Supporting Information: NMR spectra

Palladium-catalyzed *anti*-Michael reductive Heck reaction of α,β-unsaturated esters

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[‡]Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637616

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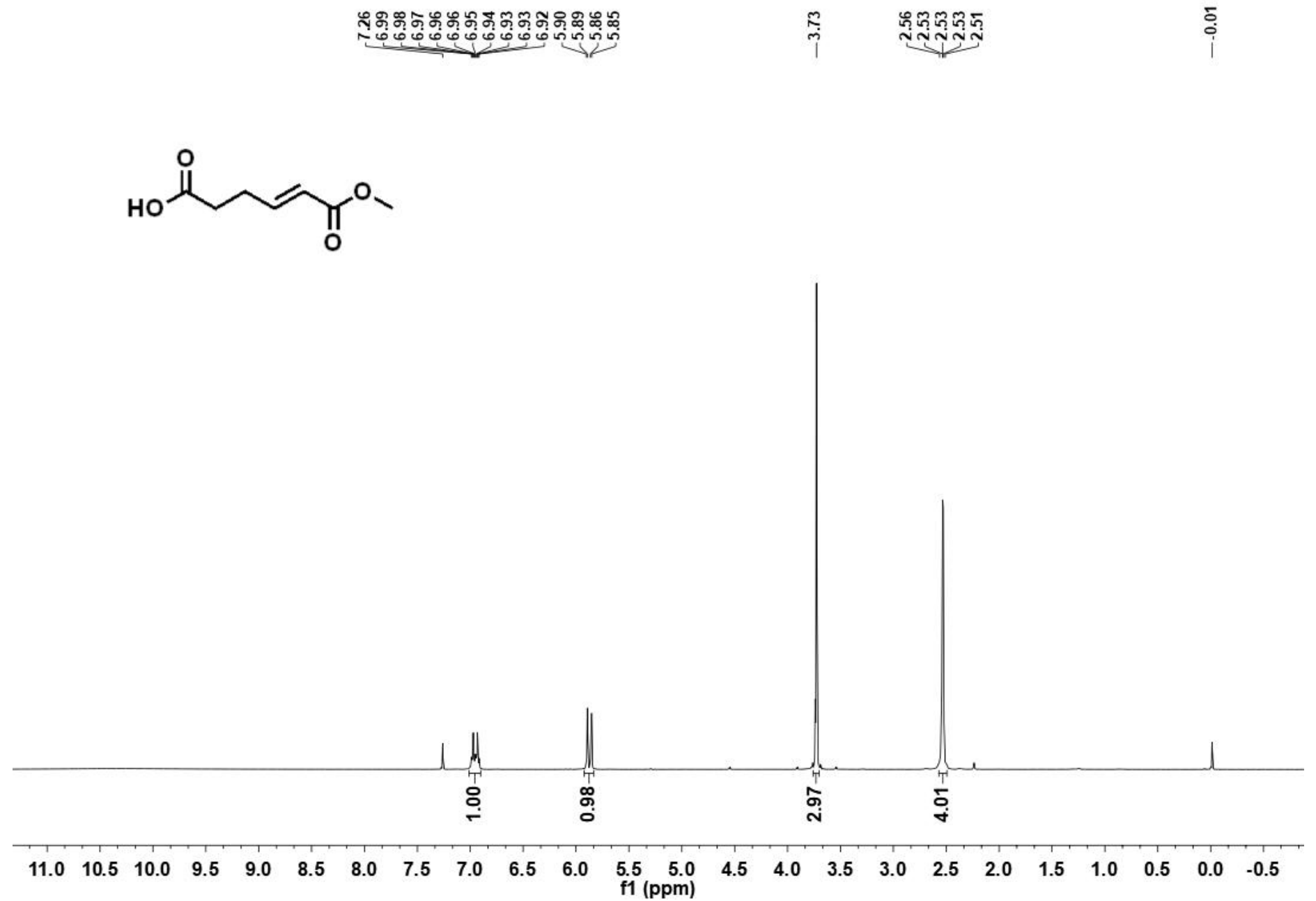
**E-mail: iamxiaojinwu@njtech.edu.cn, teckpeng@ntu.edu.sg*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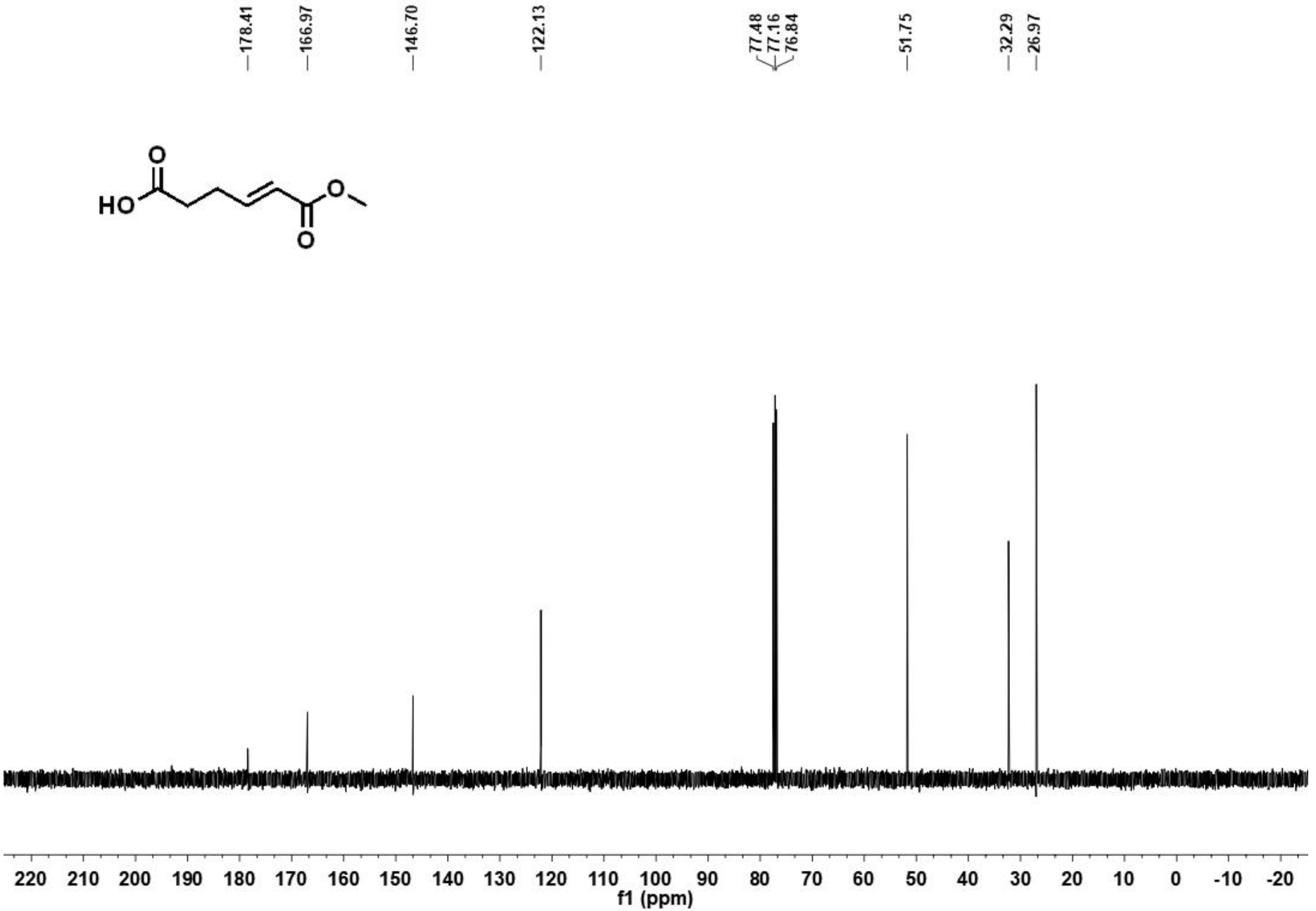
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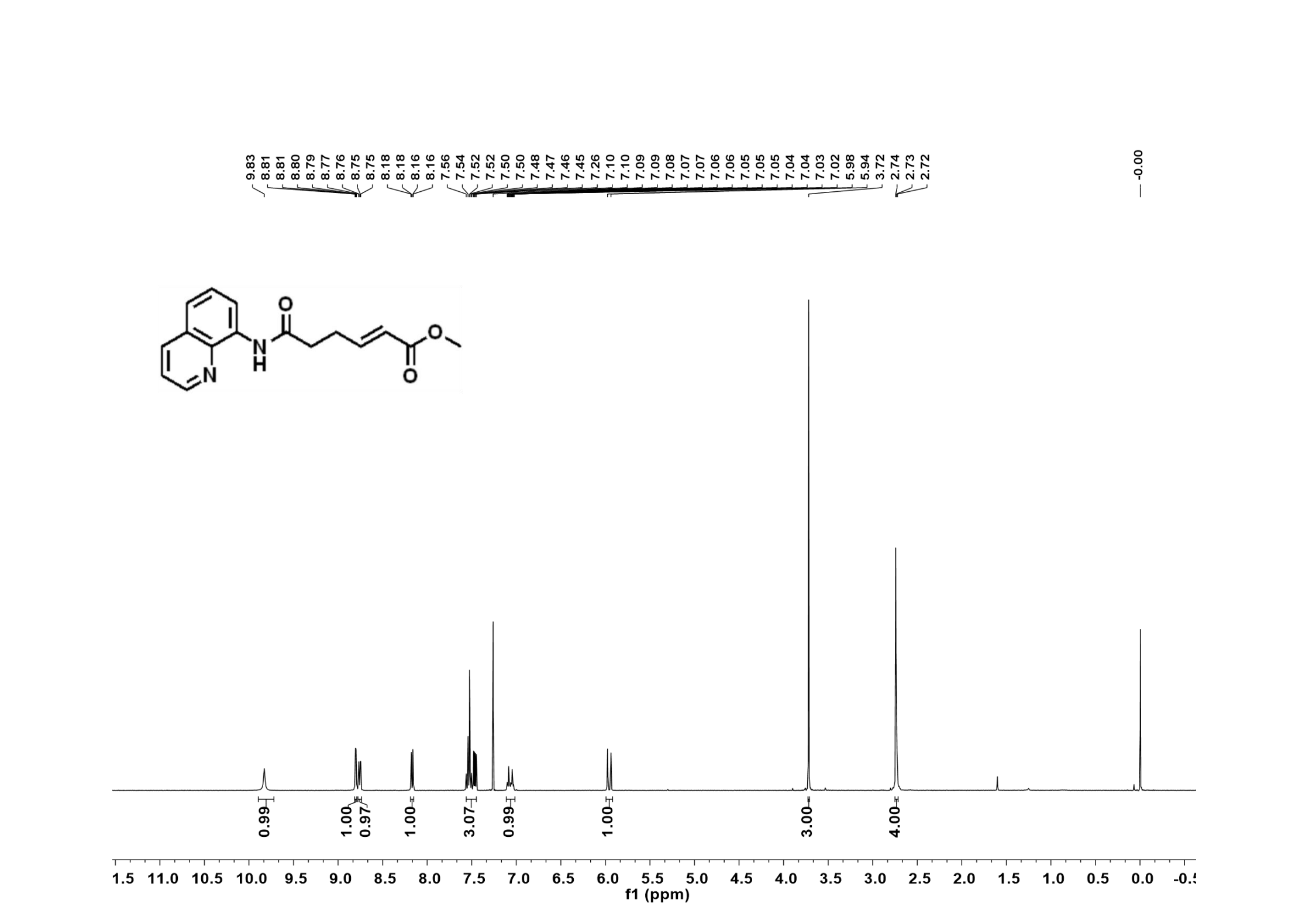
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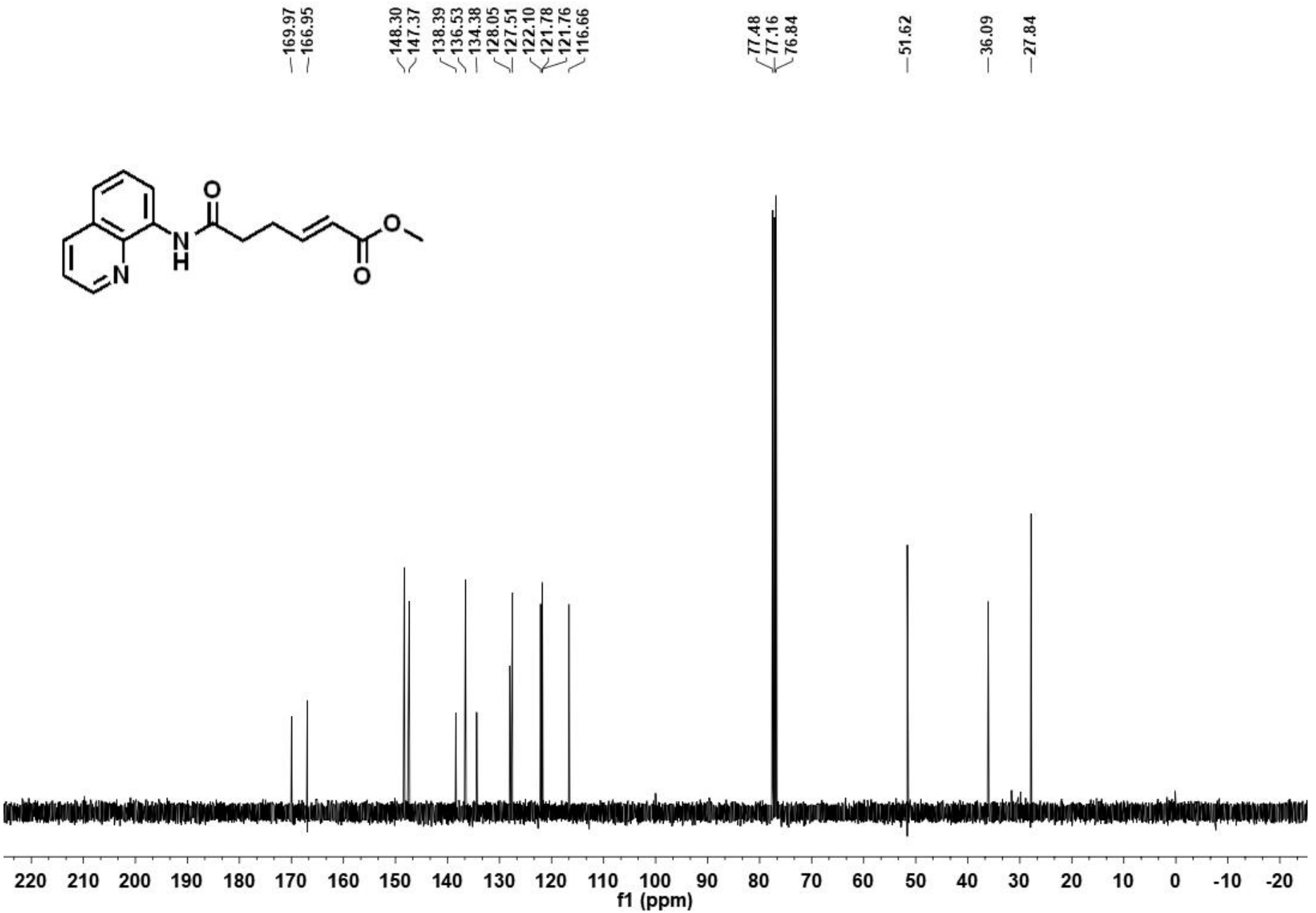
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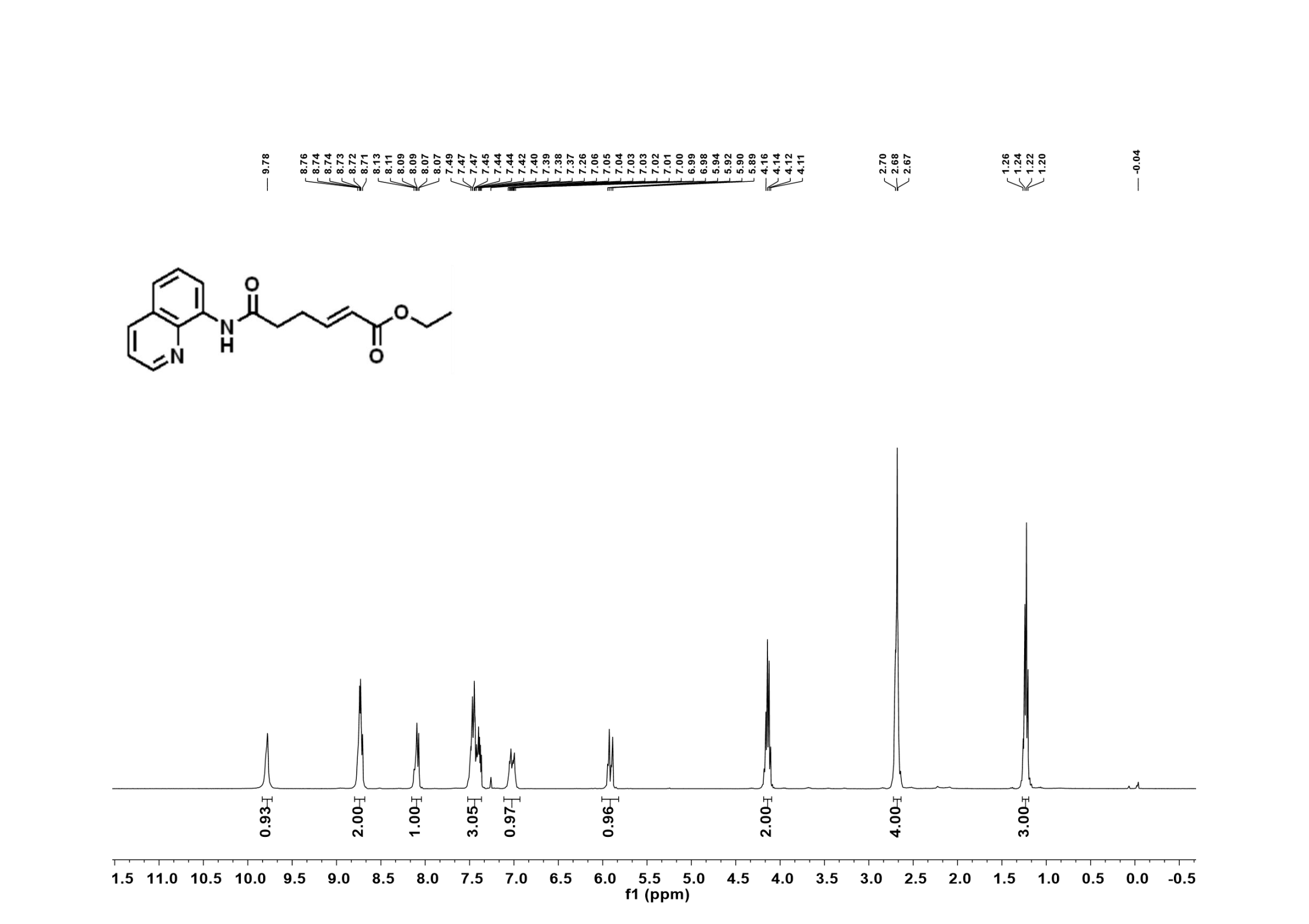
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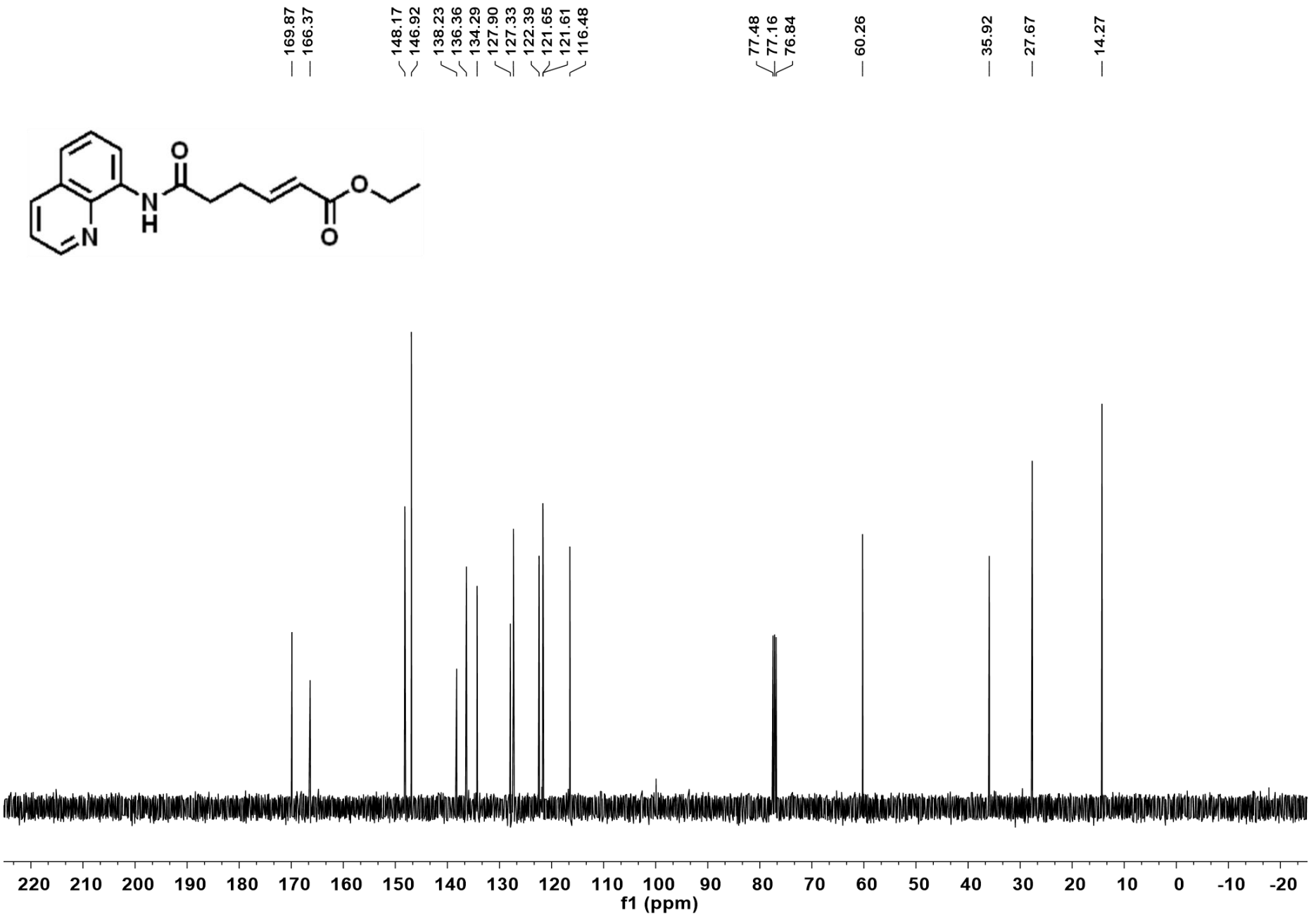
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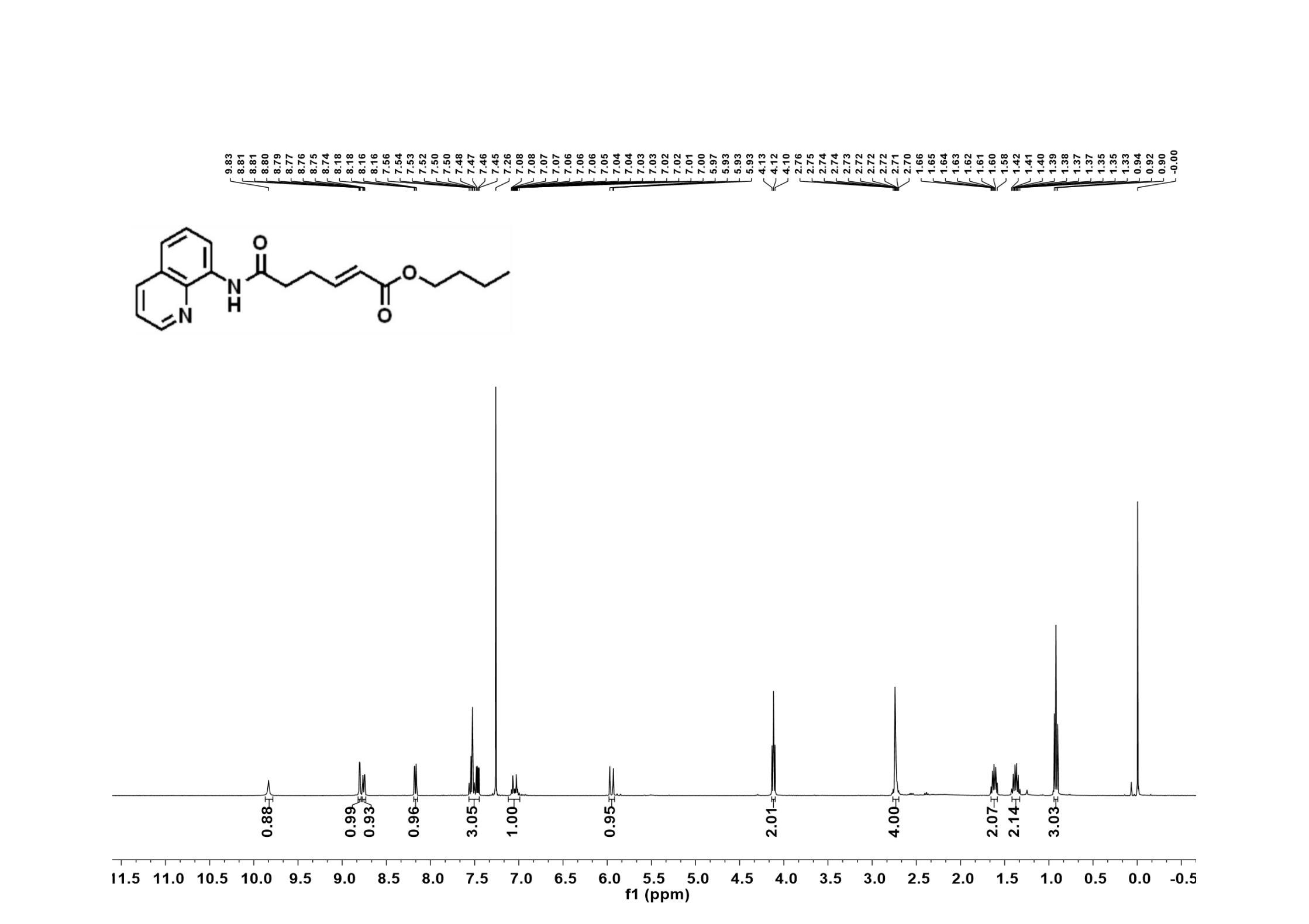
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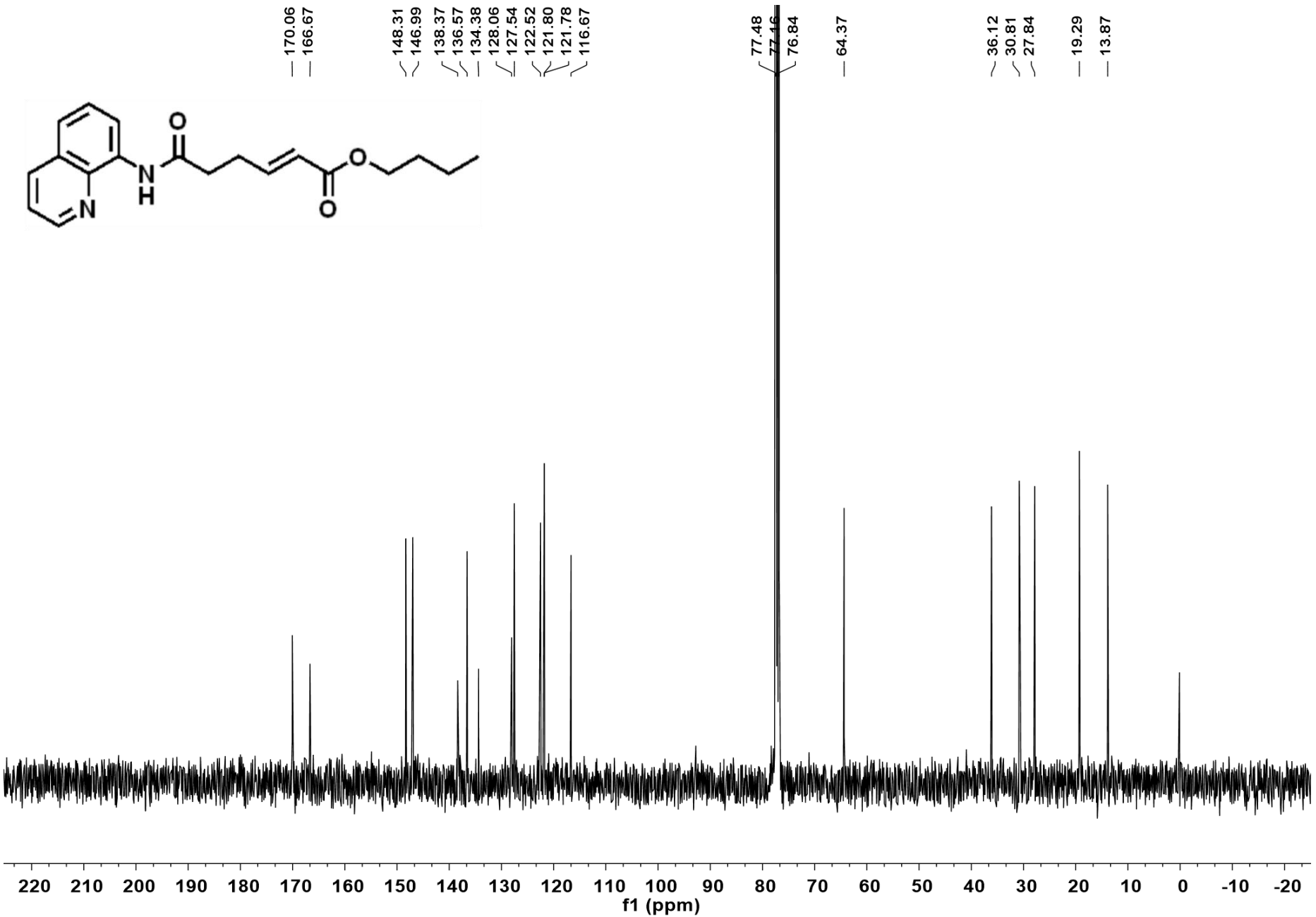
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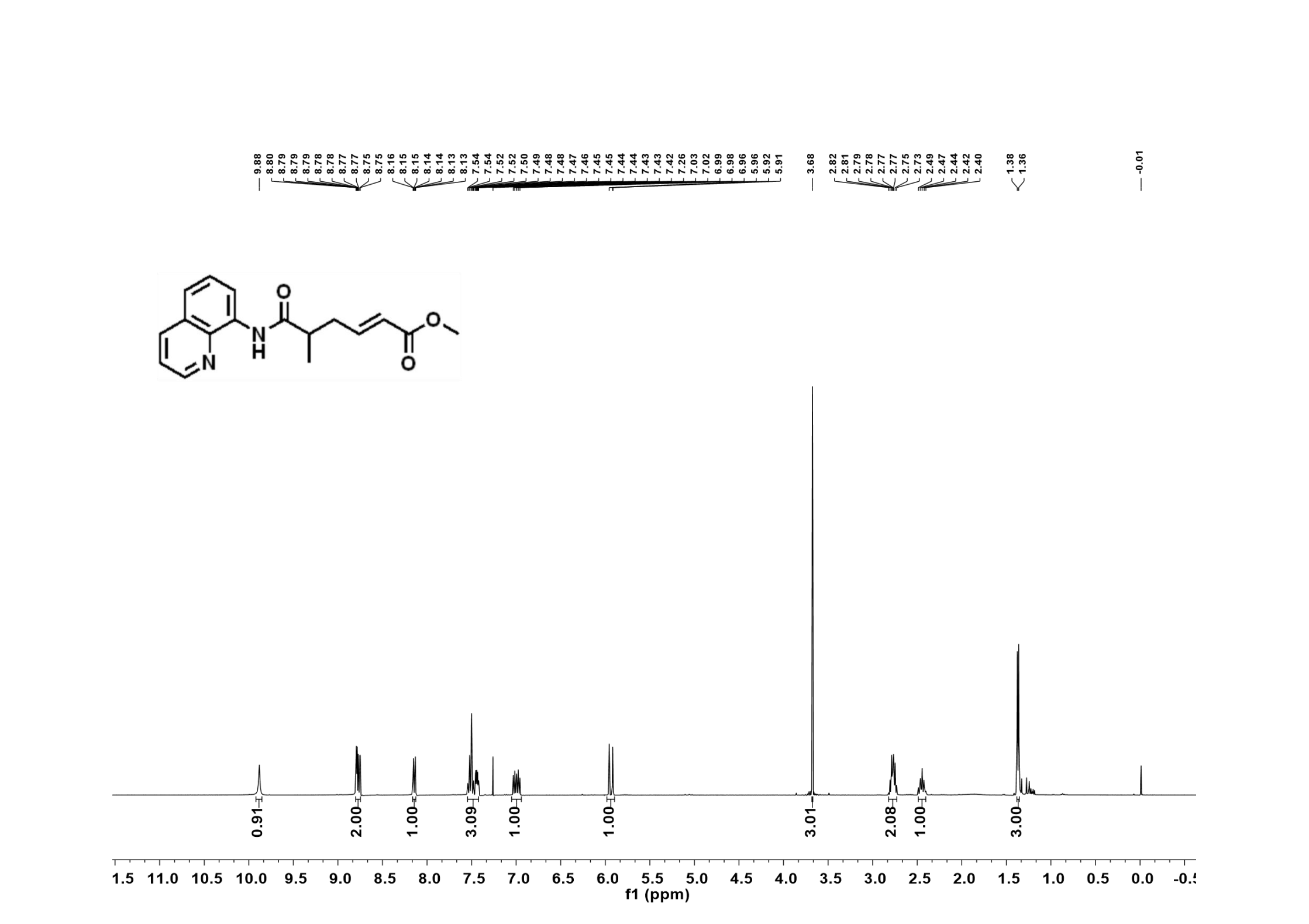
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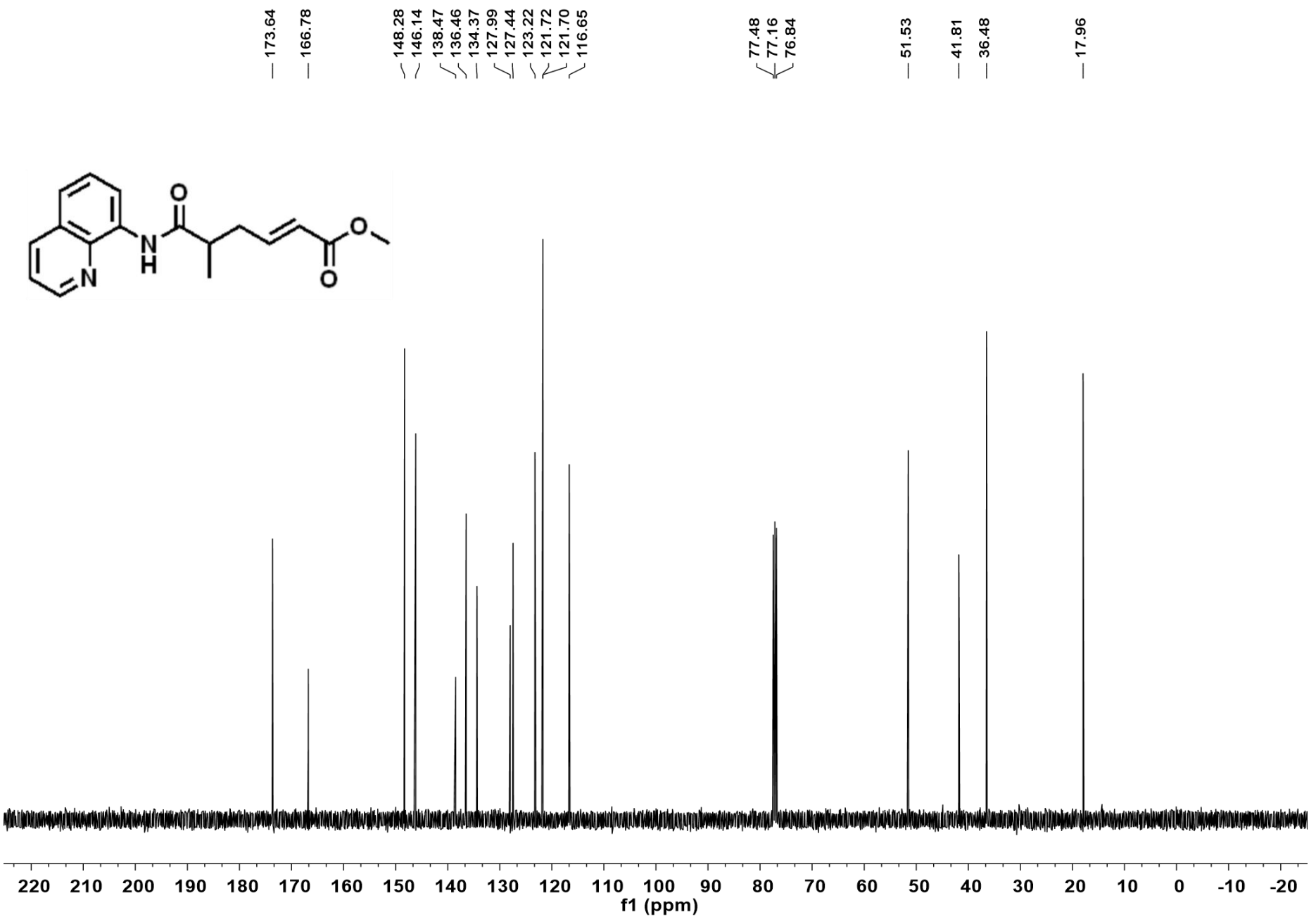
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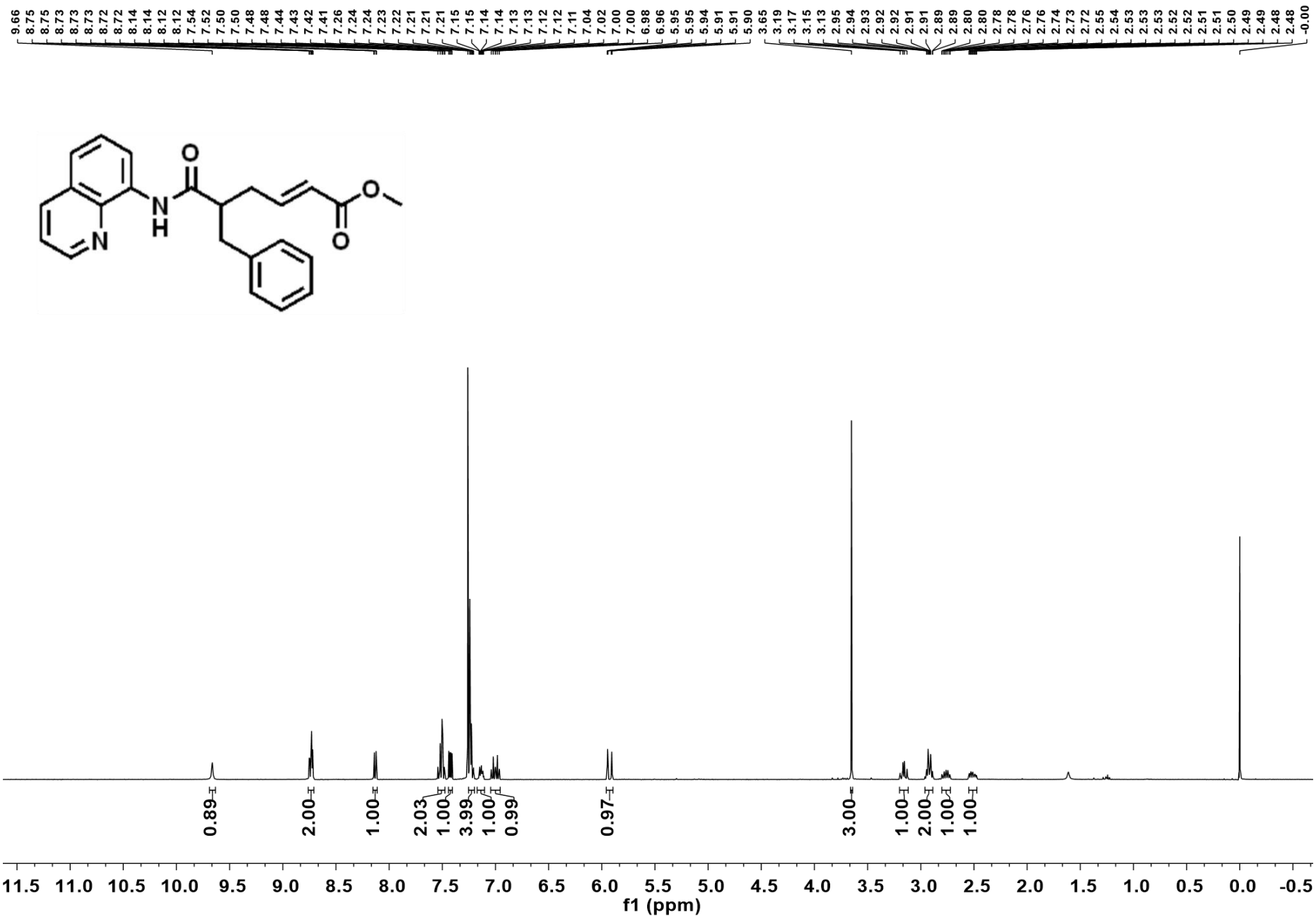
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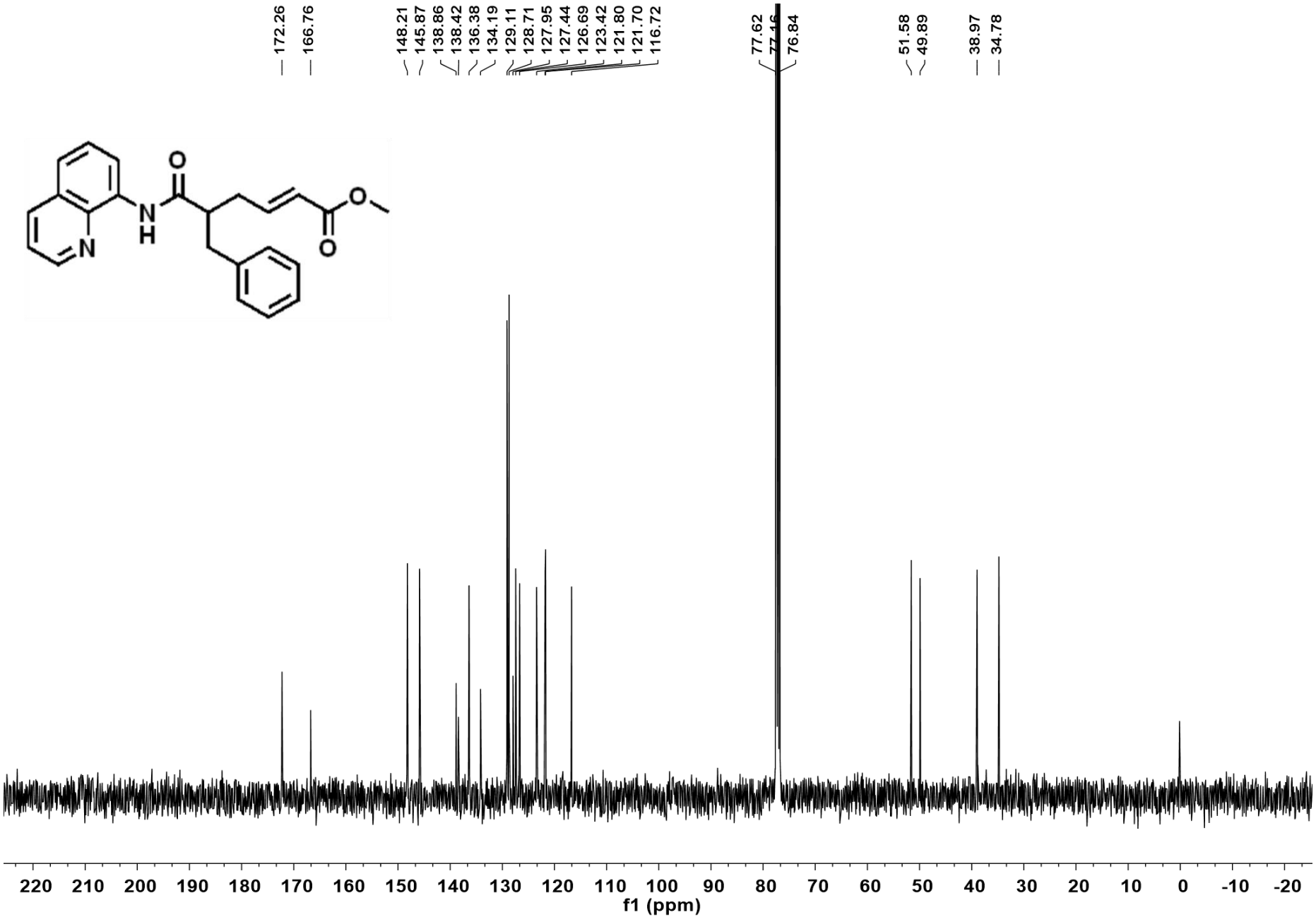
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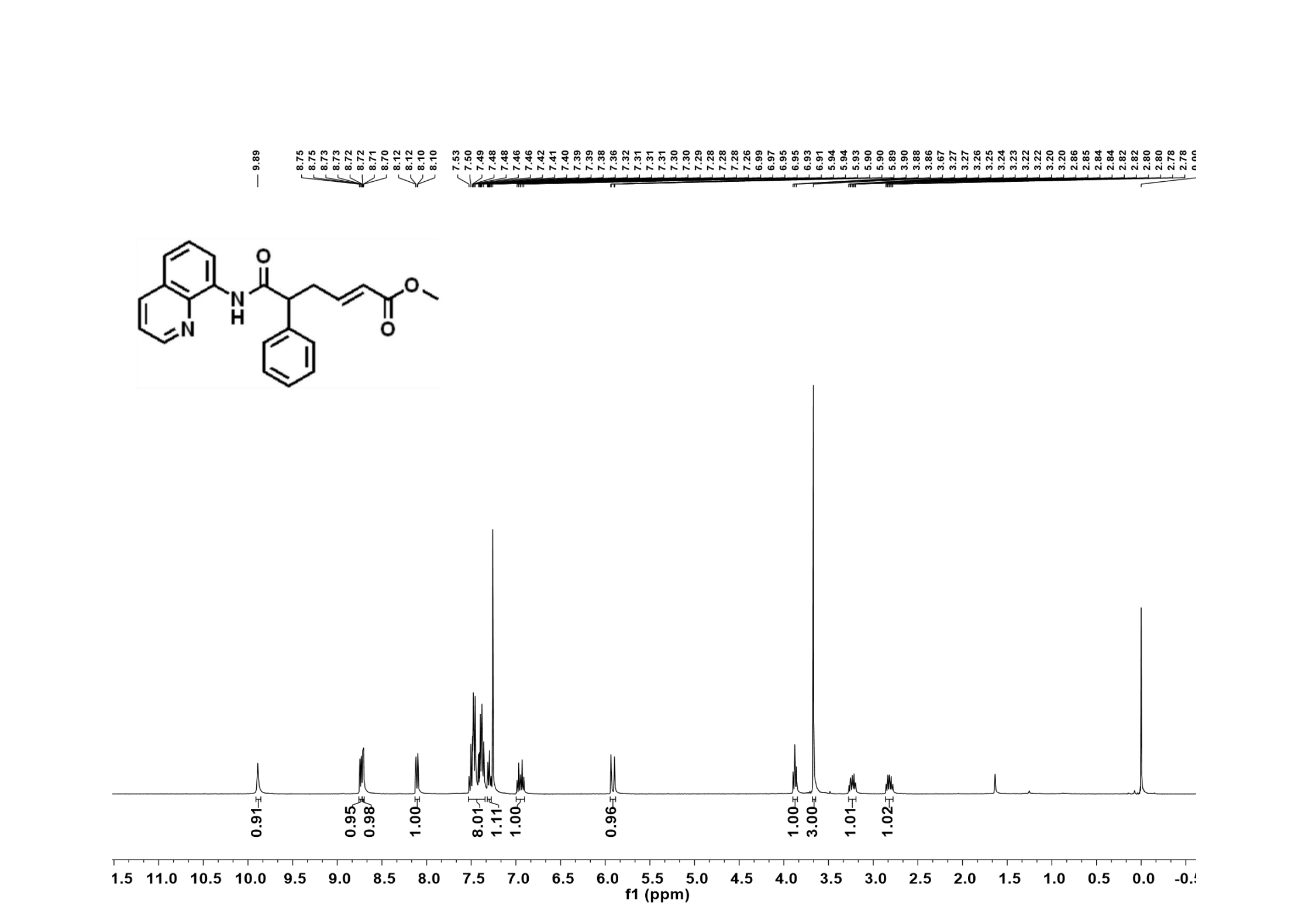
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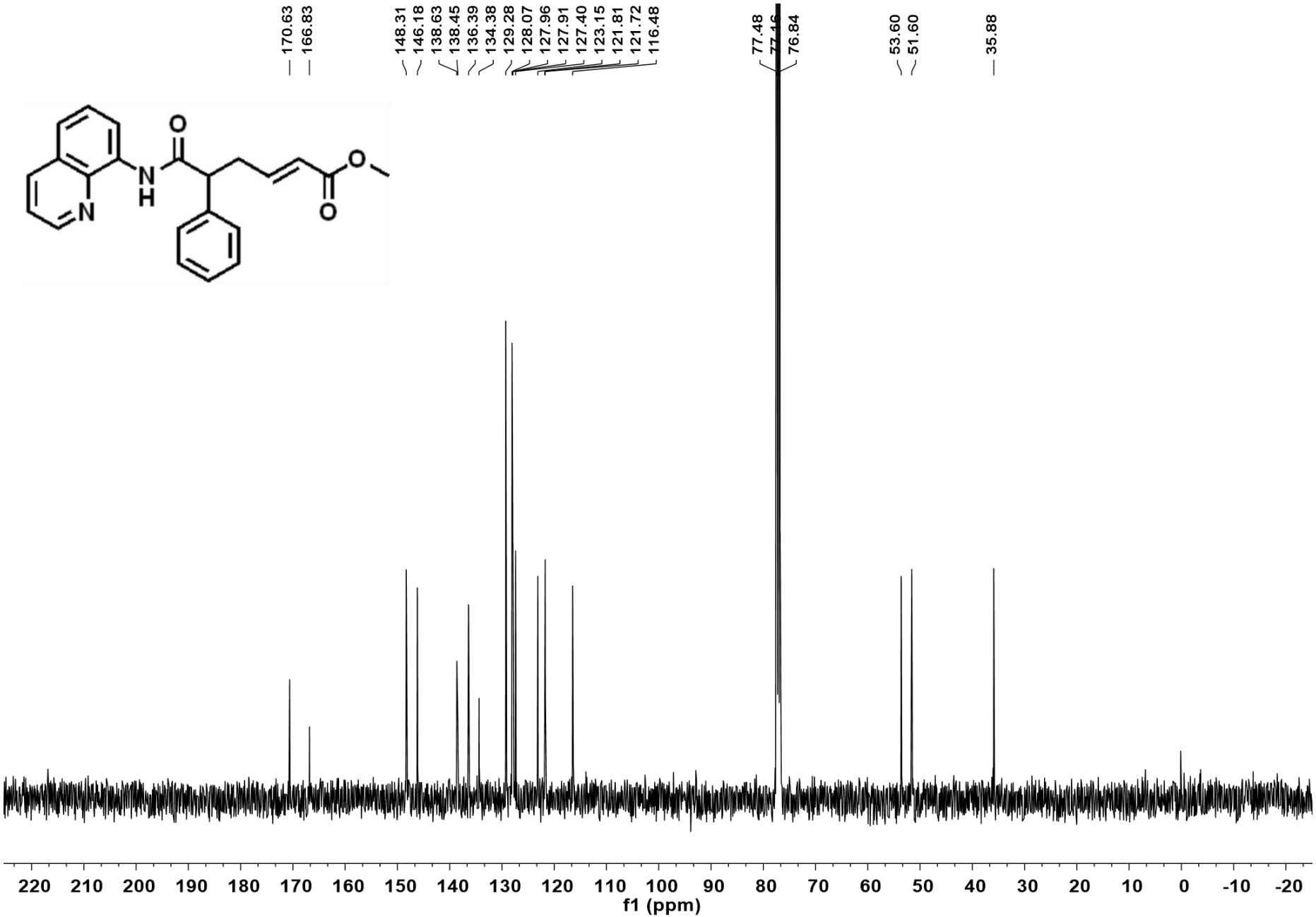
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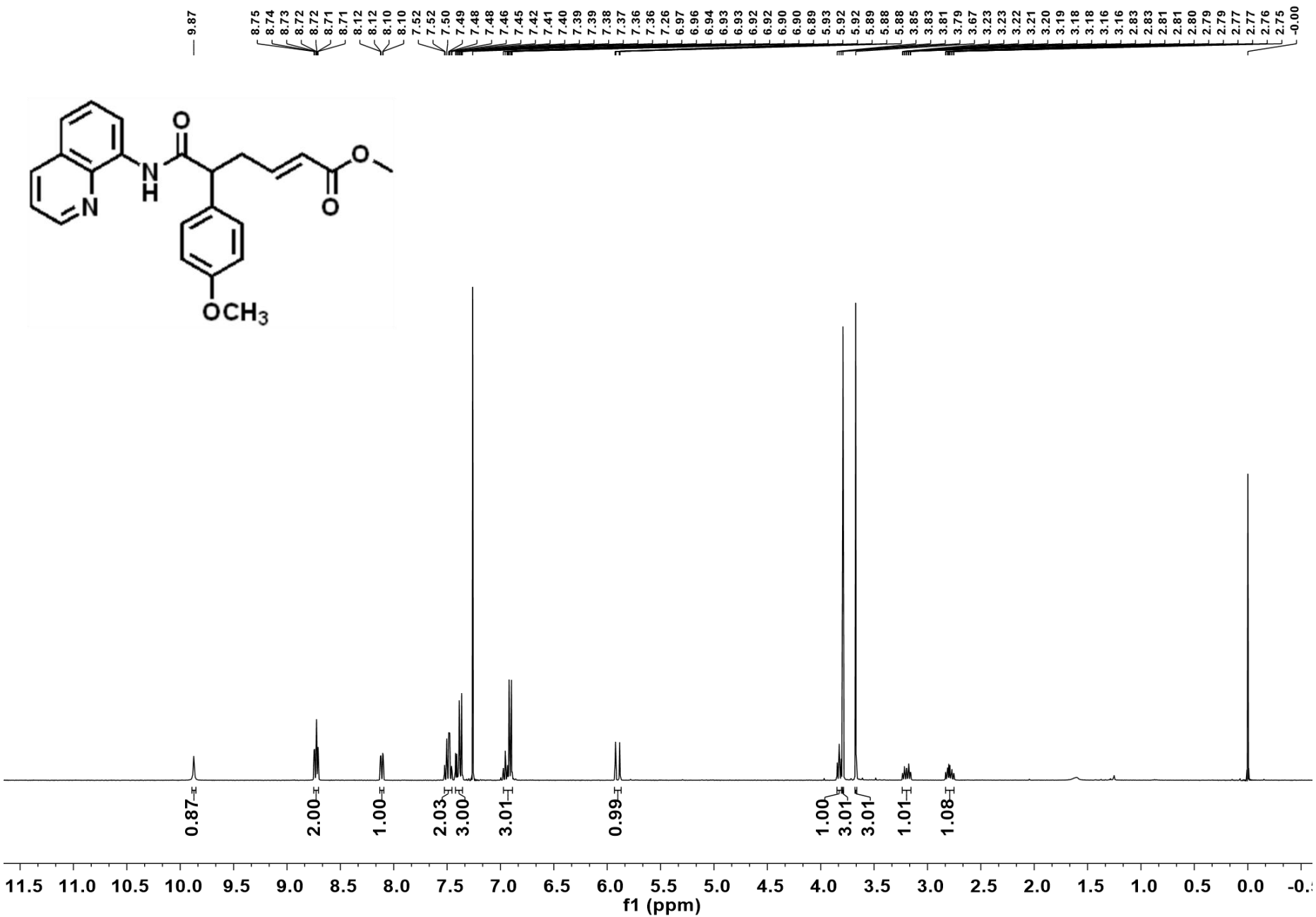
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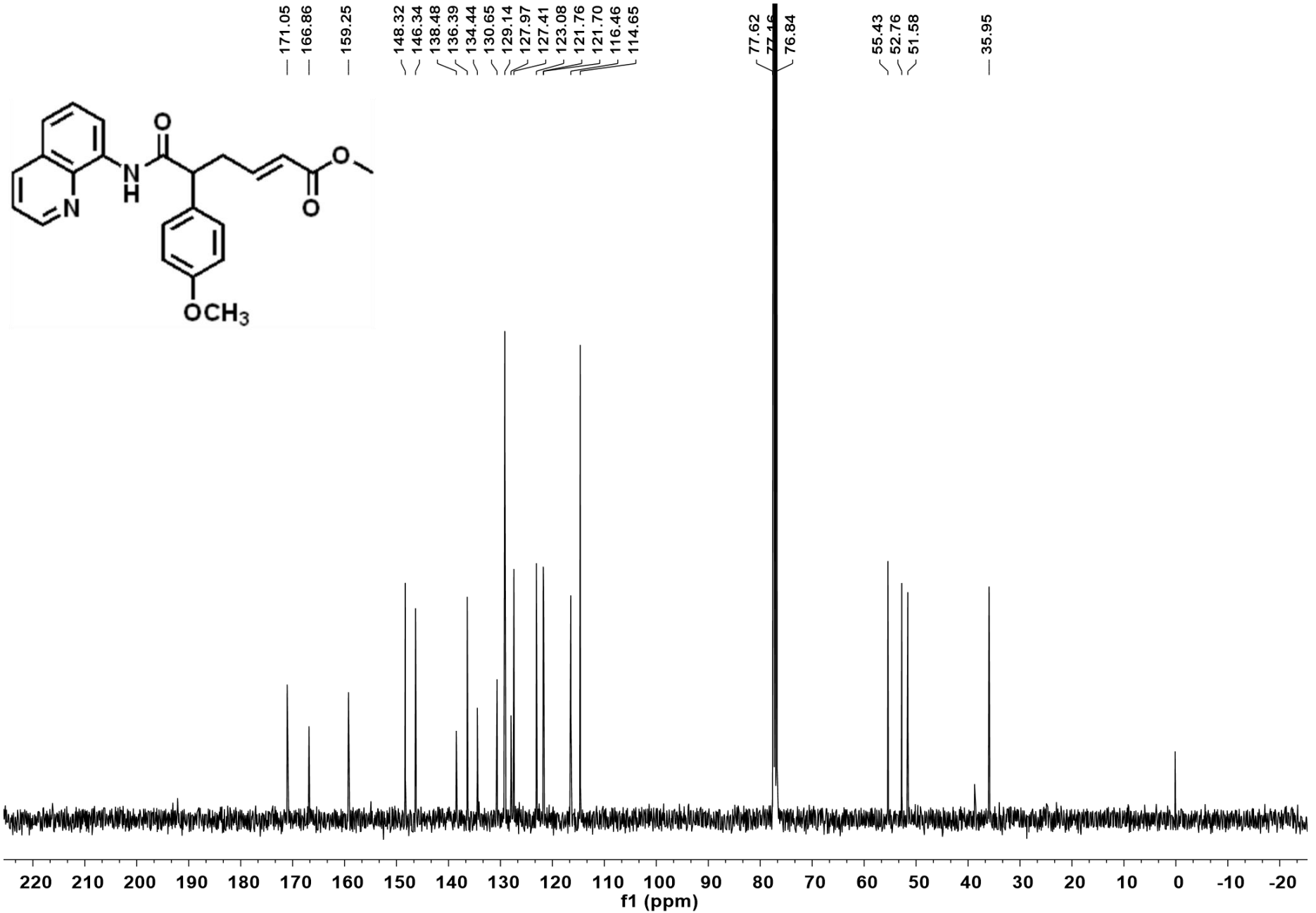
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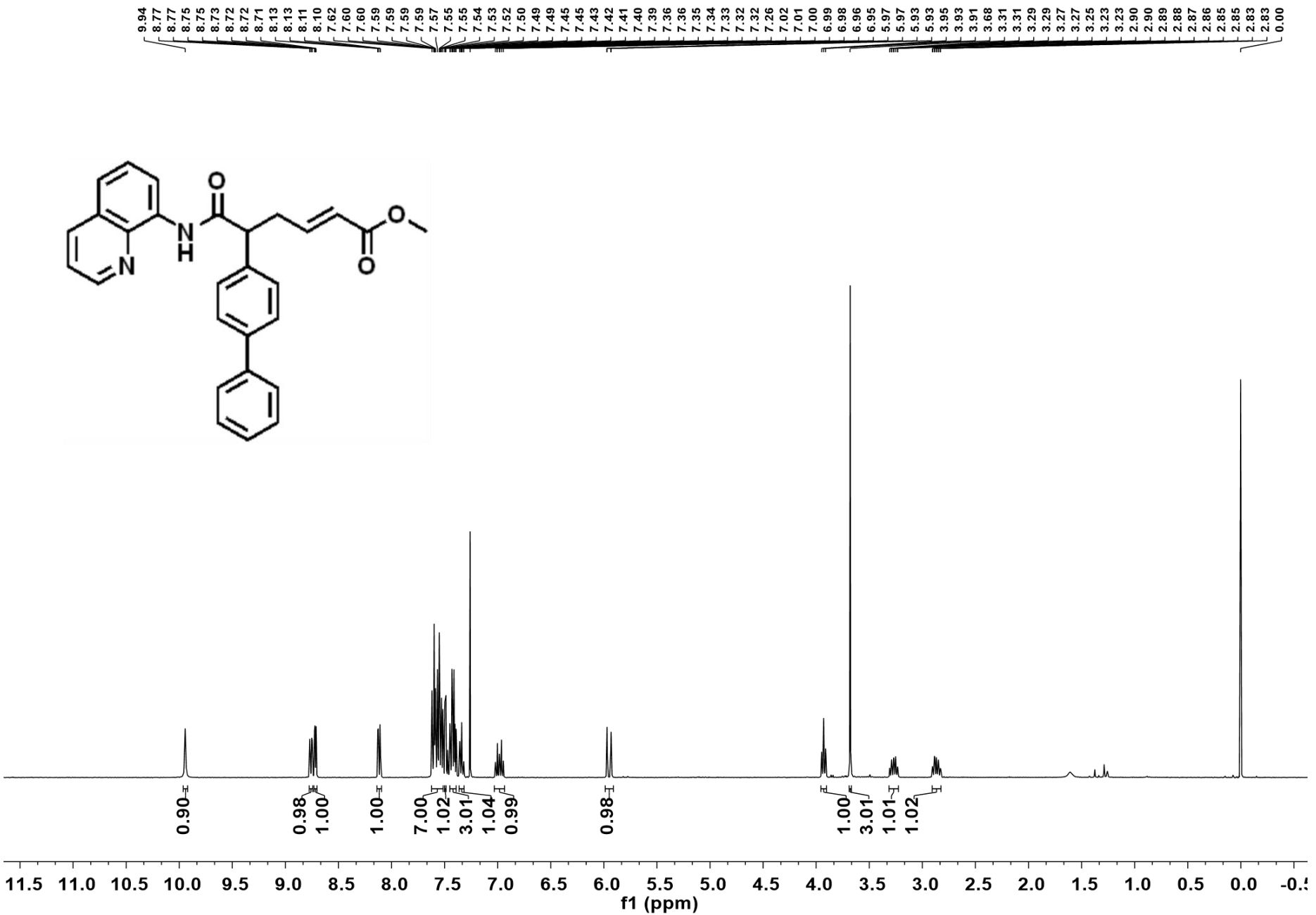
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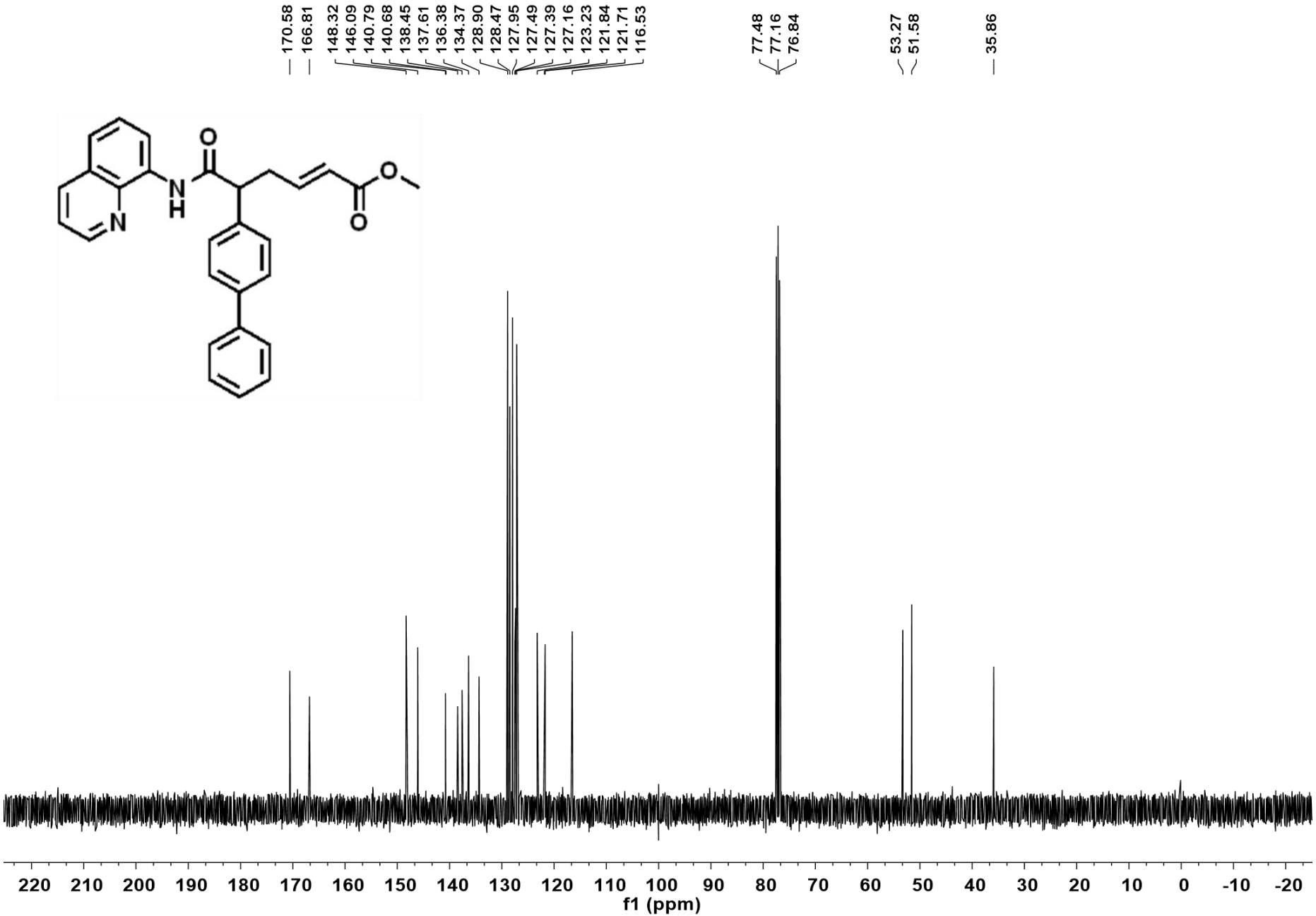
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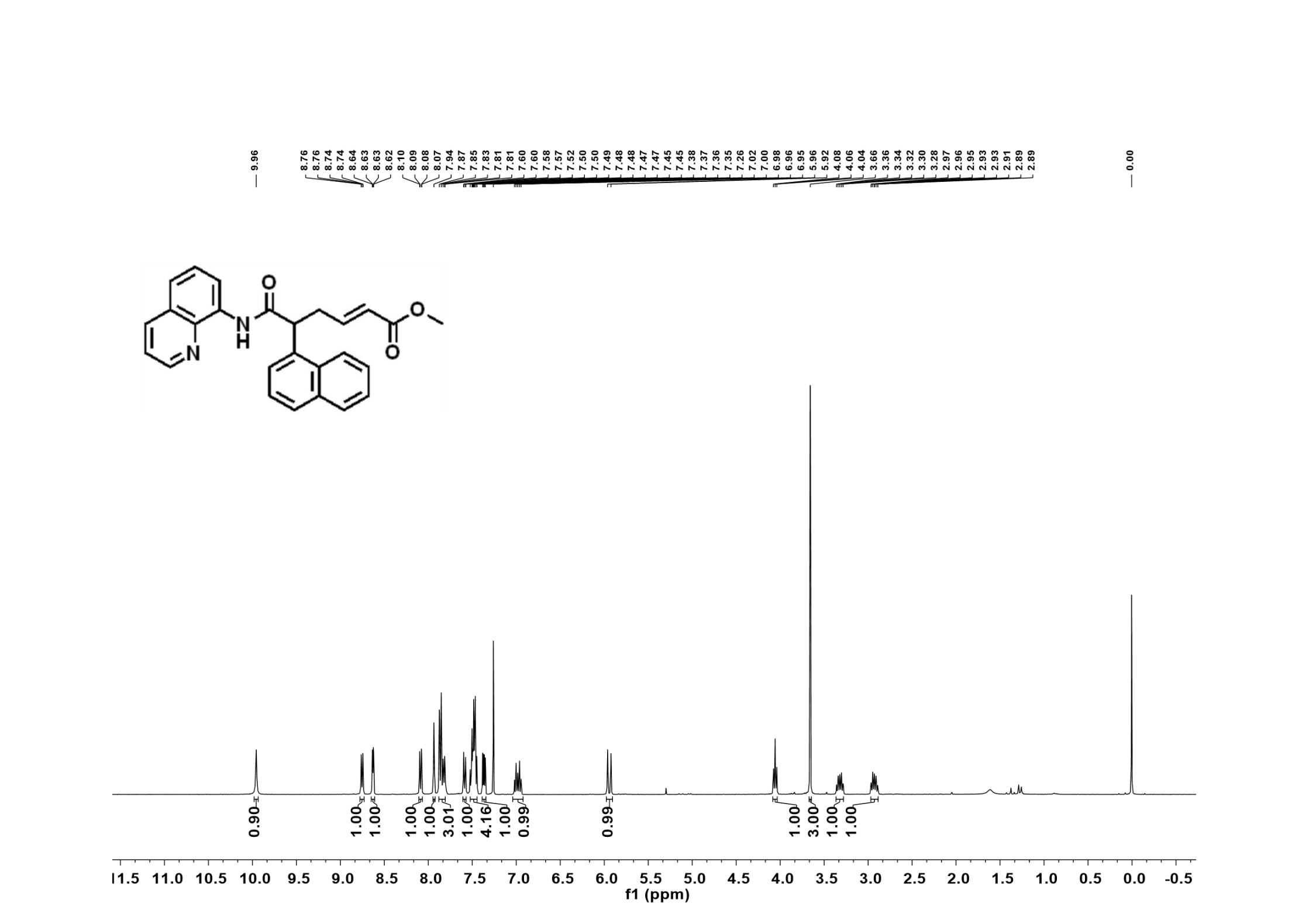
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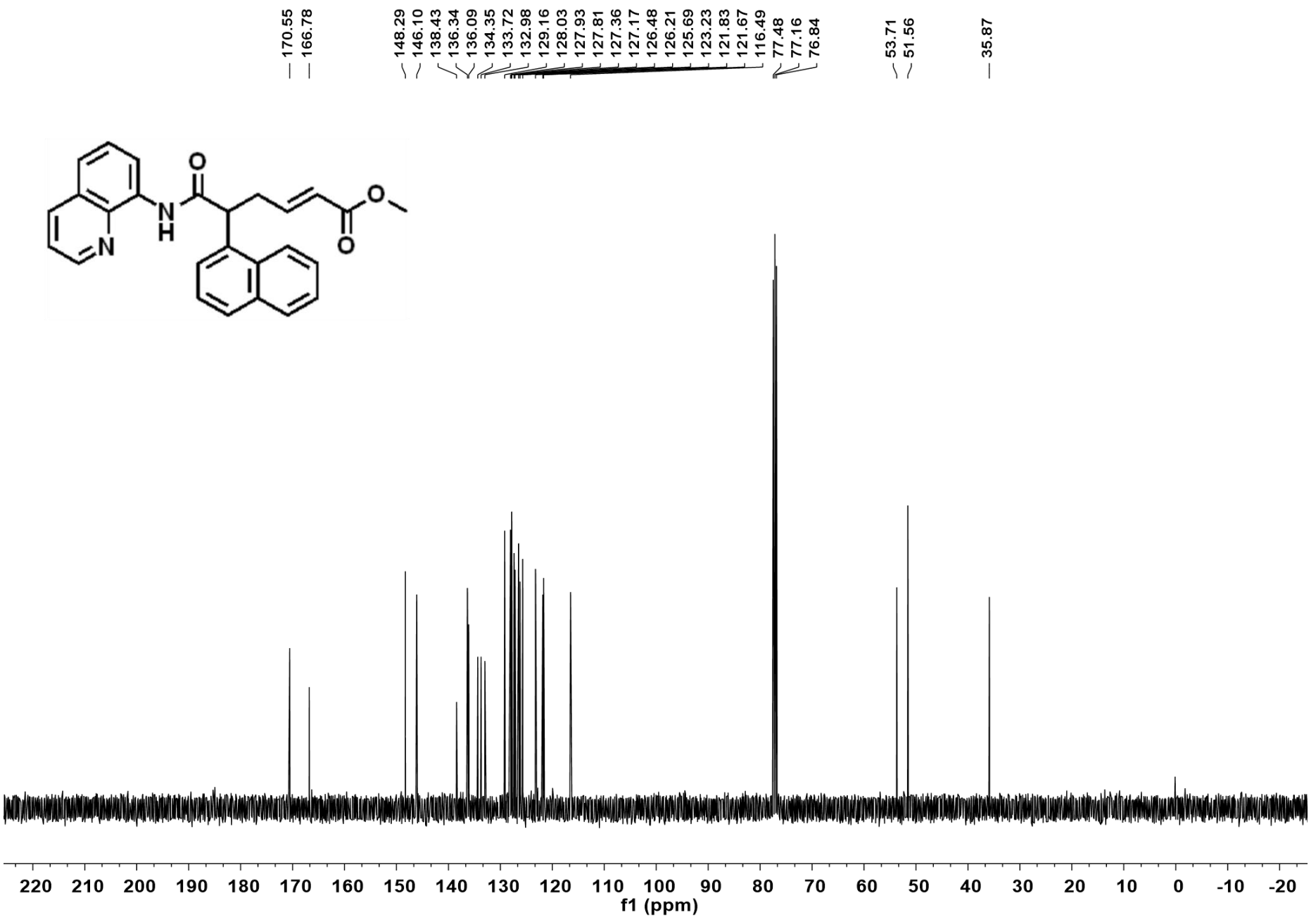
f1 (ppm)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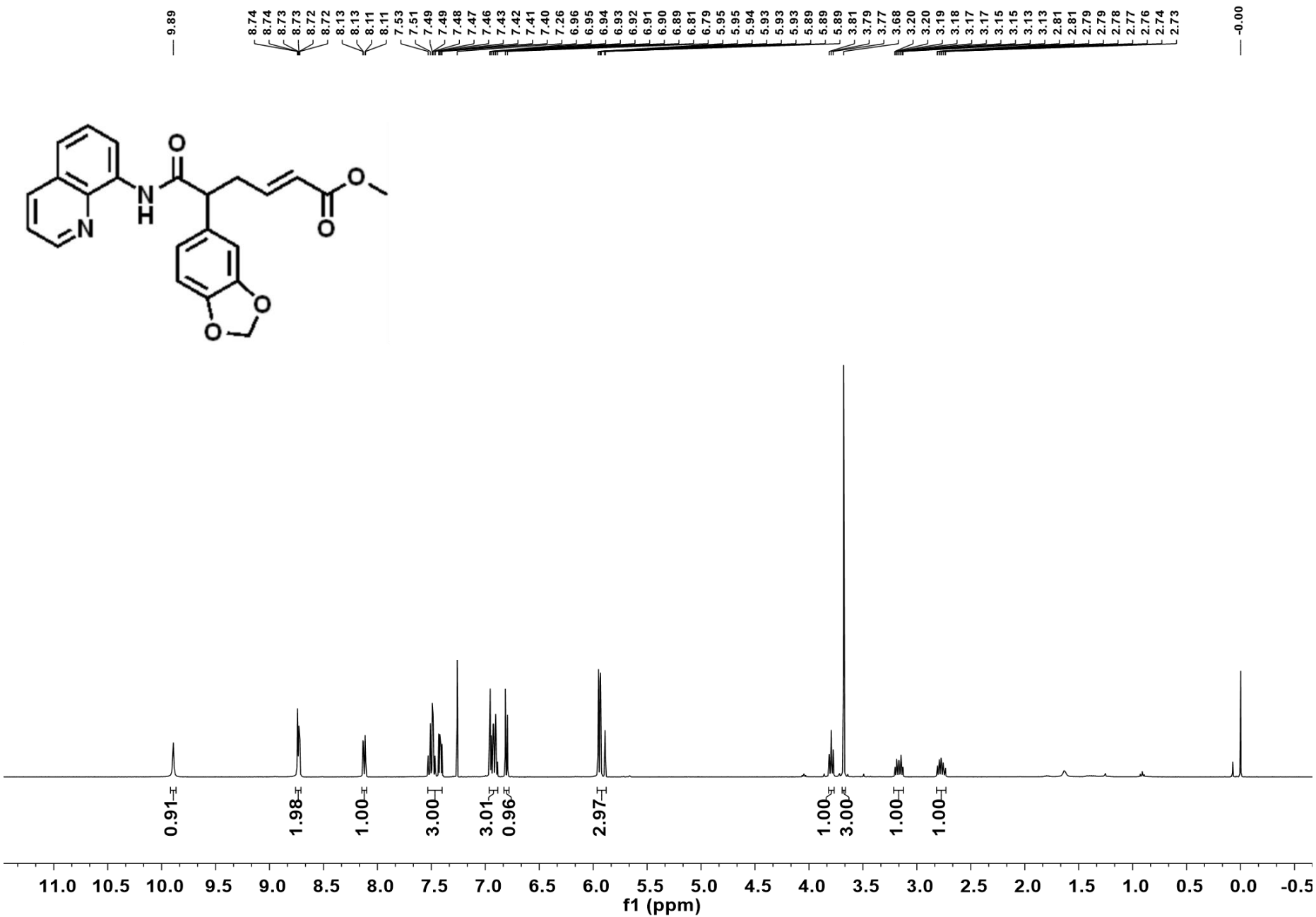
f1 (ppm)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3.13
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2.79
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2.76
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2.73
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O
O
O
O
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1.00
3.00
3.01
0.96
2.97
1.00
3.00
1.00
1.00
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10.0
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9.0
8.5
8.0
7.5
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6.5
6.0
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5.0
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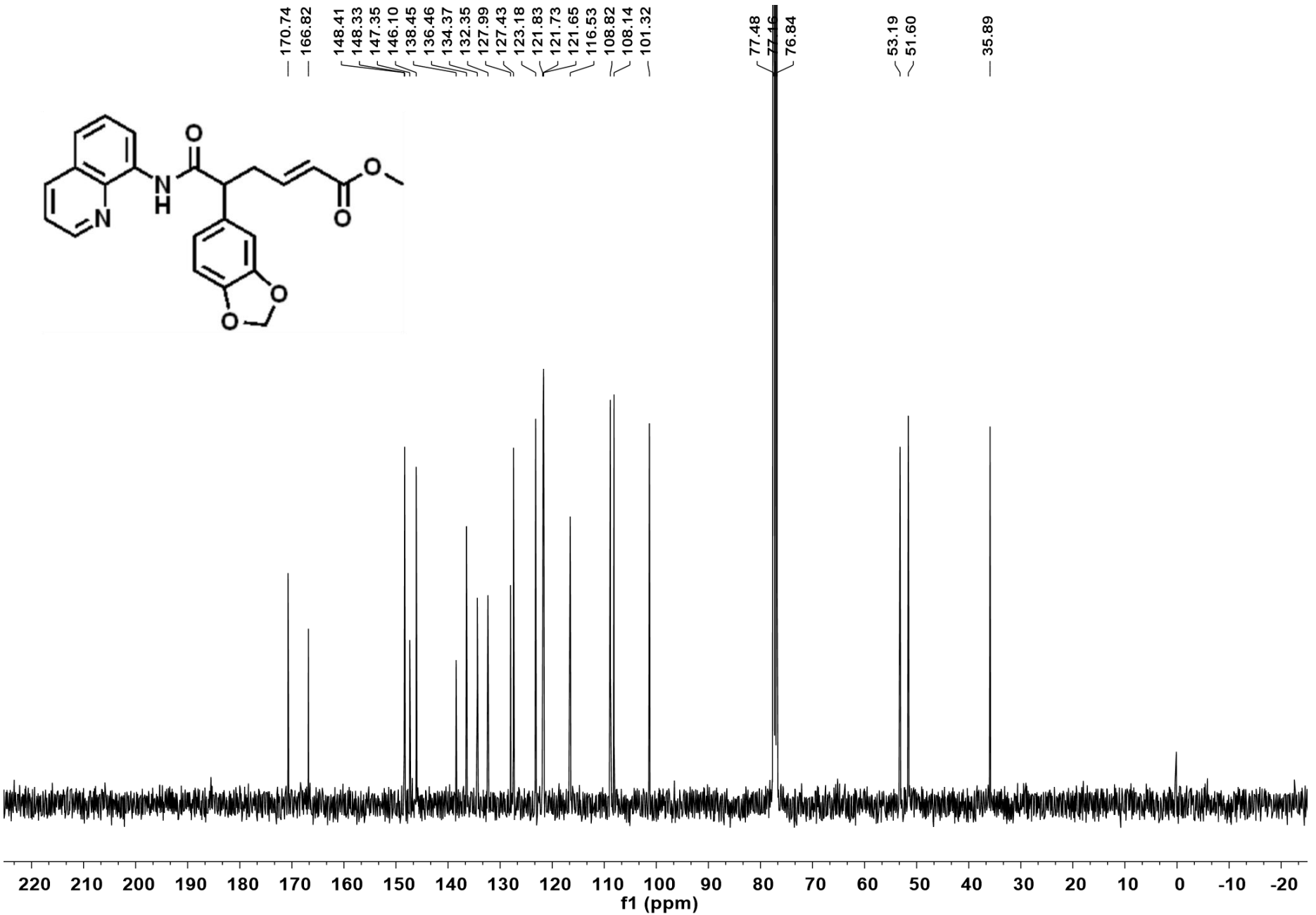
-0.5
f1 (ppm)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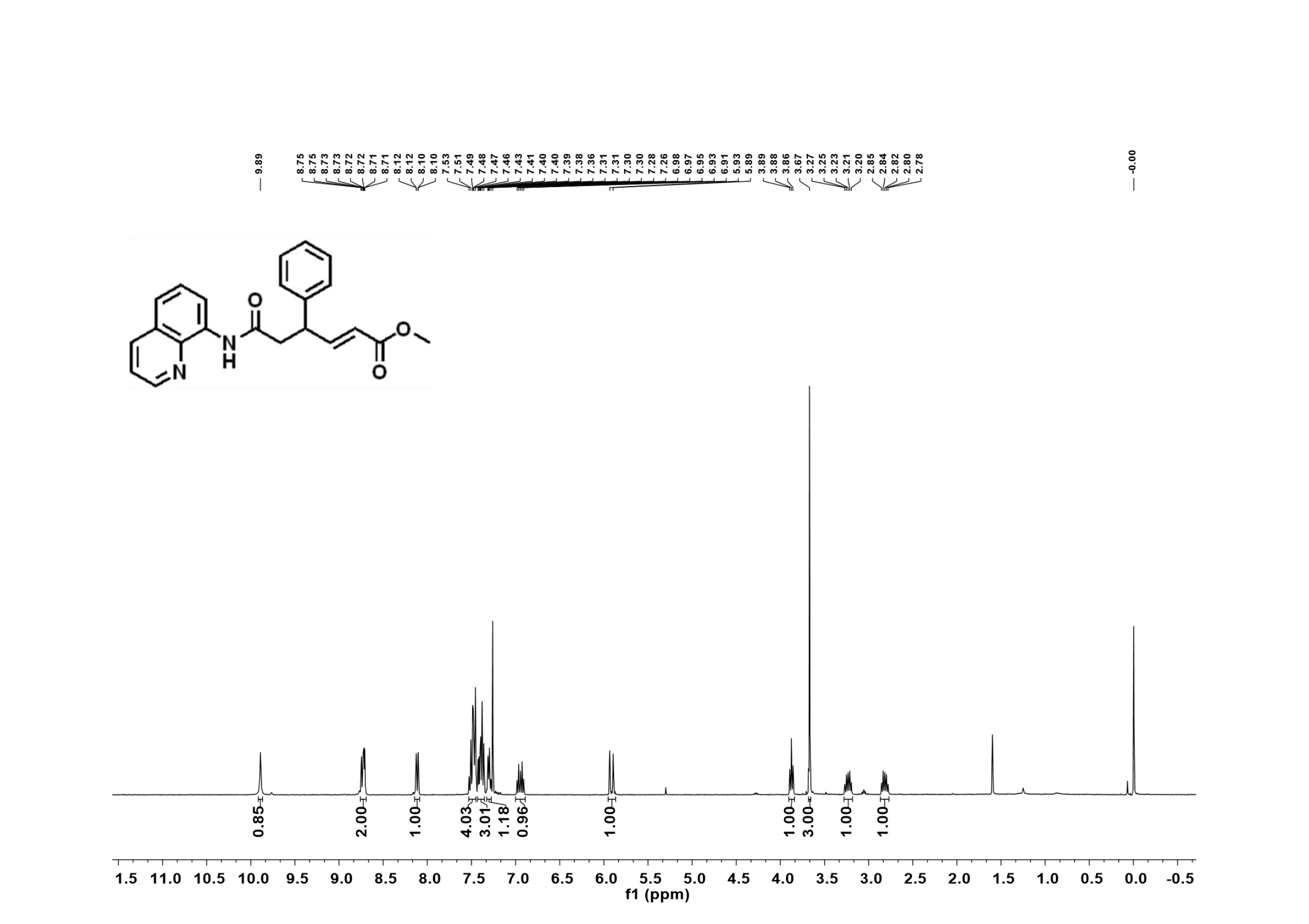
f1 (ppm)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2.78
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H
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O
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2.00
1.00
4.03
3.01
1.18
0.96
1.00
1.00
3.00
1.00
1.00
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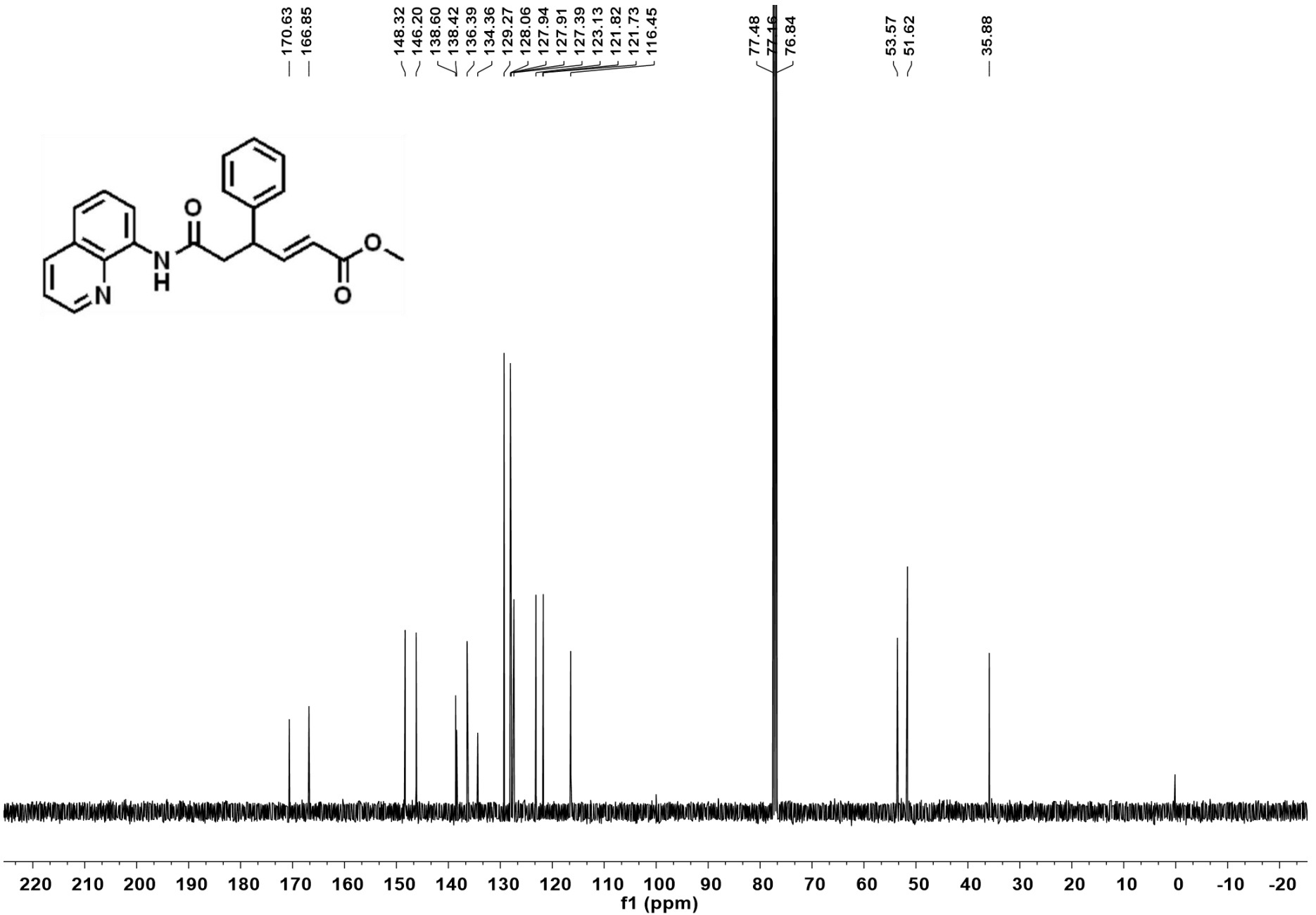
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121.73
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76.84
53.57
51.62
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H
N
O
O
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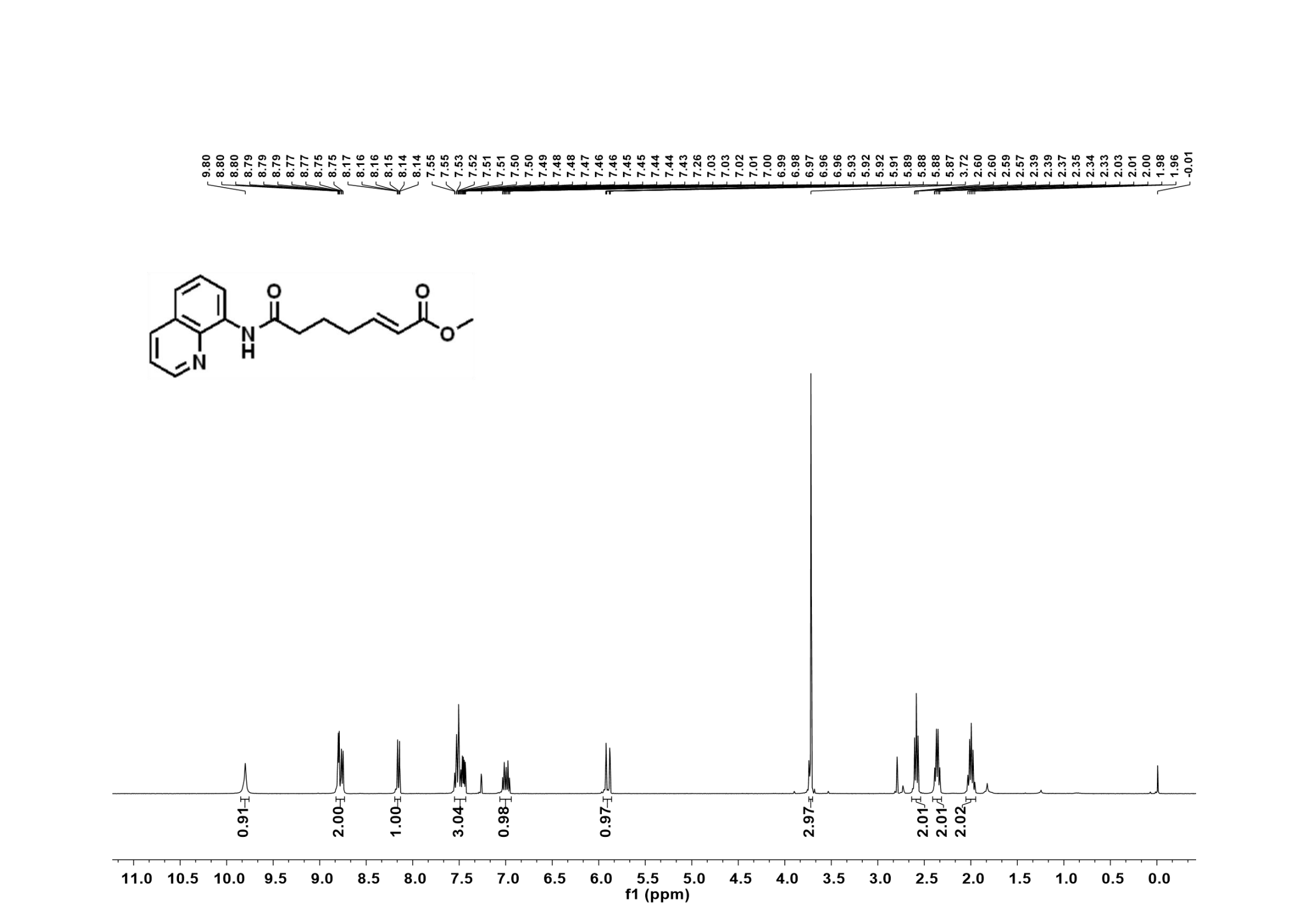
f1 (ppm)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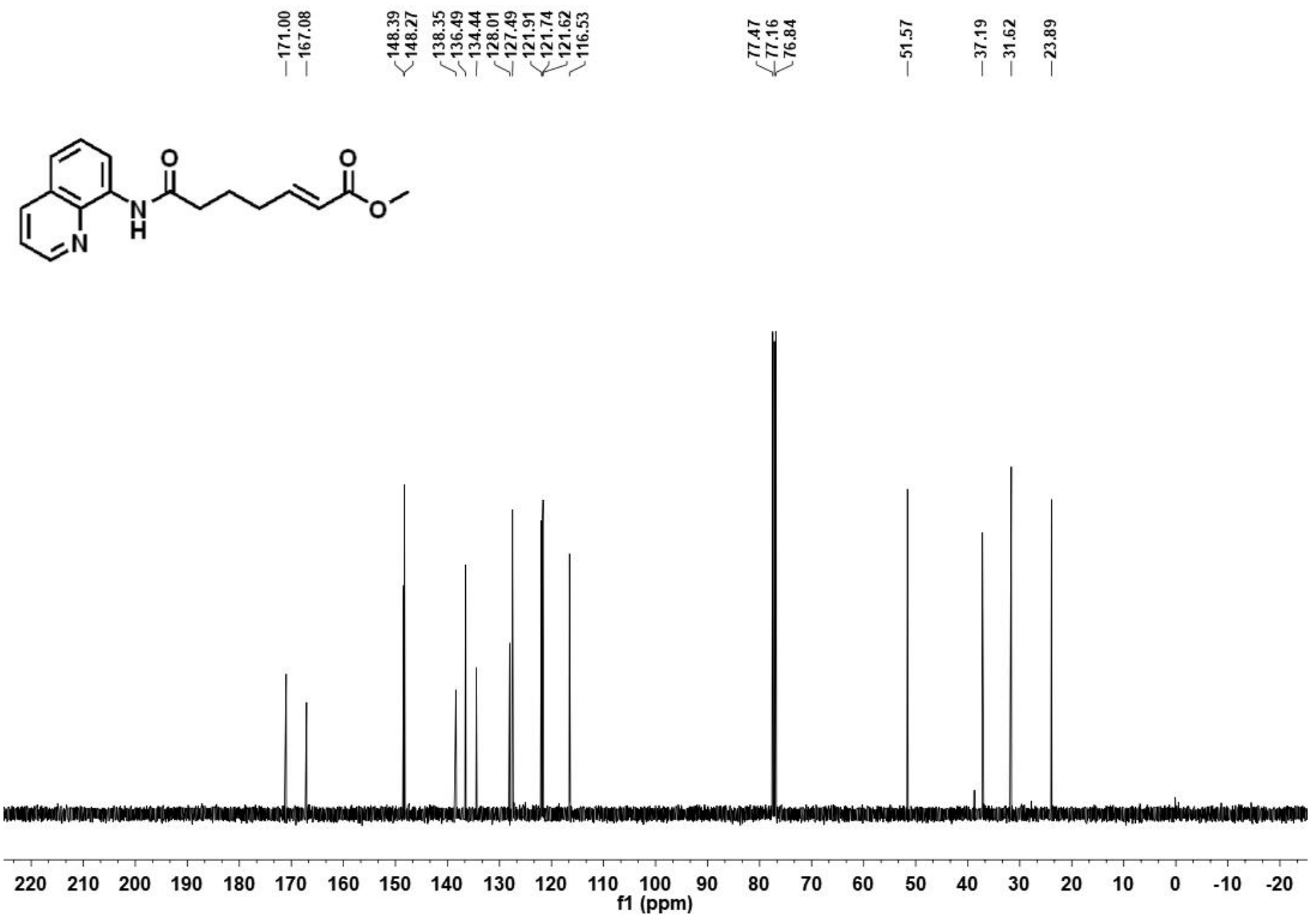
7.55 7.55 7.53 7.52 7.51 7.51 7.50 7.50 7.49 7.48 7.48 7.47 7.46 7.46 7.45 7.45 7.44 7.44 7.43 7.26 7.03 7.03 7.02 7.01 7.00 6.99 6.98 6.97 6.96 6.96 5.93 5.92 5.92 5.91 5.89 5.88 5.88 5.87 3.72 2.60 2.60 2.59 2.57 2.39 2.39 2.37 2.35 2.34 2.33 2.03 2.01 2.00 1.98 1.96 -0.01
O
O
N
H
N
0.91
2.00
1.00
3.04
0.98
0.97
2.97
2.01
2.01
2.02
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)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51.57
37.19
31.62
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N
H
N
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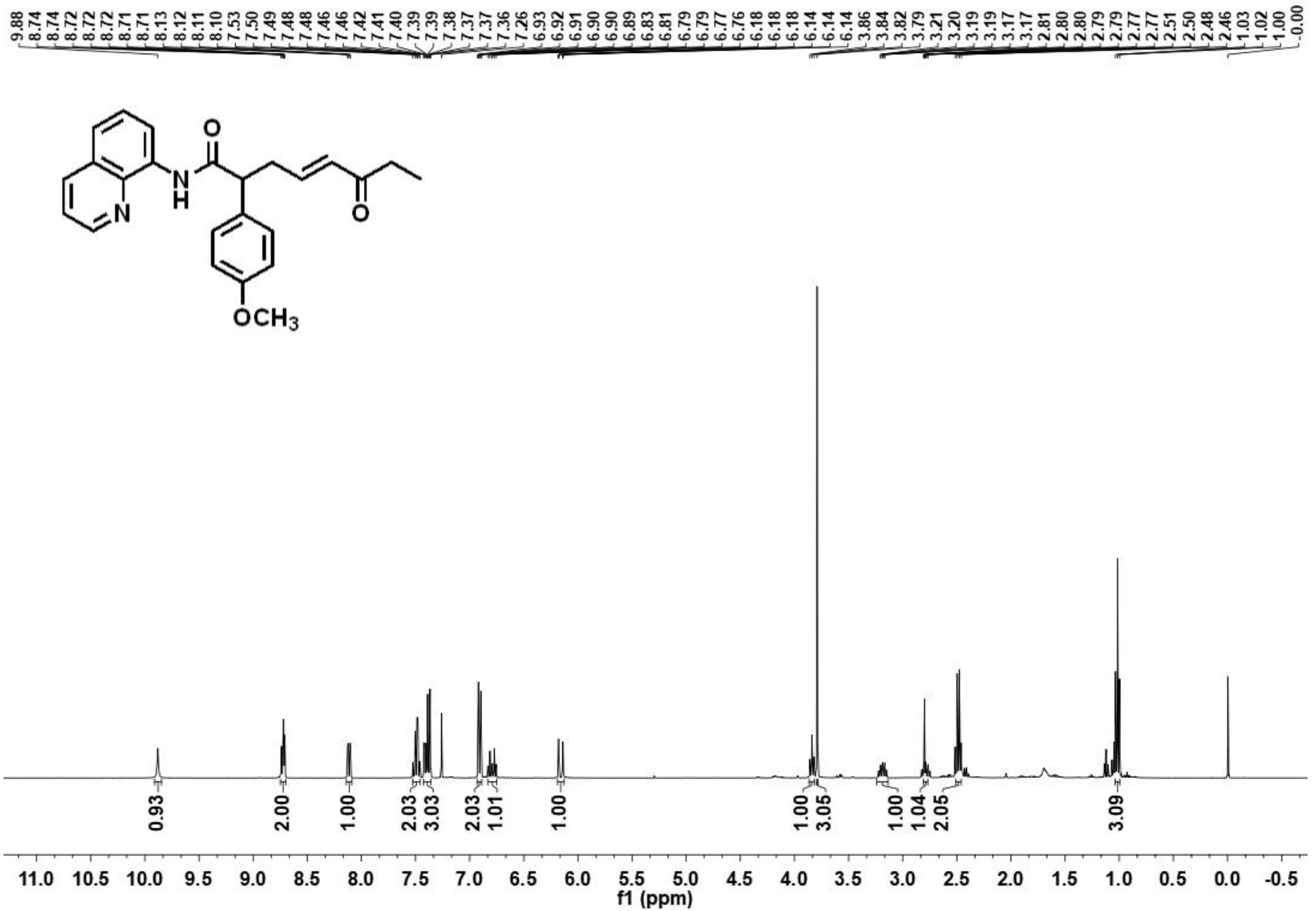
f1 (ppm)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6.18
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3.84
3.82
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3.19
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2.80
2.79
2.79
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2.51
2.50
2.48
2.46
1.03
1.02
1.00
-0.00
O
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H
N
O
OCH3
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1.00
2.03
3.03
2.03
1.01
1.00
1.00
3.05
1.00
1.04
2.05
3.09
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10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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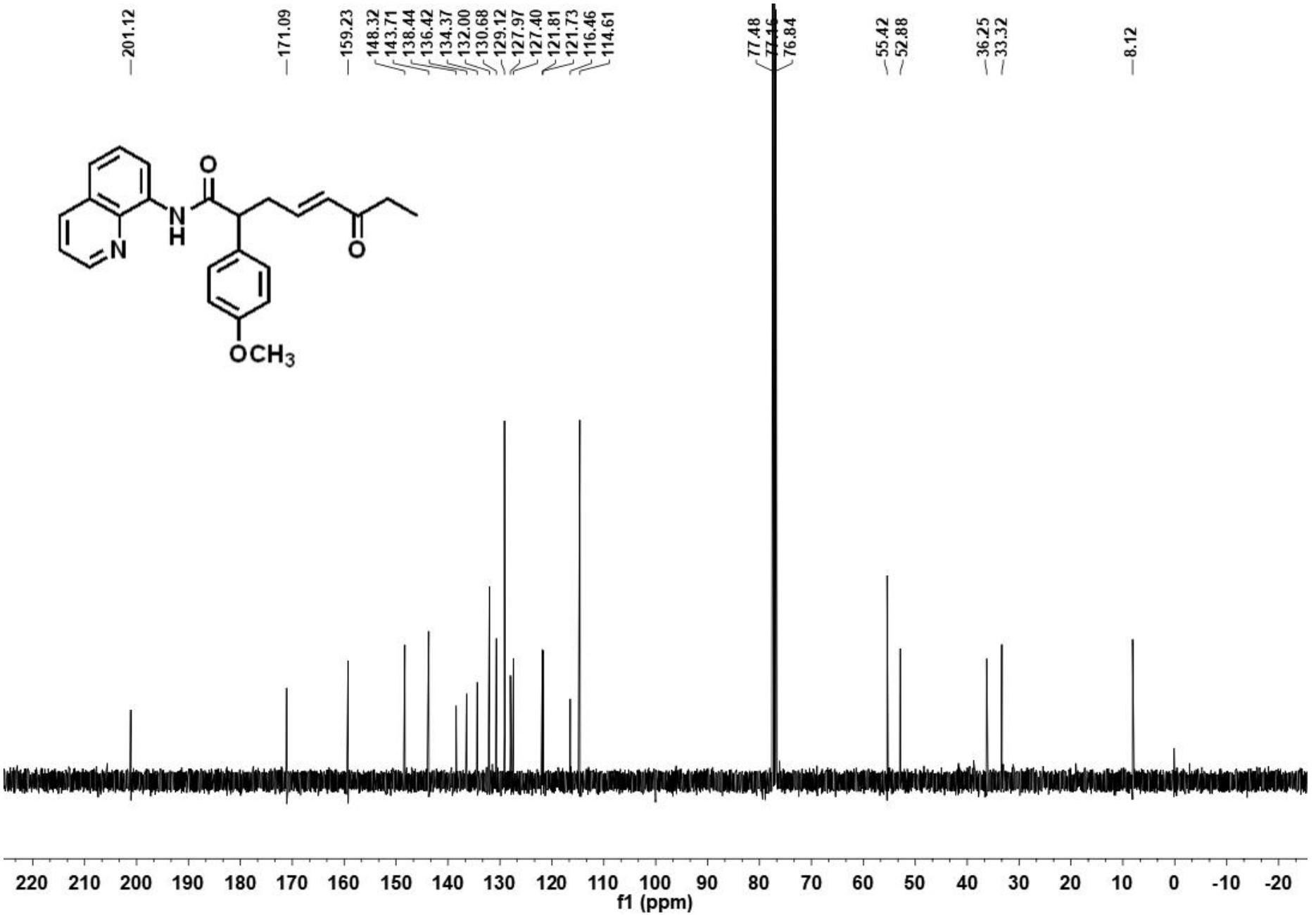
-0.5
f1 (ppm)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127.40
121.81
121.73
116.46
114.61
77.48
77.16
76.84
55.42
52.88
36.25
33.32
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O
OCH3
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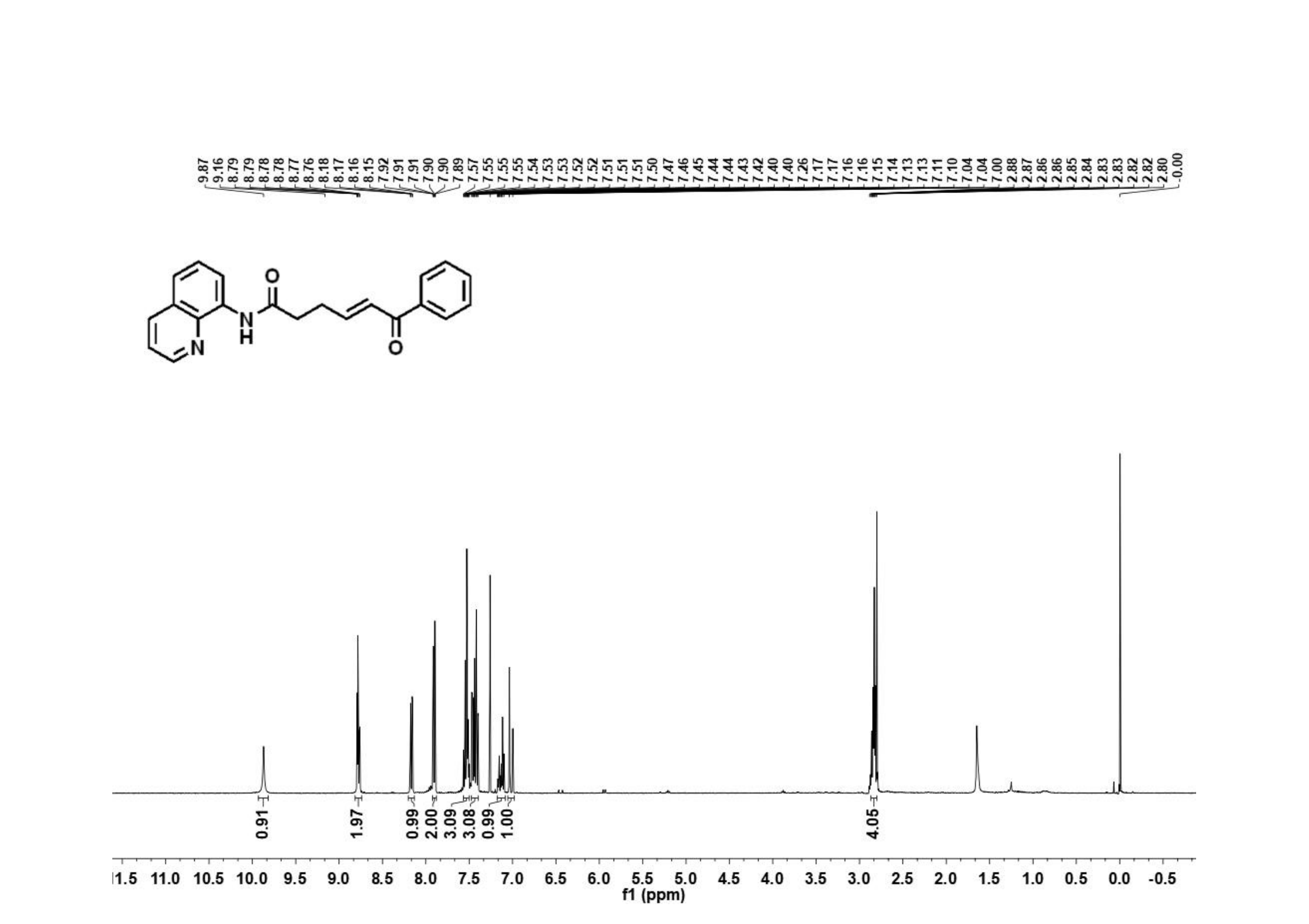
f1 (ppm)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7.11
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7.04
7.00
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2.86
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2.83
2.83
2.82
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2.80
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O
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1.97
0.99
2.00
3.09
3.08
0.99
1.00
4.05
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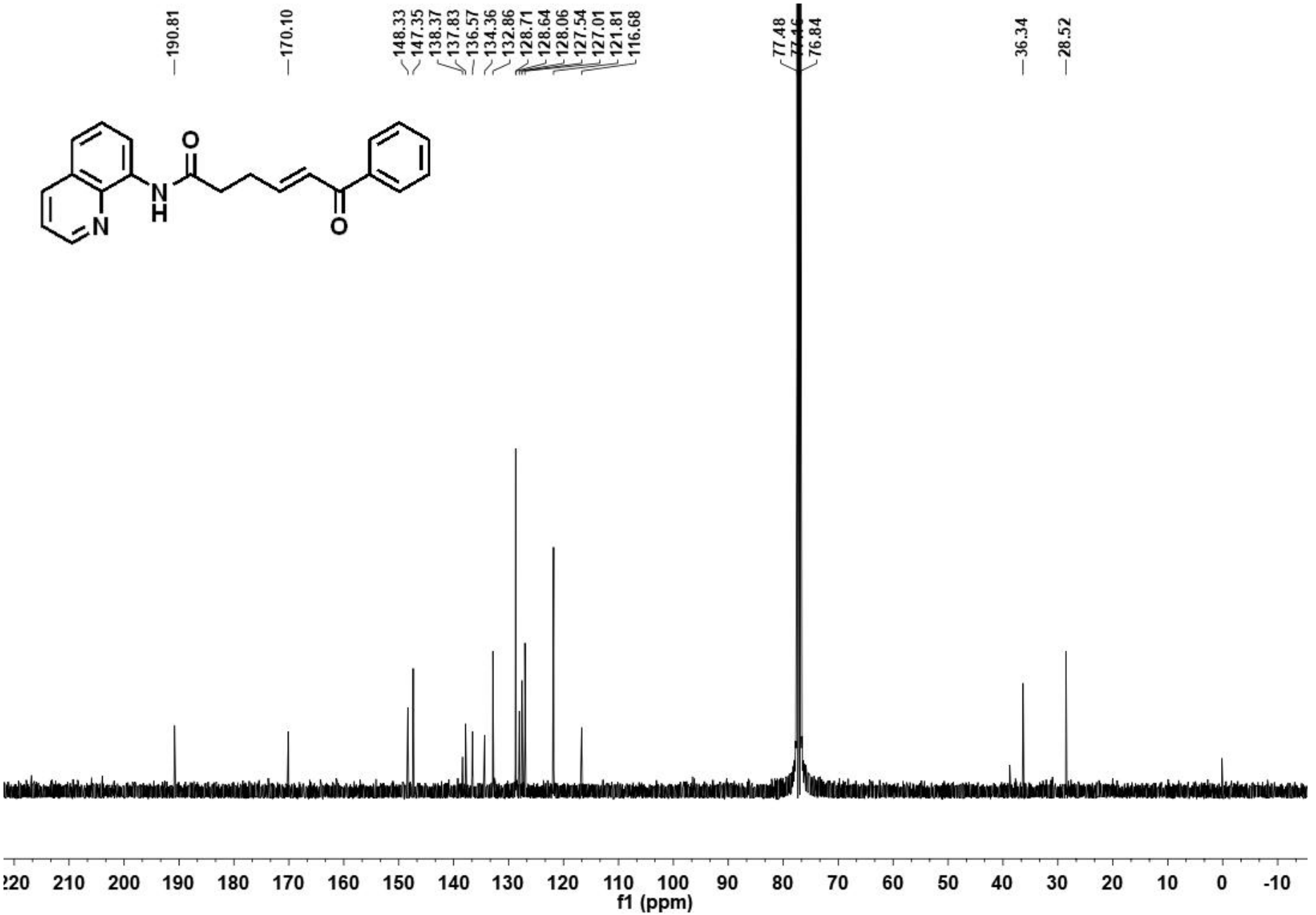
f1 (ppm)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127.54
127.01
121.81
116.68
77.48
76.84
36.34
28.52
O
N
H
N
O
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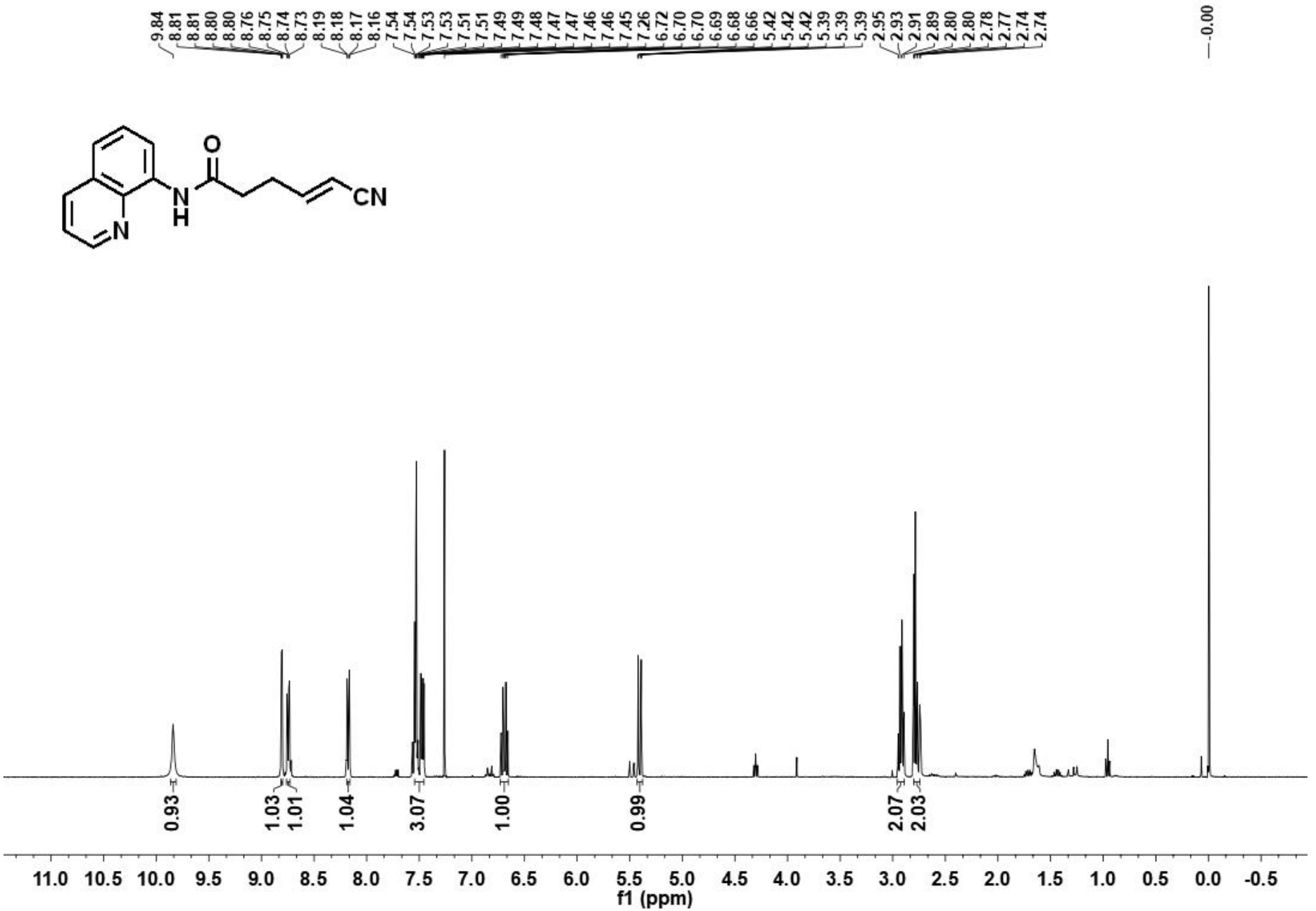
f1 (ppm)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7.47
7.46
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5.39
5.39
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2.89
2.80
2.80
2.78
2.77
2.74
2.74
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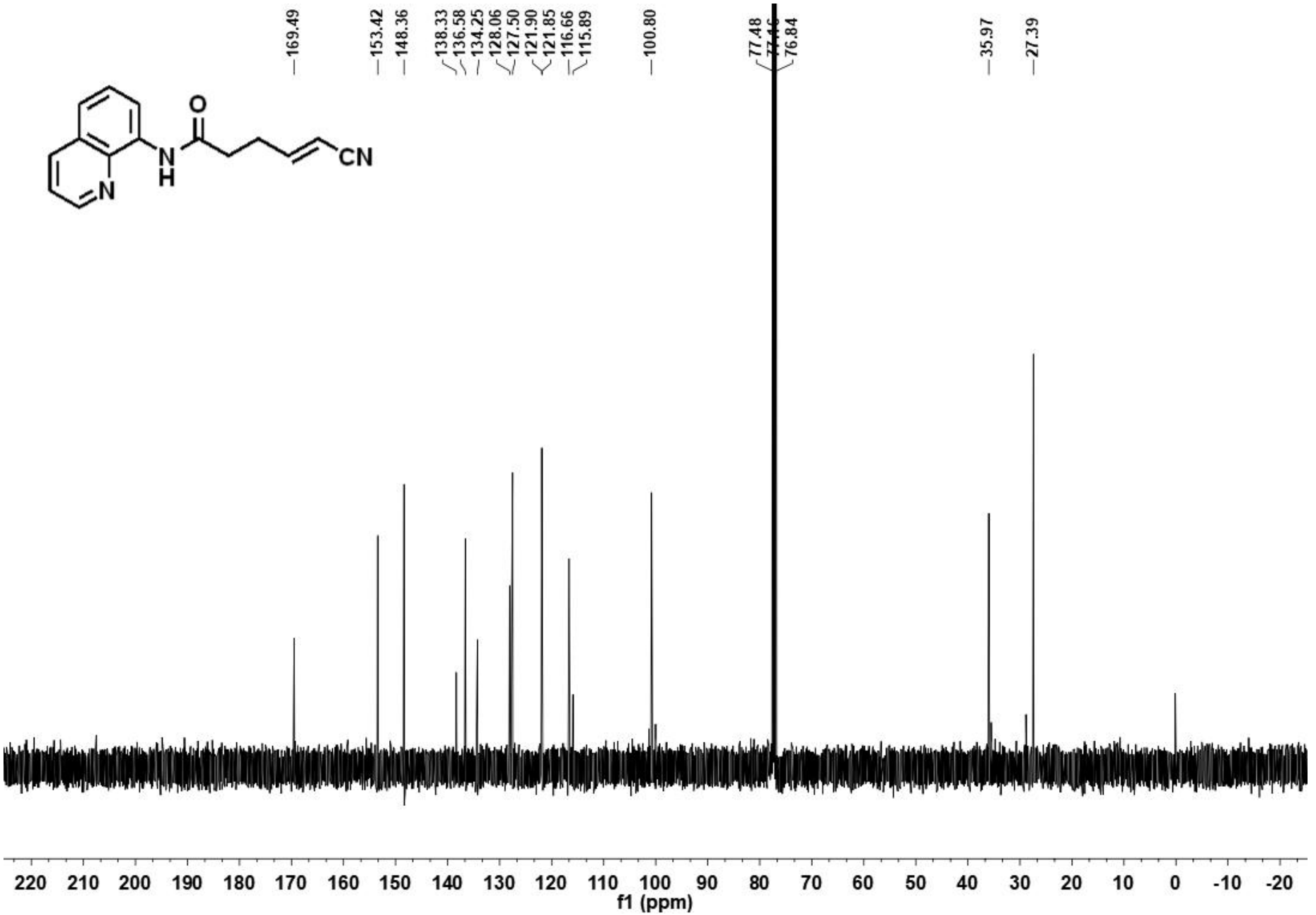
O
N
H
N
CN
0.93
1.03
1.01
1.04
3.07
1.00
0.99
2.07
2.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.48
76.84
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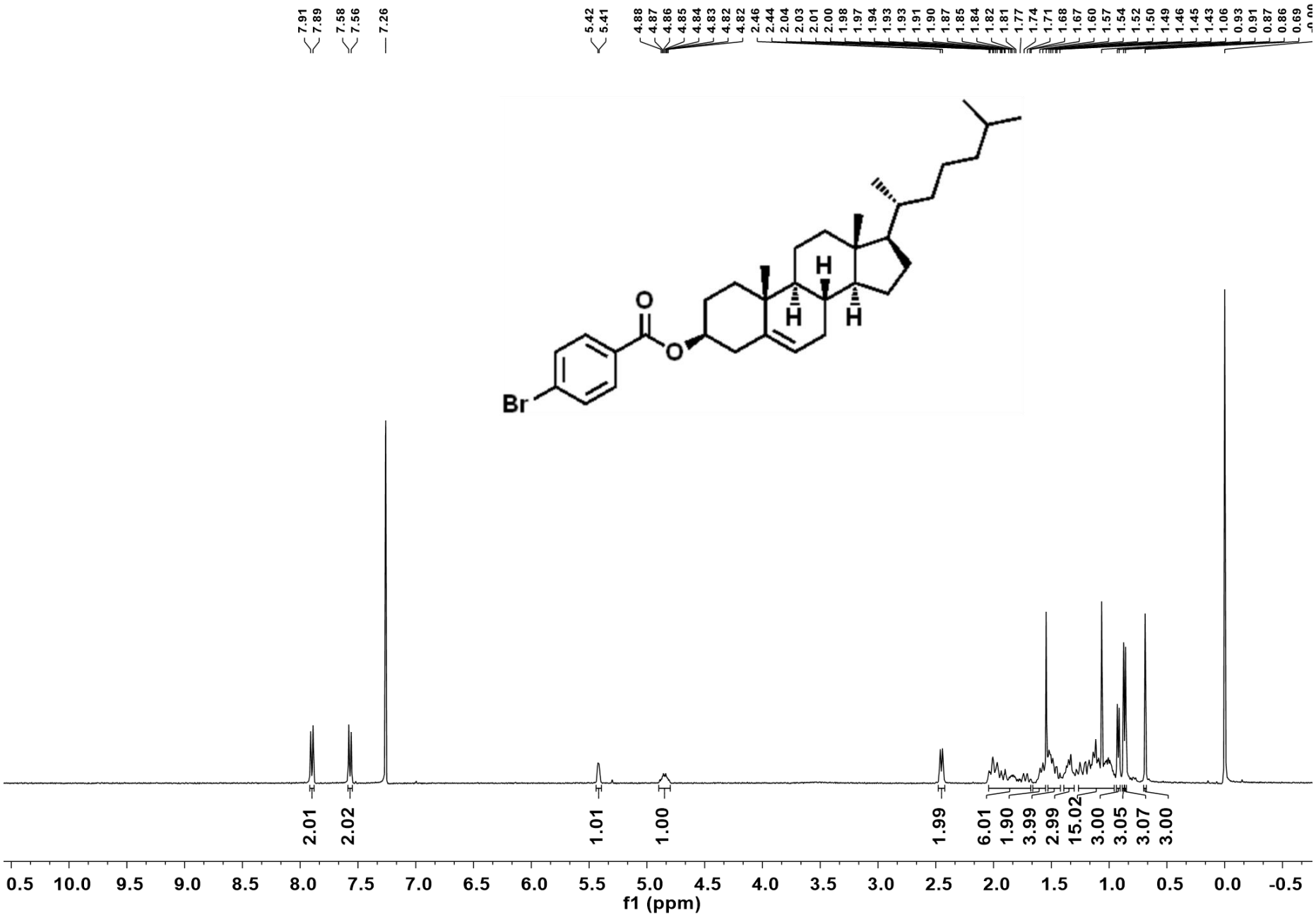
27.39
O
N
H
N
CN
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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4.86
4.85
4.84
4.83
4.82
2.46
2.44
2.04
2.03
2.01
2.00
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1.97
1.94
1.93
1.93
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1.90
1.87
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1.84
1.82
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1.77
1.74
1.71
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1.67
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1.50
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1.45
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0.86
0.69
O
O
H
H
H
Br
2.01
2.02
1.01
1.00
1.99
6.01
1.90
3.99
2.99
15.02
3.00
3.05
3.07
3.00
0.5
10.0
9.5
9.0
8.5
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7.5
7.0
