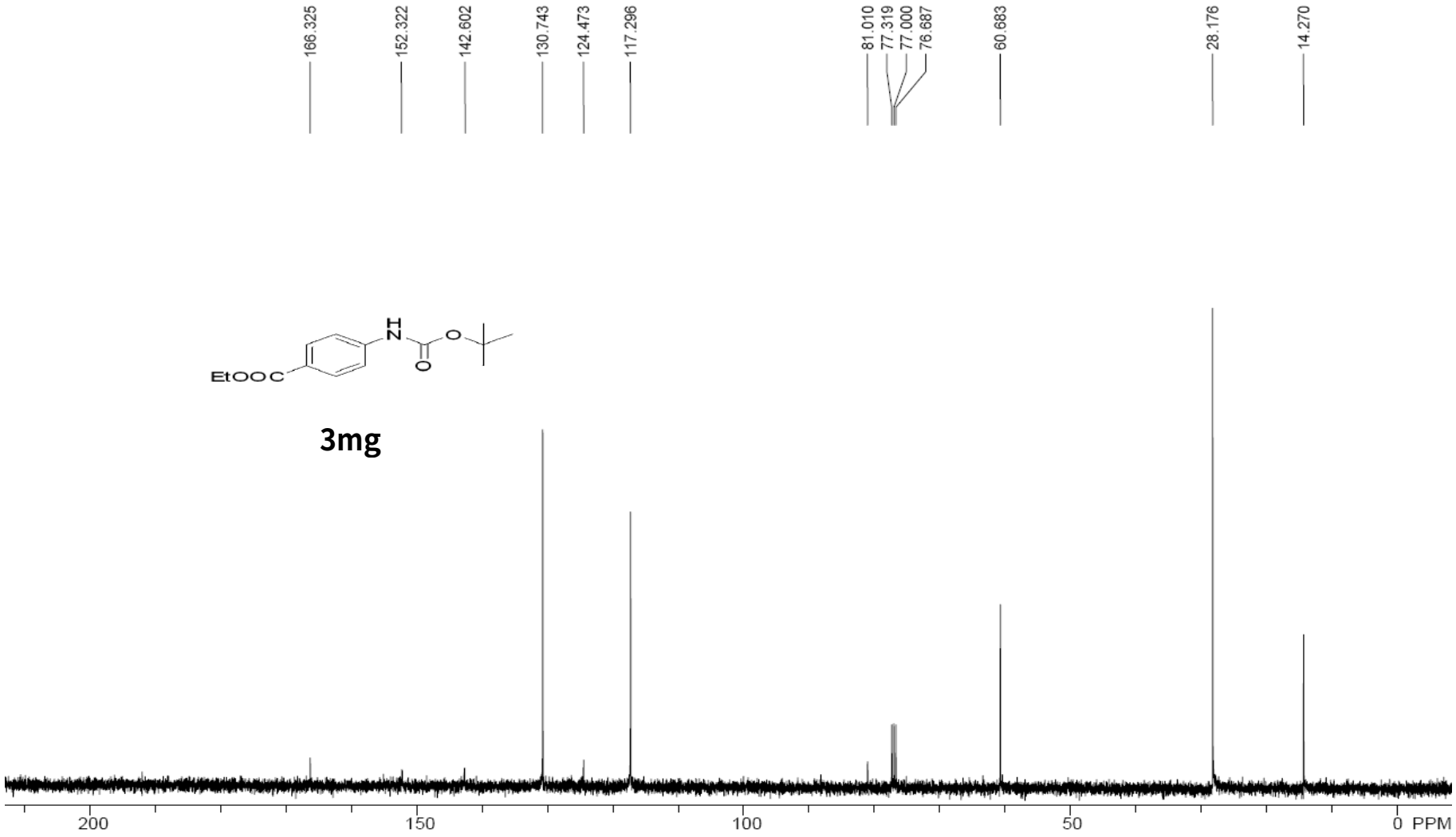
3kg

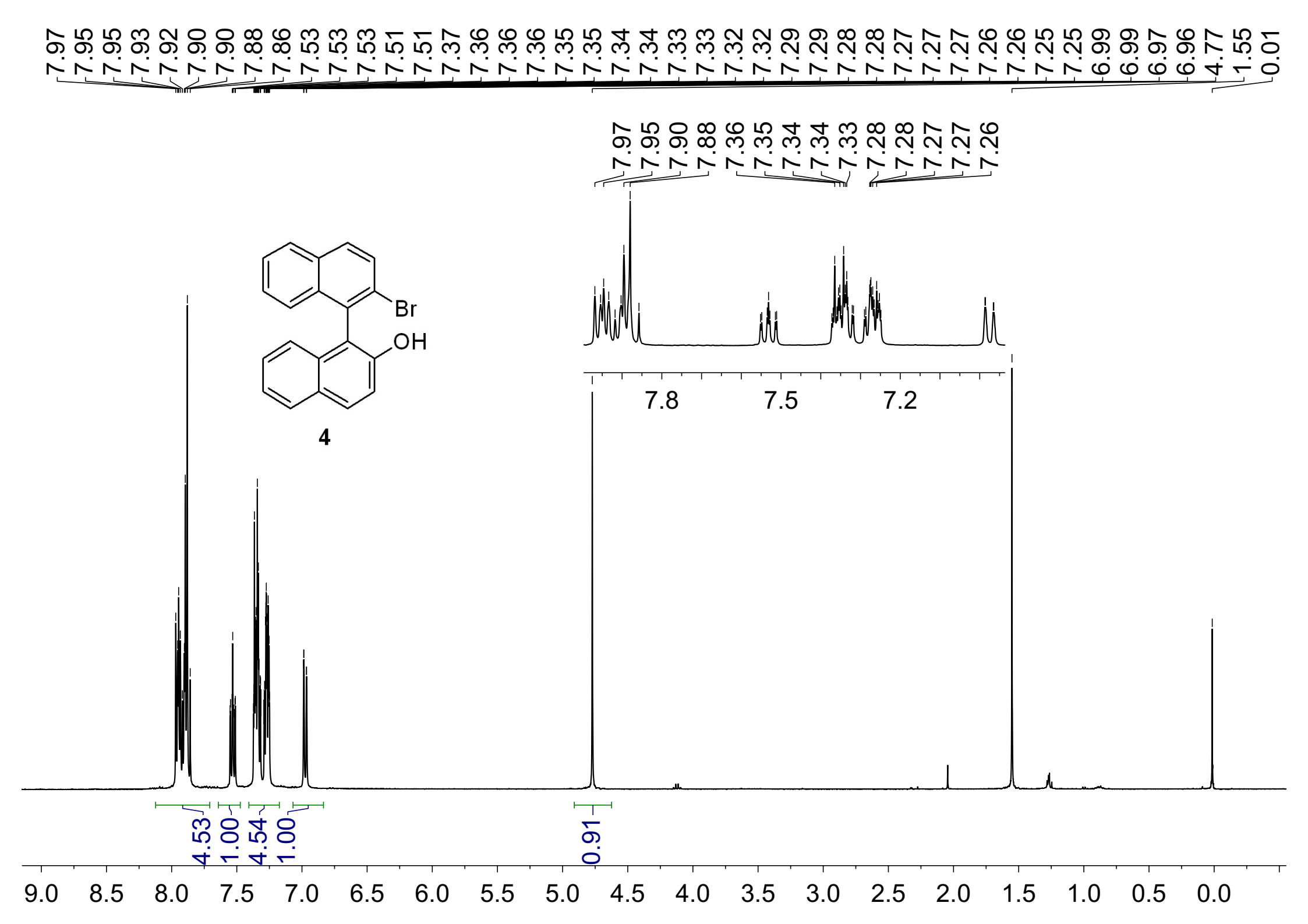

7.54
7.52
7.48
7.45
7.26
6.65
1.60
1.60
1.59
1.53
1.53
1.53
1.53
1.52
1.52
1.52
1.52
1.51
1.51
1.51
F3C
3lg
7.56
7.46
1.98
1.89
1.11
9.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