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5.0
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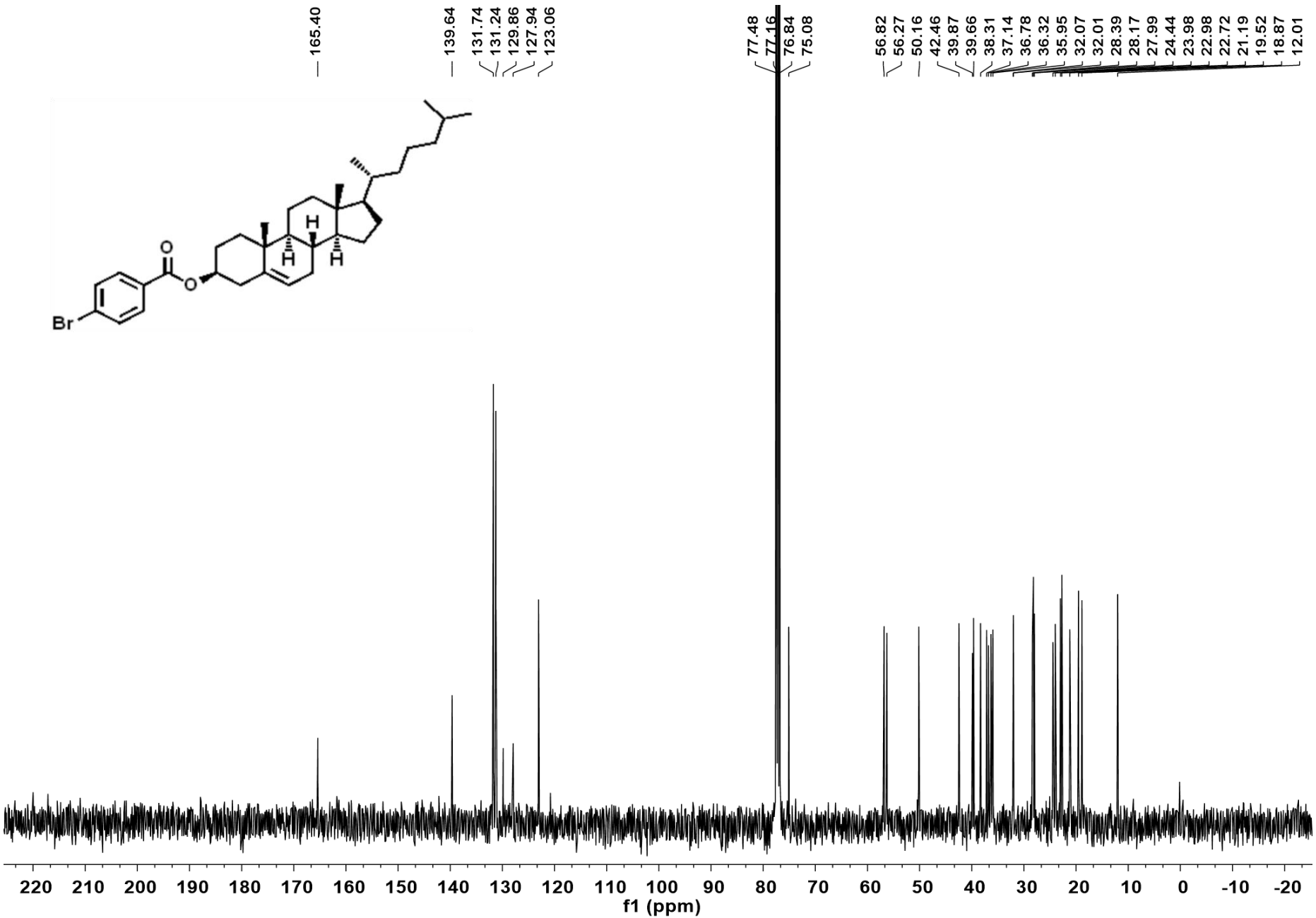
-0.5
f1 (ppm)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50.16
42.46
39.87
39.66
38.31
37.14
36.78
36.32
35.95
32.07
32.01
28.39
28.17
27.99
24.44
23.98
22.98
22.72
21.19
19.52
18.87
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Br
H
H
H
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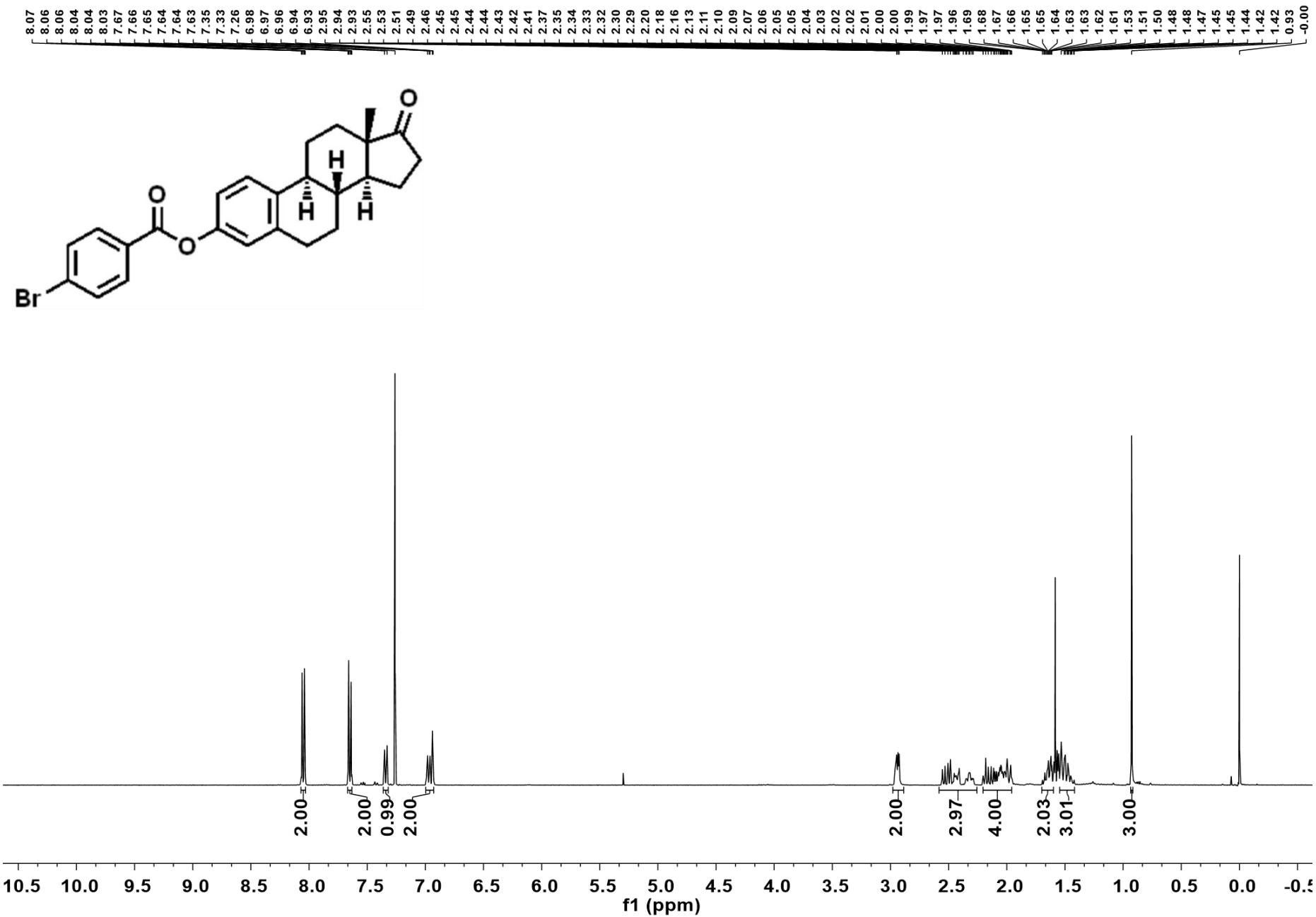
f1 (ppm)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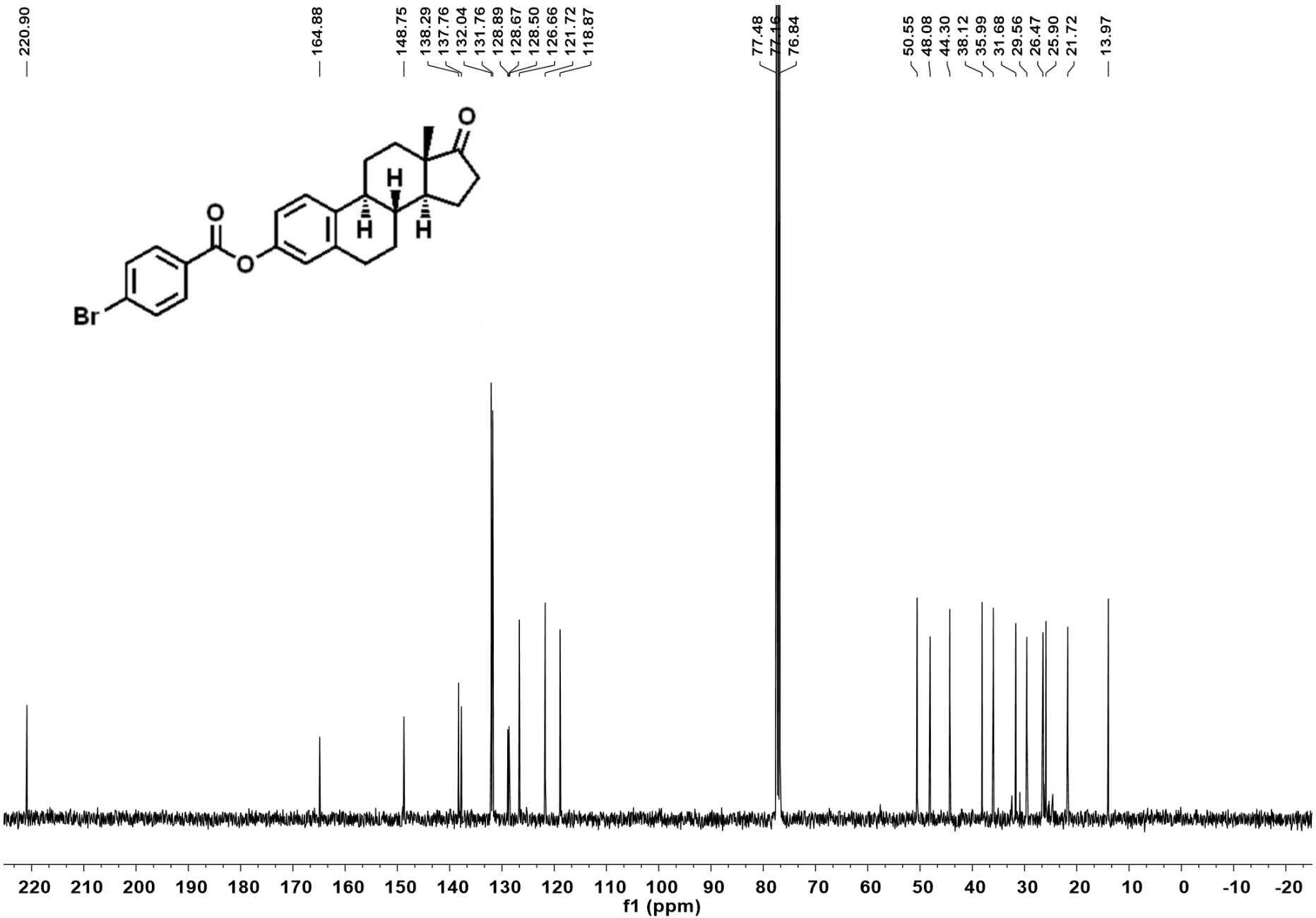
O
H
H
H
O
O
Br
2.00
2.00
0.99
2.00
2.00
2.97
4.00
2.03
3.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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121.72
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77.48
77.16
76.84
50.55
48.08
44.30
38.12
35.99
31.68
29.56
26.47
25.90
21.72
13.97
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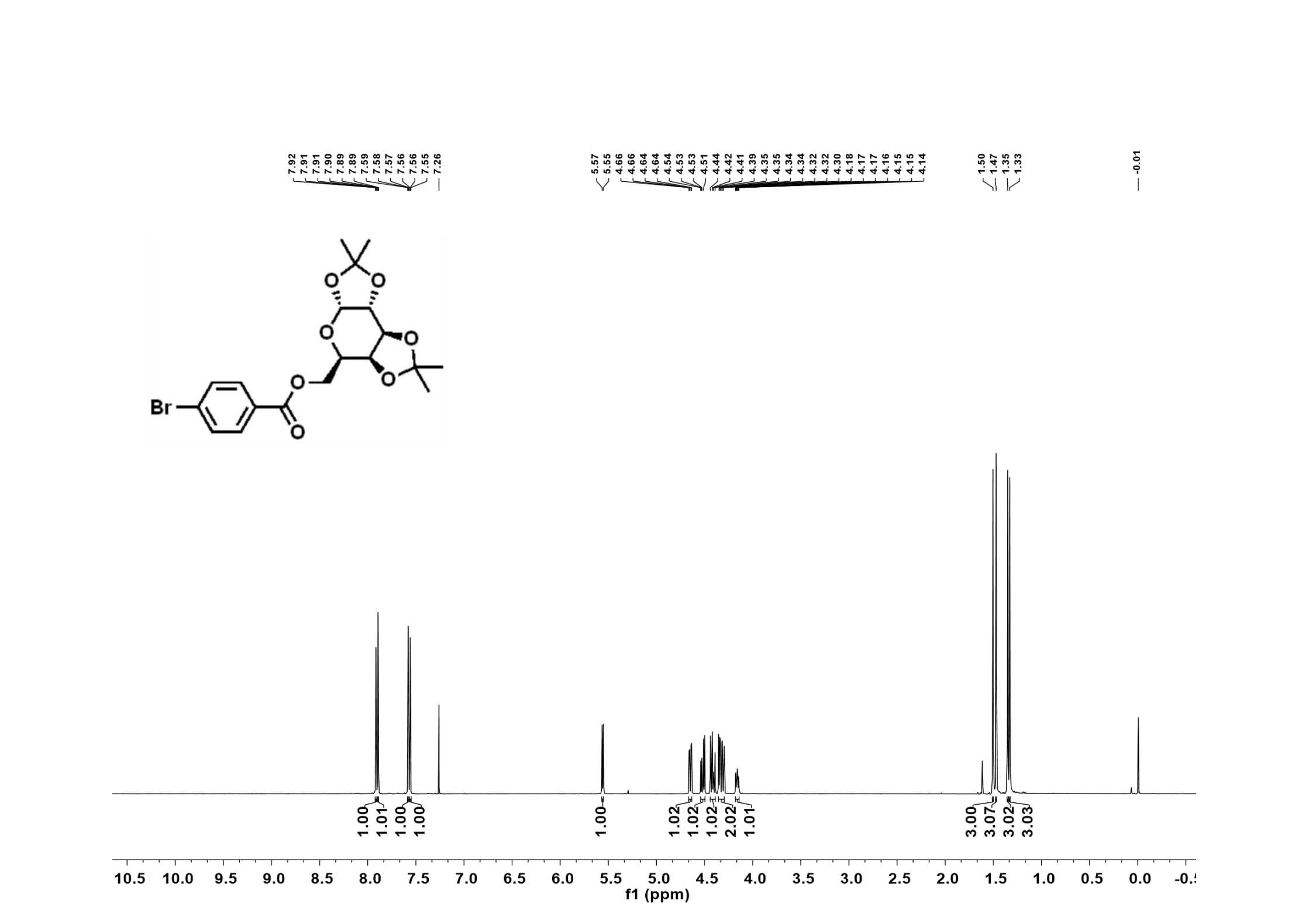
H
H
H
Br
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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2.02
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3.02
3.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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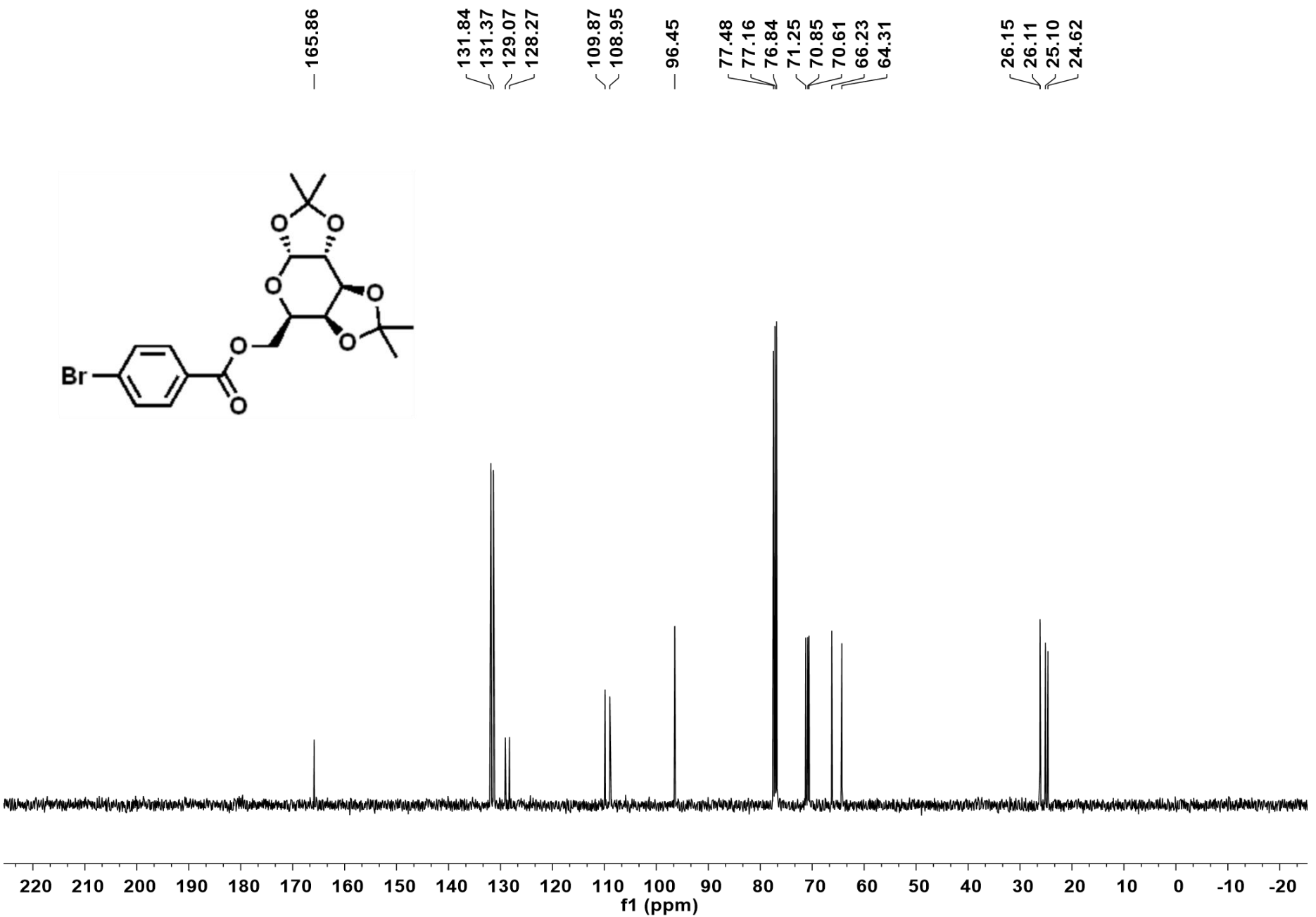
0.0
f1 (ppm)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76.84
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70.61
66.23
64.31
26.15
26.11
25.10
24.62
Br
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O
O
O
O
O
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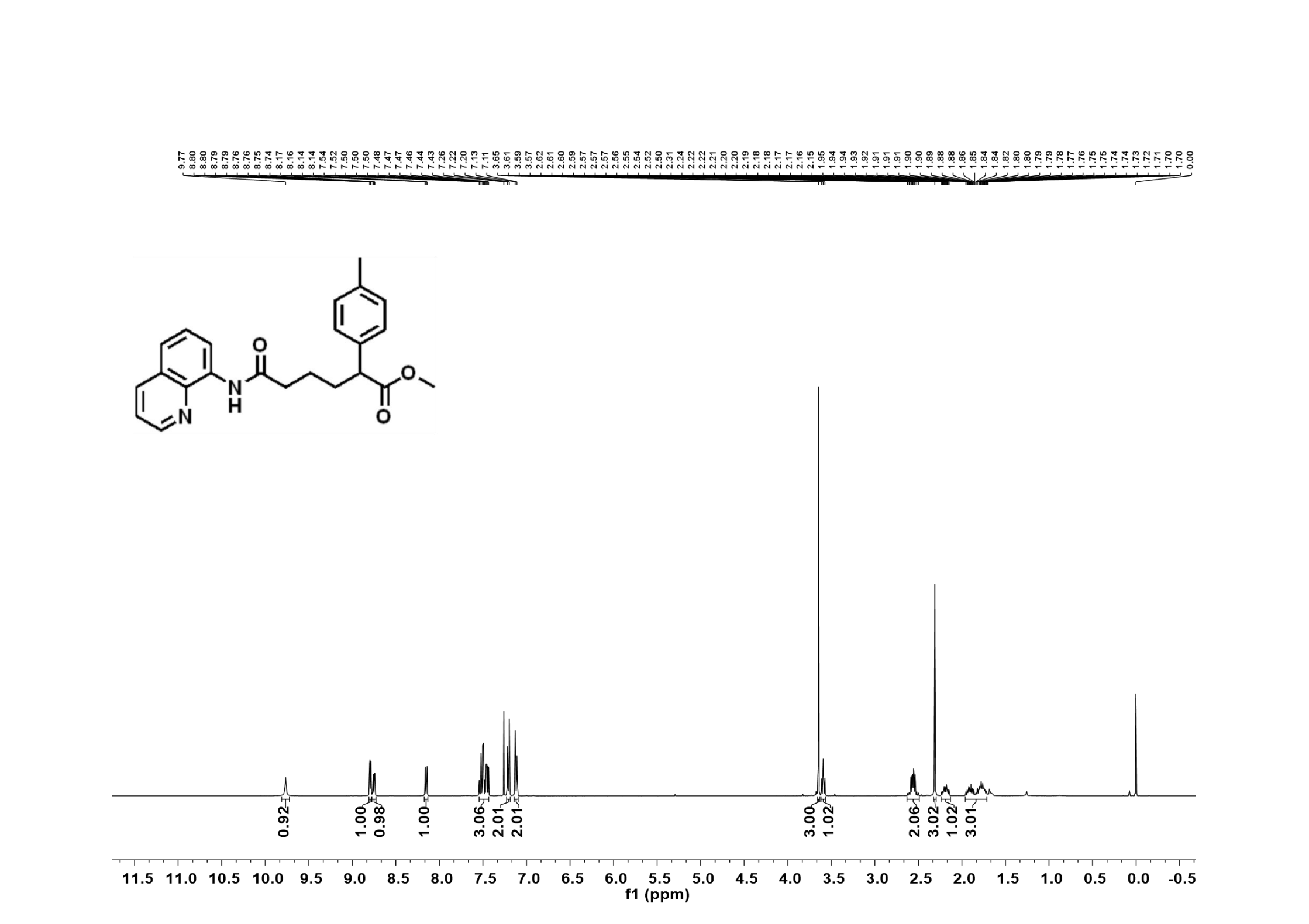
f1 (ppm)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O
N
H
N
O
O
0.92
1.00
0.98
1.00
3.06
2.01
2.01
3.00
1.02
2.06
3.02
1.02
3.01
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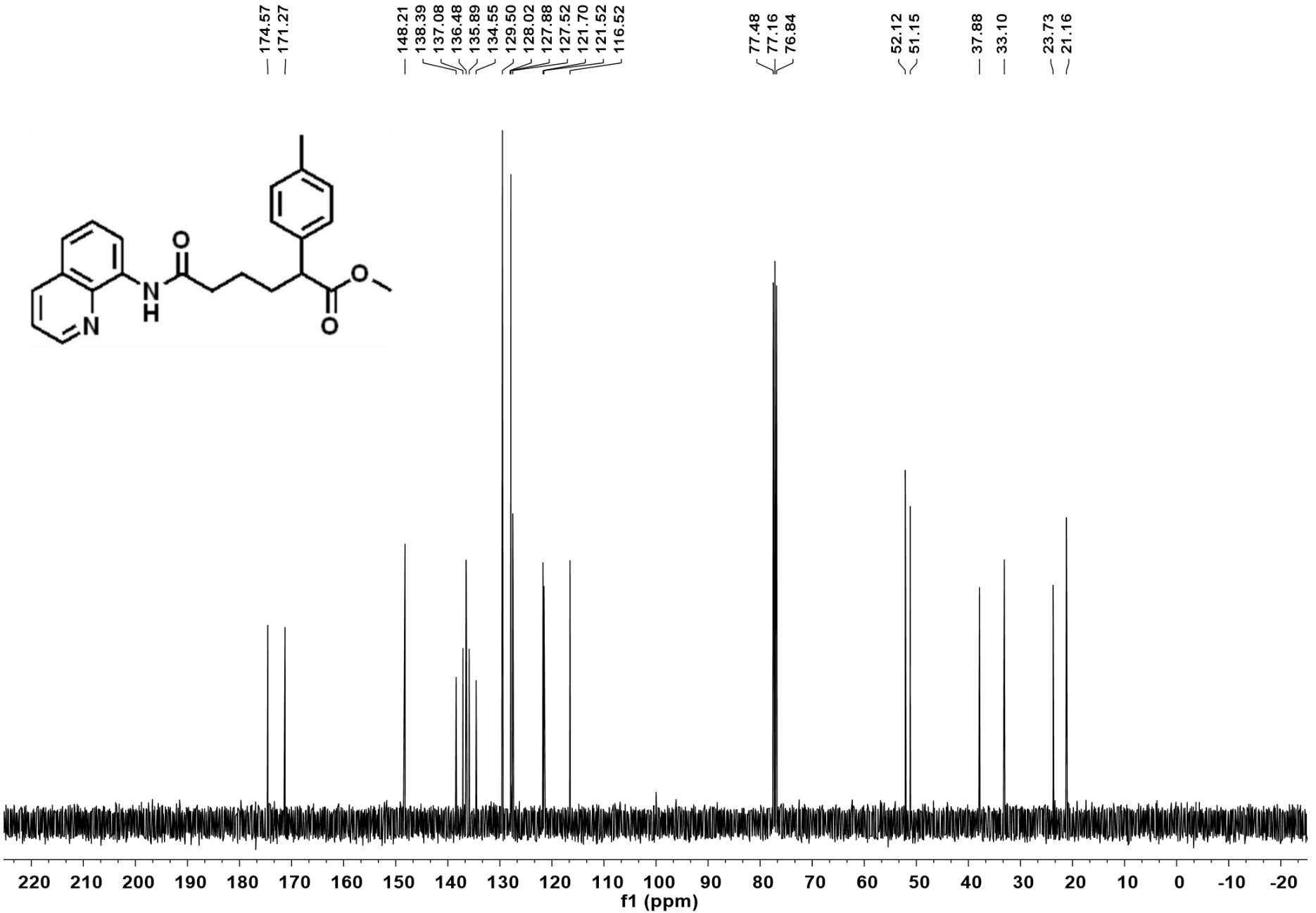
f1 (ppm)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116.52
77.48
77.16
76.84
52.12
51.15
37.88
33.10
23.73
21.16
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H
N
O
O
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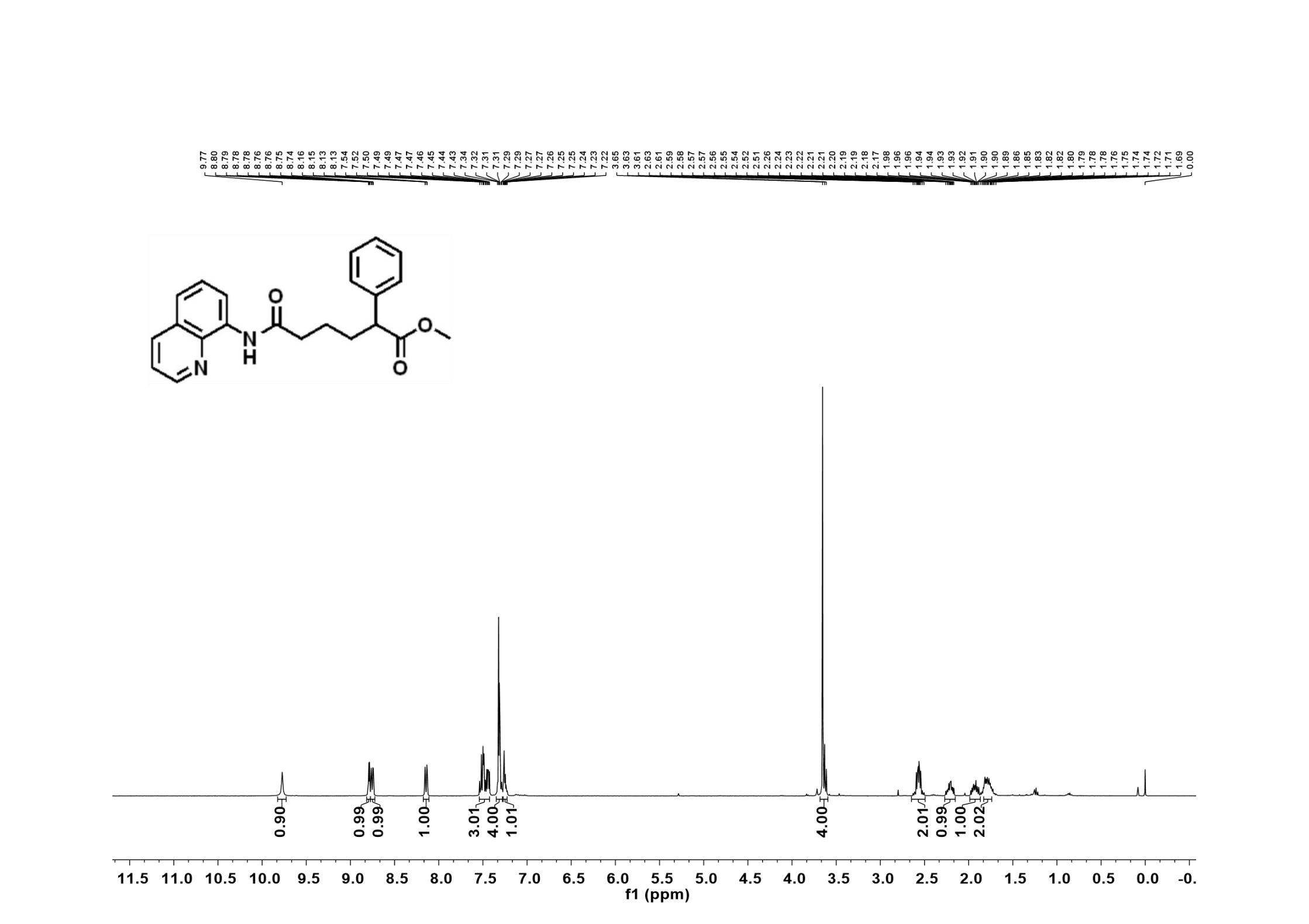
f1 (ppm)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3.65 3.63 3.61 2.63 2.61 2.59 2.58 2.57 2.57 2.56 2.55 2.54 2.52 2.51 2.26 2.24 2.23 2.22 2.21 2.21 2.20 2.19 2.19 2.18 2.17 1.98 1.96 1.96 1.94 1.94 1.93 1.93 1.92 1.91 1.90 1.90 1.89 1.86 1.85 1.83 1.82 1.82 1.80 1.79 1.78 1.78 1.76 1.75 1.74 1.74 1.72 1.71 1.69 0.00
O
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H
N
O
O
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0.99
0.99
1.00
3.01
4.00
1.01
4.00
2.01
0.99
1.00
2.02
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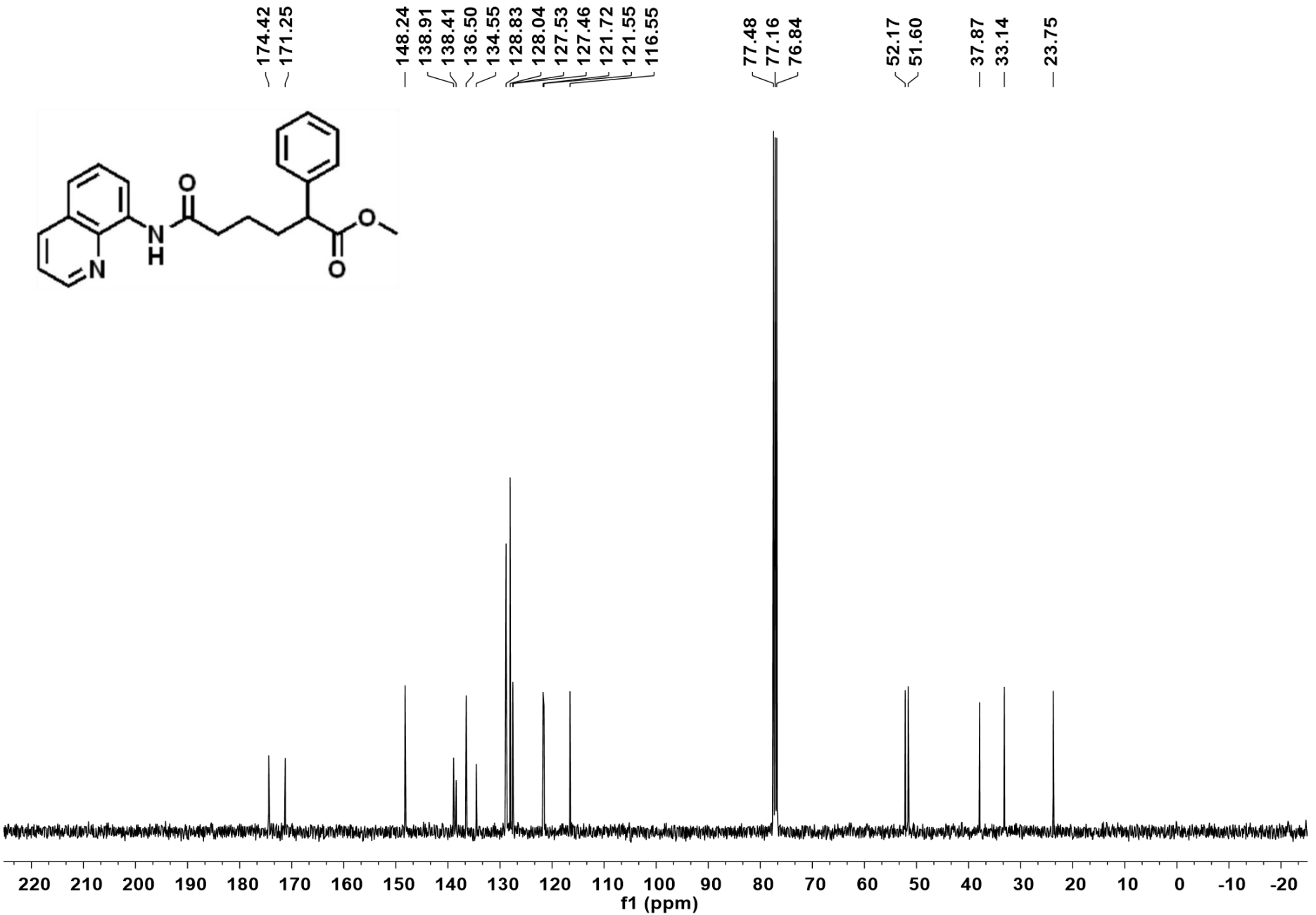
f1 (ppm)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77.48
77.16
76.84
52.17
51.60
37.87
33.14
23.75
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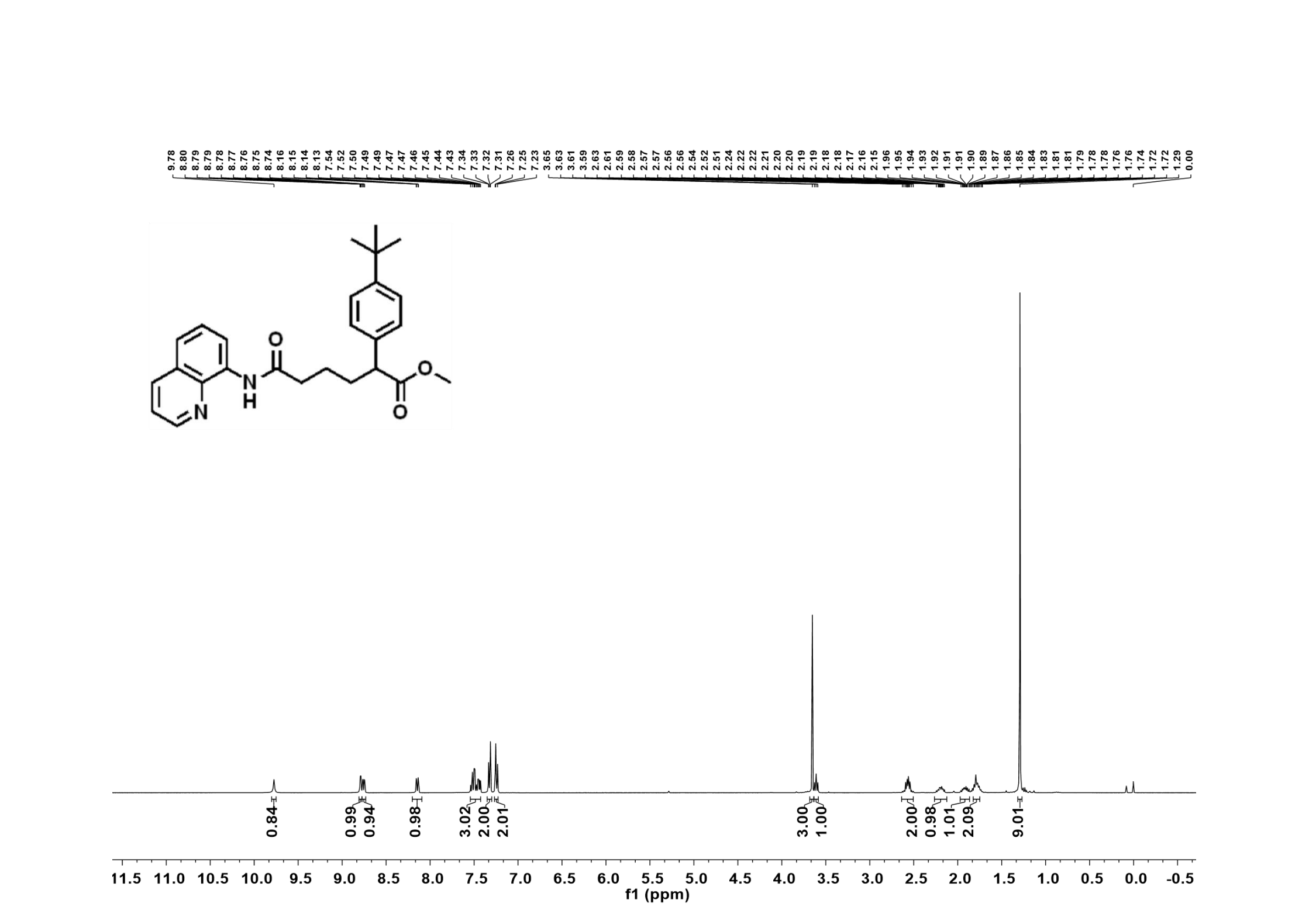
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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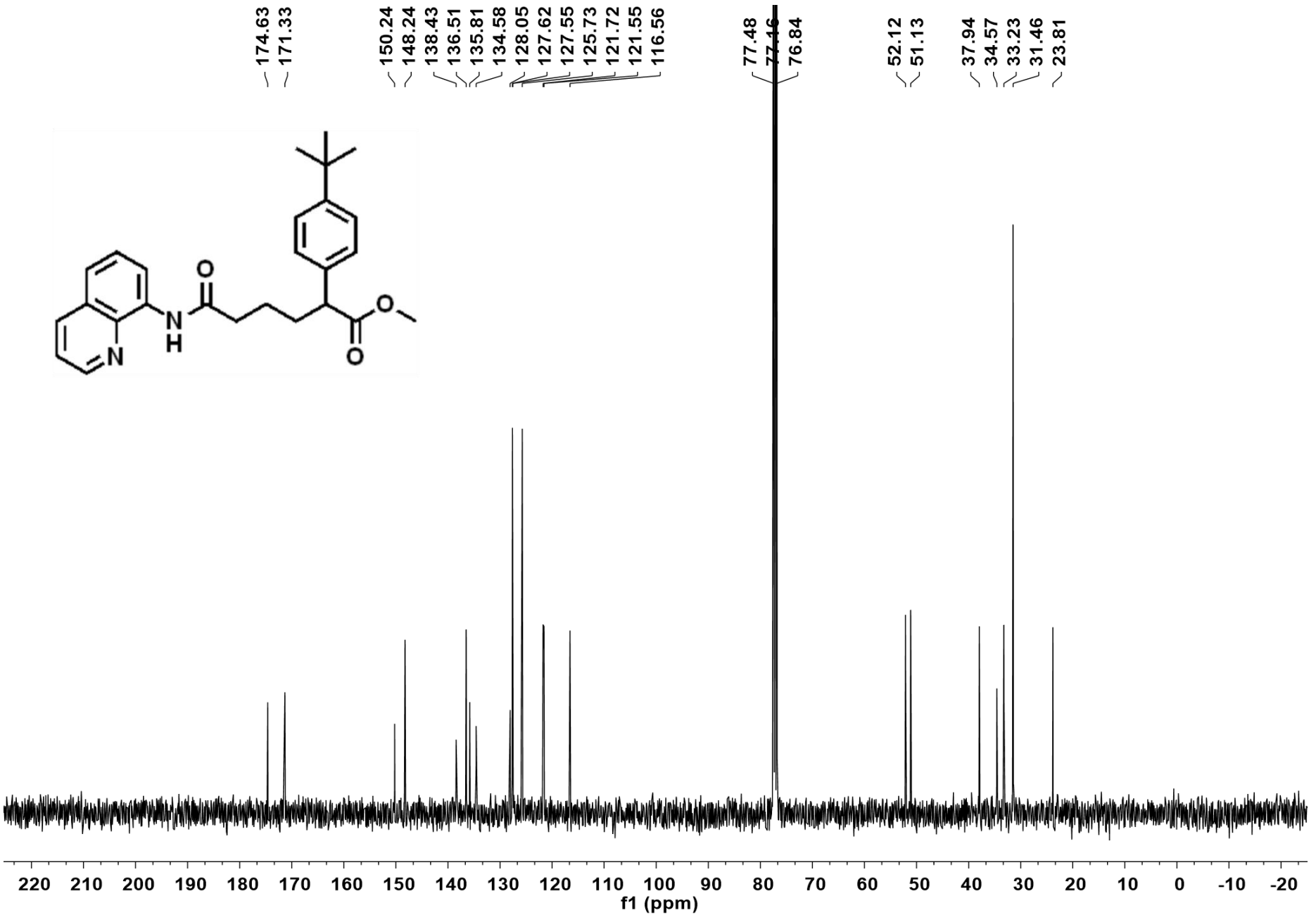
3.65 3.63 3.61 3.59 2.63 2.61 2.59 2.58 2.57 2.57 2.56 2.56 2.54 2.52 2.51 2.24 2.22 2.22 2.21 2.20 2.20 2.19 2.19 2.18 2.18 2.17 2.16 2.15 1.96 1.95 1.94 1.93 1.92 1.91 1.91 1.90 1.89 1.87 1.86 1.85 1.84 1.83 1.81 1.81 1.79 1.78 1.78 1.76 1.76 1.74 1.72 1.72 1.29 0.00
O
N
H
N
O
O
0.84 0.99 0.94 0.98 3.02 2.00 2.01 3.00 1.00 2.00 0.98 1.01 2.09 9.01
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
f1 (ppm)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134.58
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127.55
125.73
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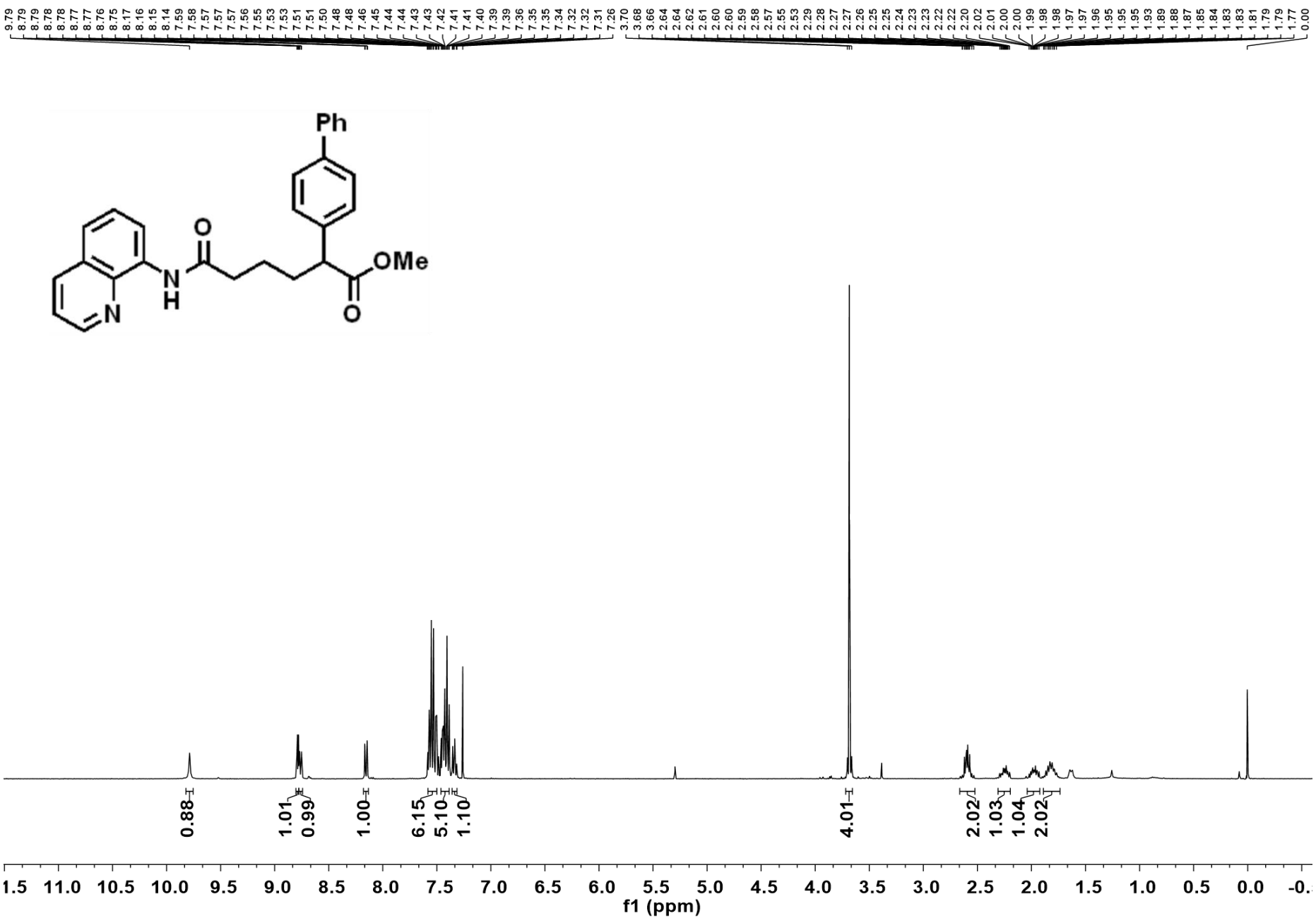
121.55
116.56
77.48
77.16
76.84
52.12
51.13
37.94
34.57
33.23
31.46
23.81
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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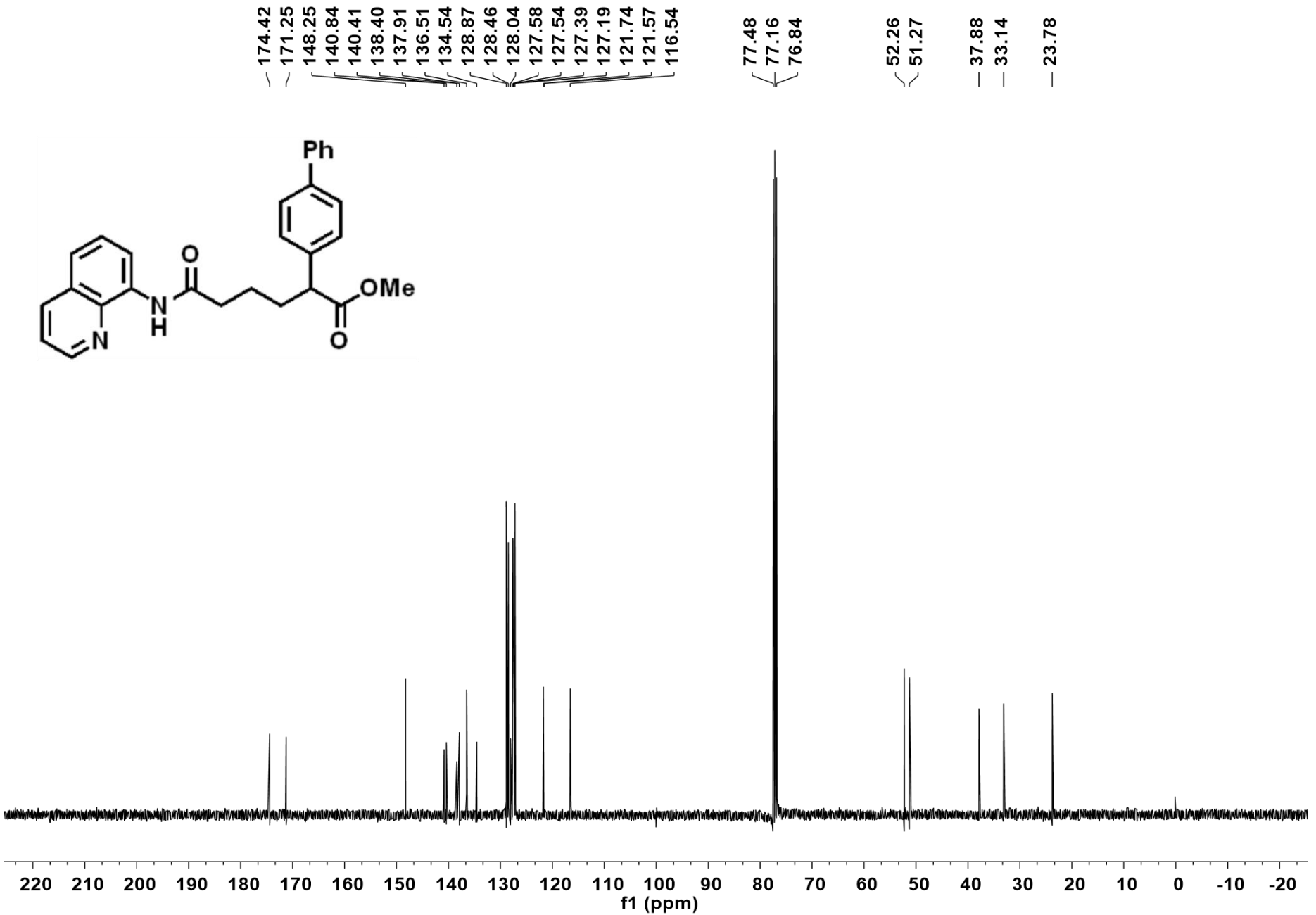
H
N
OMe
O
f1 (ppm)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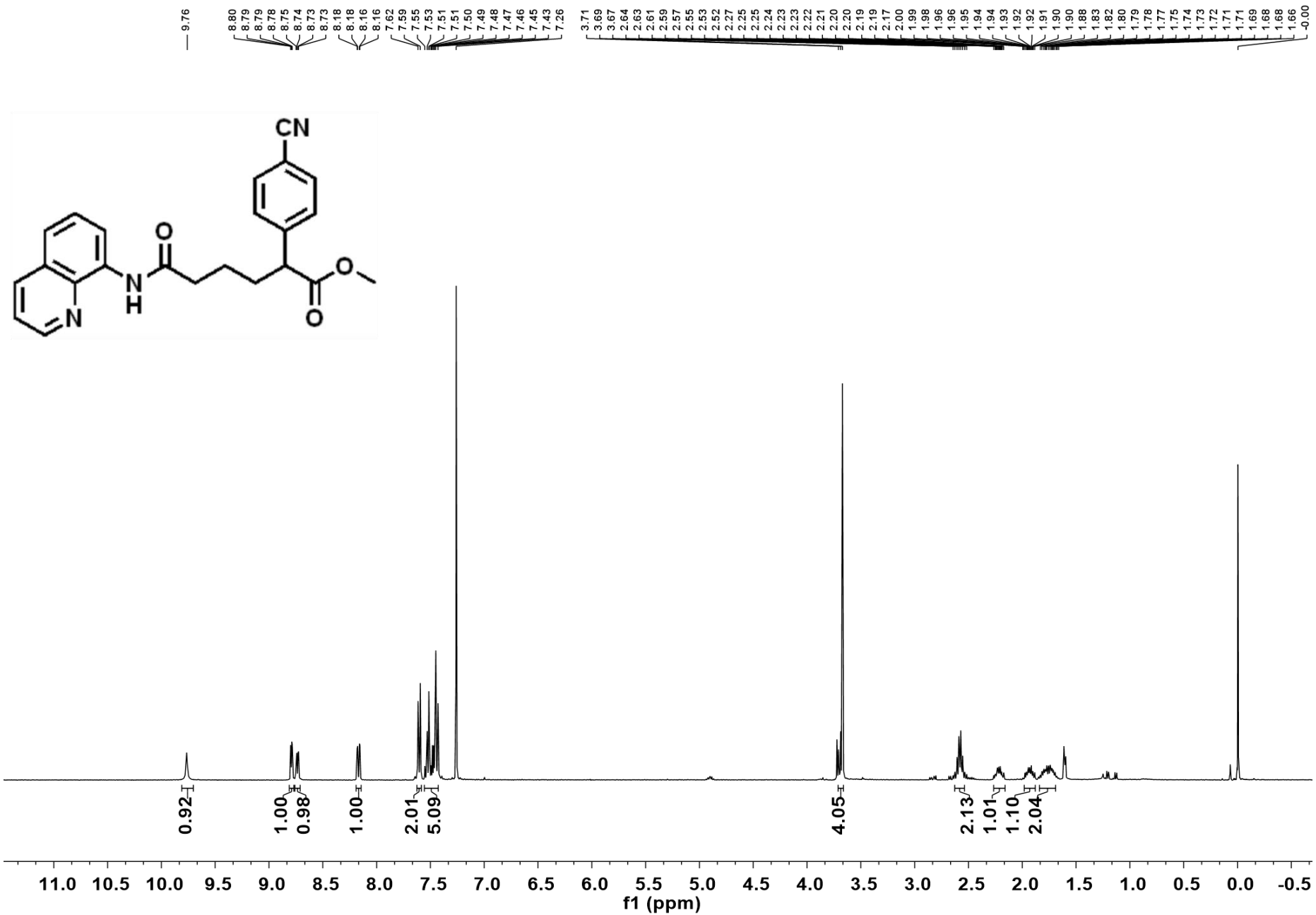
136.51
134.54
128.87
128.46
128.04
127.58
127.54
127.39
127.19
121.74
121.57
116.54
77.48
77.16
76.84
52.26
51.27
37.88
33.14
23.78
Ph
O
N
H
N
OMe
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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8.16
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7.55
7.53
7.51
7.51
7.50
7.49
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7.47
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7.45
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7.26
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1.96
1.96
1.95
1.94
1.94
1.93
1.92
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1.72
1.71
1.71
1.69
1.68
1.68
1.66
-0.00
CN
O
N
H
O
O
N
0.92
1.00
0.98
1.00
2.01
5.09
4.05
2.13
1.01
1.10
2.04
11.0
10.5
10.0
9.5
9.0
8.5
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6.5
6.0
5.5
5.0
4.5
4.0
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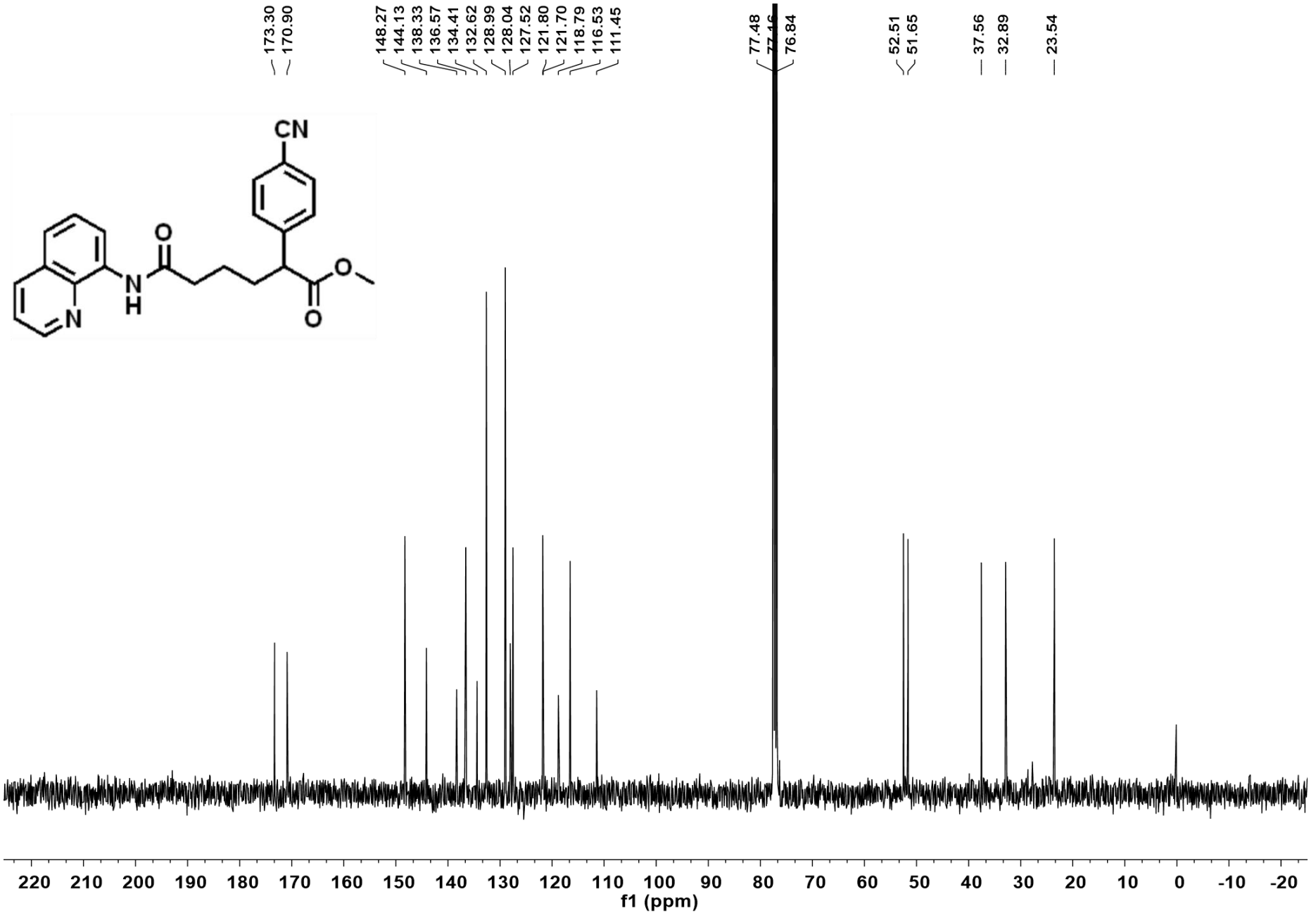
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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144.13
138.33
136.57
134.41
132.62
128.99
128.04
127.52
121.80
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118.79
116.53
111.45
77.48
77.16
76.84
52.51
51.65
37.56
32.89
23.54
CN
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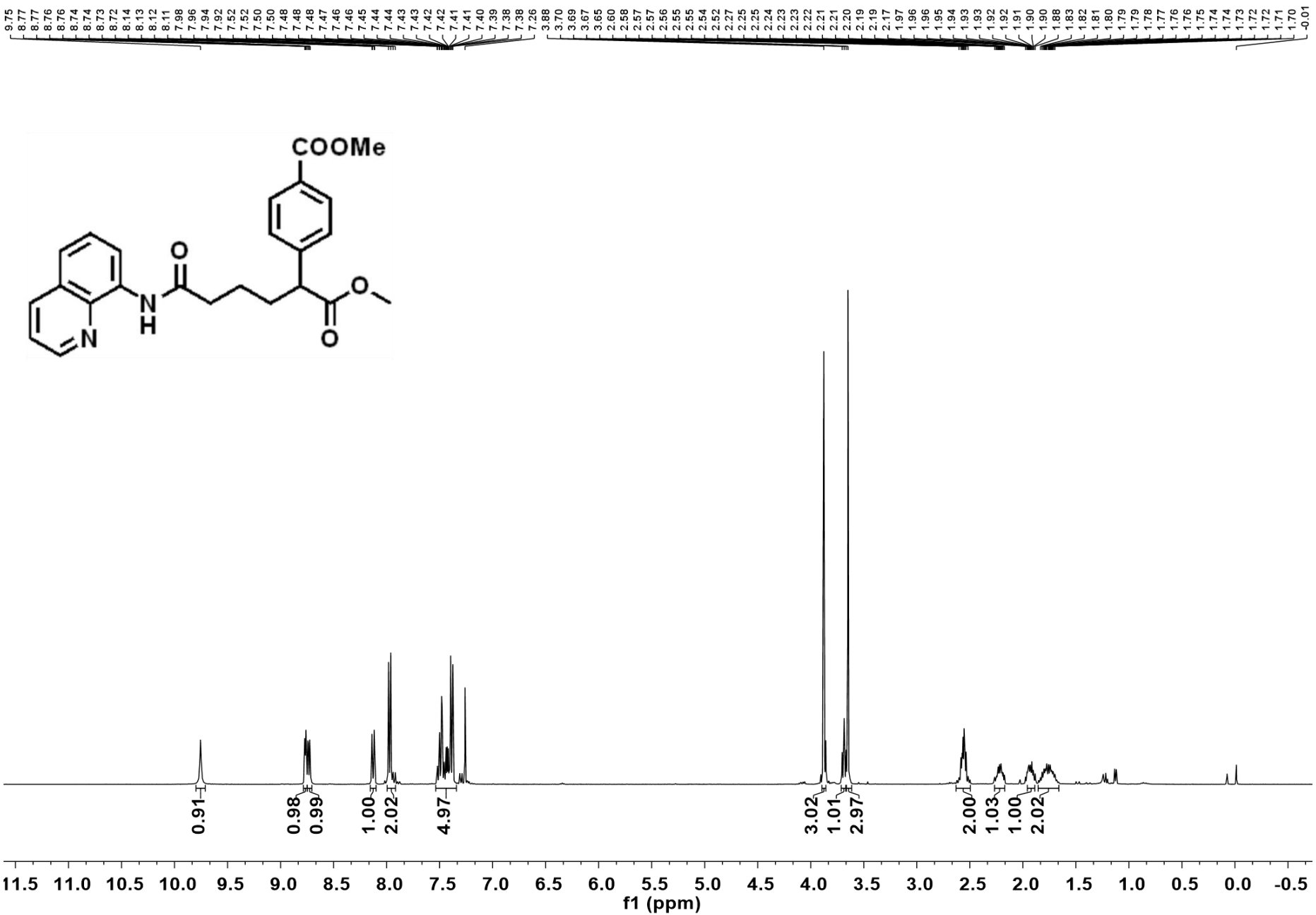
H
O
O
N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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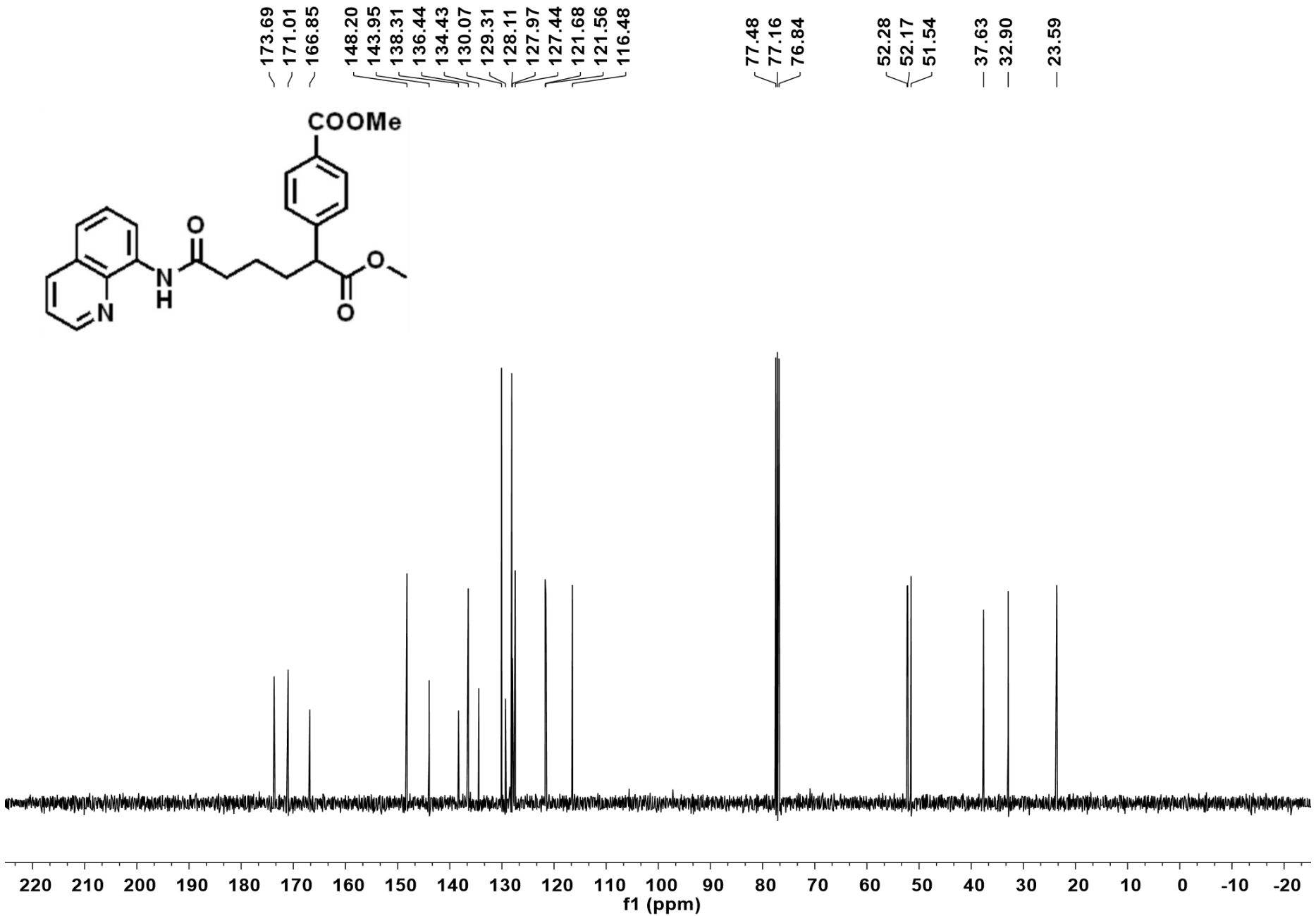
3.88 3.70 3.69 3.67 3.65 2.60 2.58 2.57 2.57 2.56 2.55 2.55 2.54 2.52 2.27 2.25 2.25 2.24 2.23 2.23 2.22 2.21 2.21 2.20 2.19 2.19 2.17 1.97 1.96 1.96 1.95 1.94 1.93 1.93 1.92 1.92 1.91 1.90 1.90 1.88 1.83 1.82 1.81 1.80 1.79 1.79 1.78 1.77 1.76 1.76 1.75 1.74 1.74 1.73 1.72 1.72 1.71 1.70 -0.01
COOMe
O
N
H
O
O
N
0.91
0.98
0.99
1.00
2.02
4.97
3.02
1.01
2.97
2.00
1.03
1.00
2.02
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
f1 (ppm)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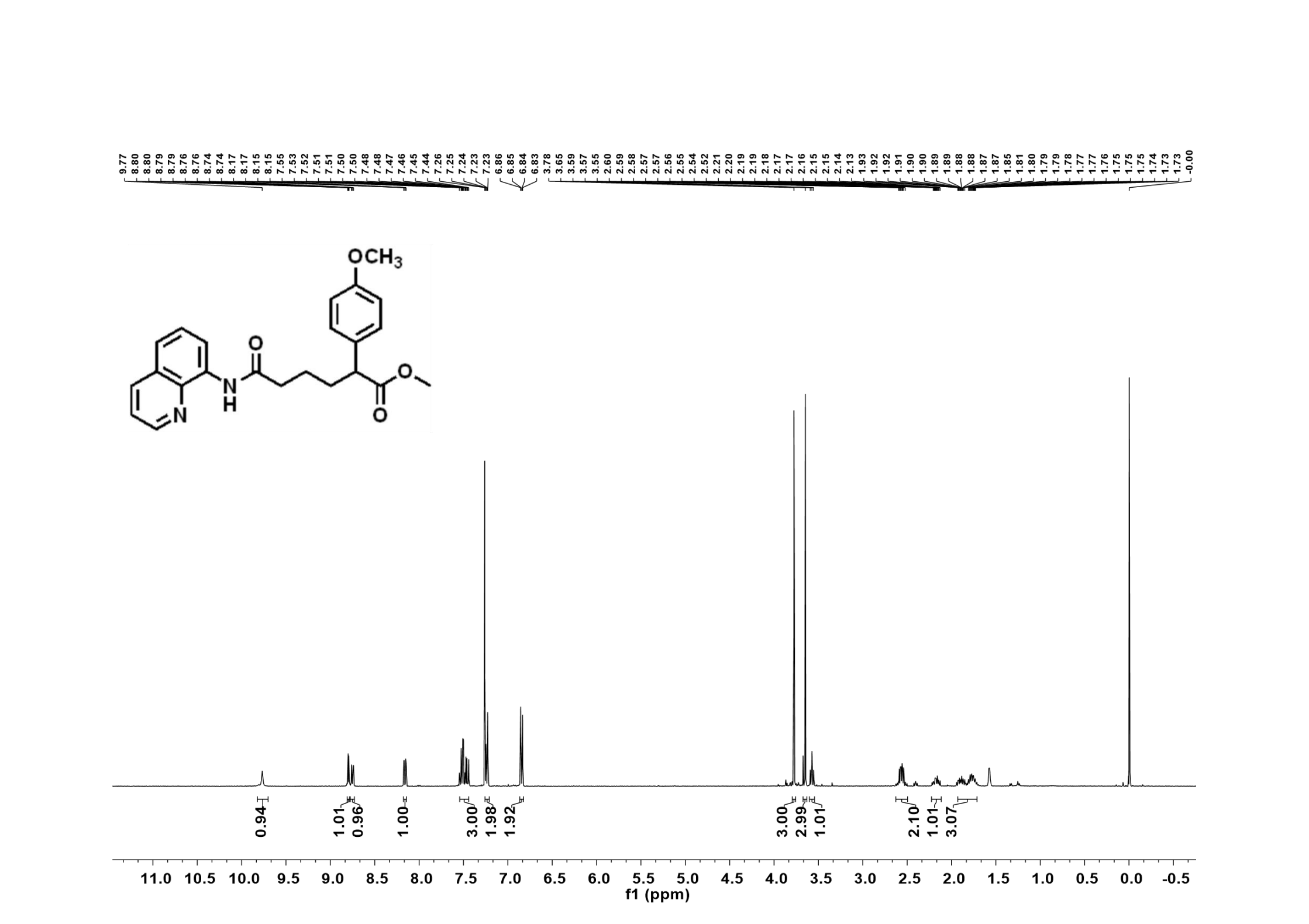
121.68
121.56
116.48
77.48
77.16
76.84
52.28
52.17
51.54
37.63
32.90
23.59
COOMe
O
N
H
O
O
N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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OCH3
O
N
H
N
O
O
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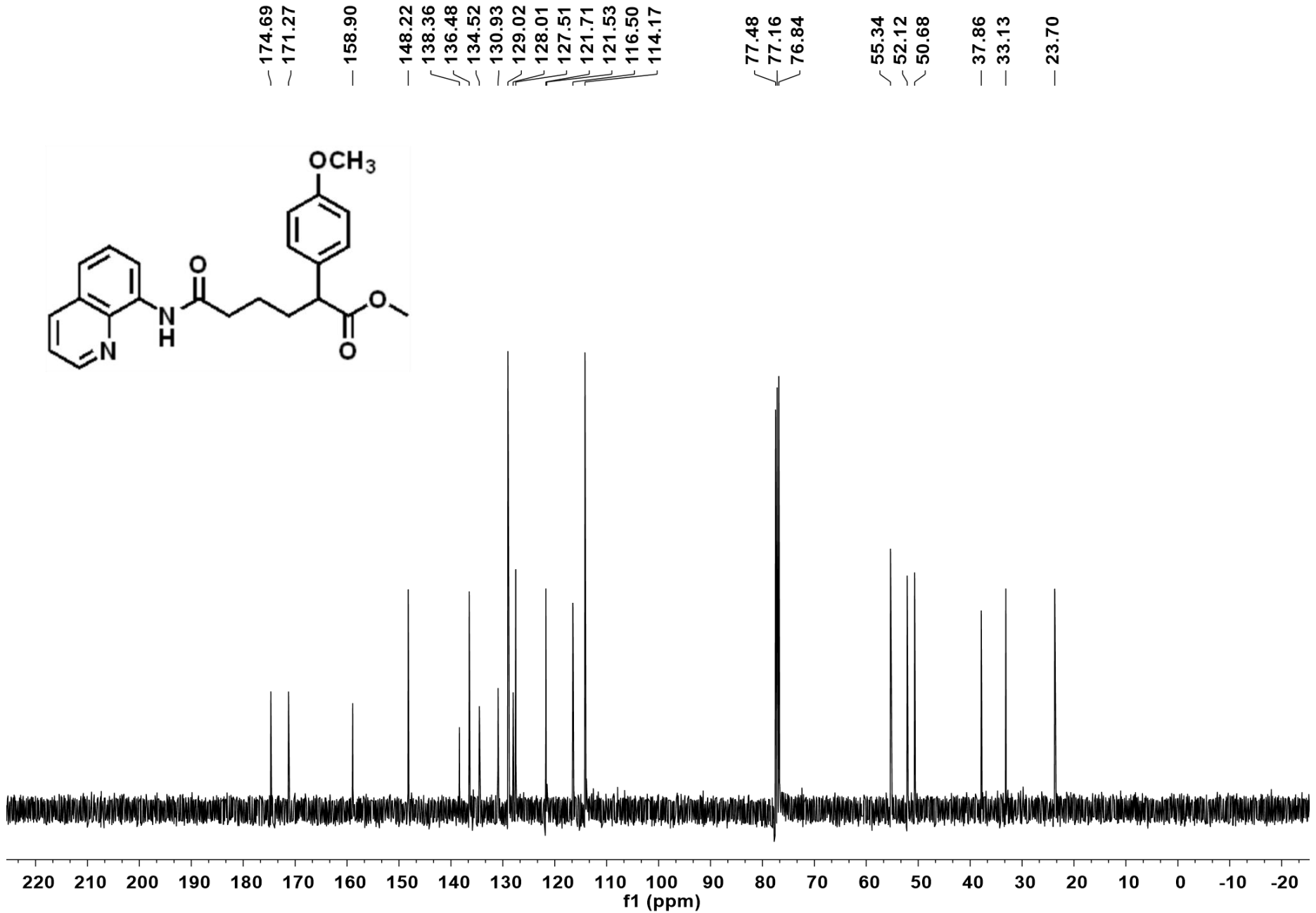
1.01
0.96
1.00
3.00
1.98
1.92
3.00
2.99
1.01
2.10
1.01
3.07
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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121.71
121.53
116.50
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77.48
77.16
76.84
55.34
52.12
50.68
37.86
33.13
23.70
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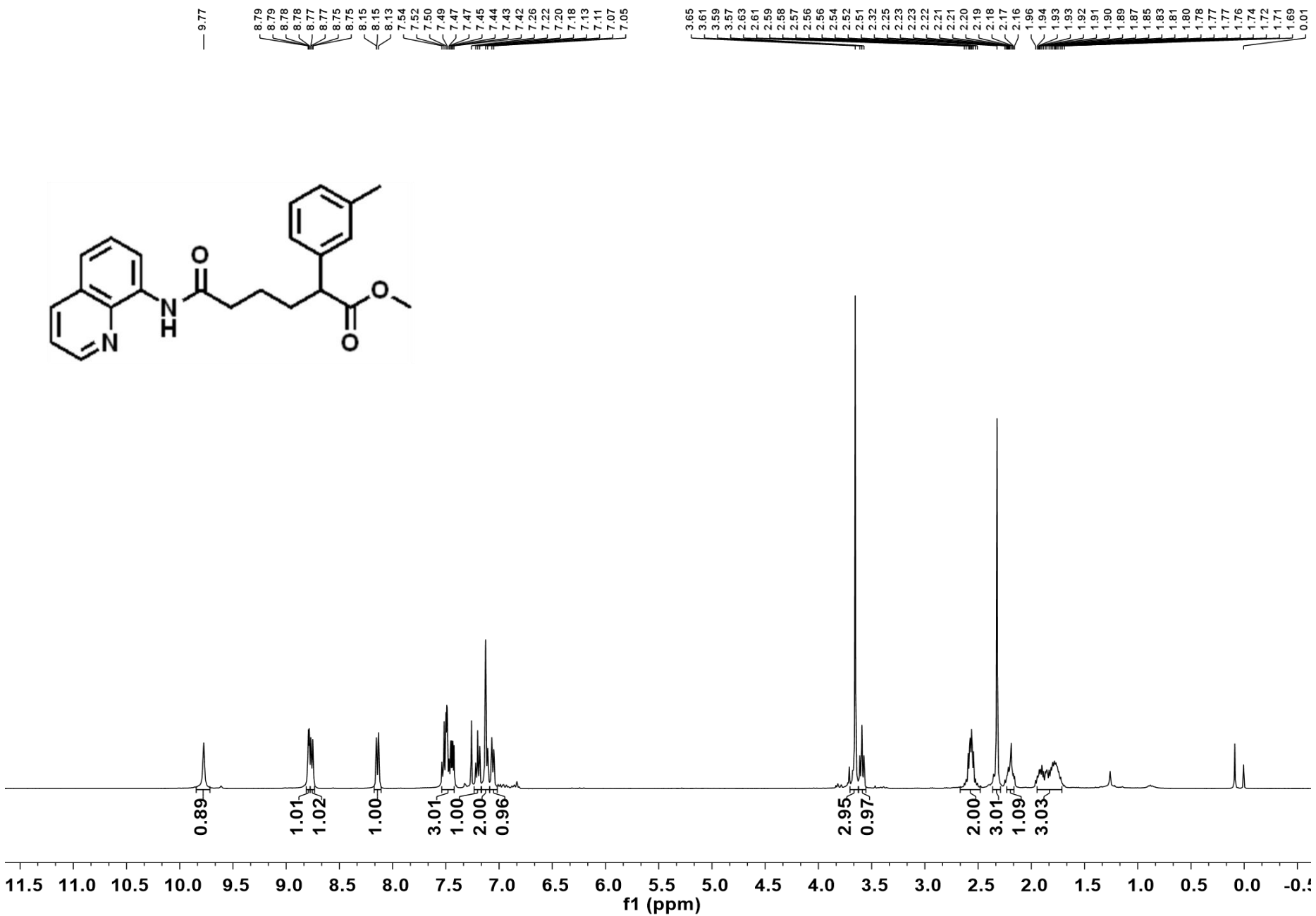
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.54
7.52
7.50
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7.47
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7.18
7.13
7.11
7.07
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2.22
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2.18
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1.93
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1.91
1.90
1.89
1.87
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1.81
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1.78
1.77
1.77
1.76
1.74
1.72
1.71
1.69
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O
N
H
N
O
O
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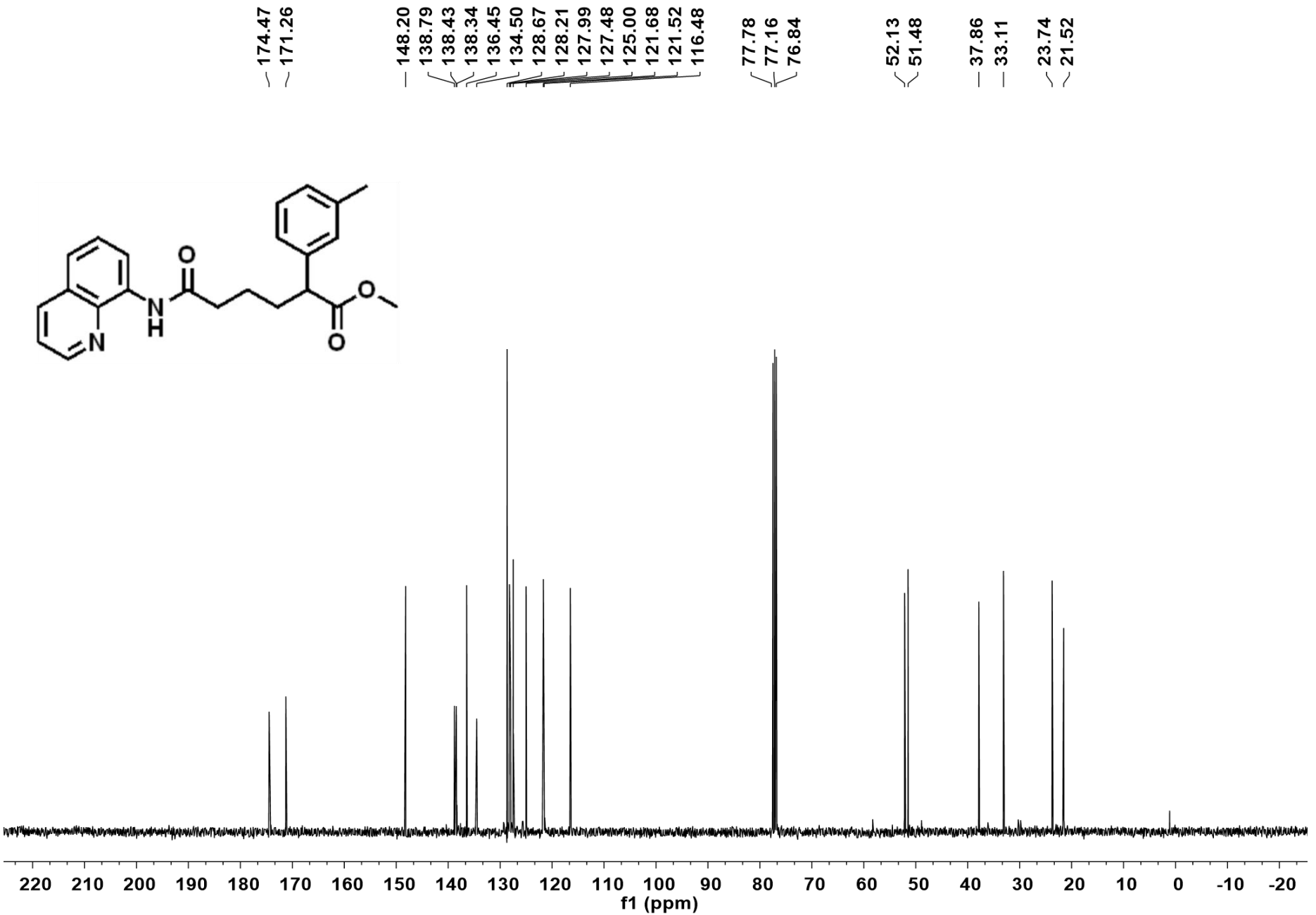
1.01
1.02
1.00
3.01
1.00
2.00
0.96
2.95
0.97
2.00
3.01
1.09
3.03
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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121.52