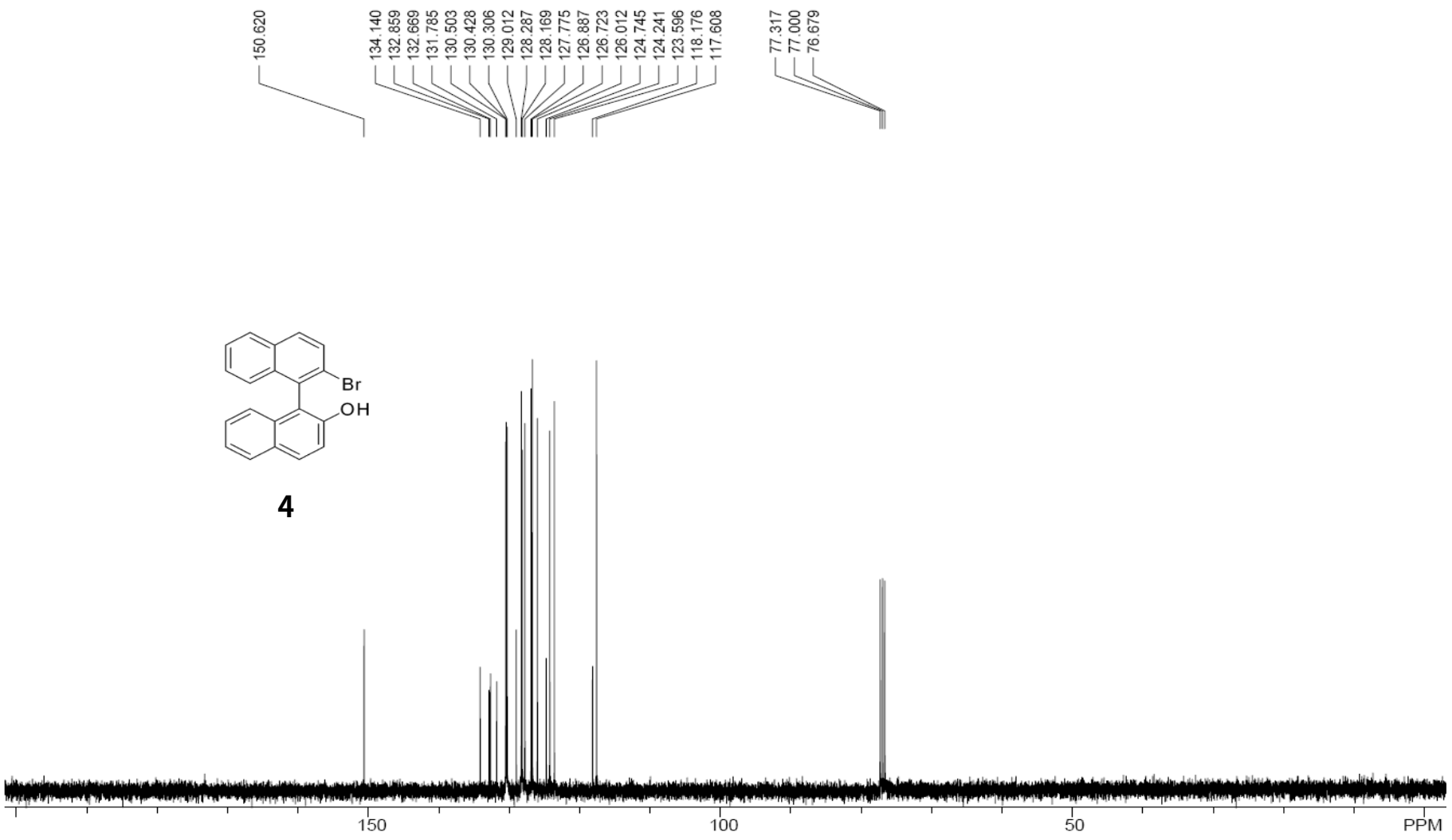

152.367
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126.217
126.179
126.140
125.562
124.897
124.567
122.877
117.890
81.237
77.316
77.000
76.680
28.252
28.230
28.210
28.182
28.155
28.141
28.121
H
N
O
O
F3C
200
150
100
50
PPM