116.48
77.78
77.16
76.84
52.13
51.48
37.86
33.11
23.74
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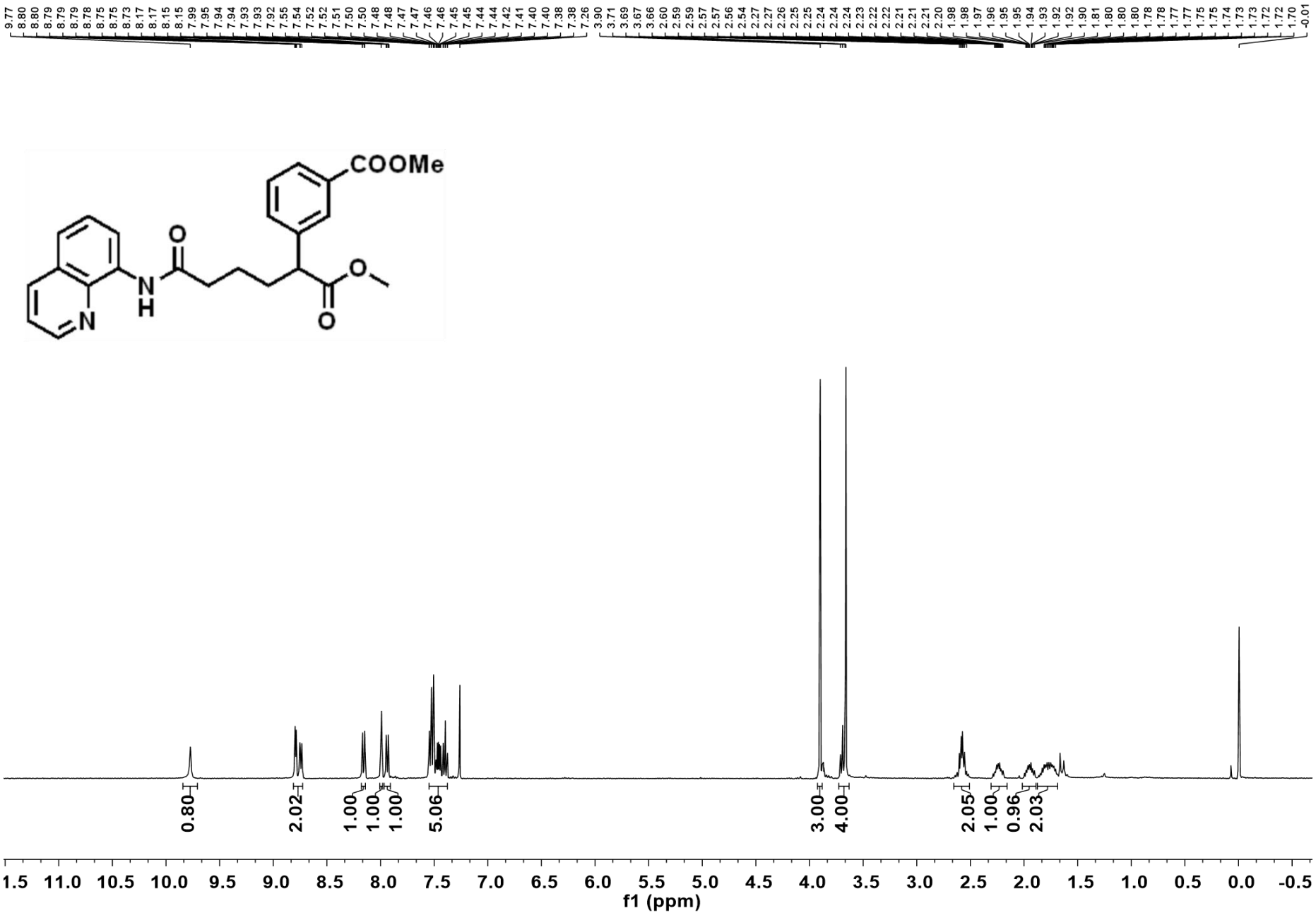
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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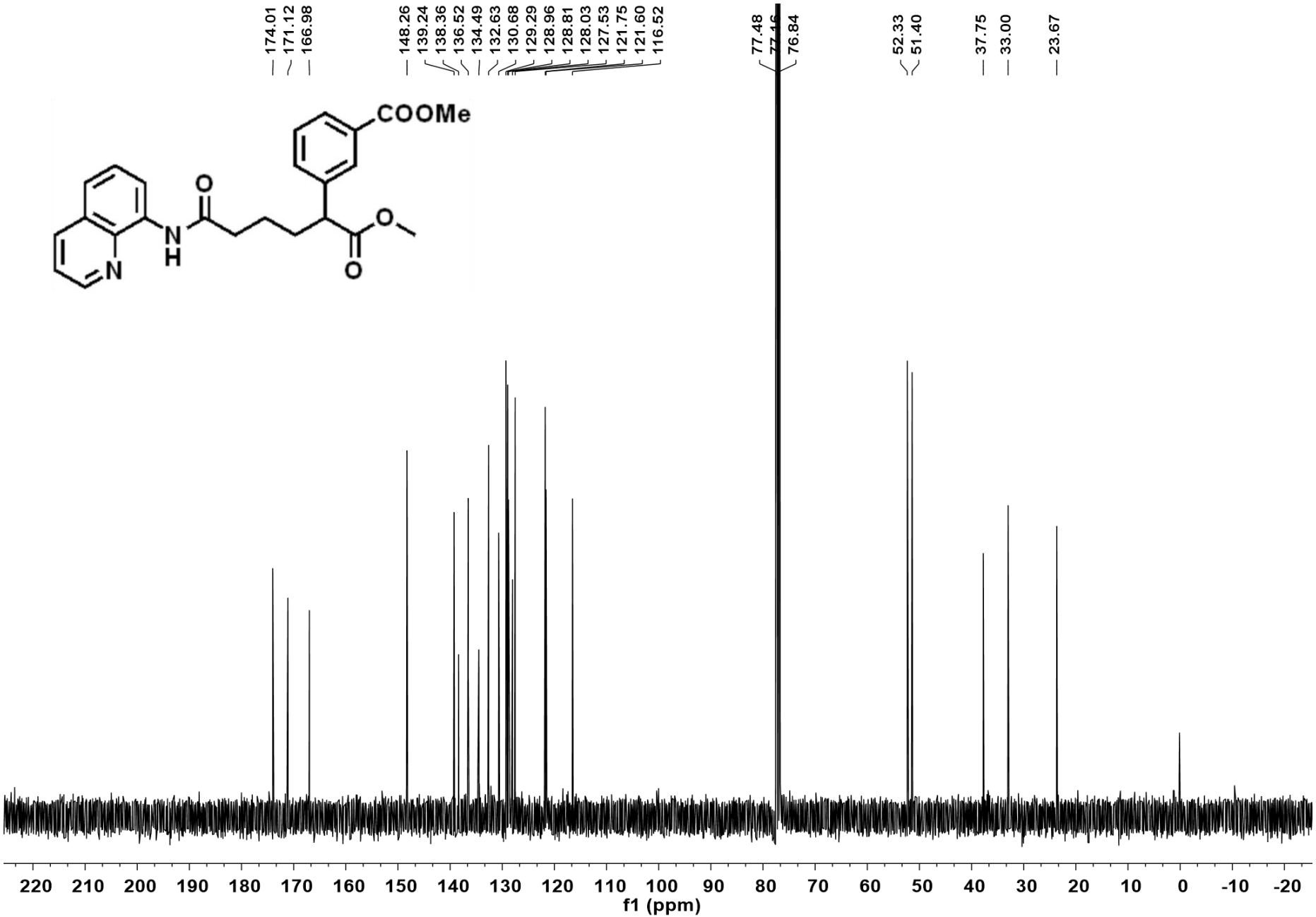
3.90 3.71 3.69 3.67 3.66 2.60 2.59 2.59 2.57 2.57 2.56 2.54 2.27 2.27 2.26 2.25 2.25 2.24 2.24 2.24 2.23 2.22 2.22 2.21 2.21 2.21 2.20 1.98 1.98 1.97 1.96 1.95 1.95 1.94 1.93 1.92 1.92 1.90 1.81 1.80 1.80 1.80 1.78 1.78 1.77 1.77 1.75 1.75 1.74 1.73 1.73 1.72 1.72 1.70 -0.01
COOMe
O
N
H
O
O
N
0.80
2.02
1.00
1.00
1.00
5.06
3.00
4.00
2.05
1.00
0.96
2.03
1.5 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
f1 (ppm)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134.49
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130.68
129.29
128.96
128.81
128.03
127.53
121.75
121.60
116.52
77.48
77.16
76.84
52.33
51.40
37.75
33.00
23.67
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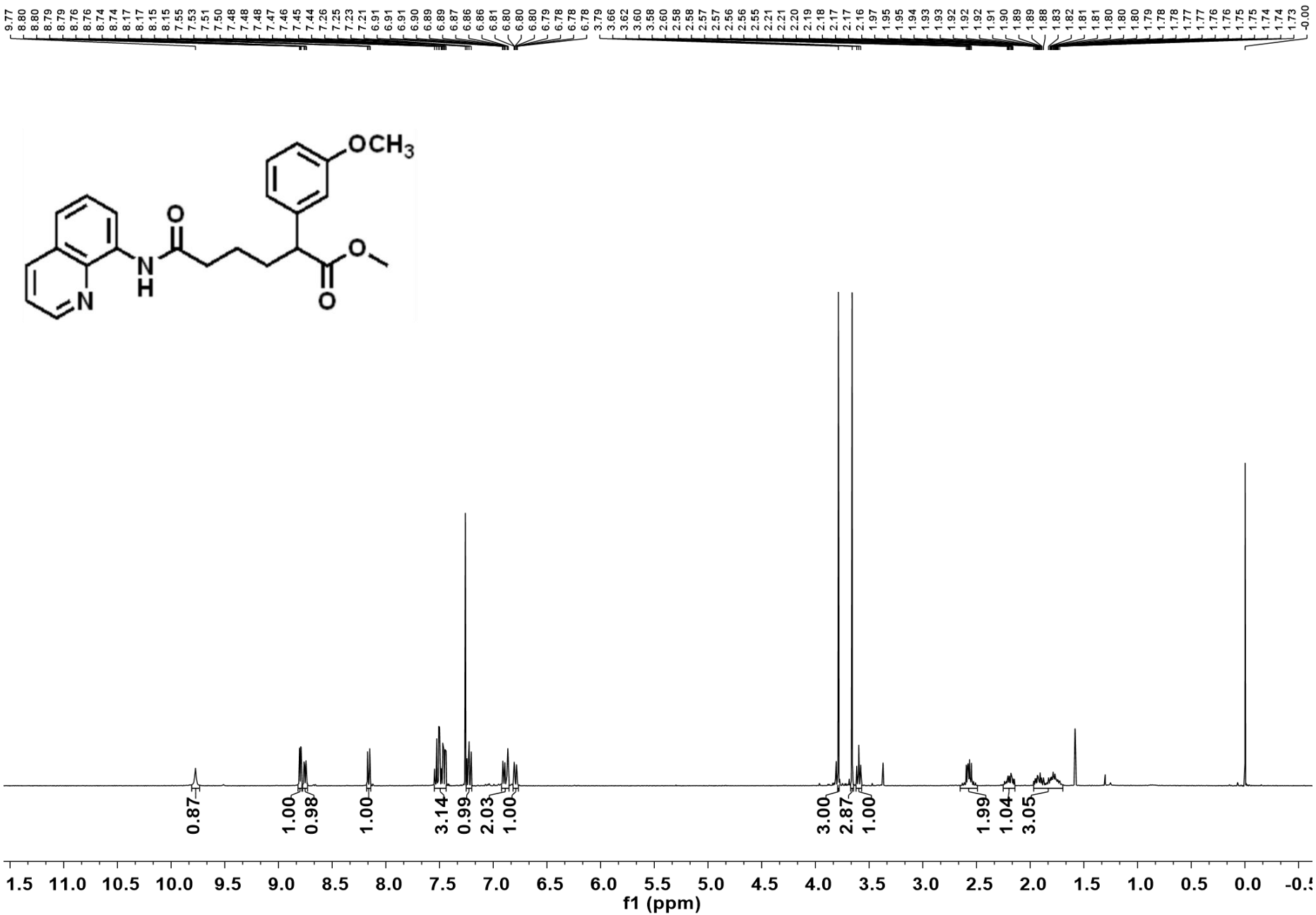
H
O
O
N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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OCH3
O
N
H
O
O
N
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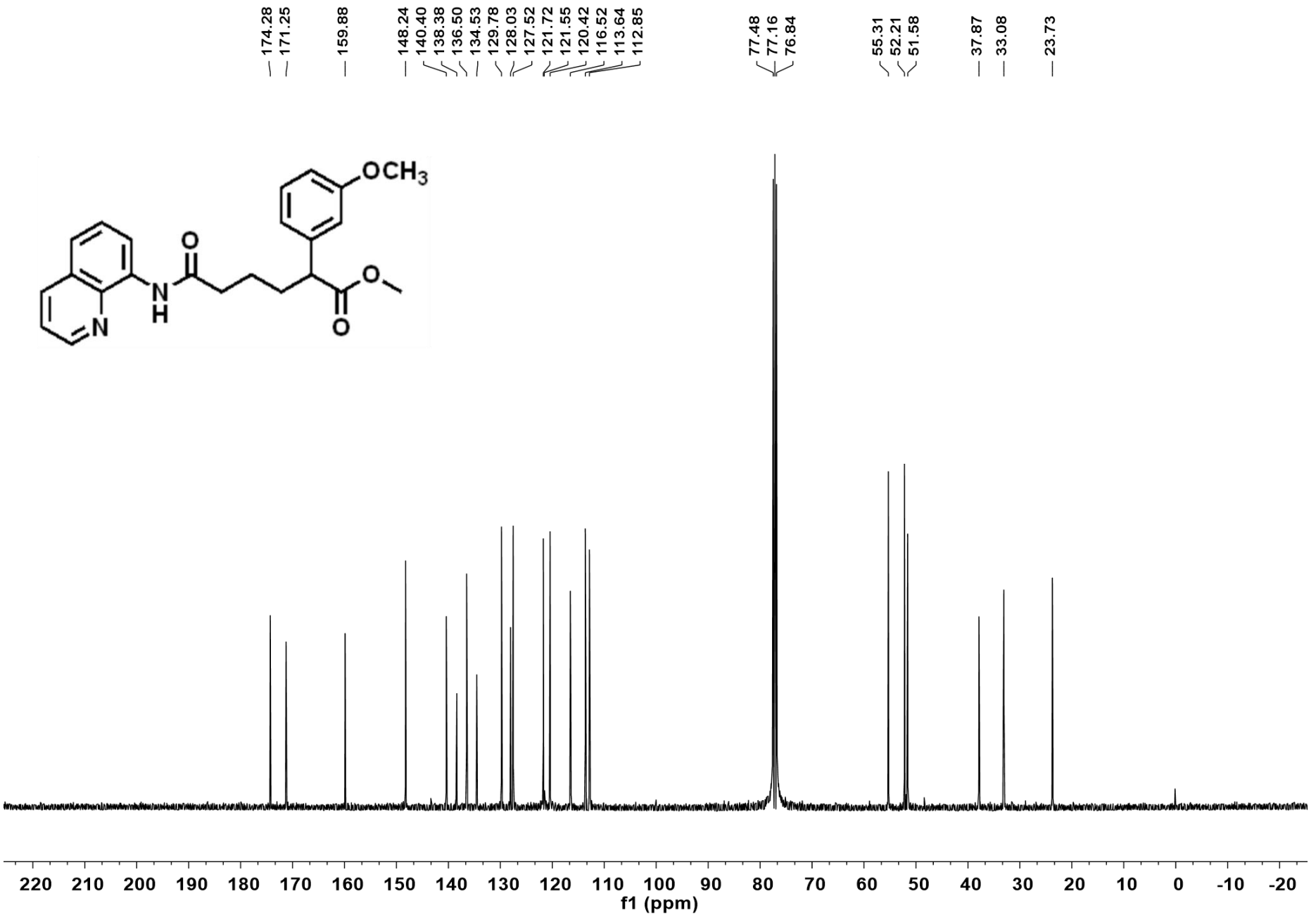
0.98
1.00
3.14
0.99
2.03
1.00
3.00
2.87
1.00
1.99
1.04
3.05
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.52
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121.55
120.42
116.52
113.64
112.85
77.48
77.16
76.84
55.31
52.21
51.58
37.87
33.08
23.73
OCH3
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H
N
O
O
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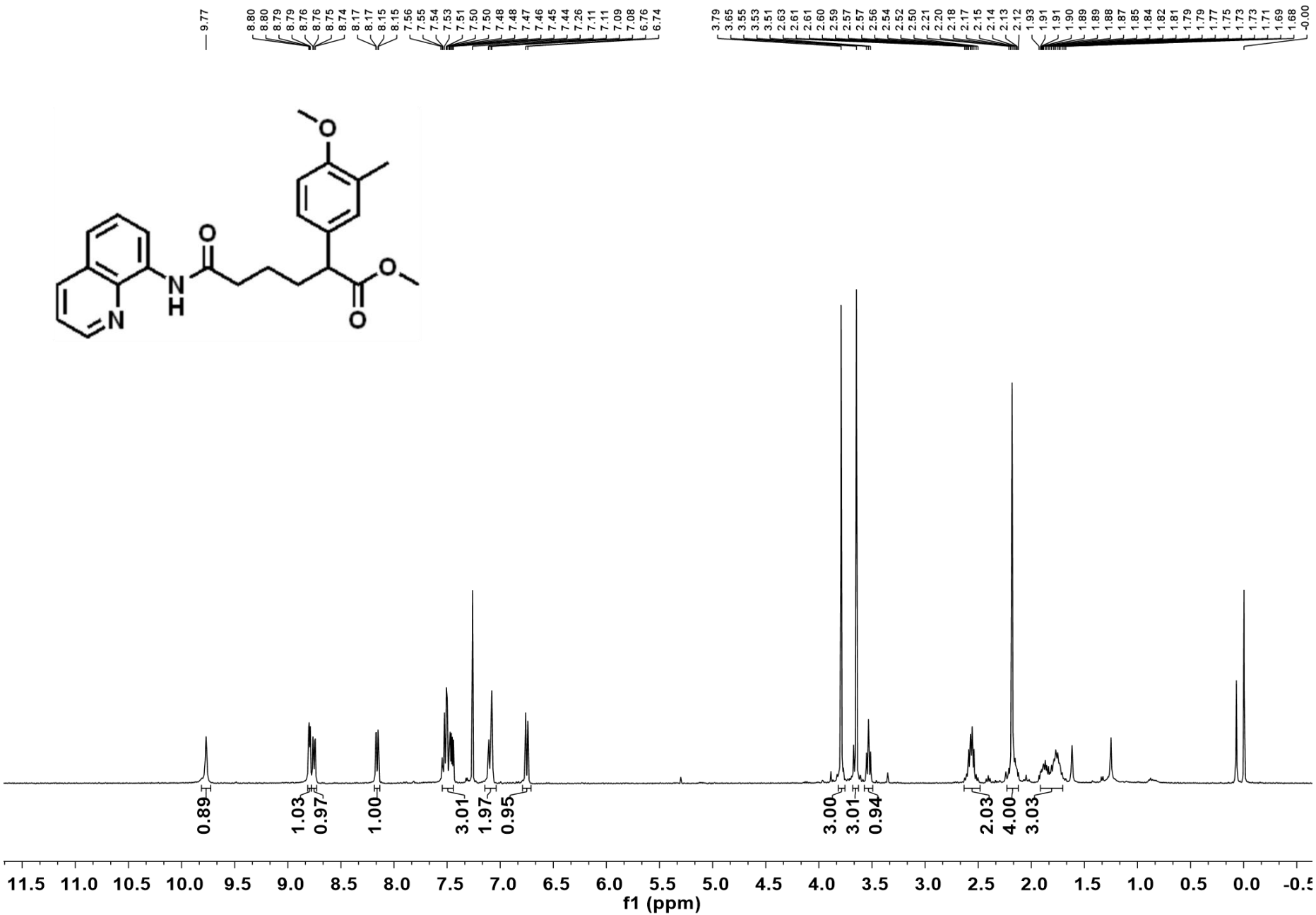
f1 (ppm)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8.15
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7.56
7.55
7.54
7.53
7.51
7.50
7.50
7.48
7.48
7.47
7.46
7.45
7.44
7.26
7.11
7.09
7.08
6.76
6.74
3.79
3.65
3.55
3.53
3.51
2.63
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1.91
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1.90
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1.89
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1.77
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1.73
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1.68
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O
O
N
H
N
O
O
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1.03
0.97
1.00
3.01
1.97
0.95
3.00
3.01
0.94
2.03
4.00
3.03
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
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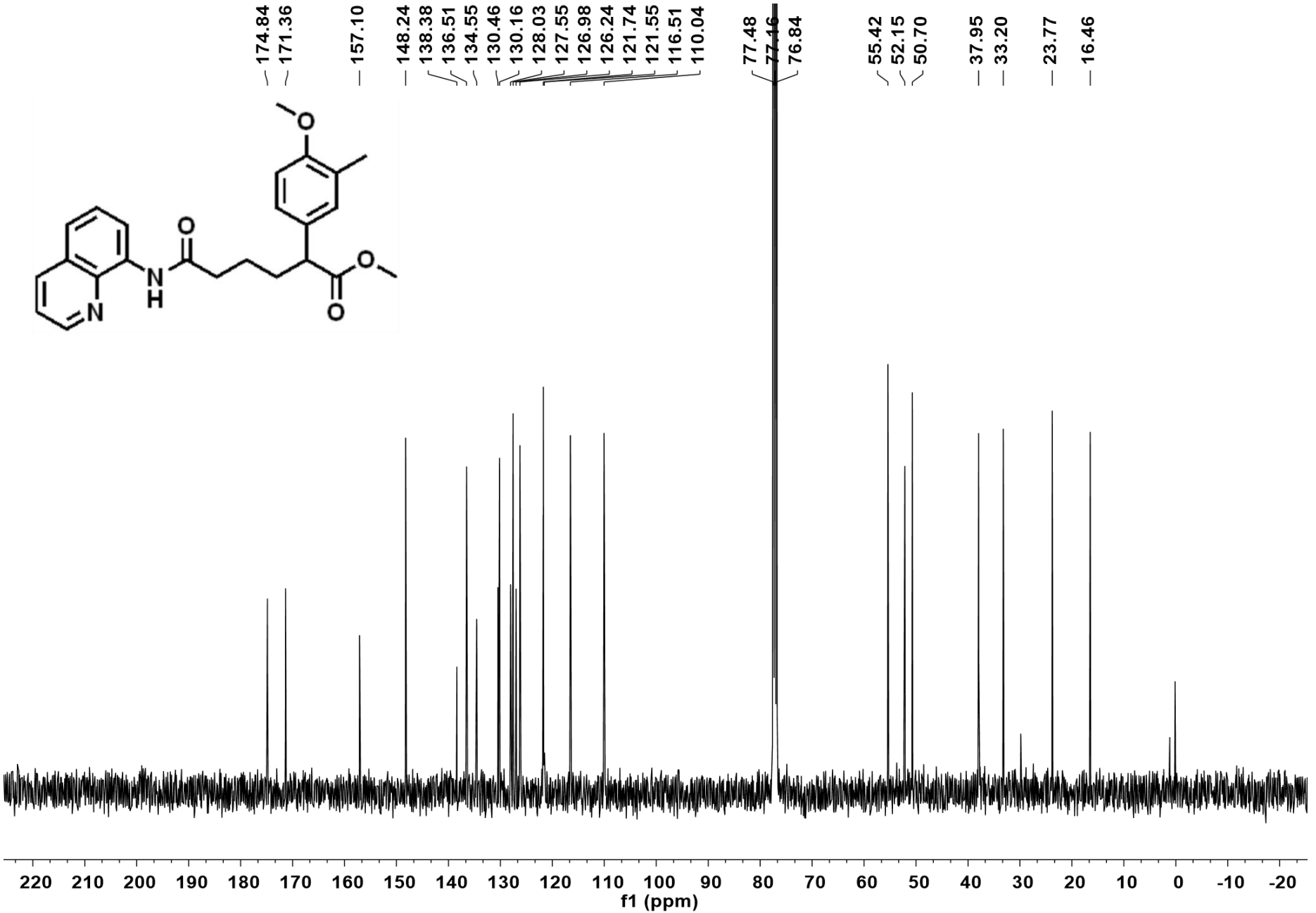
-0.5
f1 (ppm)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130.16
128.03
127.55
126.98
126.24
121.74
121.55
116.51
110.04
77.48
77.16
76.84
55.42
52.15
50.70
37.95
33.20
23.77
16.46
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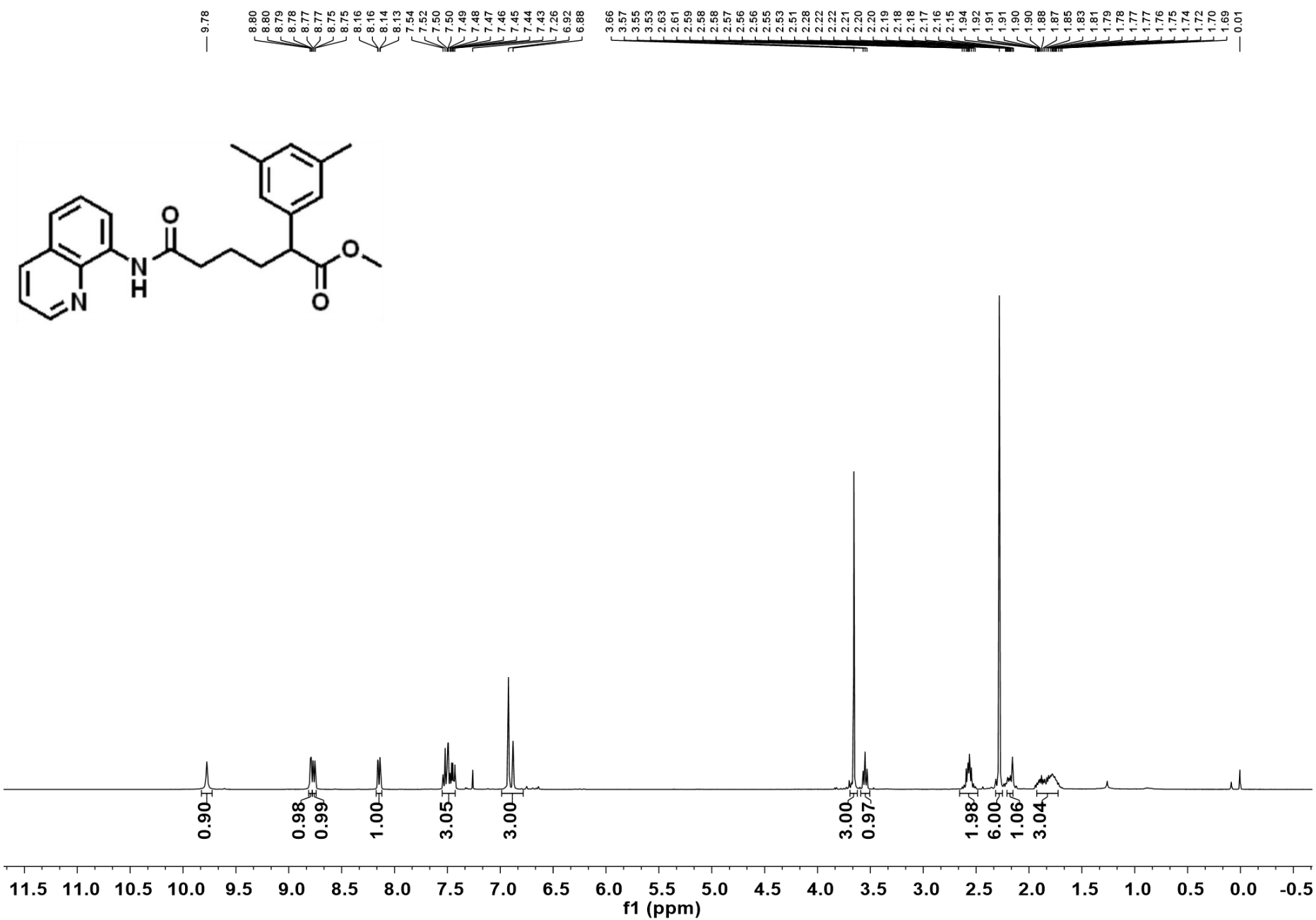
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.52
7.50
7.50
7.49
7.48
7.47
7.46
7.45
7.44
7.43
7.26
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6.88
3.66
3.57
3.55
3.53
2.63
2.61
2.59
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2.57
2.56
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2.53
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1.74
1.72
1.70
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O
N
H
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O
O
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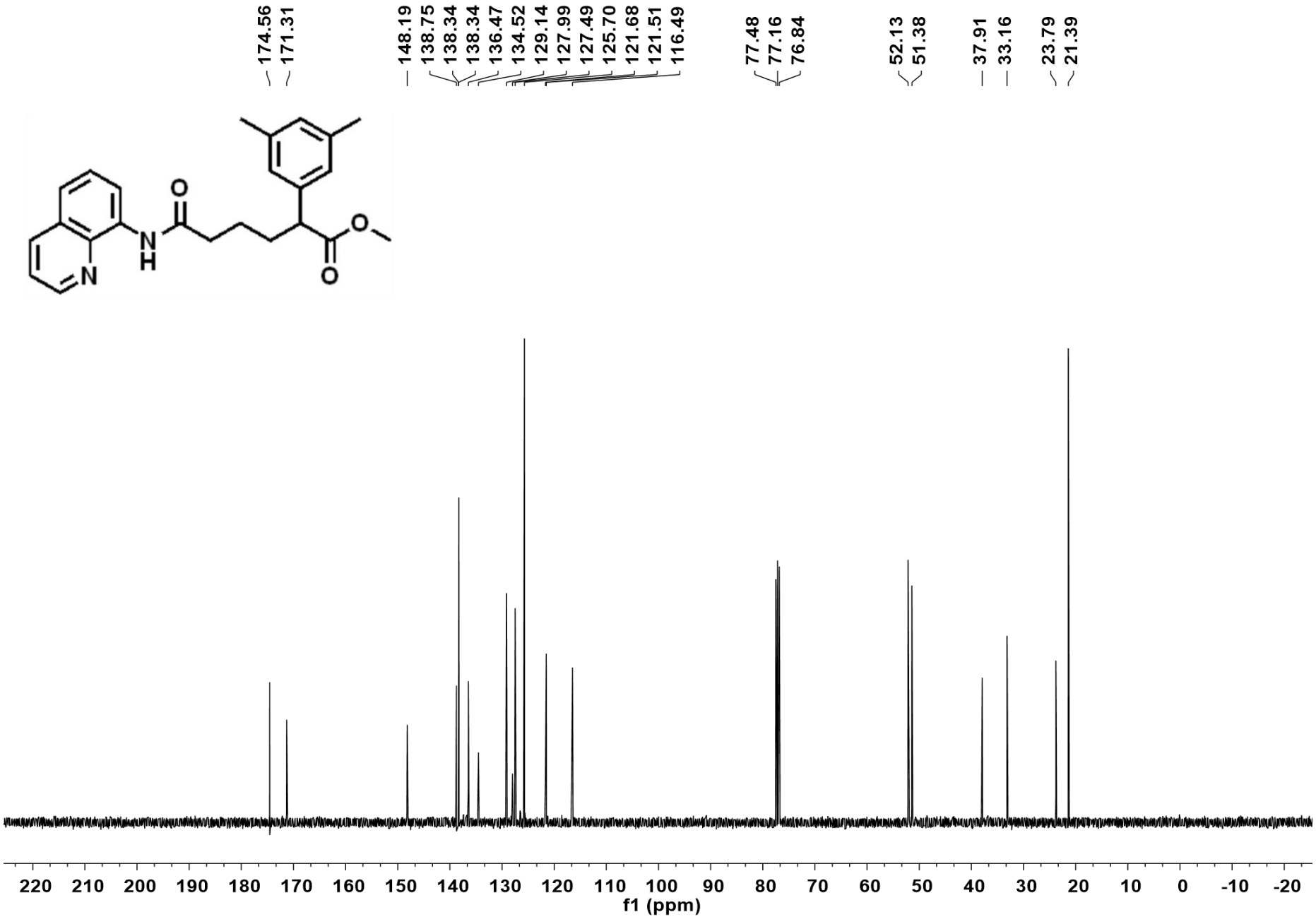
0.98
0.99
1.00
3.05
3.00
3.00
0.97
1.98
6.00
1.06
3.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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121.68
121.51
116.49
77.48
77.16
76.84
52.13
51.38
37.91
33.16
23.79
21.39
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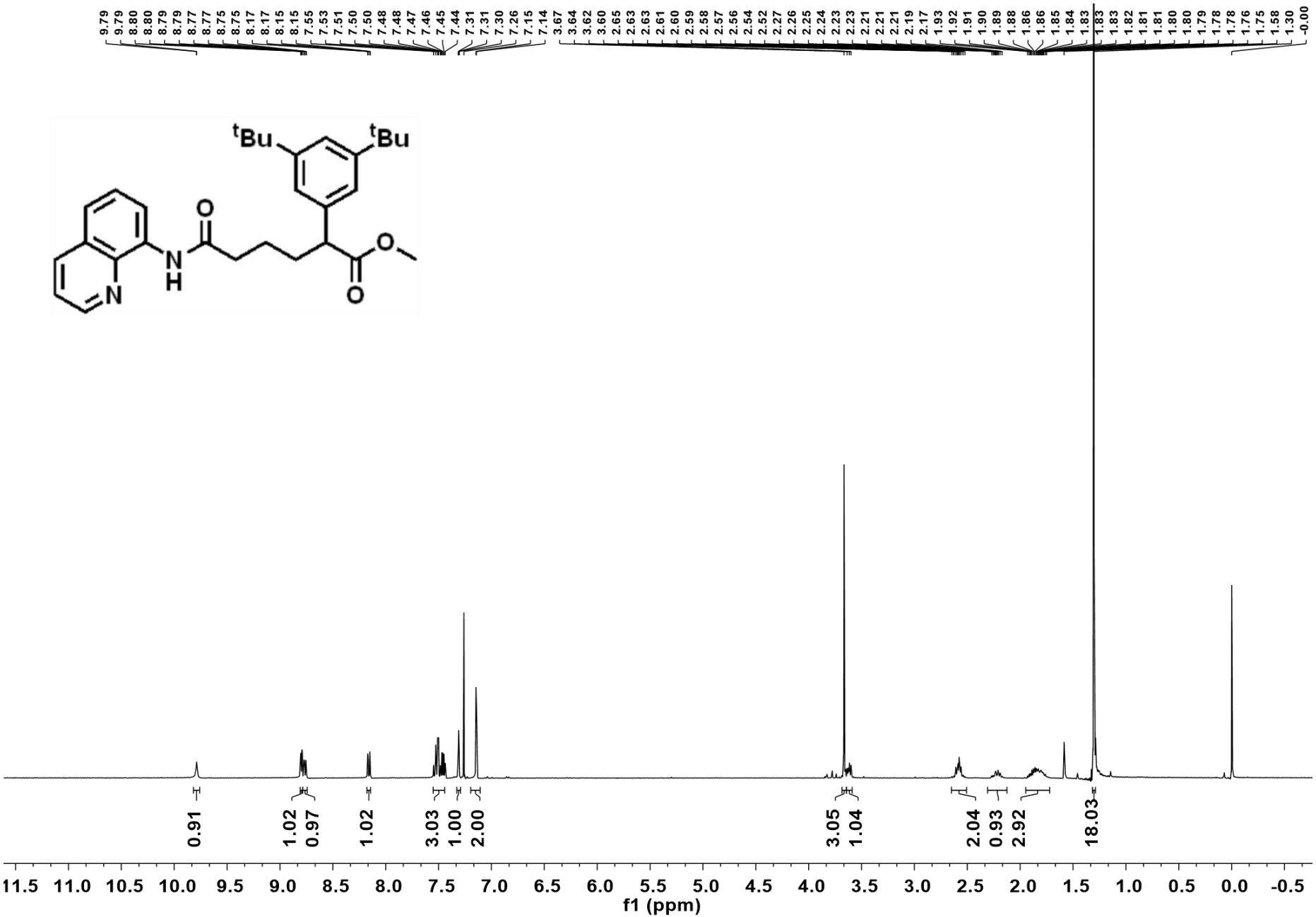
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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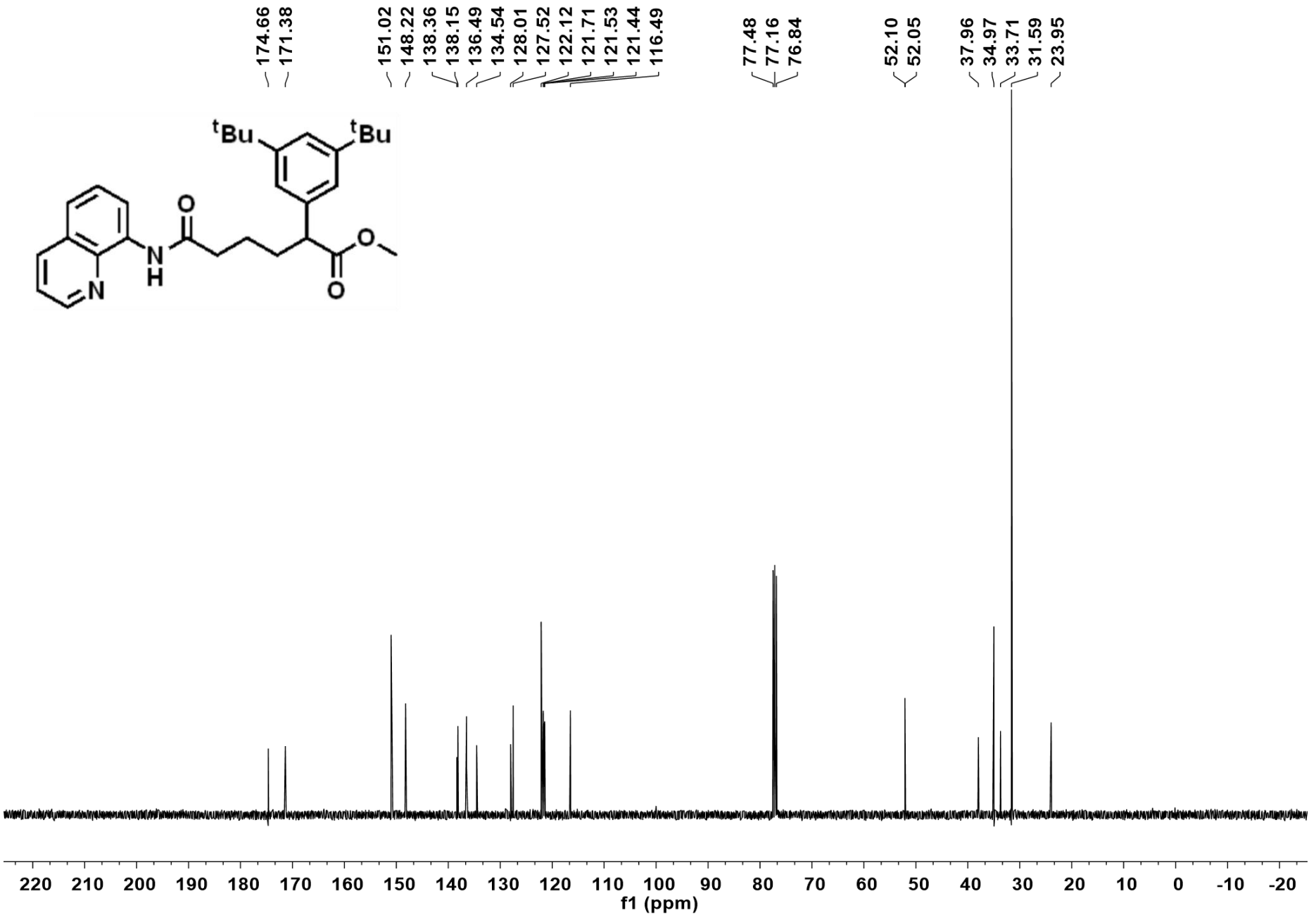
tBu
tBu
O
N
H
O
O
N
0.91
1.02
0.97
1.02
3.03
1.00
2.00
3.05
1.04
2.04
0.93
2.92
18.03
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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33.71
31.59
23.95
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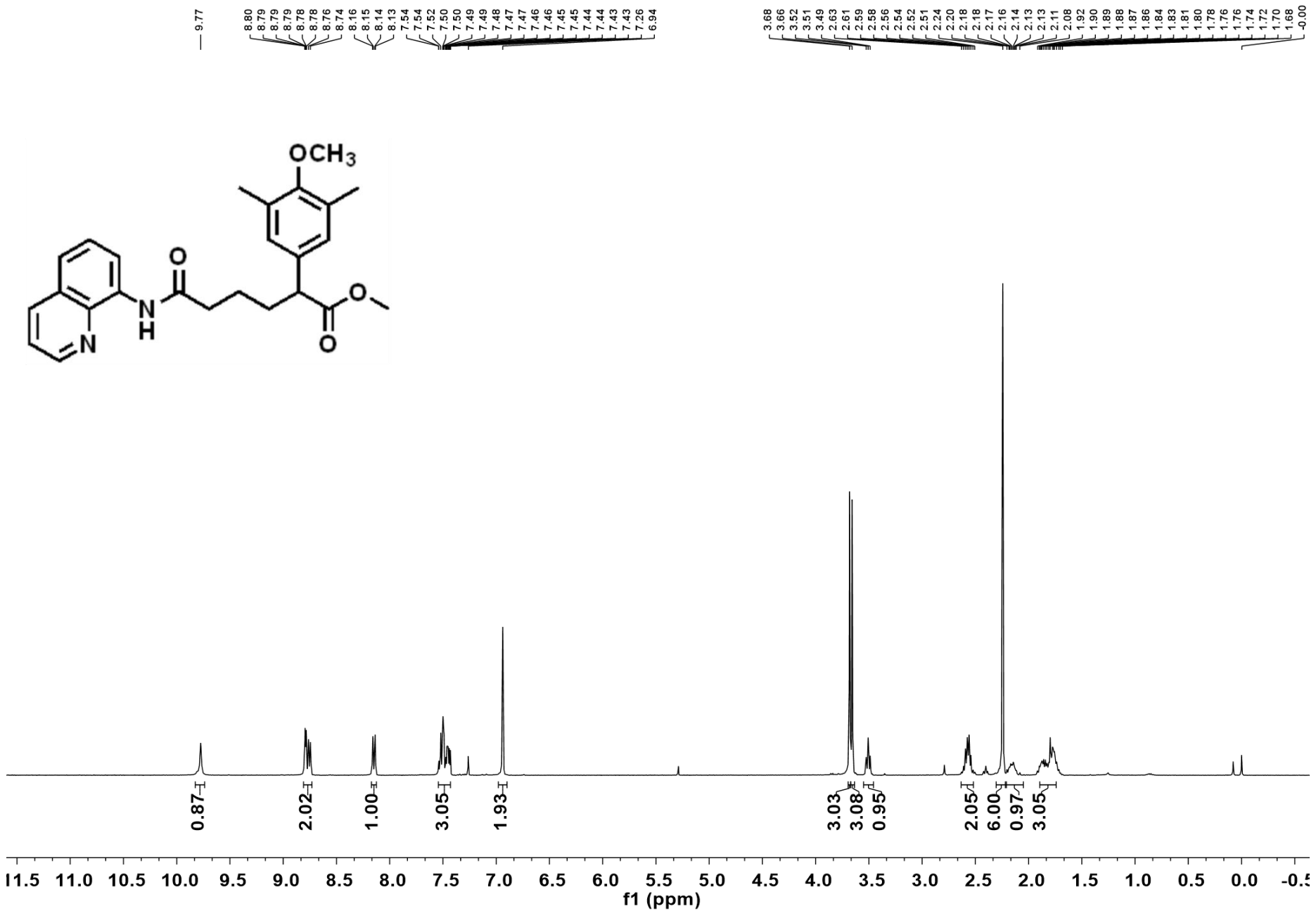
f1 (ppm)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7.54
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1.72
1.70
1.68
-0.00
OCH3
O
N
H
N
O
O
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3.05
1.93
3.03
3.08
0.95
2.05
6.00
0.97
3.05
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10.0
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7.0
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6.0
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2.0
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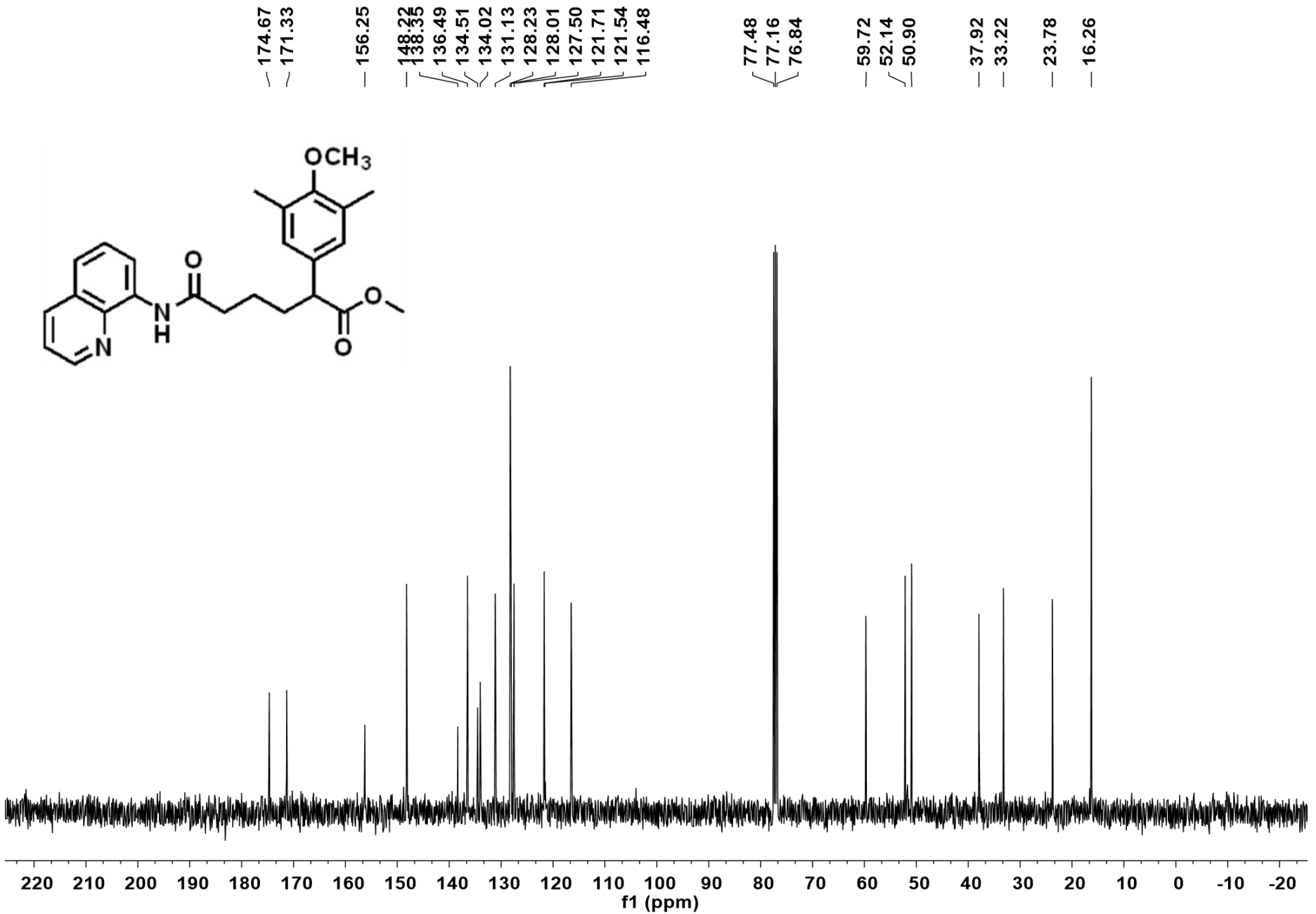
0.5
0.0
-0.5
f1 (ppm)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121.54
116.48
77.48
77.16
76.84
59.72
52.14
50.90
37.92
33.22
23.78
16.26
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H
N
O
O
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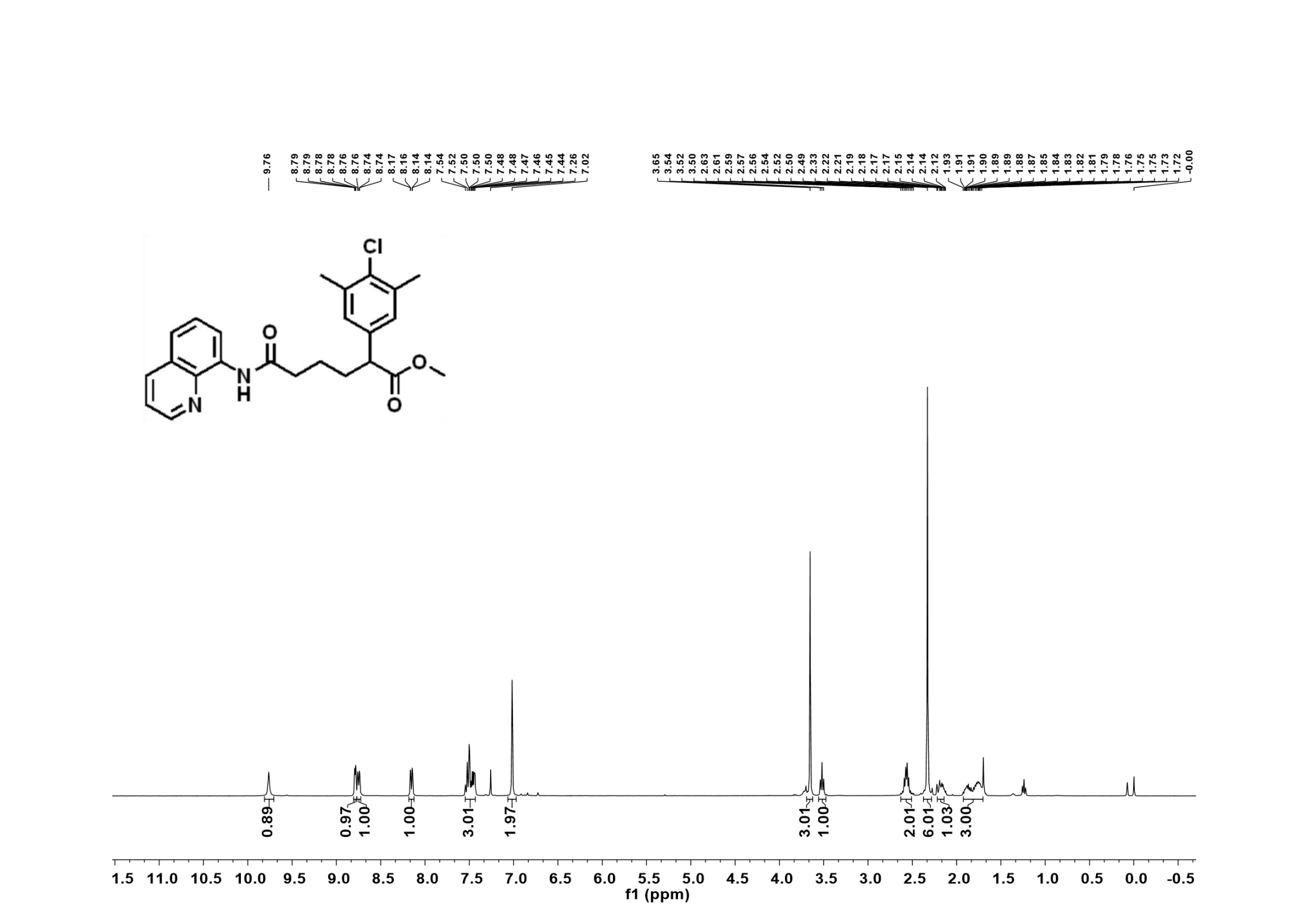
f1 (ppm)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Cl
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1.97
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2.01
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1.03
3.00
1.5
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7.5
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6.0
5.5
5.0
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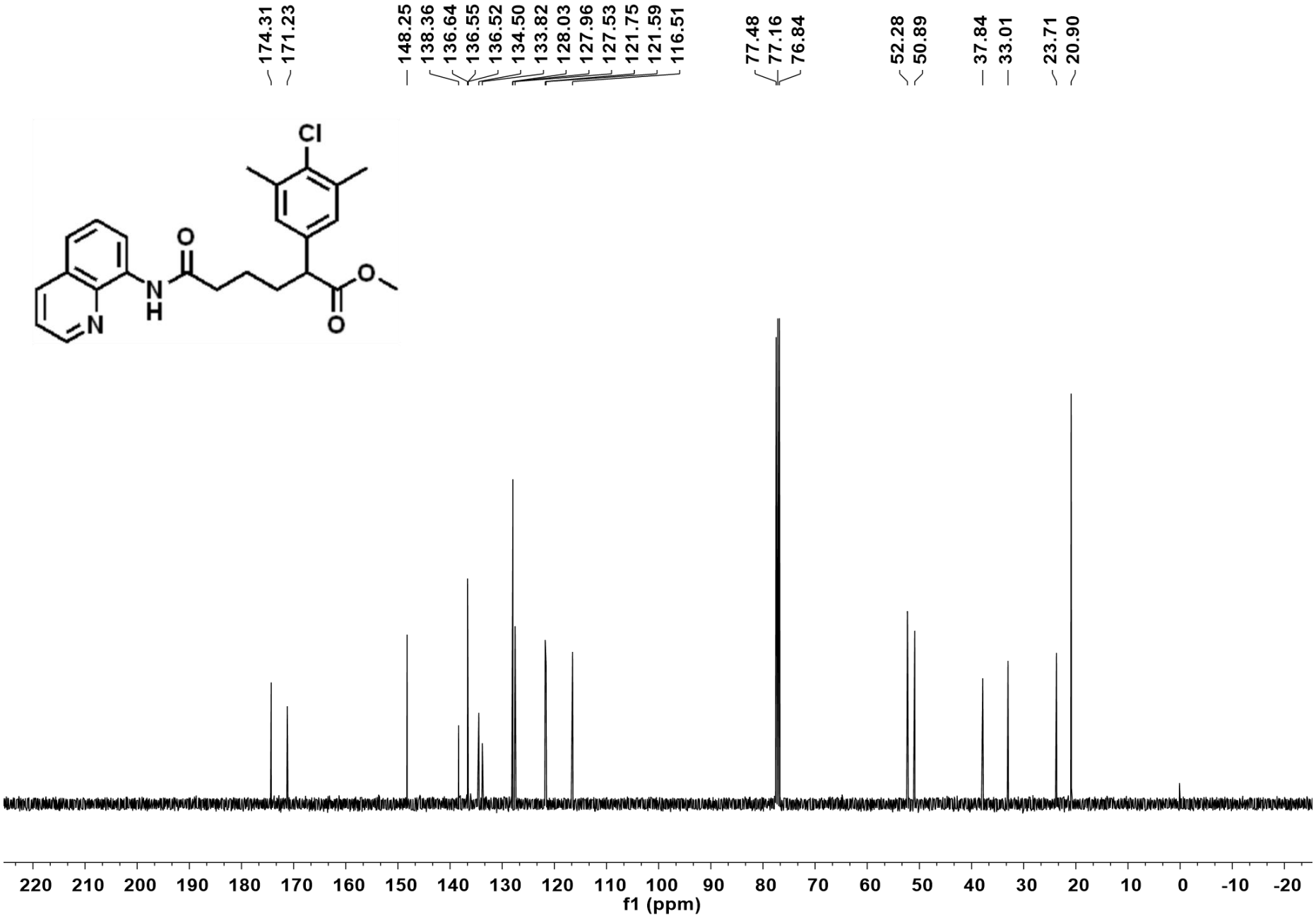
0.5
0.0
-0.5
f1 (ppm)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121.75
121.59
116.51
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77.16
76.84
52.28
50.89
37.84
33.01
23.71
20.90
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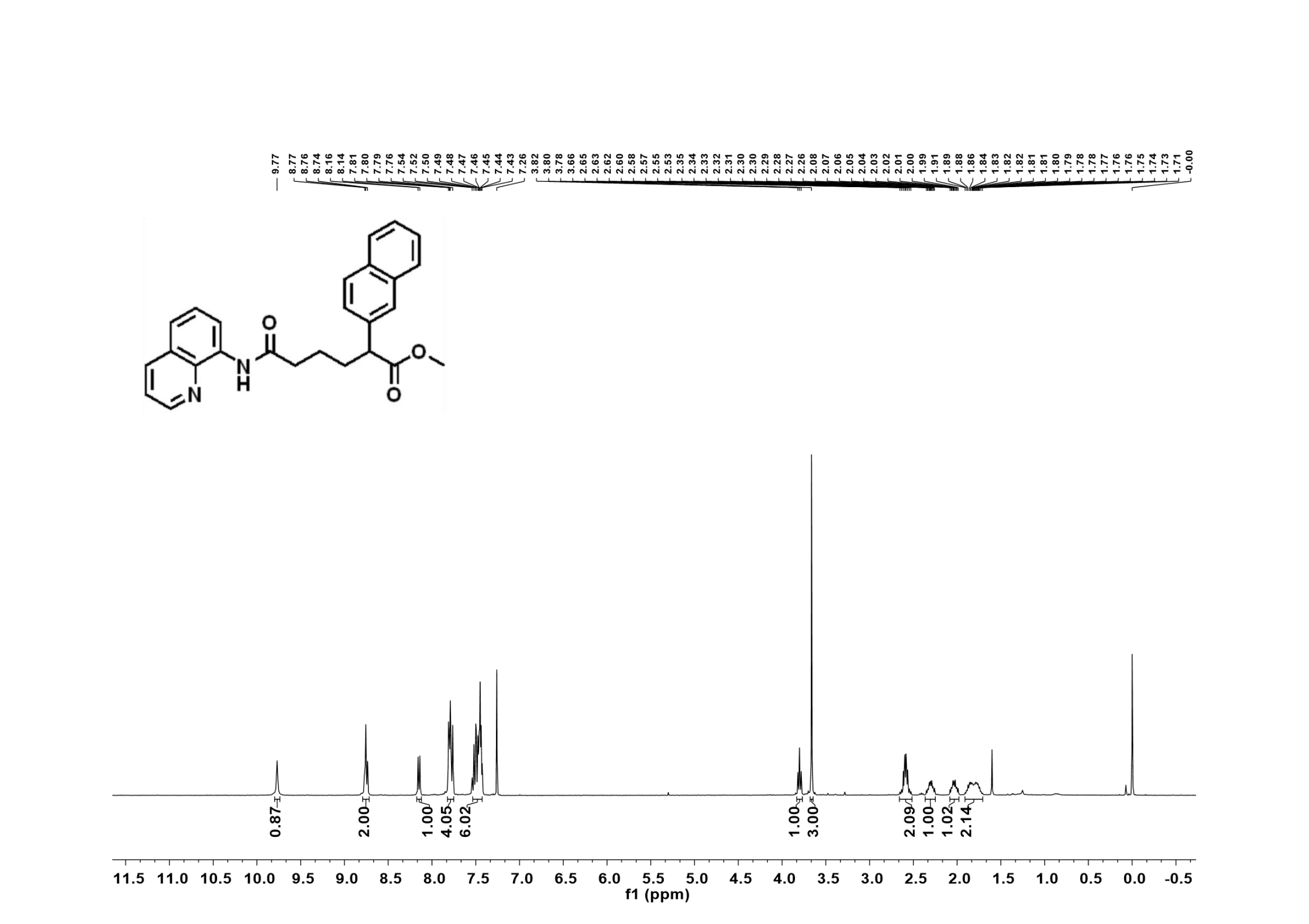
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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1.76
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1.75
1.74
1.73
1.71
-0.00
O
N
H
O
O
N
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1.00
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6.02
1.00
3.00
2.09
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1.02
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
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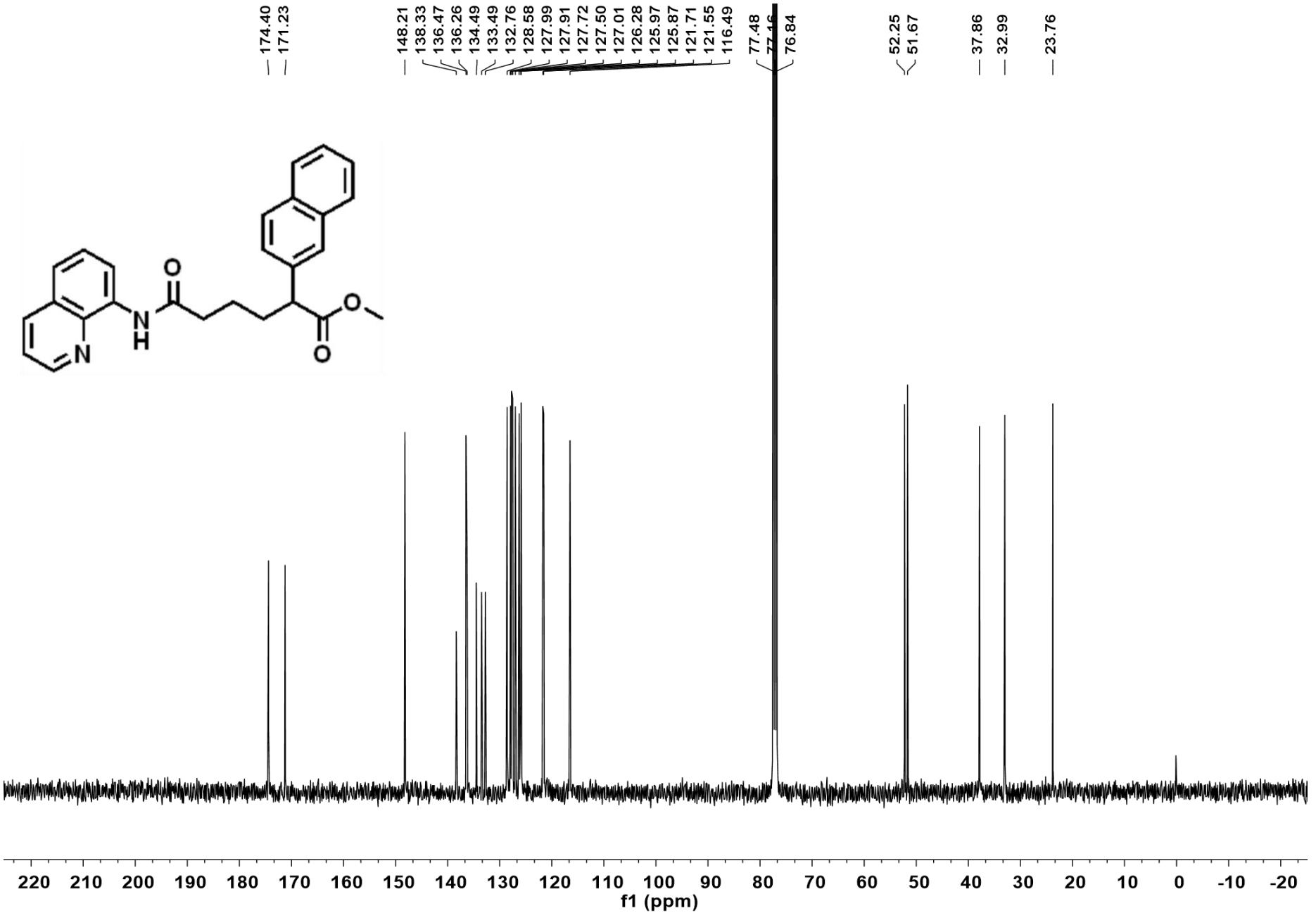
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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125.87
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77.48
77.16
76.84
52.25
51.67
37.86
32.99
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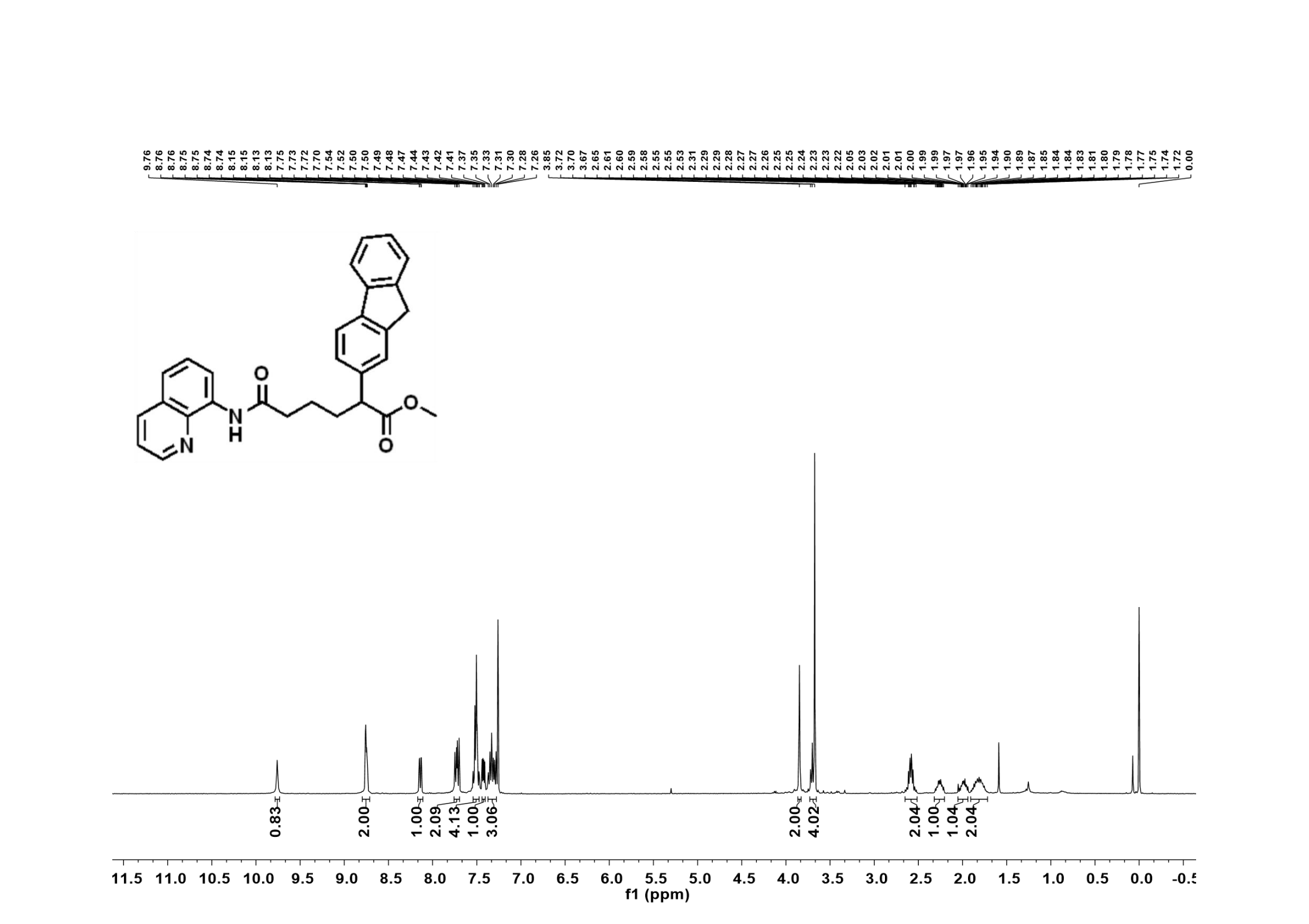
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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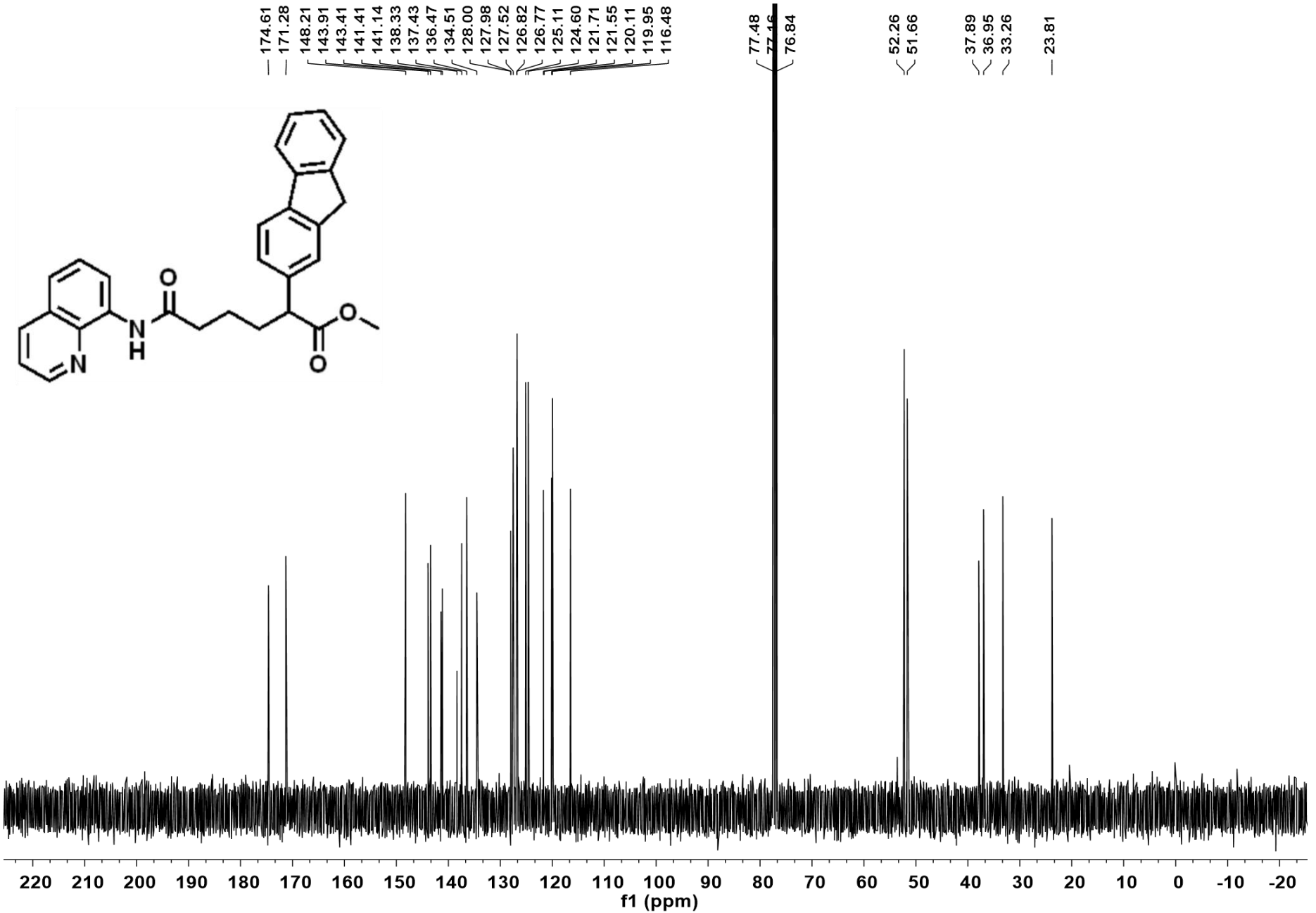
3.85 3.72 3.70 3.67 2.65 2.61 2.60 2.59 2.58 2.55 2.55 2.53 2.31 2.29 2.29 2.28 2.27 2.27 2.26 2.25 2.25 2.24 2.23 2.23 2.22 2.05 2.03 2.02 2.01 2.01 2.00 1.99 1.99 1.97 1.97 1.96 1.95 1.94 1.90 1.89 1.87 1.85 1.84 1.84 1.83 1.81 1.80 1.79 1.78 1.77 1.75 1.74 1.72 0.00
O
N
H
N
O
O
0.83
2.00
1.00
2.09
4.13
1.00
3.06
2.00
4.02
2.04
1.00
1.04
2.04
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
f1 (ppm)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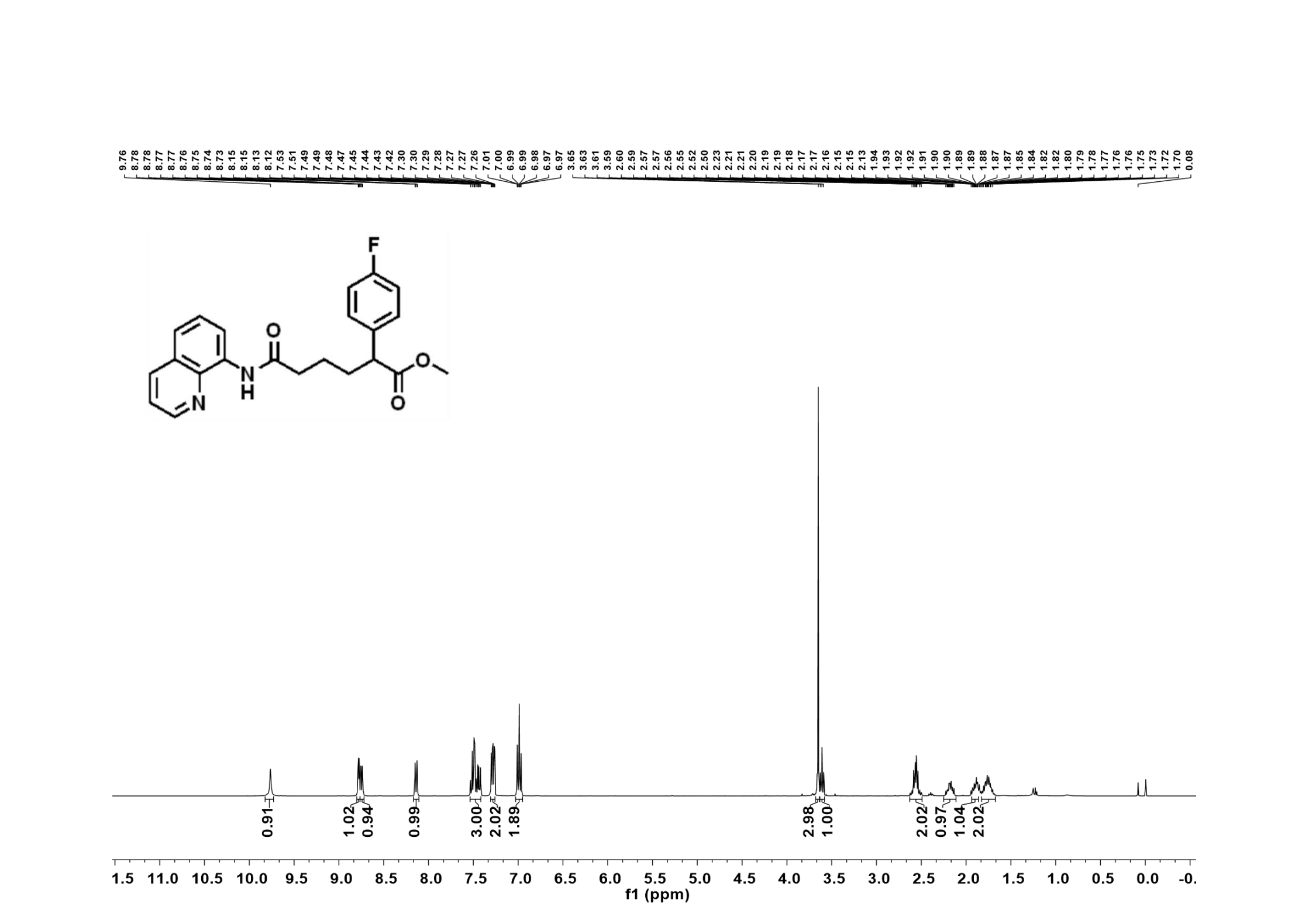
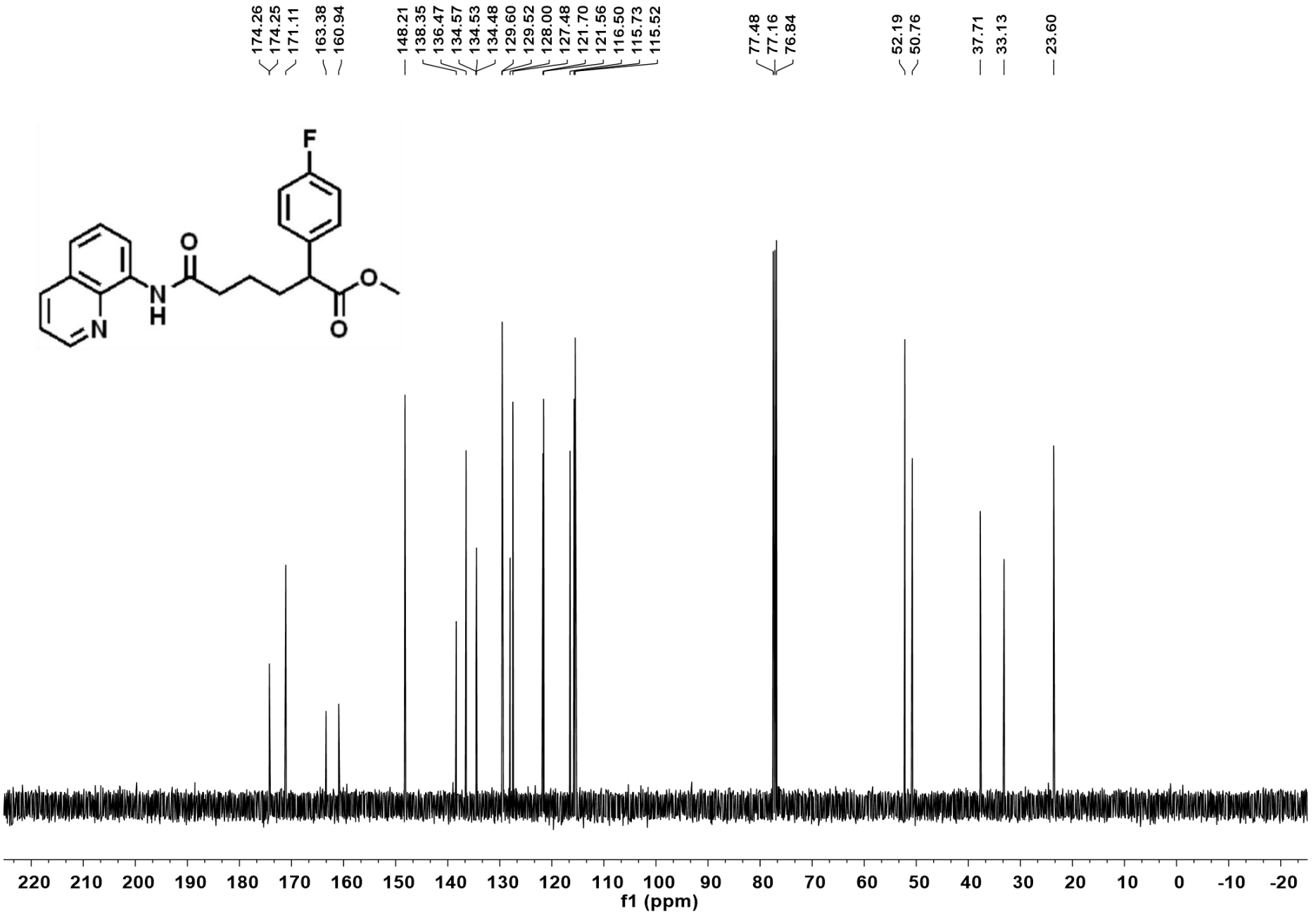
171.28
148.21
143.91
143.41
141.41
141.14
138.33
137.43
136.47
134.51
128.00
127.98
127.52
126.82
126.77
125.11
124.60
121.71
121.55
120.11
119.95
116.48
77.48
77.16
76.84
52.26
51.66
37.89
36.95
33.26
23.81
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