3lg

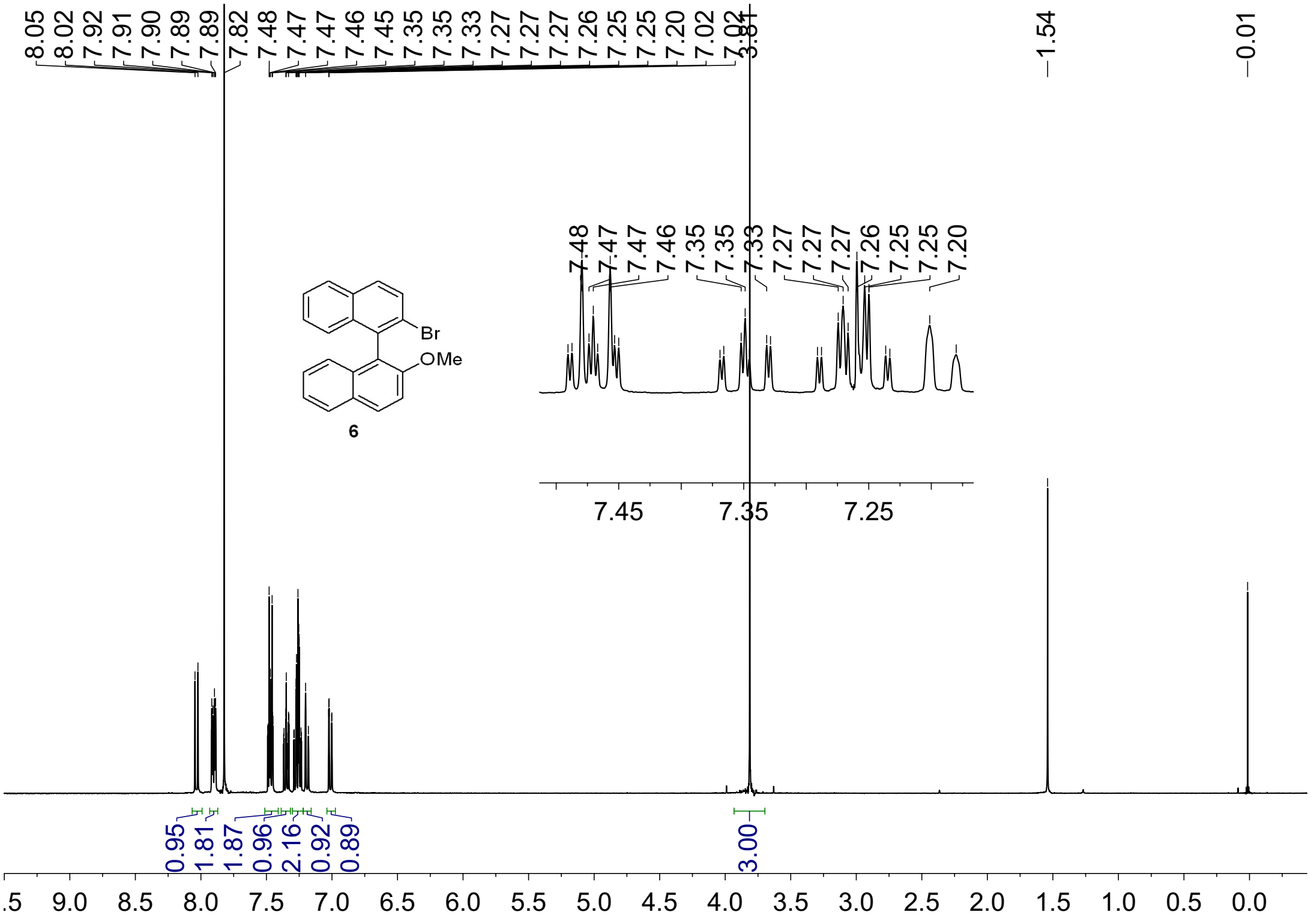

7.98
7.98
7.97
7.96
7.43
7.41
7.26
6.69
4.37
4.35
4.34
4.32
1.62
1.60
1.60
1.52
1.39
1.38
1.36
0.01
7.98
7.98
7.97
7.96
7.43
7.41
7.9
7.7
7.5
EtO2C
3mg
1.99
1.90
1.03
2.09
3.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