9.76 8.78 8.78 8.77 8.77 8.76 8.75 8.74 8.73 8.15 8.15 8.13 8.12 7.53 7.51 7.49 7.49 7.48 7.47 7.45 7.44 7.43 7.42 7.30 7.30 7.29 7.28 7.27 7.27 7.26 7.01 7.00 6.99 6.99 6.98 6.97 6.97
3.65 3.63 3.61 3.59 2.60 2.59 2.57 2.57 2.56 2.55 2.52 2.50 2.23 2.21 2.21 2.20 2.19 2.19 2.18 2.17 2.17 2.16 2.15 2.15 2.13 1.94 1.93 1.92 1.92 1.91 1.90 1.90 1.89 1.89 1.88 1.87 1.87 1.85 1.84 1.82 1.82 1.80 1.79 1.78 1.77 1.76 1.76 1.75 1.73 1.72 1.70 0.08
F
O
N
H
N
O
O
0.91
1.02
0.94
0.99
3.00
2.02
1.89
2.98
1.00
2.02
0.97
1.04
2.02
1.5 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.
f1 (ppm)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174.25
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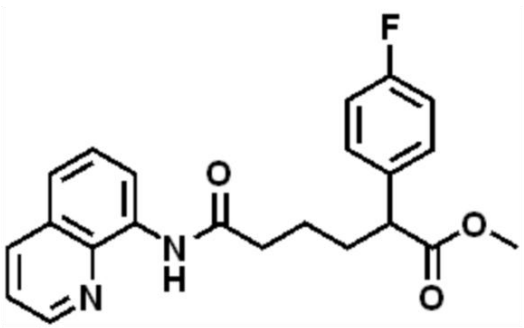
136.47
134.57
134.53
134.48
129.60
129.52
128.00
127.48
121.70
121.56
116.50
115.73
115.52
77.48
77.16
76.84
52.19
50.76
37.71
33.13
23.60
F
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)