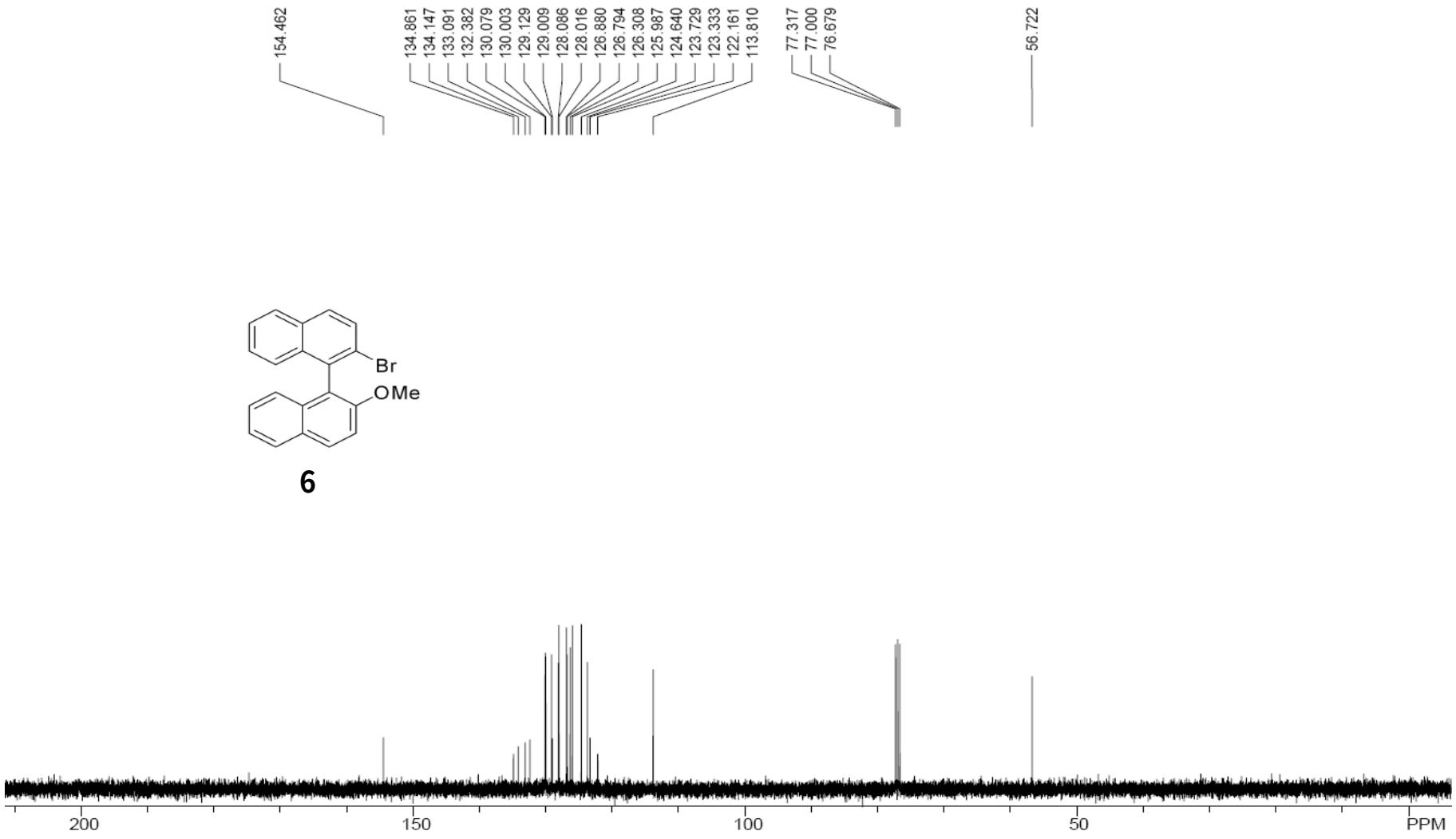

166.325
152.322
142.602
130.743
124.473
117.296
81.010
77.319
77.000
76.687
60.683
28.176
14.270
EtOOC
3mg
200
150
100
50
0 PPM


7.97 7.95 7.95 7.93 7.92 7.90 7.90 7.88 7.86 7.53 7.53 7.53 7.51 7.51 7.37 7.36 7.36 7.36 7.35 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.29 7.29 7.28 7.28 7.27 7.27 7.27 7.26 7.26 7.25 7.25 6.99 6.99 6.97 6.96 4.77 1.55 0.01
7.97 7.95 7.90 7.88 7.36 7.35 7.34 7.34 7.33 7.28 7.28 7.27 7.27 7.26
Br
OH
4
7.8
7.5
7.2
4.53
1.00
4.54
1.00
0.91
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