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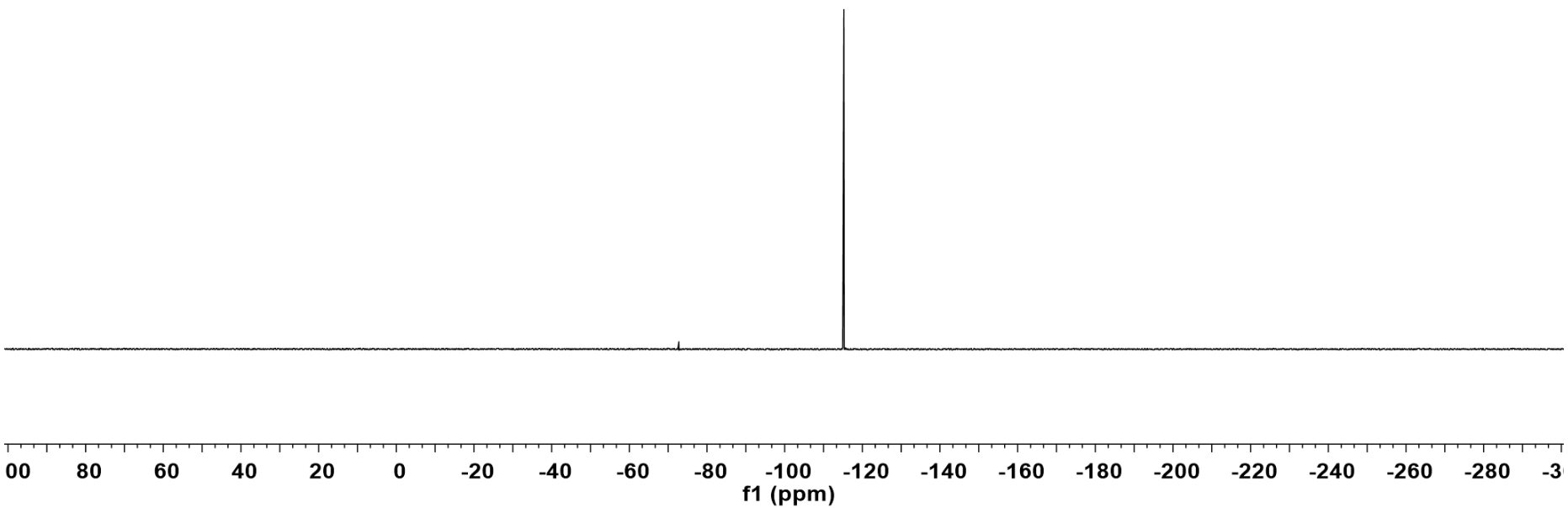
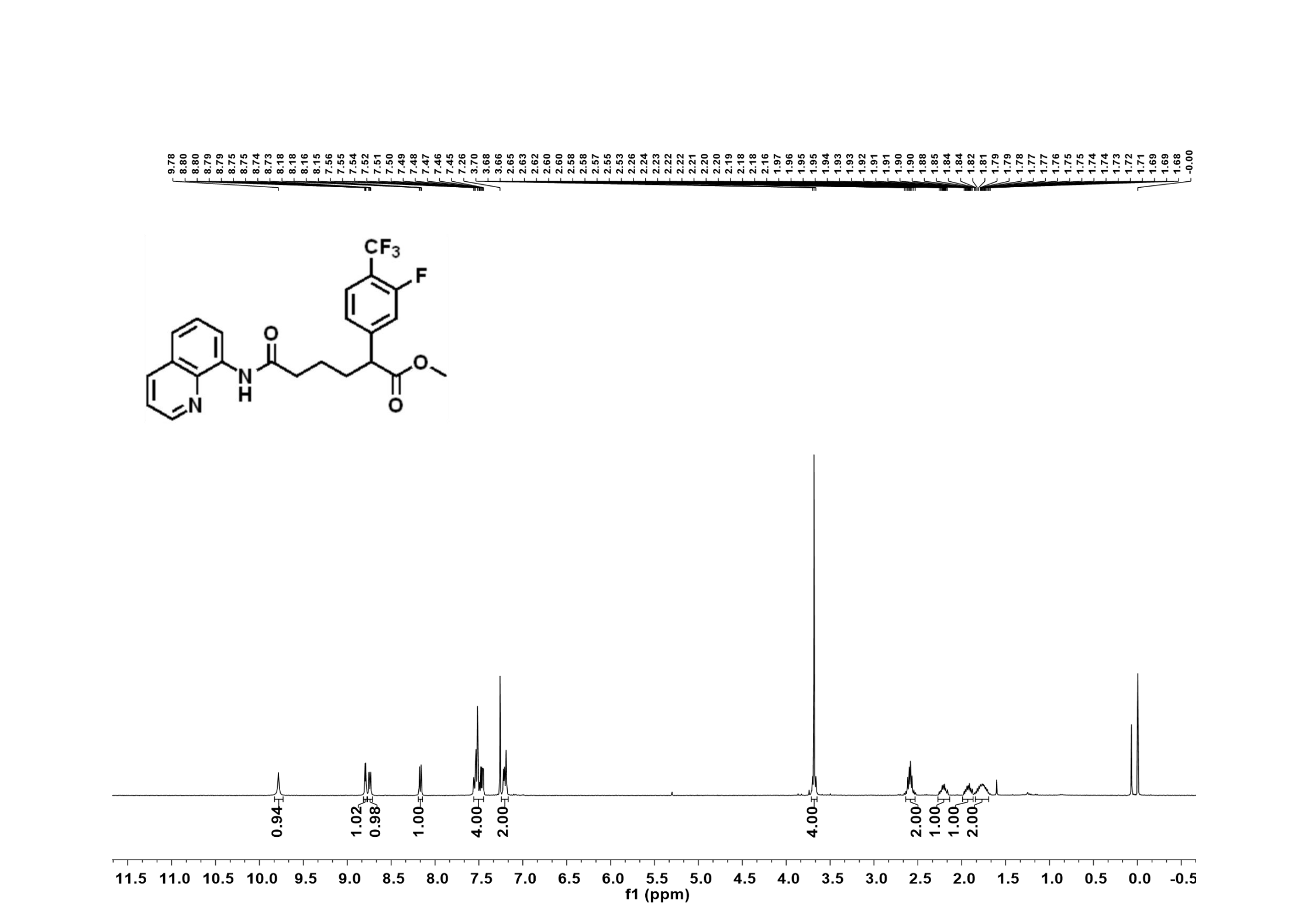
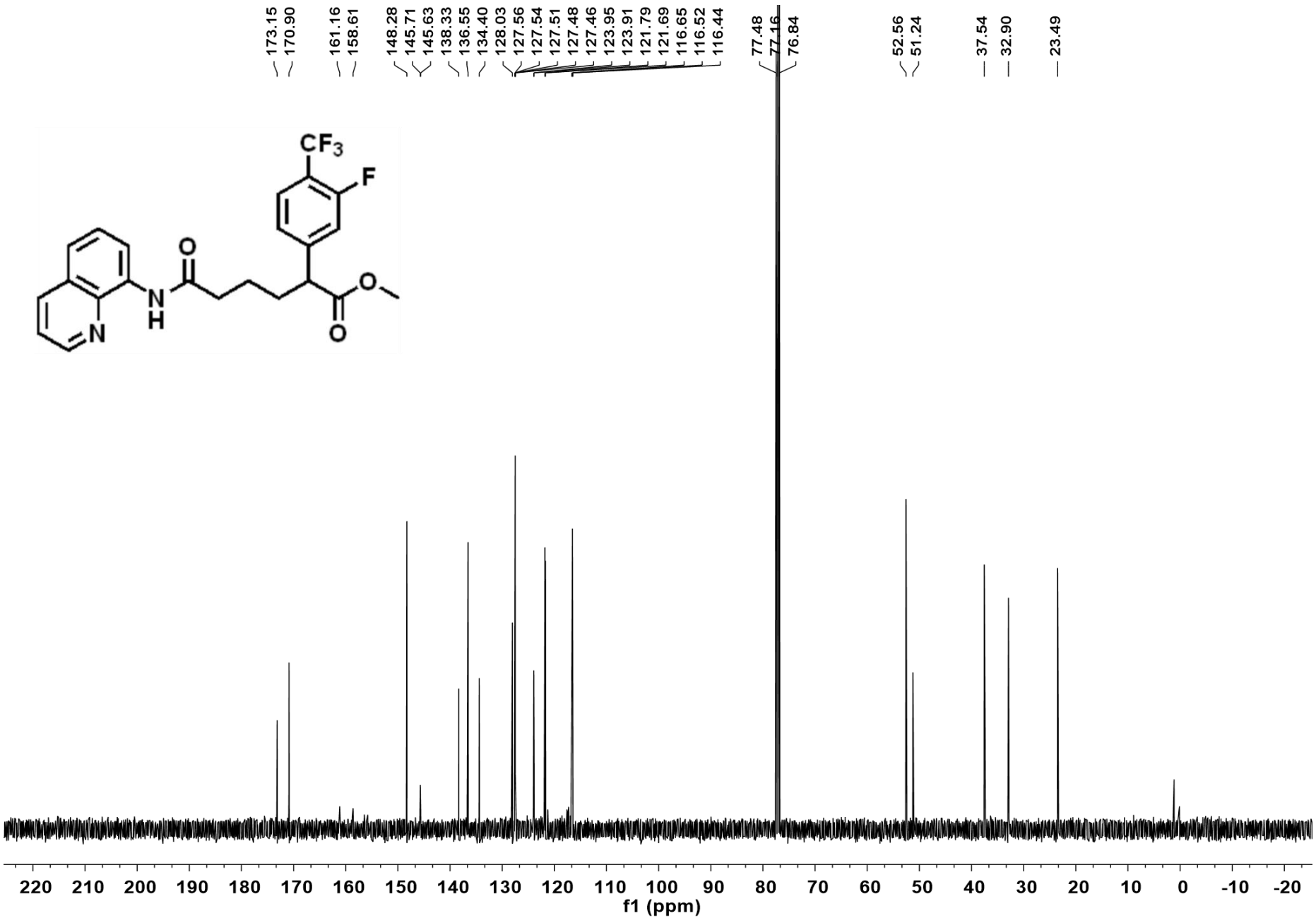
-115.22
-115.23
-115.24
-115.25
-115.25
-115.26
-115.27
-115.28