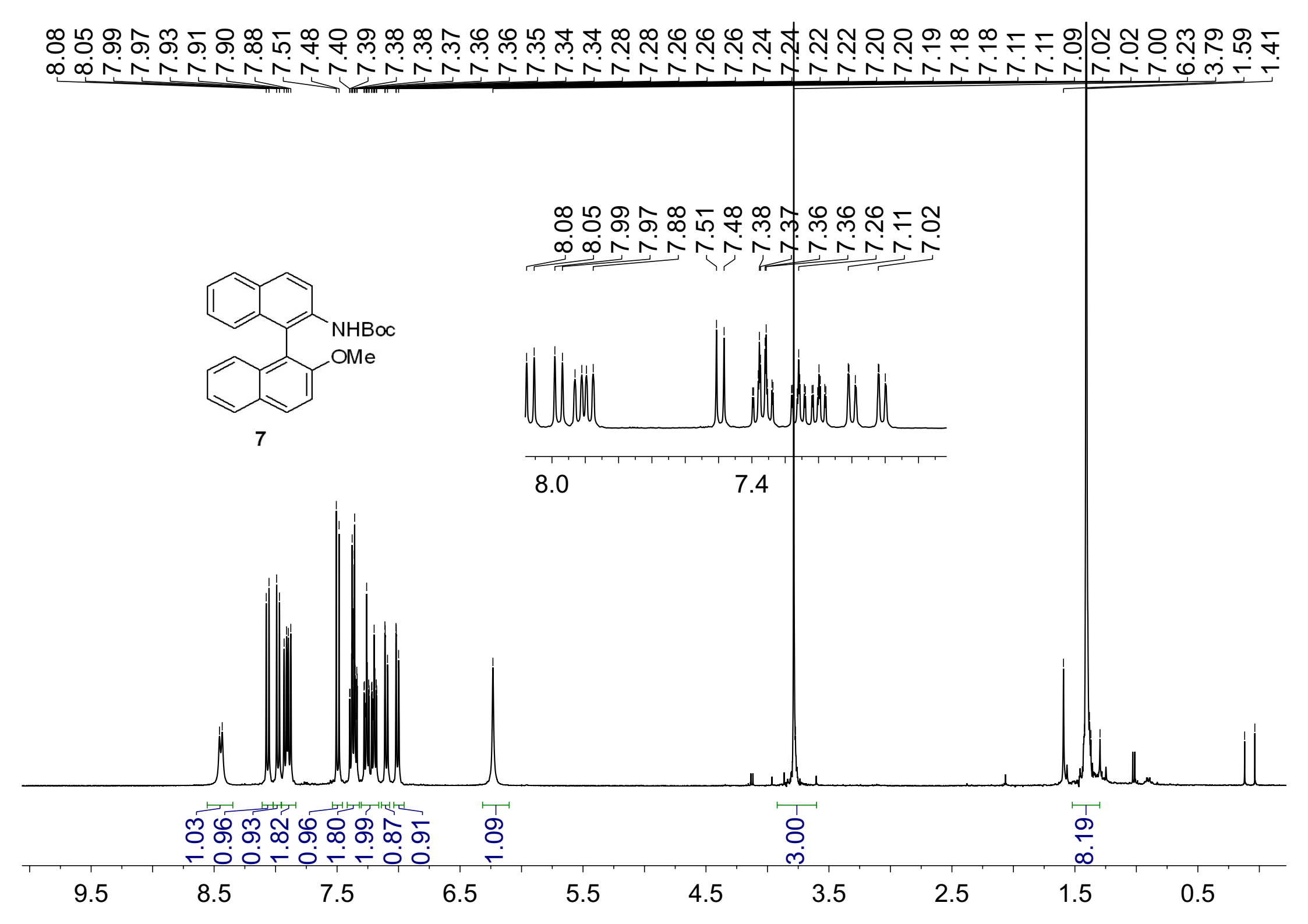

150.620
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132.859
132.669
131.785
130.503
130.428
130.306
129.012
128.287
128.169
127.775
126.887
126.723
126.012
124.745
124.241
123.596
118.176
117.608
77.317
77.000
76.679
Br
OH
150
100
50
PPM