9.78 8.80 8.80 8.79 8.79 8.75 8.75 8.74 8.73 8.18 8.18 8.16 8.15 7.56 7.55 7.54 7.52 7.51 7.50 7.49 7.48 7.47 7.46 7.45 7.26 3.70 3.68 3.66 2.65 2.63 2.62 2.60 2.60 2.58 2.58 2.57 2.55 2.53 2.26 2.24 2.23 2.22 2.22 2.21 2.20 2.20 2.19 2.18 2.18 2.16 1.97 1.96 1.95 1.95 1.94 1.93 1.93 1.92 1.91 1.91 1.90 1.90 1.88 1.85 1.84 1.84 1.82 1.81 1.79 1.79 1.78 1.77 1.77 1.76 1.75 1.75 1.74 1.74 1.73 1.72 1.71 1.69 1.69 1.68 -0.00
CF3
F
O
N
H
O
O
N
0.94
1.02
0.98
1.00
4.00
2.00
4.00
2.00
1.00
1.00
2.00
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
f1 (ppm)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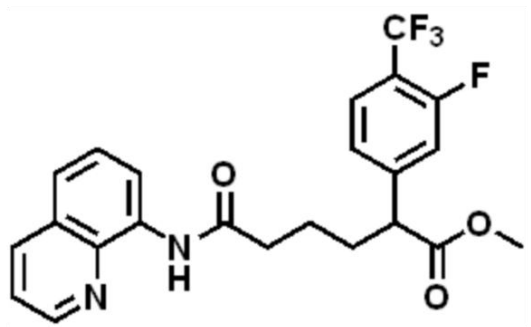
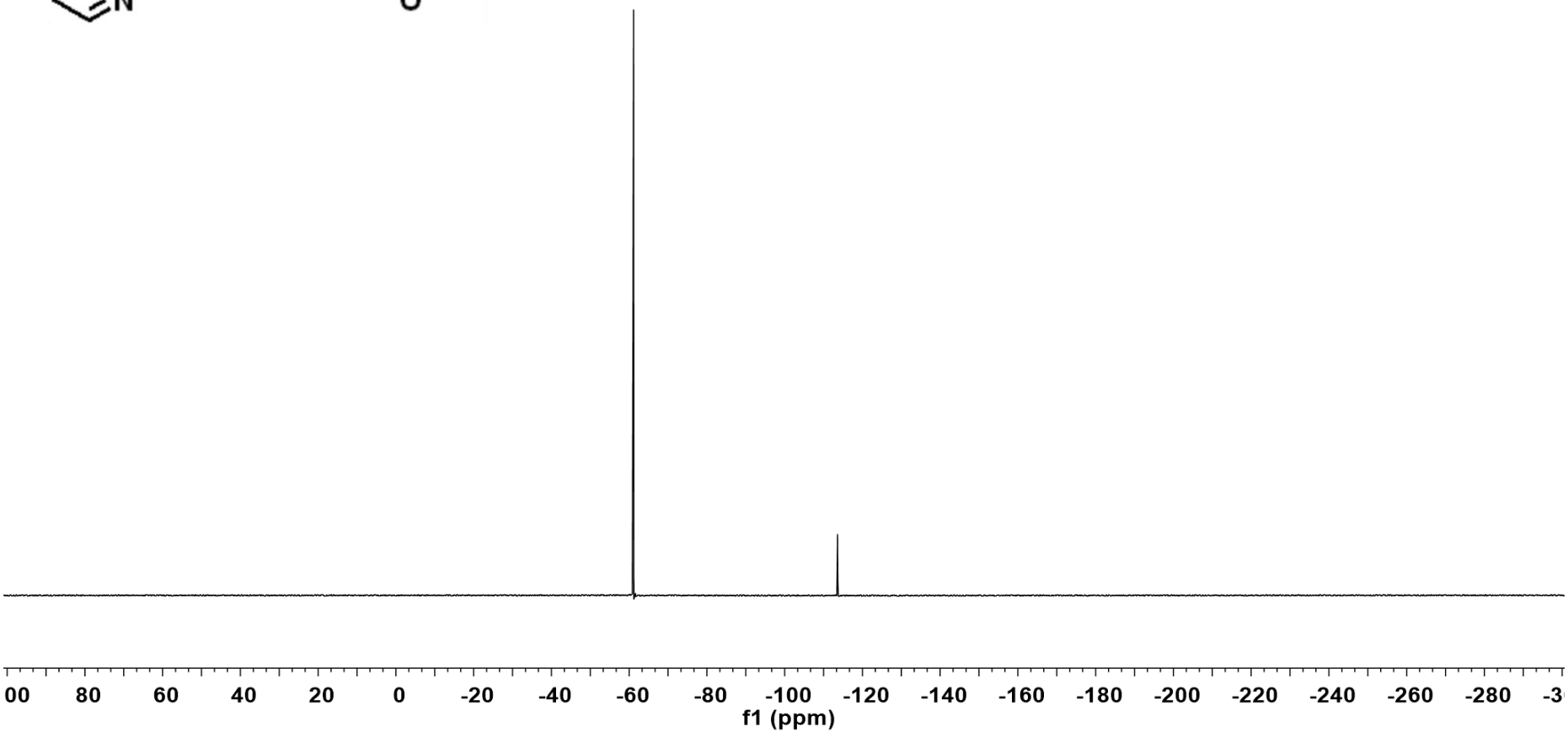
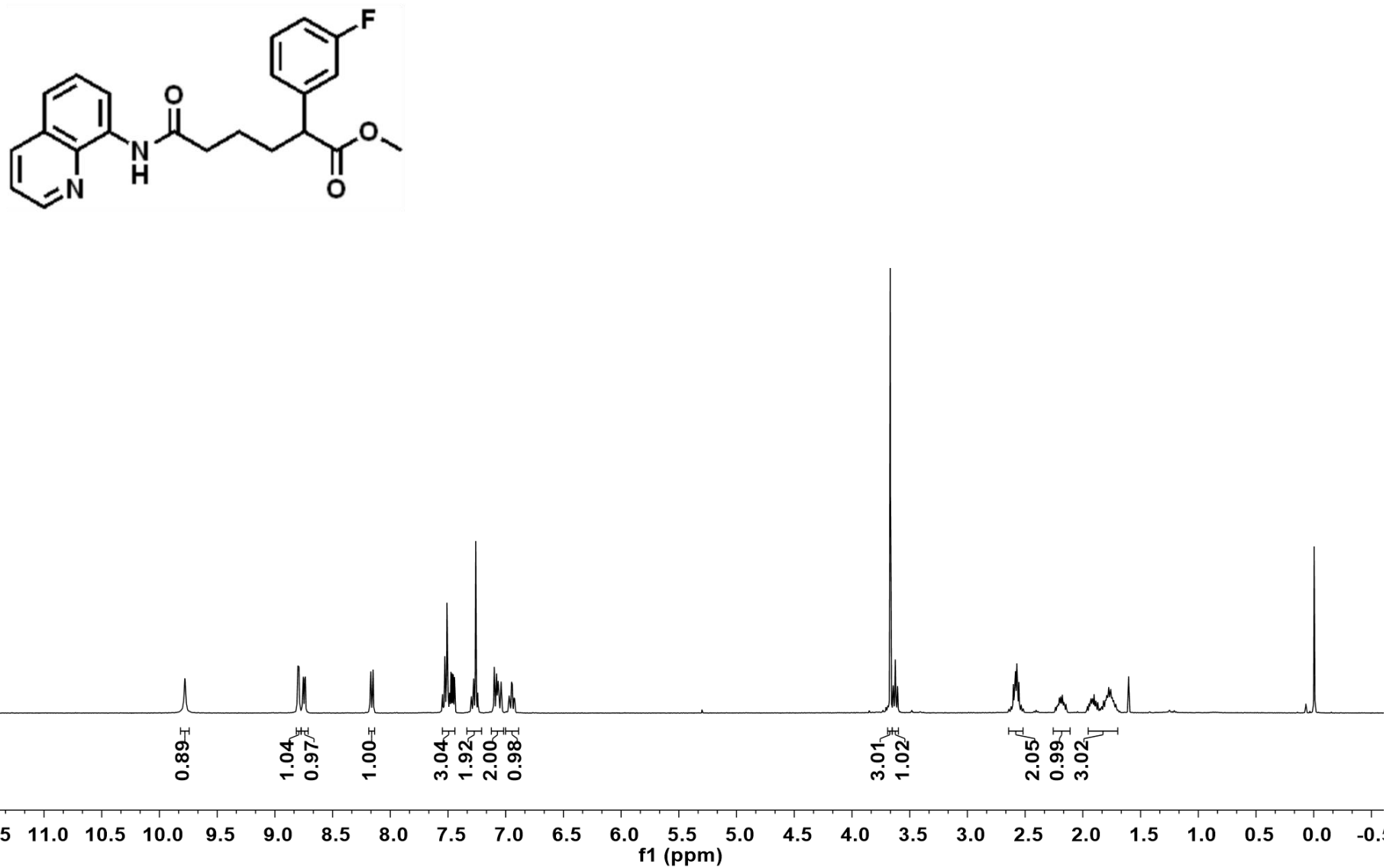
170.90
161.16
158.61
148.28
145.71
145.63
138.33
136.55
134.40
128.03
127.56
127.54
127.51
127.48
127.46
123.95
123.91
121.79
121.69
116.65
116.52
116.44
77.48
77.16
76.84
52.56
51.24
37.54
32.90
23.49
CF3
F
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

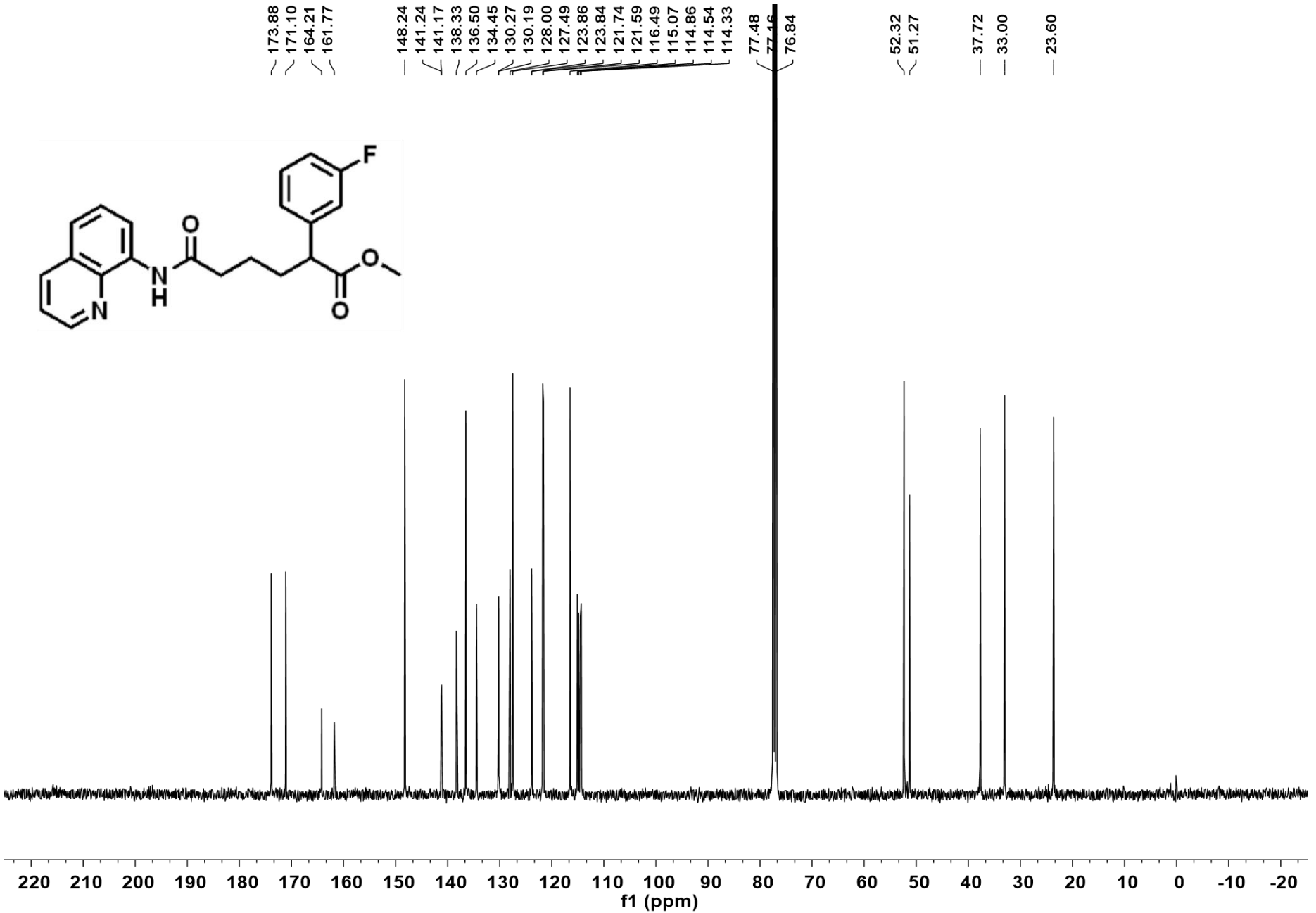


-61.15
-61.18

-113.54
-113.58
-113.60
-113.61
-113.63
-113.64
-113.66
-113.69




9.78 8.80 8.80 8.79 8.79 8.76 8.75 8.74 8.74 8.17 8.17 8.15 8.15 7.55 7.53 7.51 7.50 7.49 7.48 7.47 7.47 7.45 7.44 7.30 7.28 7.26 7.24 7.10 7.08 7.07 7.06 7.04 6.97 6.96 6.95 6.94 6.93 6.92 3.67 3.64 3.62 3.61 2.64 2.62 2.60 2.59 2.58 2.57 2.56 2.55 2.54 2.53 2.52 2.24 2.22 2.22 2.21 2.20 2.20 2.19 2.18 2.18 2.17 2.17 2.16 2.15 1.96 1.95 1.94 1.94 1.93 1.92 1.92 1.90 1.90 1.89 1.87 1.85 1.84 1.84 1.82 1.80 1.79 1.78 1.76 1.75 1.73 1.72 1.70 1.70 1.68 -0.00
F
O
N
H
N
O
O
0.89
1.04
0.97
1.00
3.04
1.92
2.00
0.98
3.01
1.02
2.05
0.99
3.02
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
f1 (ppm)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171.10
164.21
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141.24
141.17
138.33
136.50
134.45
130.27
130.19
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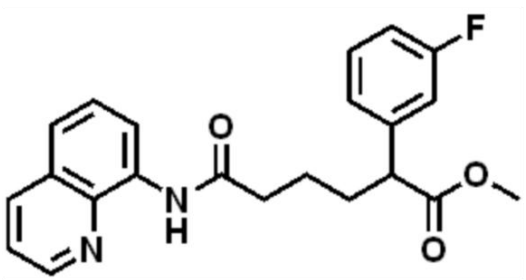
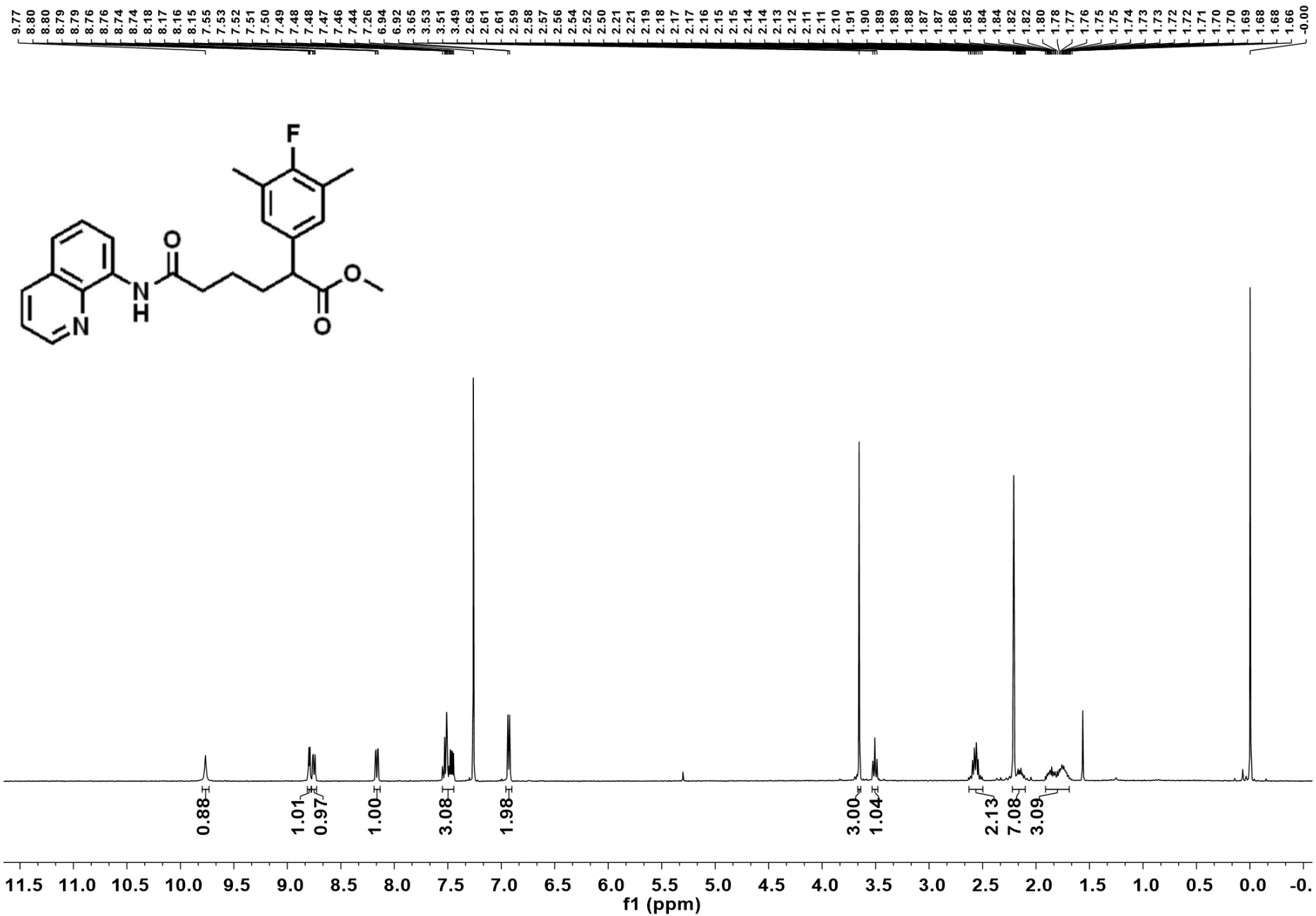
127.49
123.86
123.84
121.74
121.59
116.49
115.07
114.86
114.54
114.33
77.48
77.16
76.84
52.32
51.27
37.72
33.00
23.60
F
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

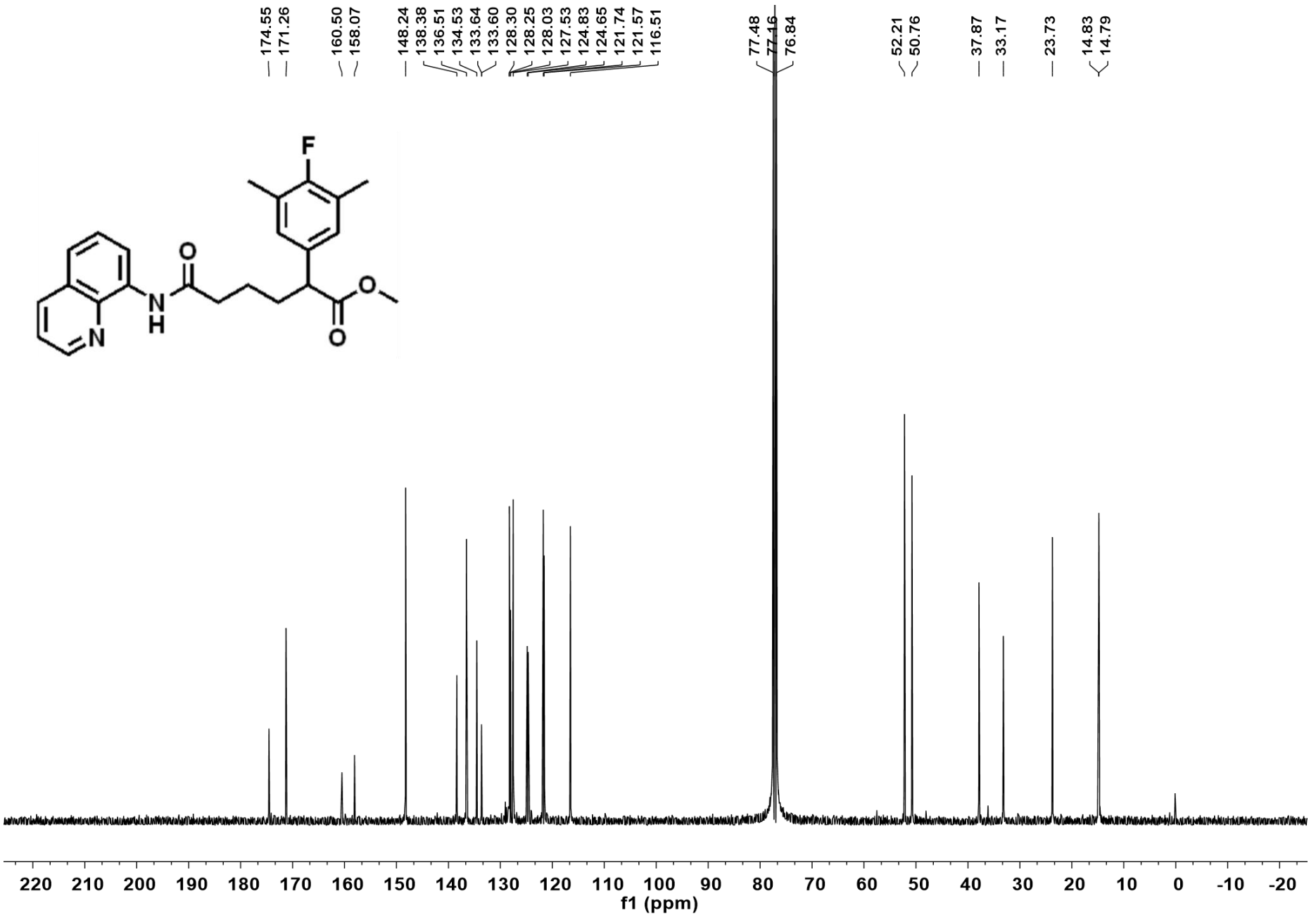


-112.55
-112.56
-112.57
-112.59
-112.60
-112.61

100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300

f1 (ppm)


9.77 8.80 8.80 8.79 8.79 8.76 8.76 8.74 8.74 8.18 8.17 8.16 8.15 7.55 7.53 7.52 7.51 7.50 7.49 7.48 7.48 7.47 7.46 7.44 7.26 6.94 6.92 3.65 3.53 3.51 3.49 2.63 2.61 2.61 2.59 2.58 2.57 2.56 2.54 2.52 2.50 2.21 2.21 2.19 2.18 2.17 2.17 2.16 2.15 2.15 2.14 2.14 2.13 2.12 2.11 2.11 2.10 1.91 1.90 1.89 1.89 1.88 1.87 1.87 1.86 1.85 1.84 1.84 1.82 1.82 1.80 1.78 1.77 1.76 1.75 1.75 1.74 1.73 1.73 1.72 1.72 1.71 1.70 1.70 1.69 1.68 1.68 1.66 -0.00
F
O
N
H
N
O
O
0.88
1.01
0.97
1.00
3.08
1.98
3.00
1.04
2.13
7.08
3.09
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.
f1 (ppm)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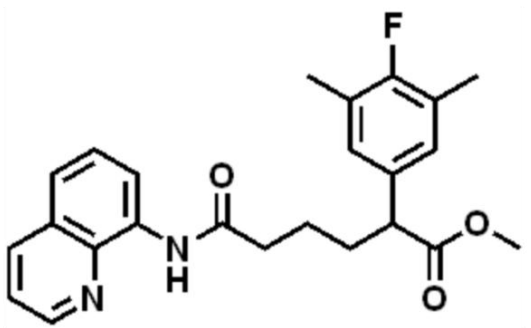
160.50
158.07
148.24
138.38
136.51
134.53
133.64
133.60
128.30
128.25
128.03
127.53
124.83
124.65
121.74
121.57
116.51
77.48
77.16
76.84
52.21
50.76
37.87
33.17
23.73
14.83
14.79
F
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)



-123.70

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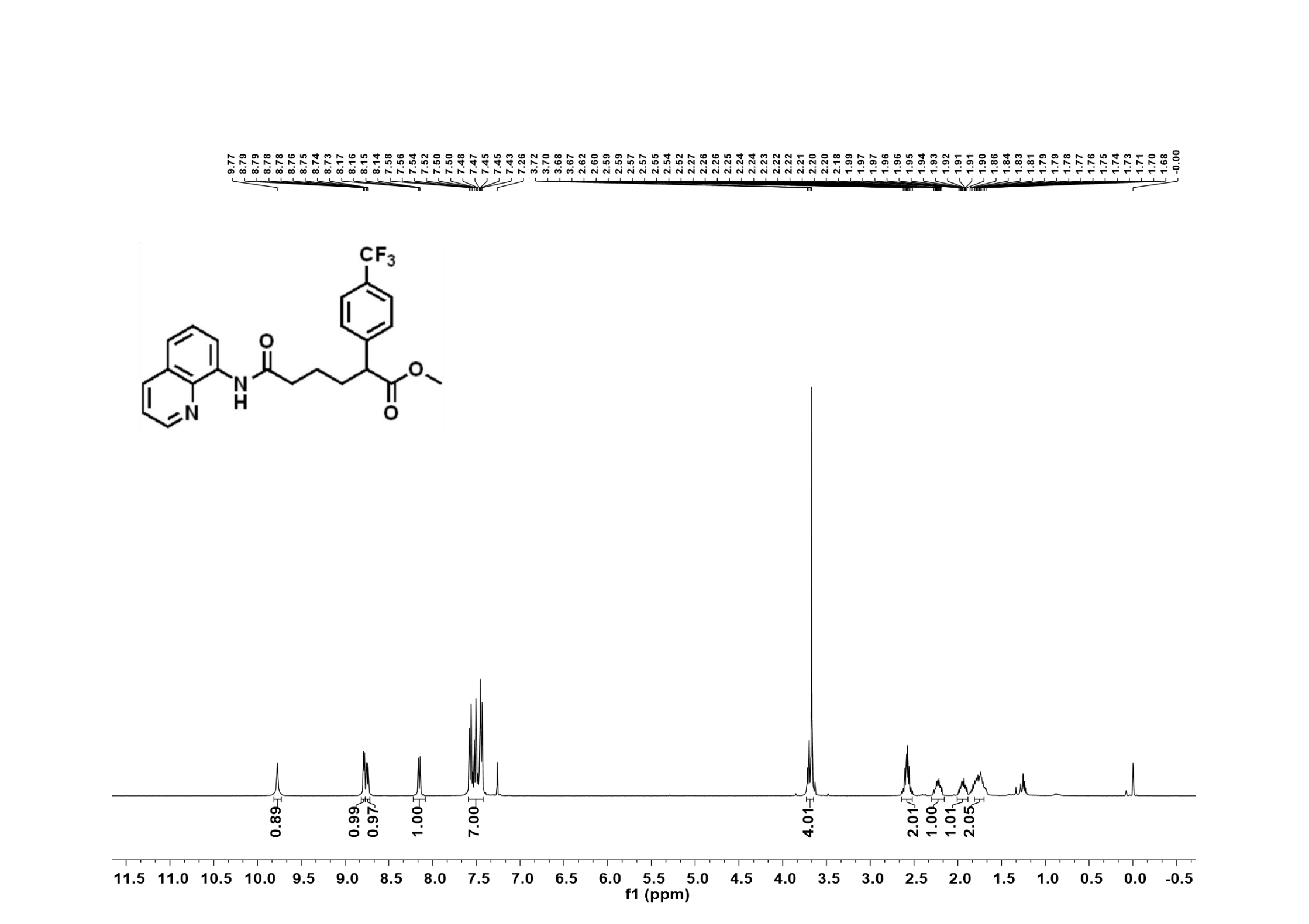
f1 (ppm)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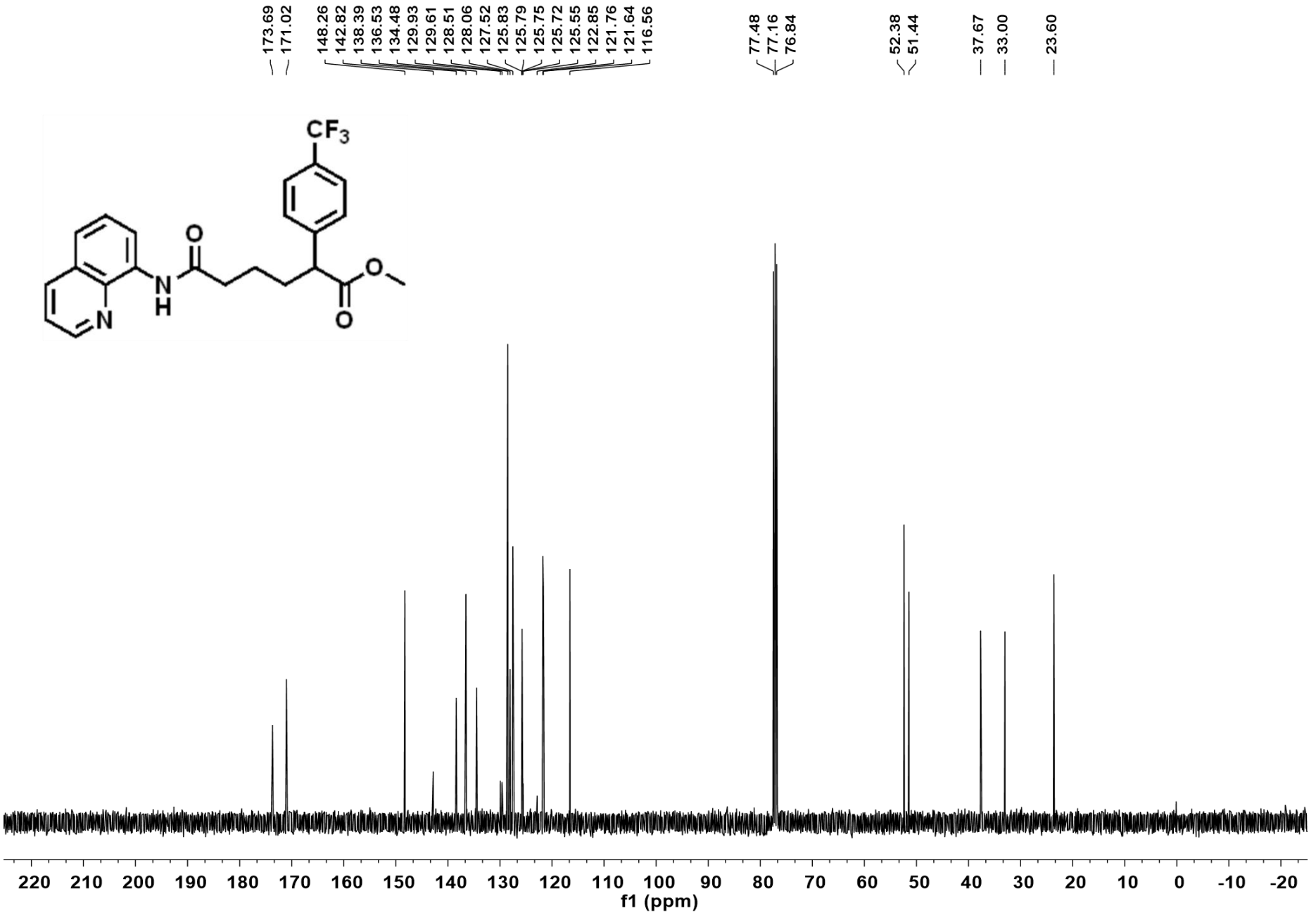
CF3
O
N
H
O
O
N
0.89
0.99
0.97
1.00
7.00
4.01
2.01
1.00
1.01
2.05
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.48
129.93
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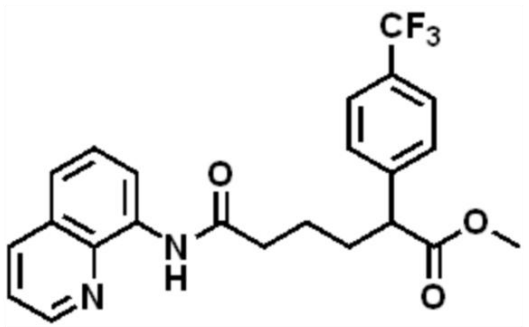
128.51
128.06
127.52
125.83
125.79
125.75
125.72
125.55
122.85
121.76
121.64
116.56
77.48
77.16
76.84
52.38
51.44
37.67
33.00
23.60
CF3
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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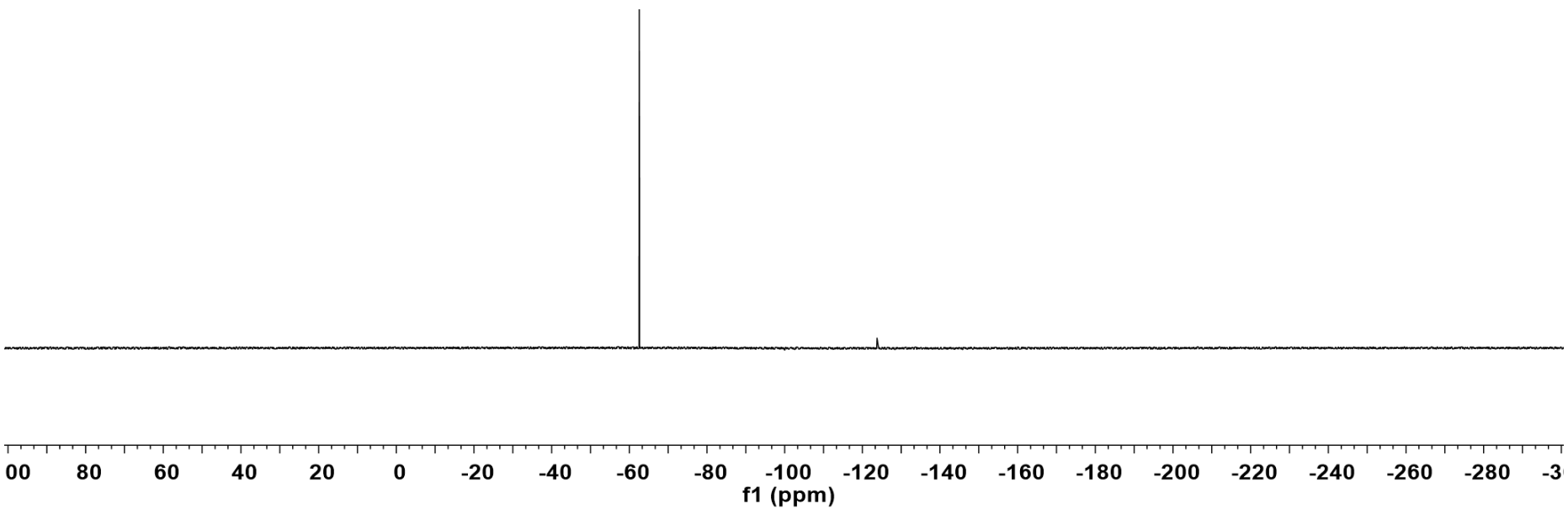
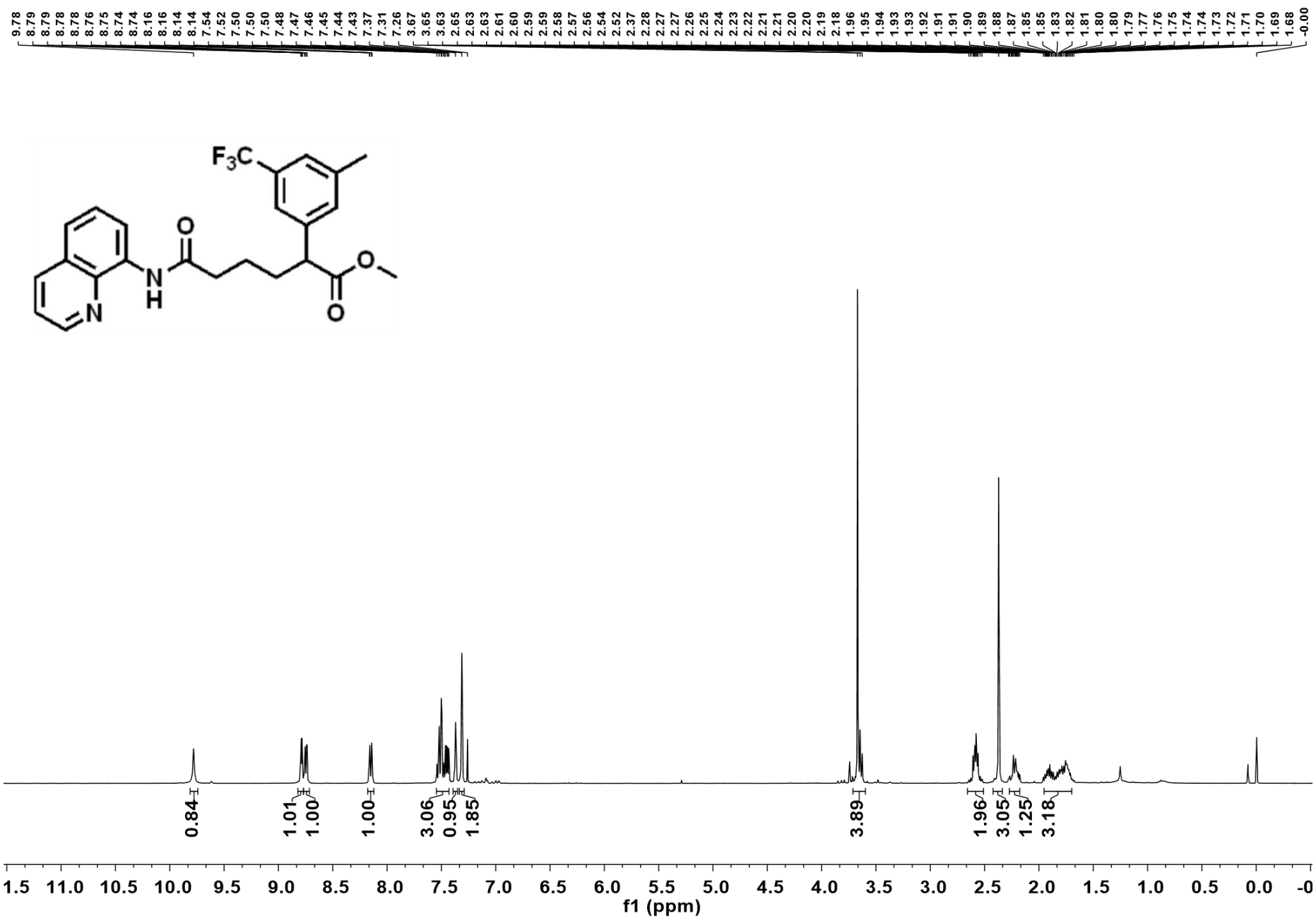
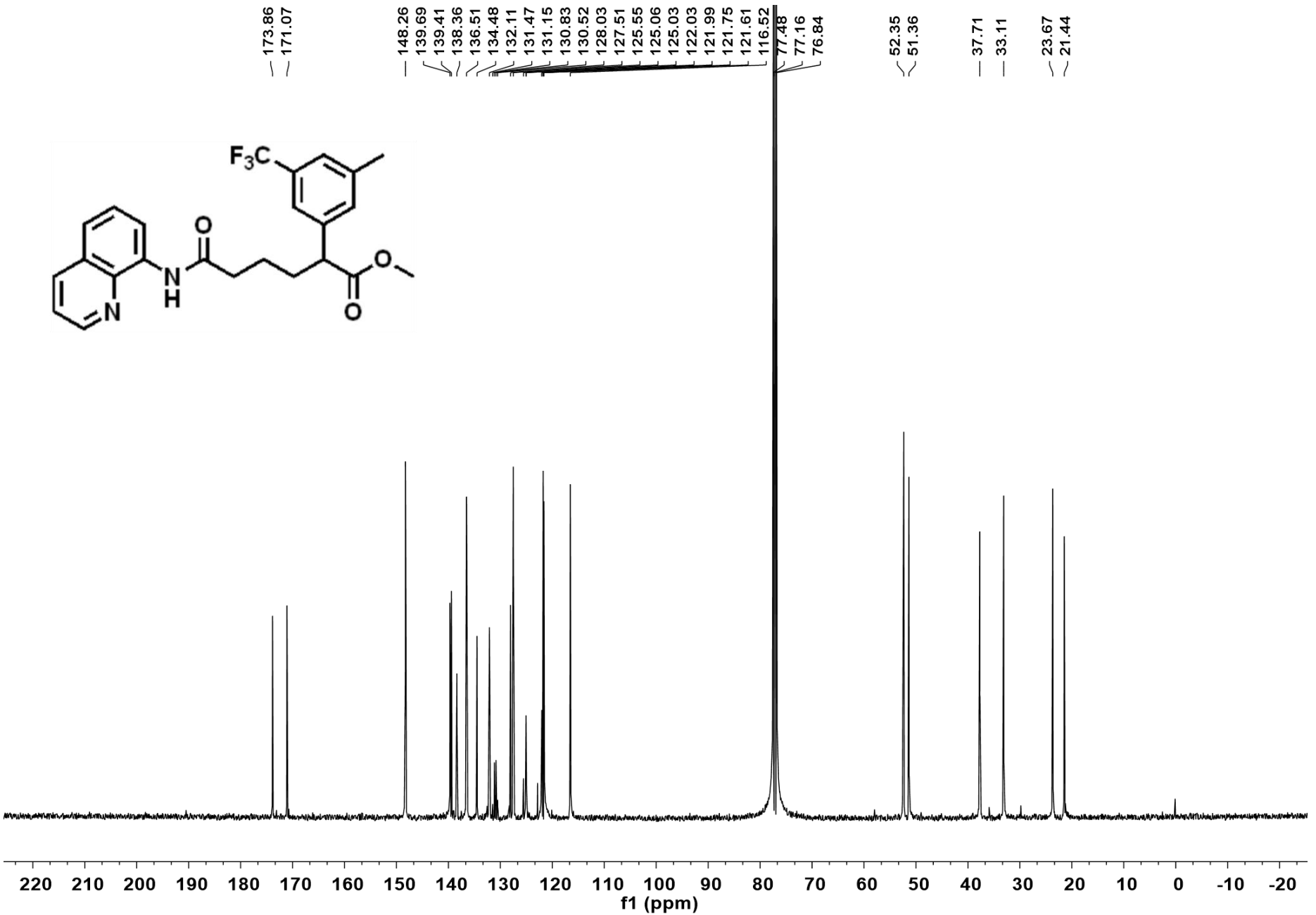
H
O
O
N

-62.57


00
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-3
f1 (ppm)


9.78 8.79 8.79 8.78 8.78 8.76 8.75 8.74 8.74 8.16 8.16 8.14 8.14 7.54 7.52 7.50 7.50 7.50 7.48 7.47 7.46 7.45 7.44 7.43 7.37 7.31 7.26 3.67 3.65 3.63 2.65 2.63 2.63 2.61 2.60 2.59 2.59 2.58 2.57 2.56 2.54 2.52 2.37 2.28 2.27 2.27 2.26 2.25 2.24 2.23 2.22 2.21 2.21 2.20 2.20 2.19 2.18 1.96 1.95 1.94 1.93 1.93 1.92 1.91 1.91 1.90 1.89 1.88 1.87 1.85 1.85 1.83 1.82 1.81 1.80 1.80 1.79 1.77 1.76 1.75 1.74 1.74 1.73 1.72 1.71 1.70 1.69 1.68 -0.00
F3C
O
N
H
O
O
N
0.84
1.01
1.00
1.00
3.06
0.95
1.85
3.89
1.96
3.05
1.25
3.18
1.5 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
f1 (ppm)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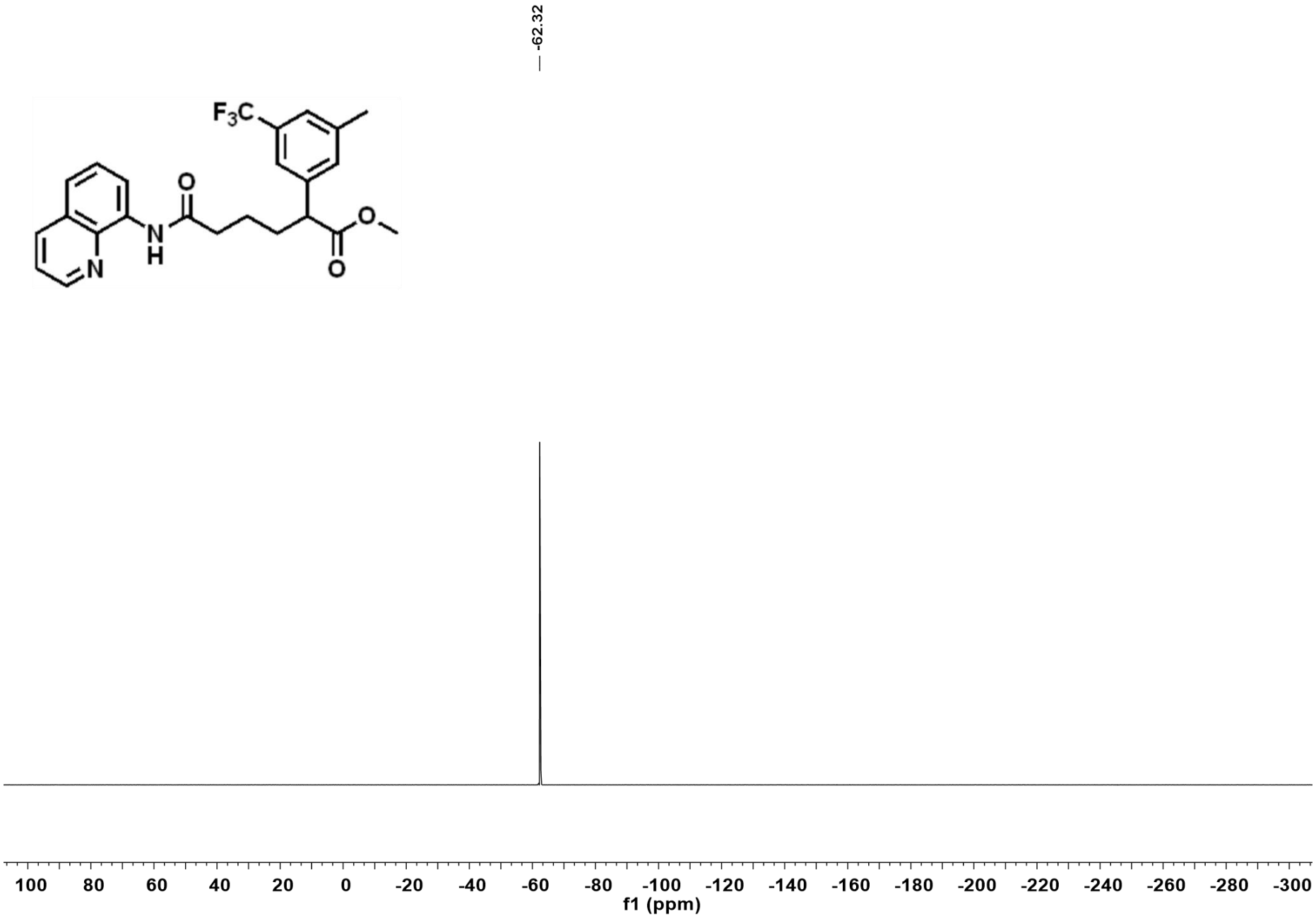
131.15
130.83
130.52
128.03
127.51
125.55
125.06
125.03
122.03
121.99
121.75
121.61
116.52
77.48
77.16
76.84
52.35
51.36
37.71
33.11
23.67
21.44
F3C
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

F3C
O
N
H
O
O
N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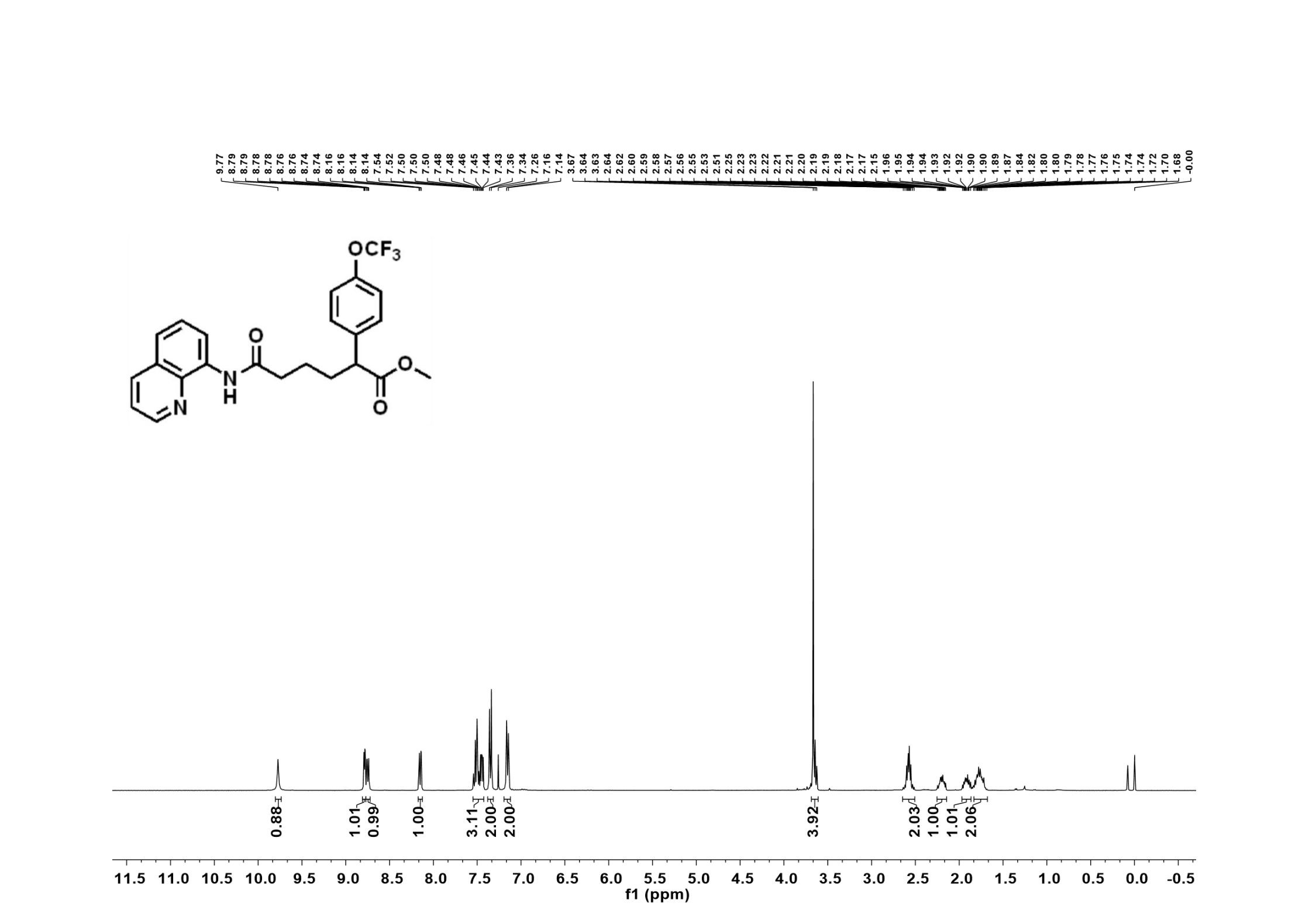
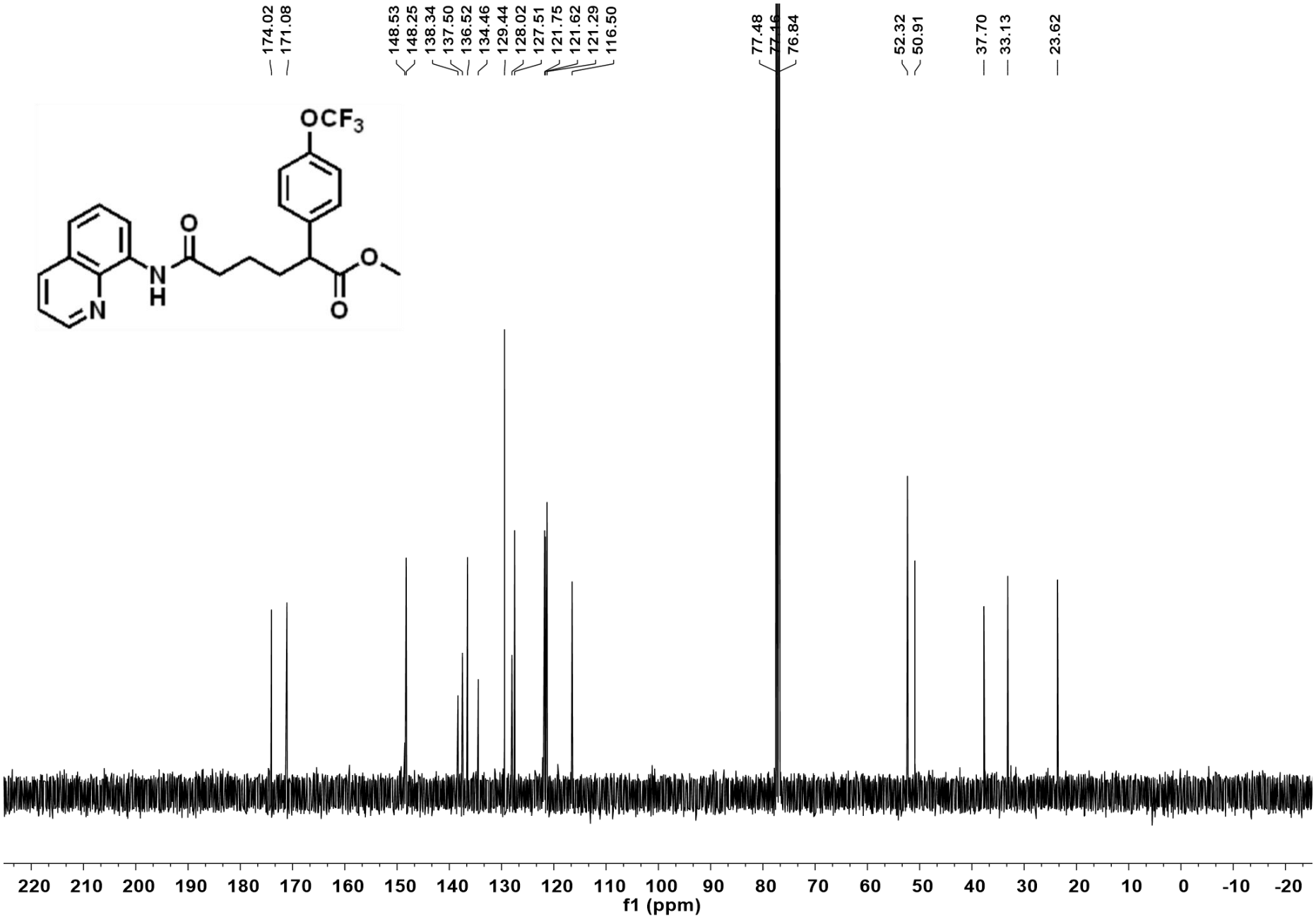
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)


9.77 8.79 8.79 8.78 8.78 8.76 8.76 8.74 8.74 8.16 8.16 8.14 8.14 7.54 7.52 7.50 7.50 7.48 7.48 7.46 7.45 7.44 7.43 7.36 7.34 7.26 7.16 7.14
3.67 3.64 3.63 2.64 2.62 2.60 2.59 2.58 2.57 2.56 2.55 2.53 2.51 2.25 2.23 2.23 2.22 2.21 2.21 2.20 2.19 2.19 2.18 2.17 2.17 2.15 1.96 1.95 1.94 1.94 1.93 1.92 1.92 1.90 1.90 1.89 1.87 1.84 1.82 1.80 1.80 1.79 1.78 1.77 1.76 1.75 1.74 1.74 1.72 1.70 1.68 -0.00
OCF3
O
N
H
O
O
N
0.88
1.01
0.99
1.00
3.11
2.00
2.00
3.92
2.03
1.00
1.01
2.06
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
f1 (ppm)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171.08
148.53
148.25
138.34
137.50
136.52
134.46
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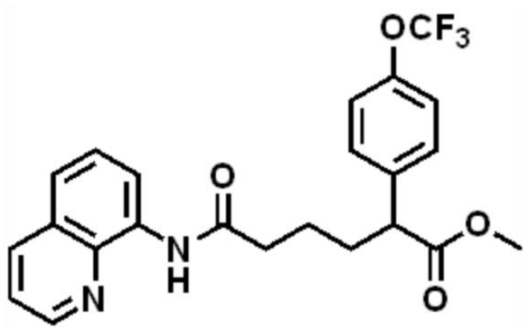
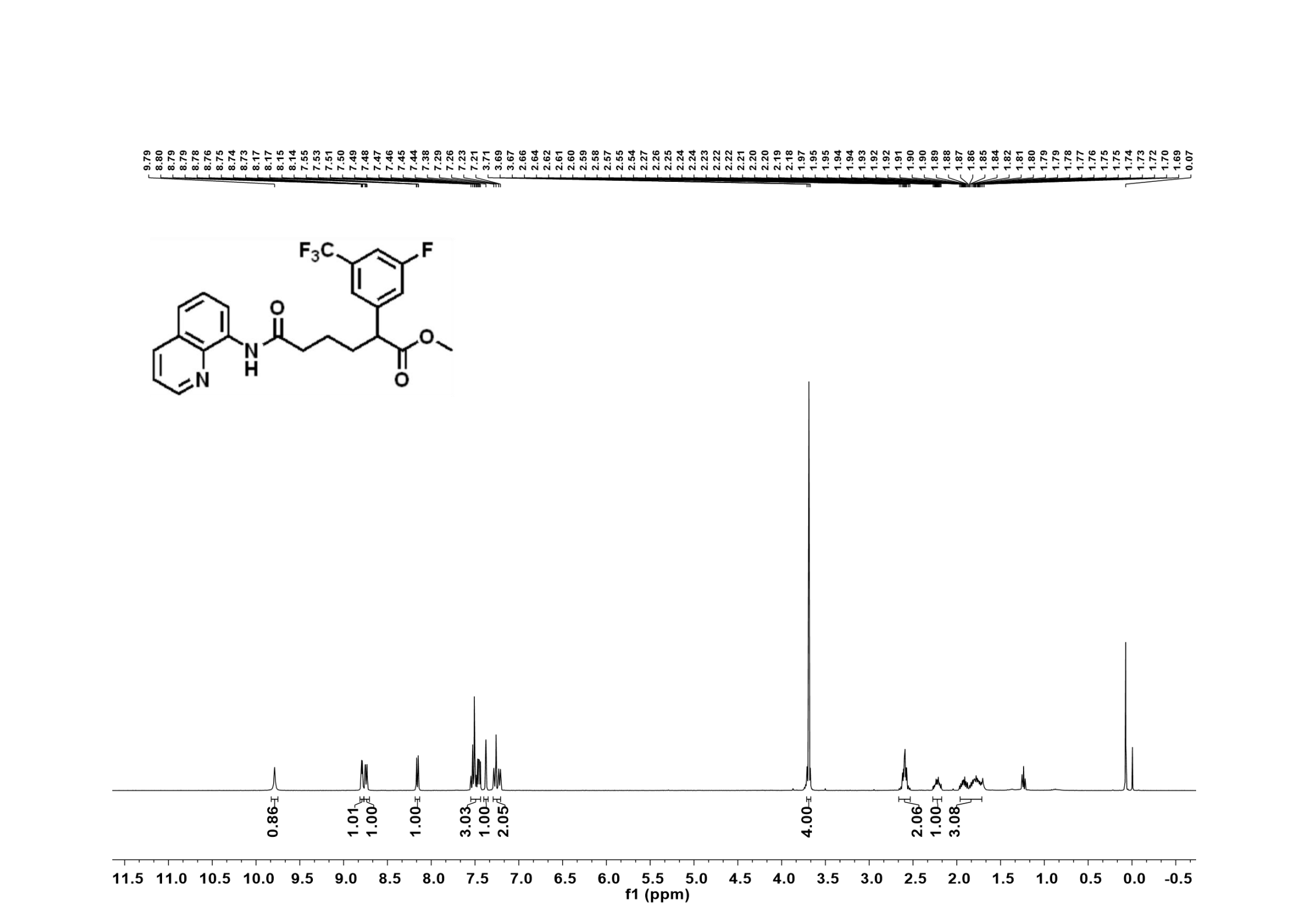
128.02
127.51
121.75
121.62
121.29
116.50
77.48
77.16
76.84
52.32
50.91
37.70
33.13
23.62
OCF3
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)