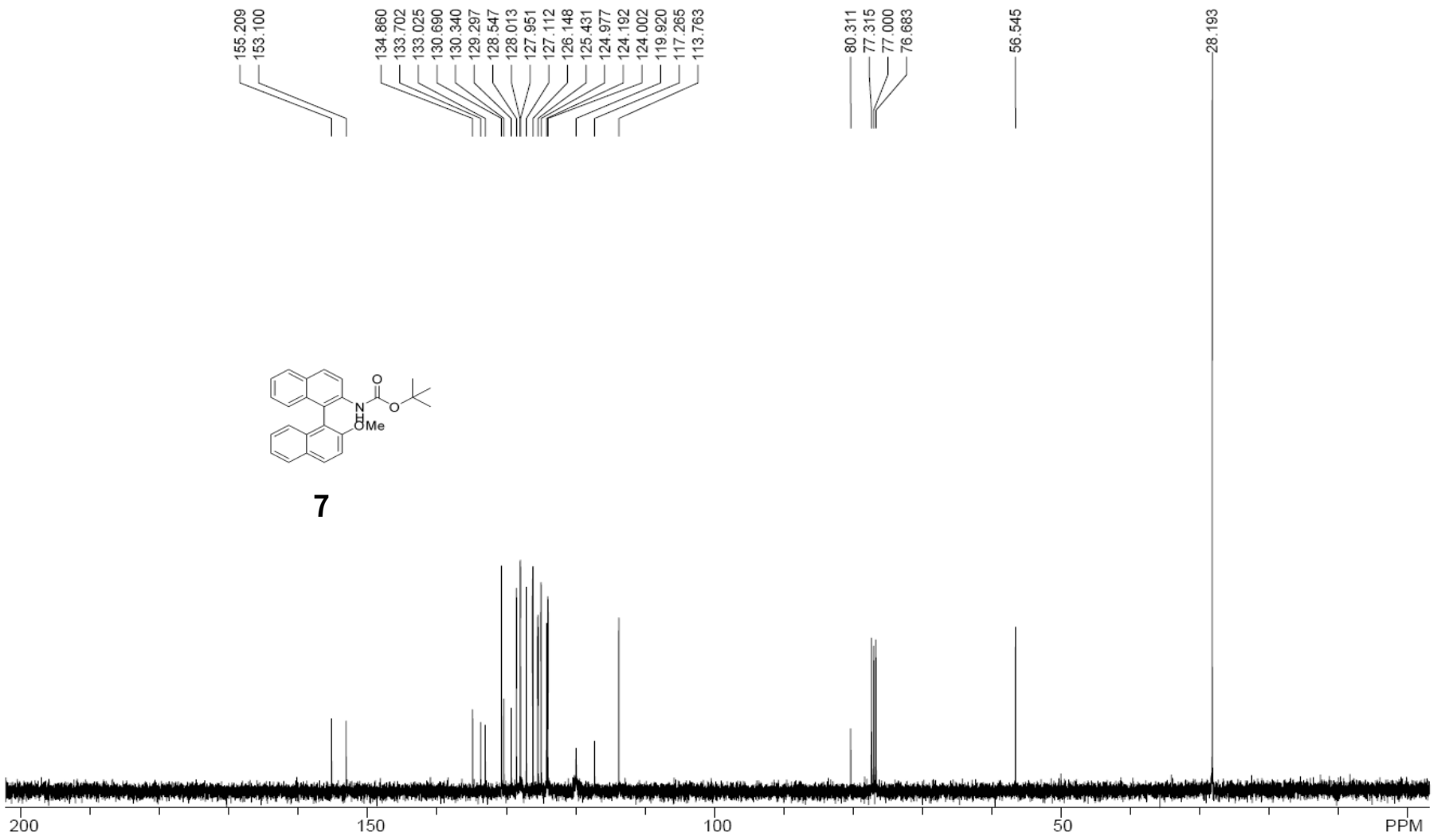
4


8.05
8.02
7.92
7.91
7.90
7.89
7.89
7.82
7.48
7.47
7.47
7.46
7.45
7.35
7.35
7.33
7.27
7.27
7.27
7.26
7.25
7.25
7.20
7.02
3.81
1.54
0.01
Br
OMe
6
7.45
7.35
7.25
0.95
1.81
1.87
0.96
2.16
0.92
0.89
3.00
.5
9.0
8.5
8.0
7.5
7.0
6.5
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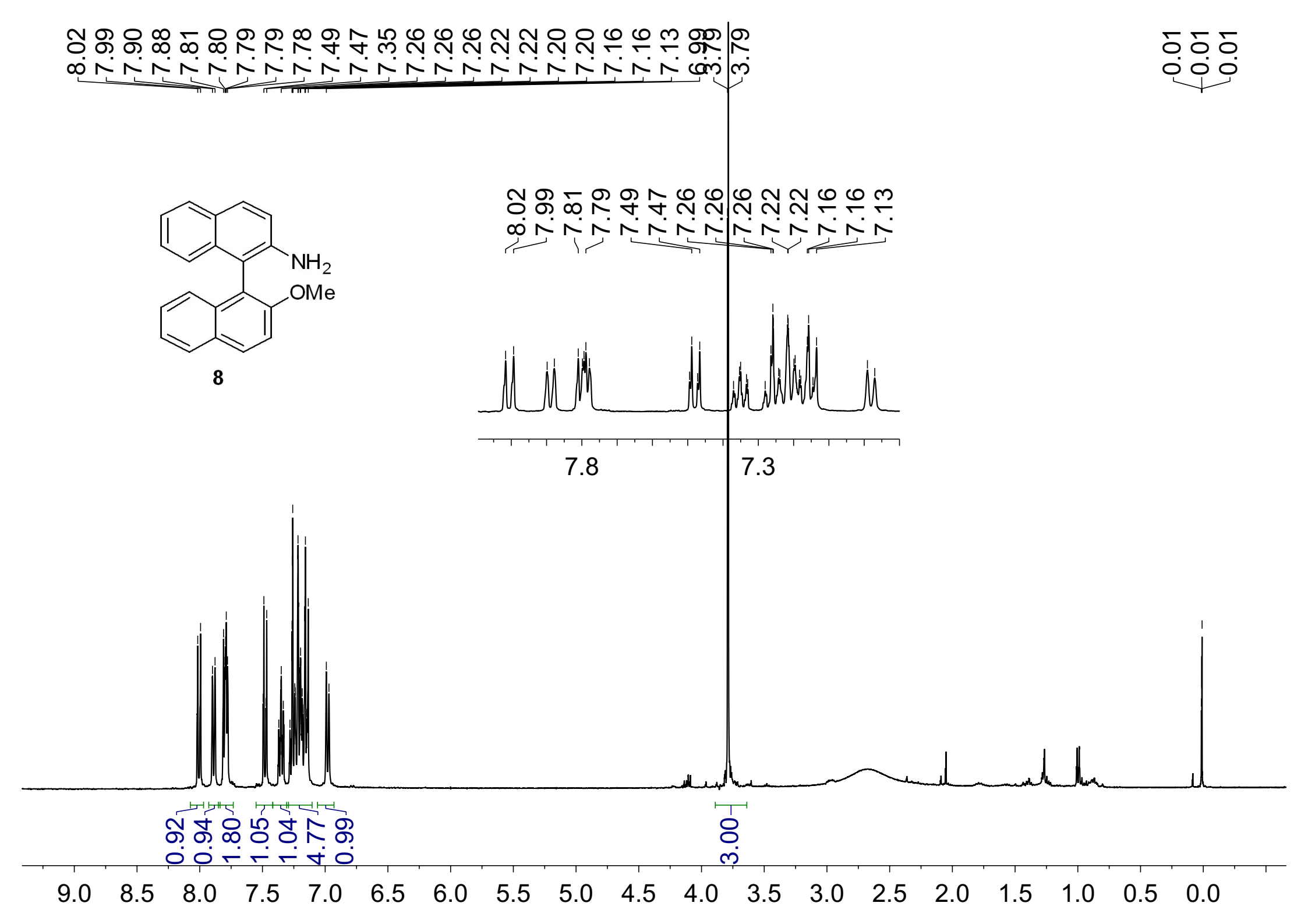

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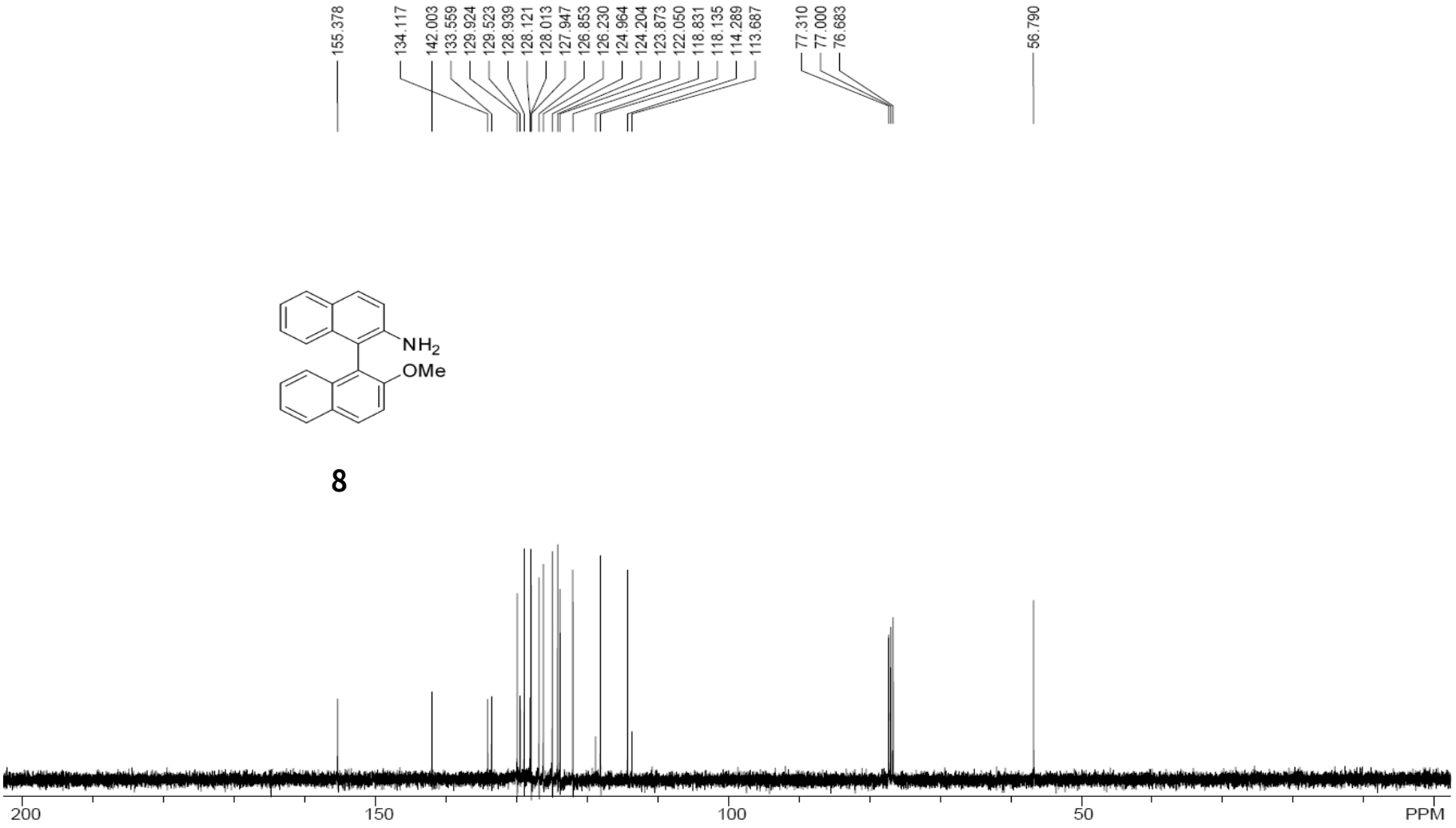
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