-57.72

100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300

f1 (ppm)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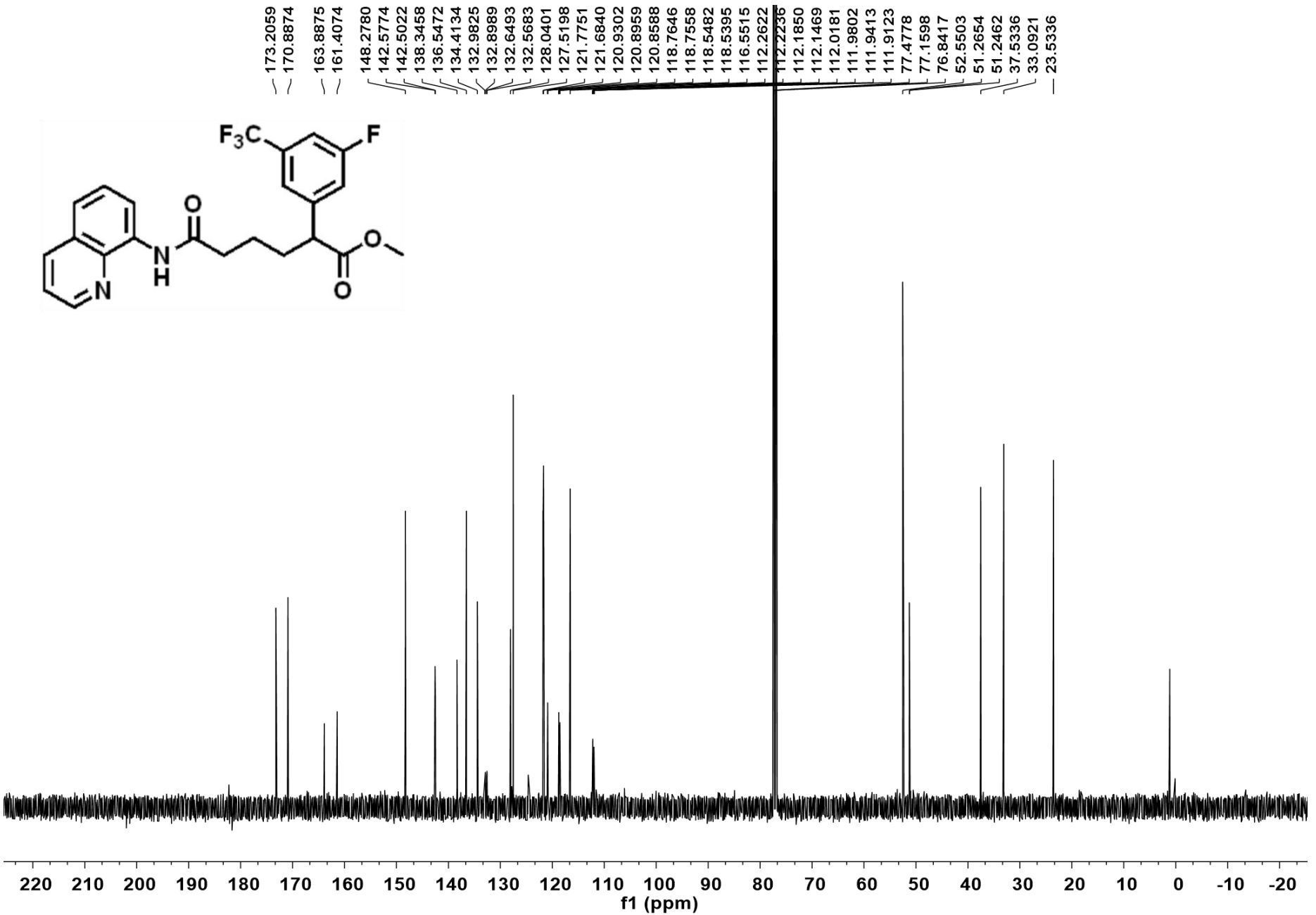
F3C
F
O
N
H
N
O
O
0.86
1.01
1.00
1.00
3.03
1.00
2.05
4.00
2.06
1.00
3.08
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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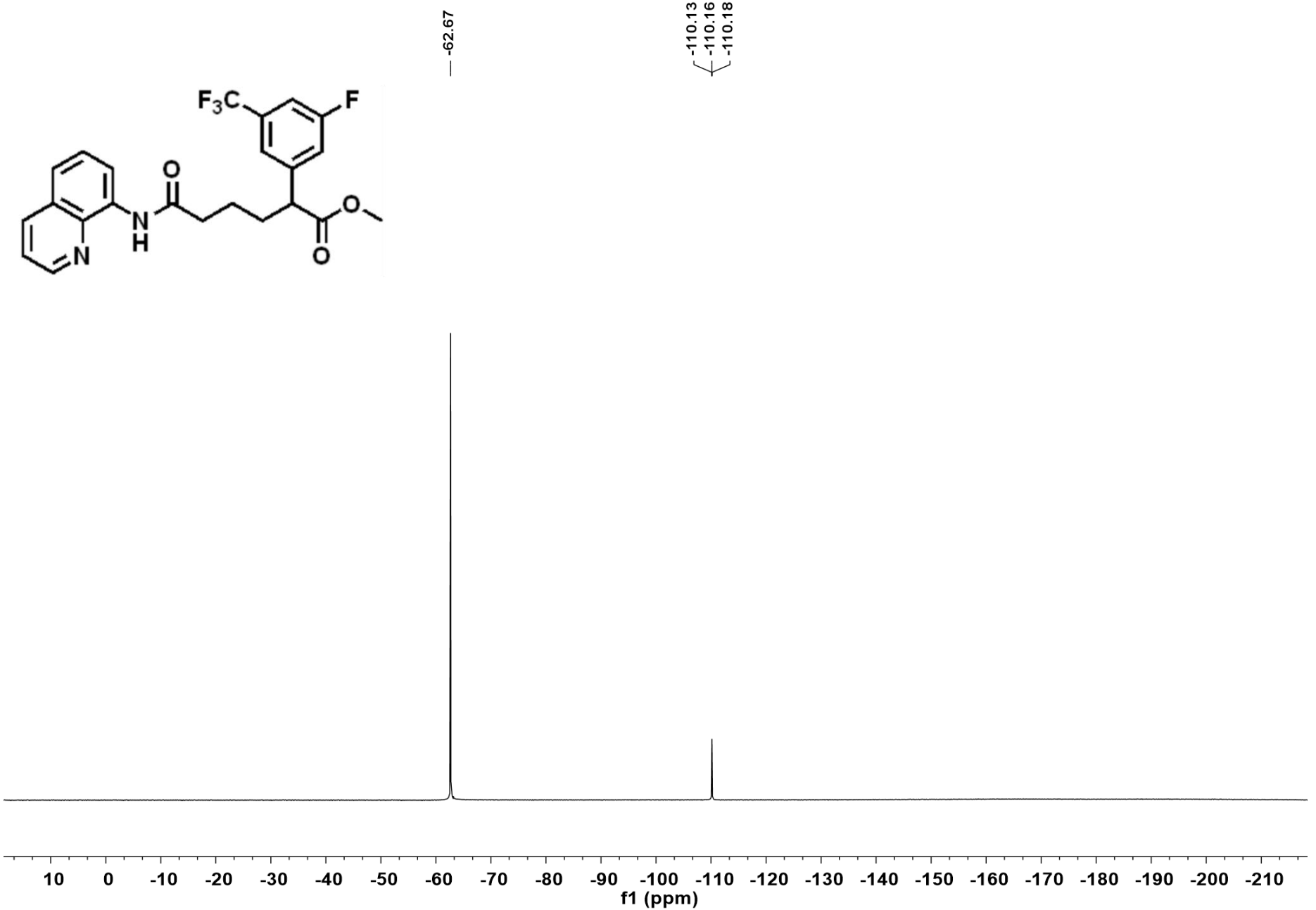
132.9825
132.8989
132.6493
132.5683
128.0401
127.5198
121.7751
121.6840
120.9302
120.8959
120.8588
118.7646
118.7558
118.5482
118.5395
116.5515
112.2622
112.2236
112.1850
112.1469
112.0181
111.9802
111.9413
111.9123
77.4778
77.1598
76.8417
52.5503
51.2654
51.2462
37.5336
33.0921
23.5336
F3C
F
O
N
H
N
O
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

F3C
F
O
N
H
N
O
O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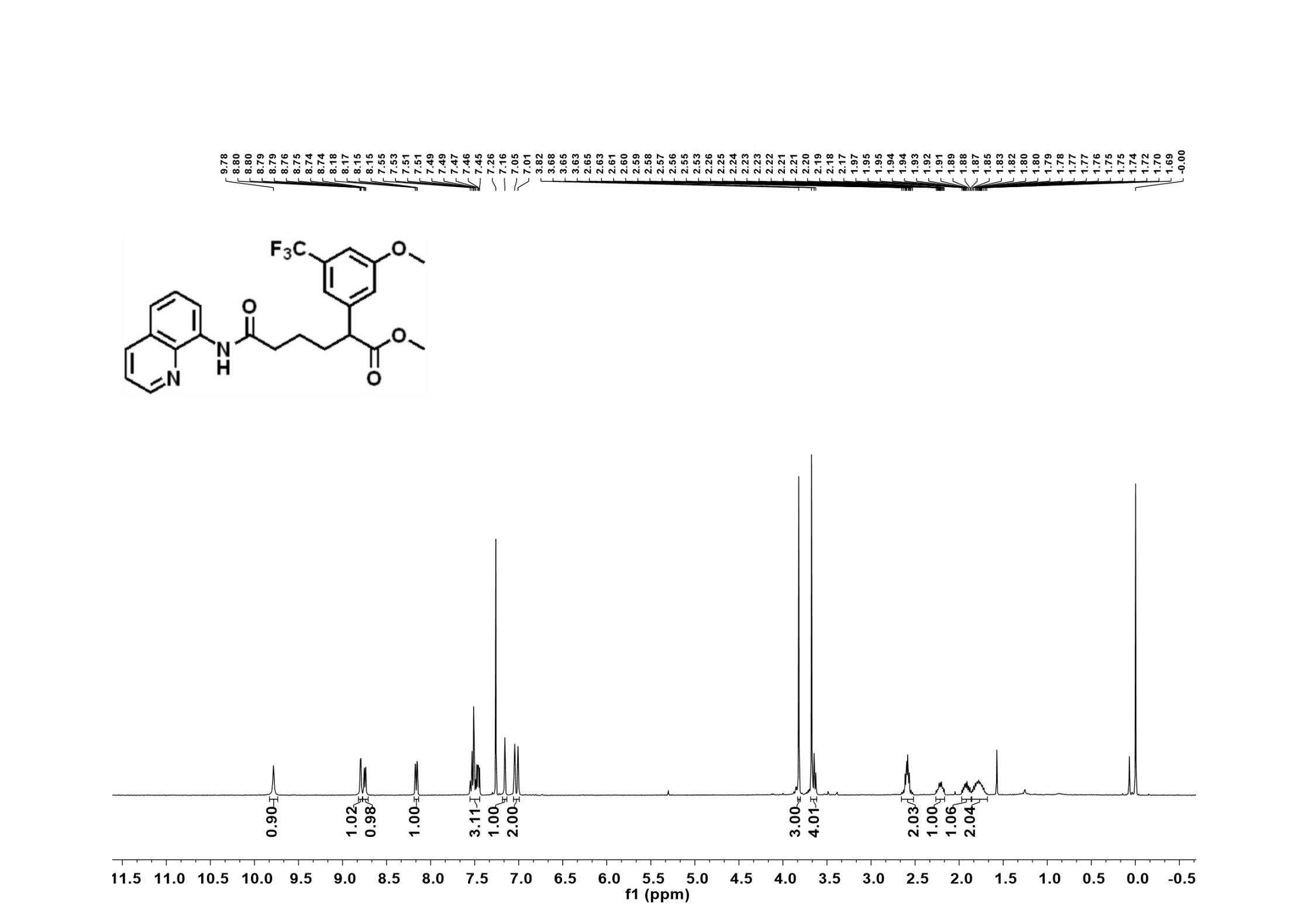
-110.13
-110.16
-110.18
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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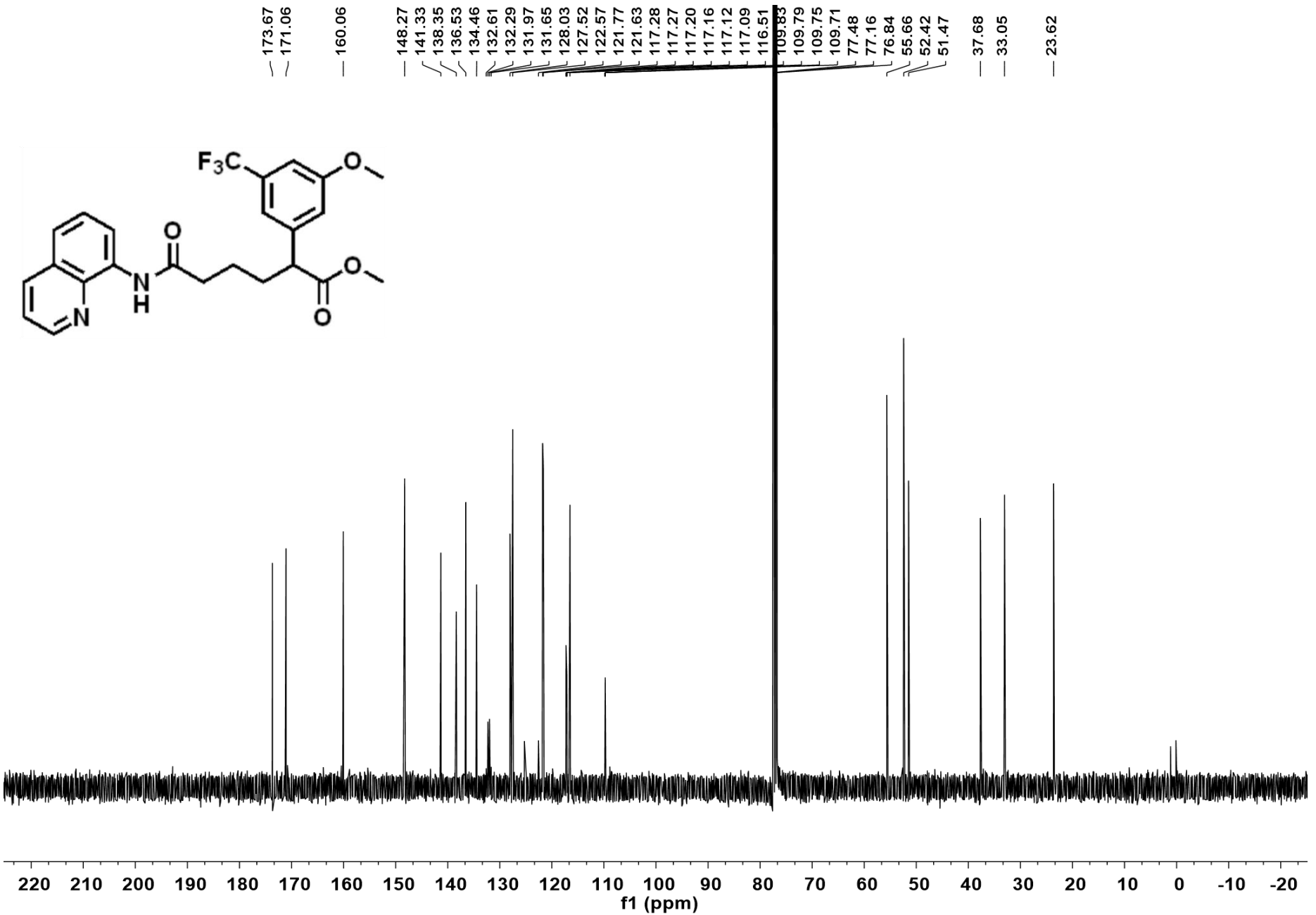
F3C
O
O
N
H
N
O
O
0.90
1.02
0.98
1.00
3.11
1.00
2.00
3.00
4.01
2.03
1.00
1.06
2.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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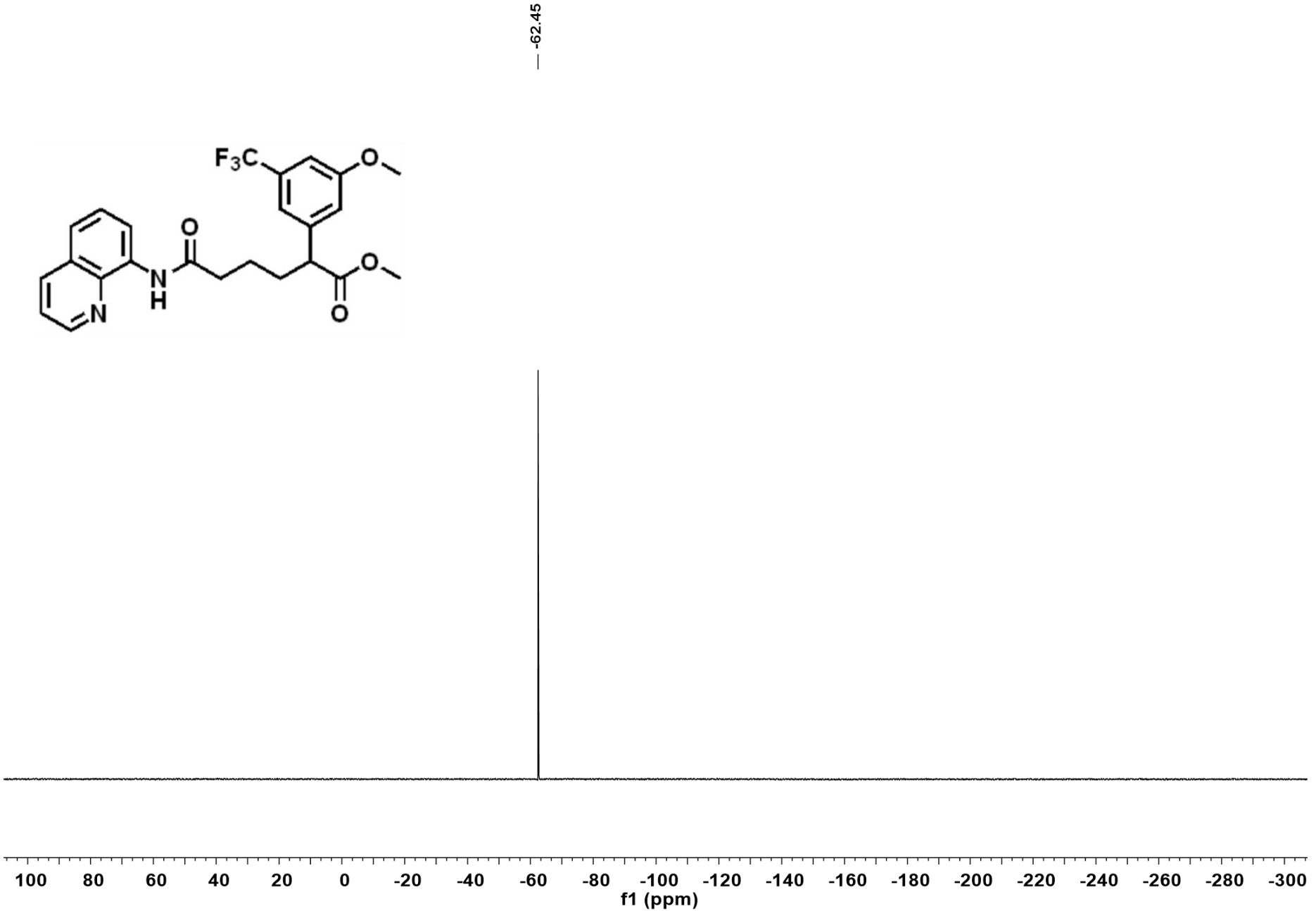
171.06
160.06
148.27
141.33
138.35
136.53
134.46
132.61
132.29
131.97
131.65
128.03
127.52
122.57
121.77
121.63
117.28
117.27
117.20
117.16
117.12
117.09
116.51
109.83
109.79
109.75
109.71
77.48
77.16
76.84
55.66
52.42
51.47
37.68
33.05
23.62
F3C
O
O
N
H
O
N
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

F3C
O
O
N
H
N
O
O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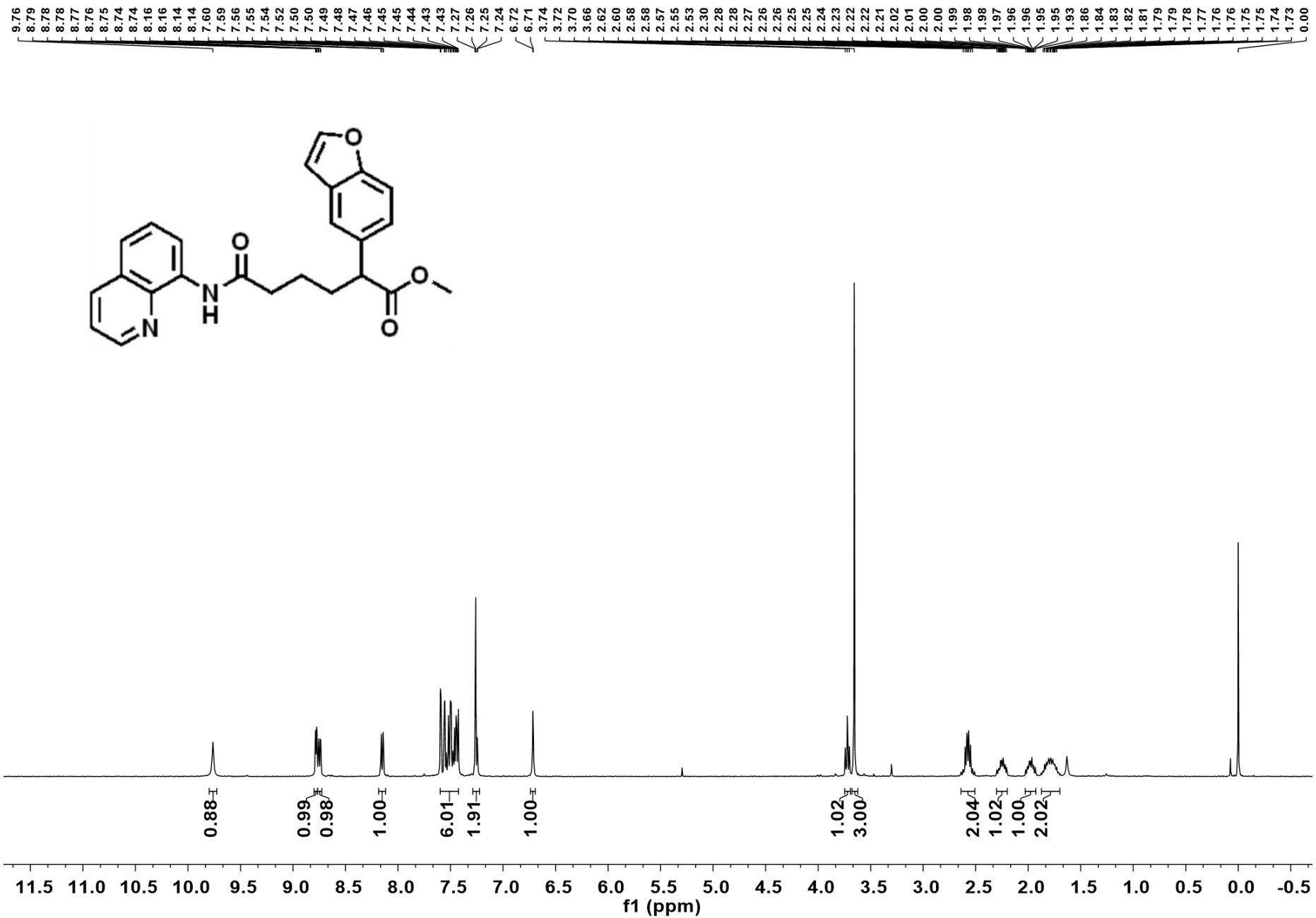
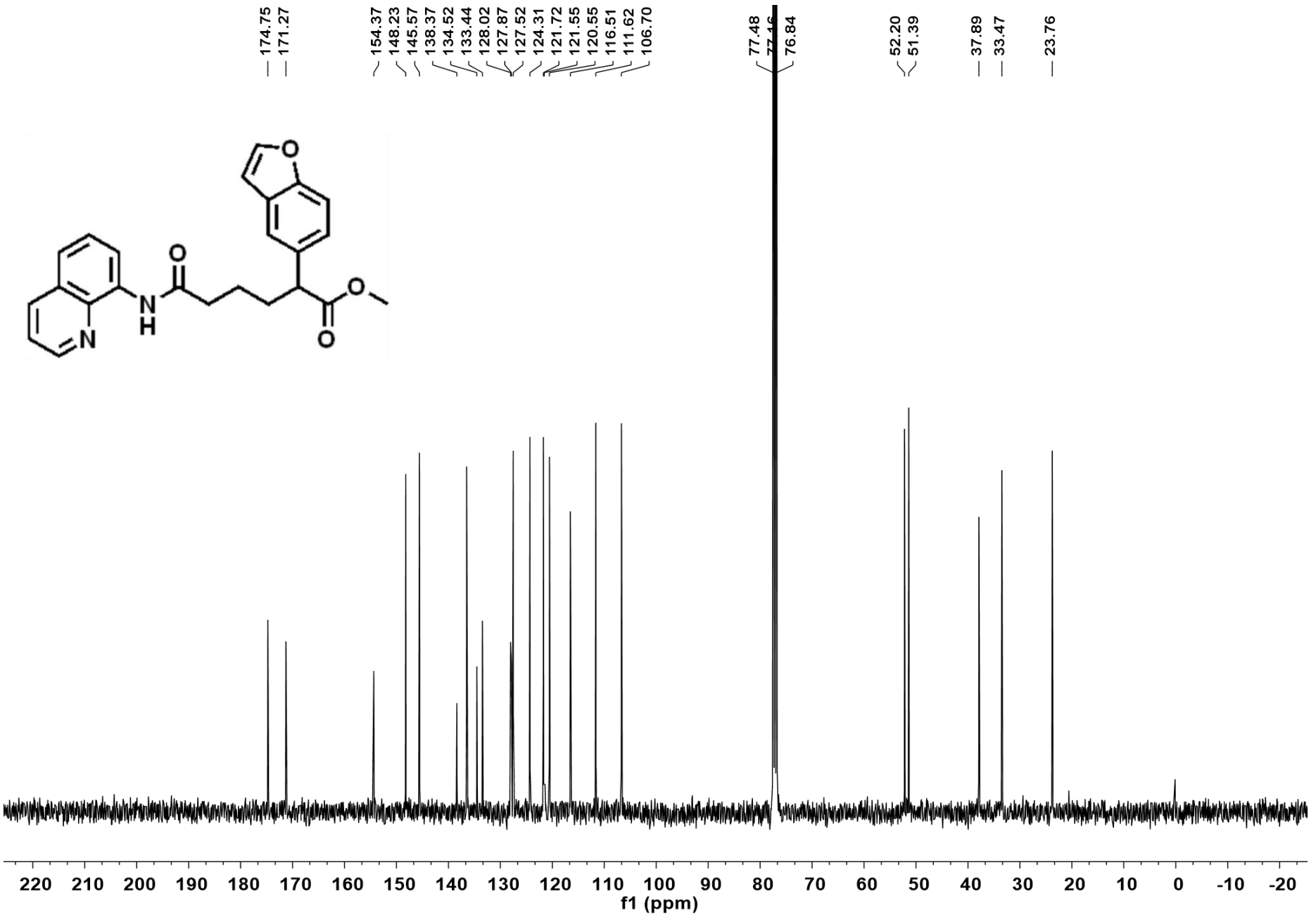
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)


9.76 8.79 8.78 8.78 8.77 8.76 8.75 8.74 8.74 8.16 8.16 8.14 8.14 7.60 7.59 7.56 7.55 7.54 7.52 7.50 7.50 7.49 7.48 7.47 7.46 7.45 7.45 7.44 7.43 7.43 7.27 7.26 7.25 7.24 6.72 6.71 3.74 3.72 3.70 3.66 2.62 2.60 2.58 2.58 2.57 2.55 2.53 2.30 2.28 2.28 2.27 2.26 2.26 2.25 2.25 2.24 2.23 2.22 2.22 2.21 2.02 2.01 2.00 2.00 1.99 1.98 1.98 1.97 1.96 1.96 1.95 1.95 1.93 1.86 1.84 1.83 1.82 1.81 1.79 1.79 1.78 1.77 1.76 1.76 1.75 1.75 1.74 1.73 0.00
O
N
H
O
O
O
N
0.88
0.99
0.98
1.00
6.01
1.91
1.00
1.02
3.00
2.04
1.02
1.00
2.02
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
f1 (ppm)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145.57
138.37
134.52
133.44
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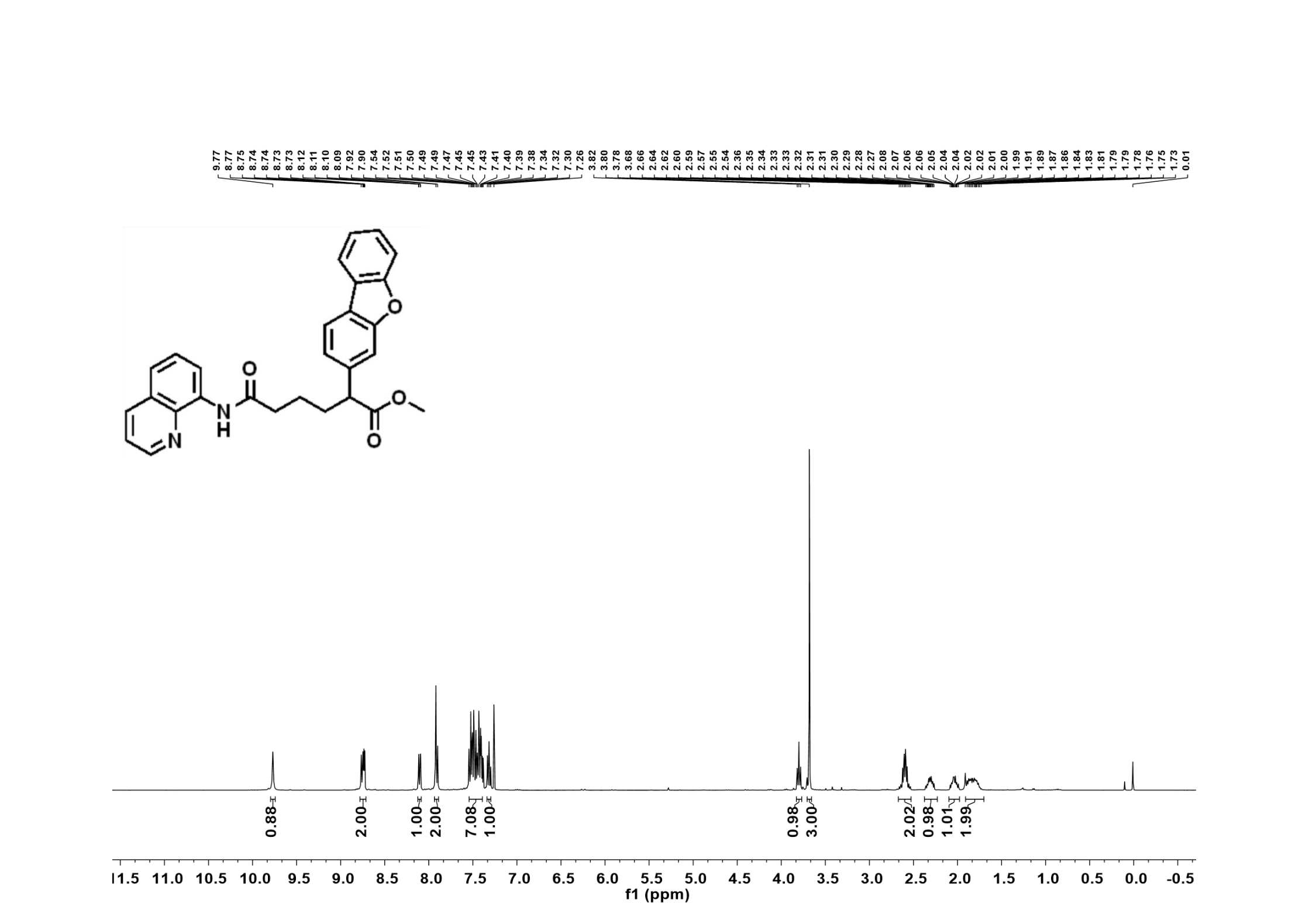
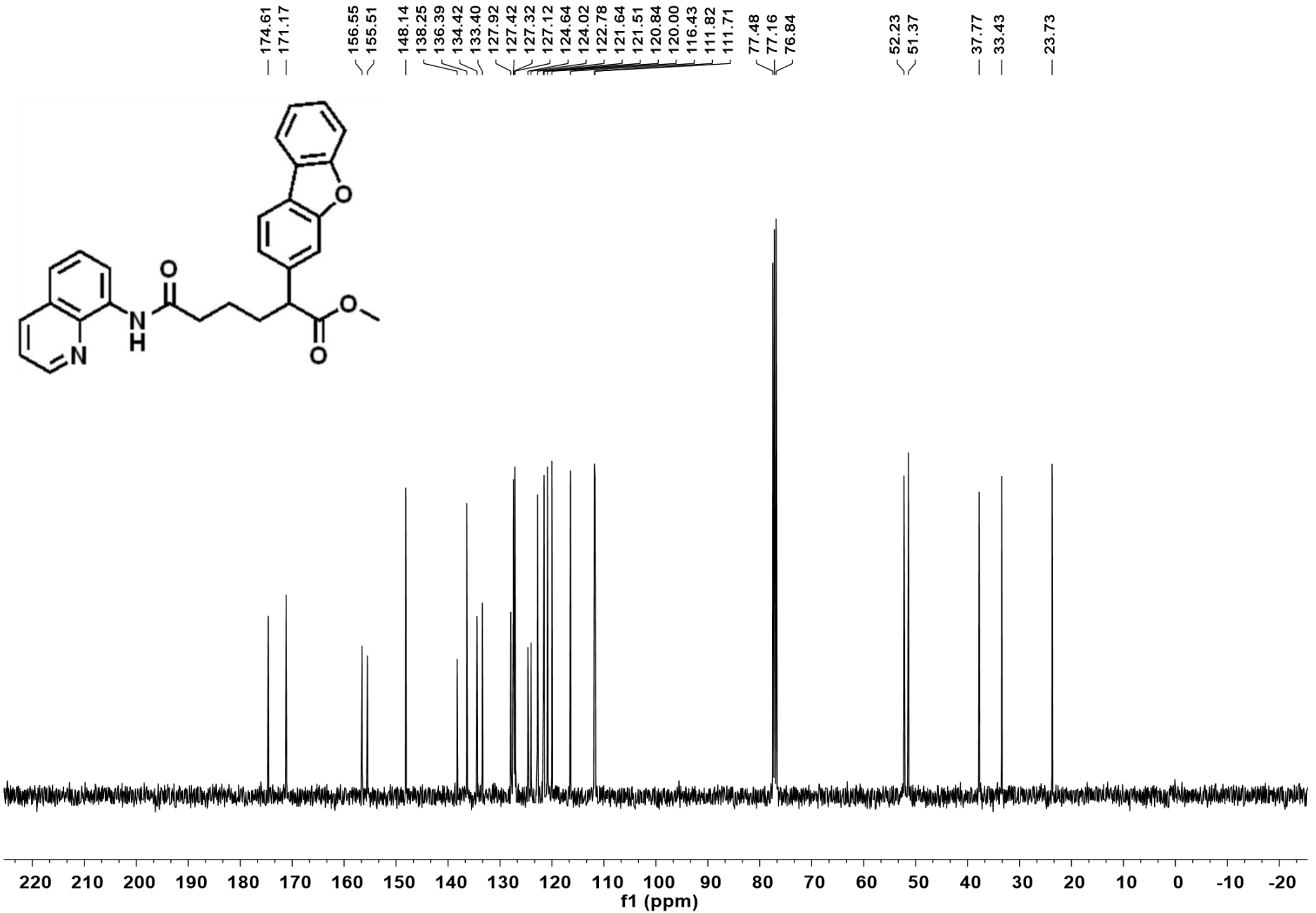
127.87
127.52
124.31
121.72
121.55
120.55
116.51
111.62
106.70
77.48
77.16
76.84
52.20
51.39
37.89
33.47
23.76
O
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


9.77 8.77 8.75 8.74 8.74 8.73 8.73 8.12 8.11 8.10 8.09 7.92 7.90 7.54 7.52 7.51 7.50 7.49 7.49 7.47 7.45 7.45 7.43 7.41 7.40 7.39 7.38 7.34 7.32 7.30 7.26
3.82 3.80 3.78 3.68 2.66 2.64 2.62 2.60 2.59 2.57 2.55 2.54 2.36 2.35 2.34 2.33 2.33 2.32 2.31 2.31 2.30 2.29 2.28 2.27 2.08 2.07 2.06 2.06 2.05 2.04 2.04 2.02 2.02 2.01 2.00 1.99 1.91 1.89 1.87 1.86 1.84 1.83 1.81 1.79 1.79 1.78 1.76 1.75 1.73 0.01
O
N
H
N
O
O
0.88
2.00
1.00
2.00
7.08
1.00
0.98
3.00
2.02
0.98
1.01
1.99
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
f1 (ppm)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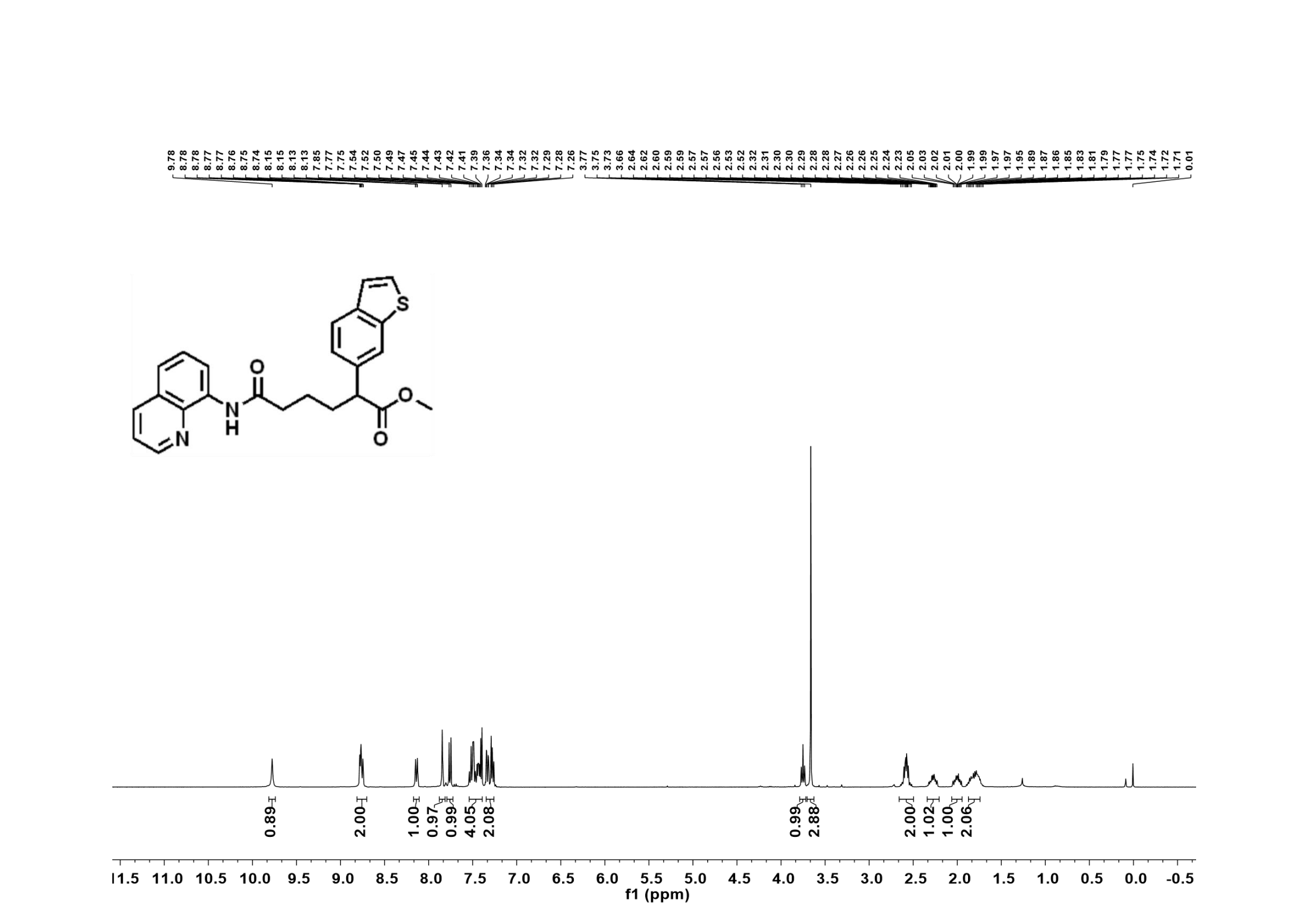
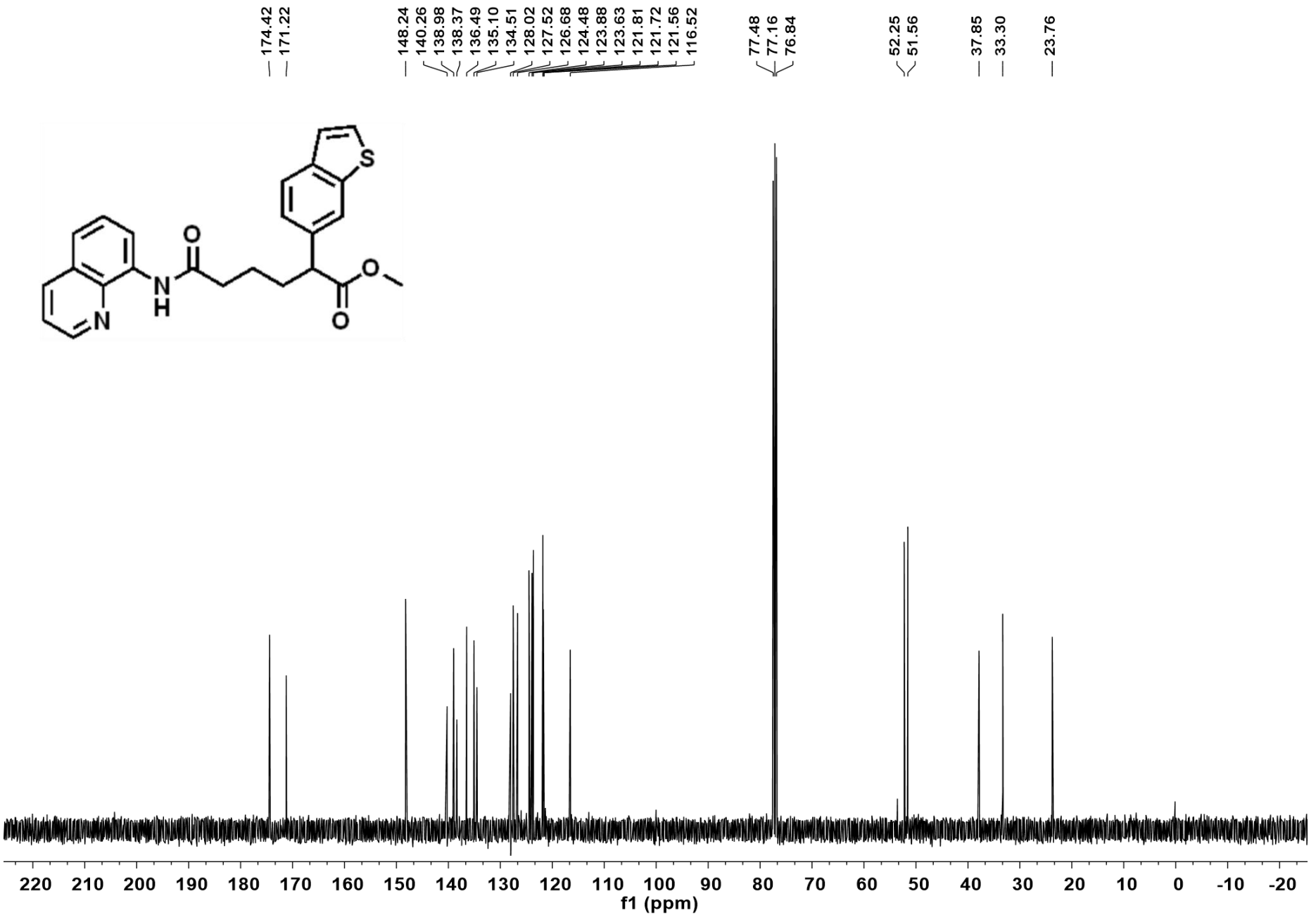
134.42
133.40
127.92
127.42
127.32
127.12
124.64
124.02
122.78
121.64
121.51
120.84
120.00
116.43
111.82
111.71
77.48
77.16
76.84
52.23
51.37
37.77
33.43
23.73
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


9.78 8.78 8.78 8.77 8.77 8.76 8.75 8.74 8.15 8.15 8.13 8.13 7.85 7.77 7.75 7.54 7.52 7.50 7.49 7.47 7.45 7.44 7.43 7.42 7.41 7.39 7.36 7.34 7.34 7.32 7.32 7.29 7.28 7.26
3.77 3.75 3.73 3.66 2.64 2.62 2.60 2.59 2.59 2.57 2.57 2.56 2.53 2.52 2.32 2.31 2.30 2.30 2.29 2.28 2.28 2.27 2.26 2.26 2.25 2.24 2.23 2.05 2.03 2.02 2.01 2.00 1.99 1.99 1.97 1.97 1.95 1.89 1.87 1.86 1.85 1.83 1.81 1.79 1.77 1.77 1.75 1.74 1.72 1.71 0.01
S
O
N
H
N
O
O
0.89 2.00 1.00 0.97 0.99 4.05 2.08 0.99 2.88 2.00 1.02 1.00 2.06
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
f1 (ppm)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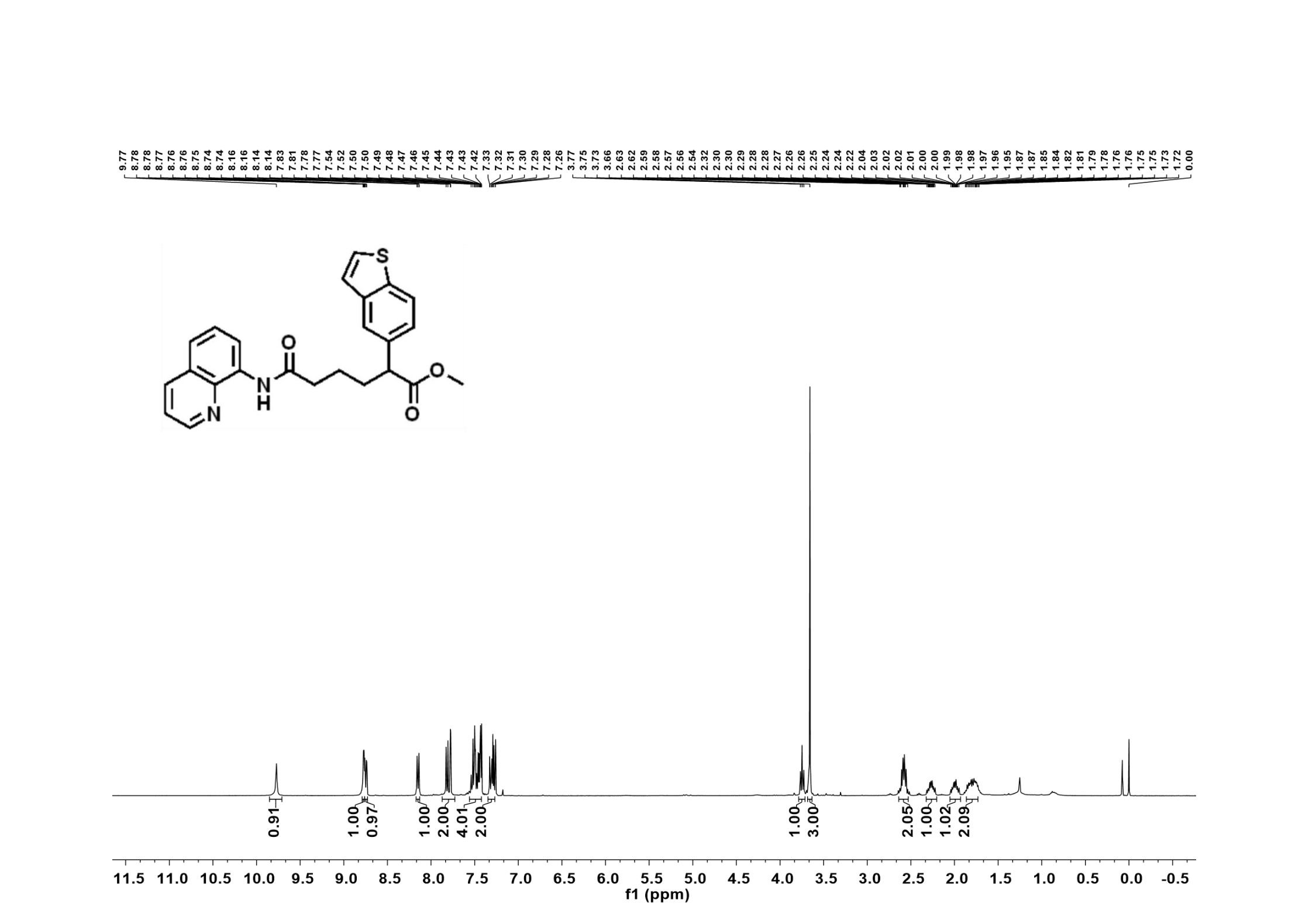
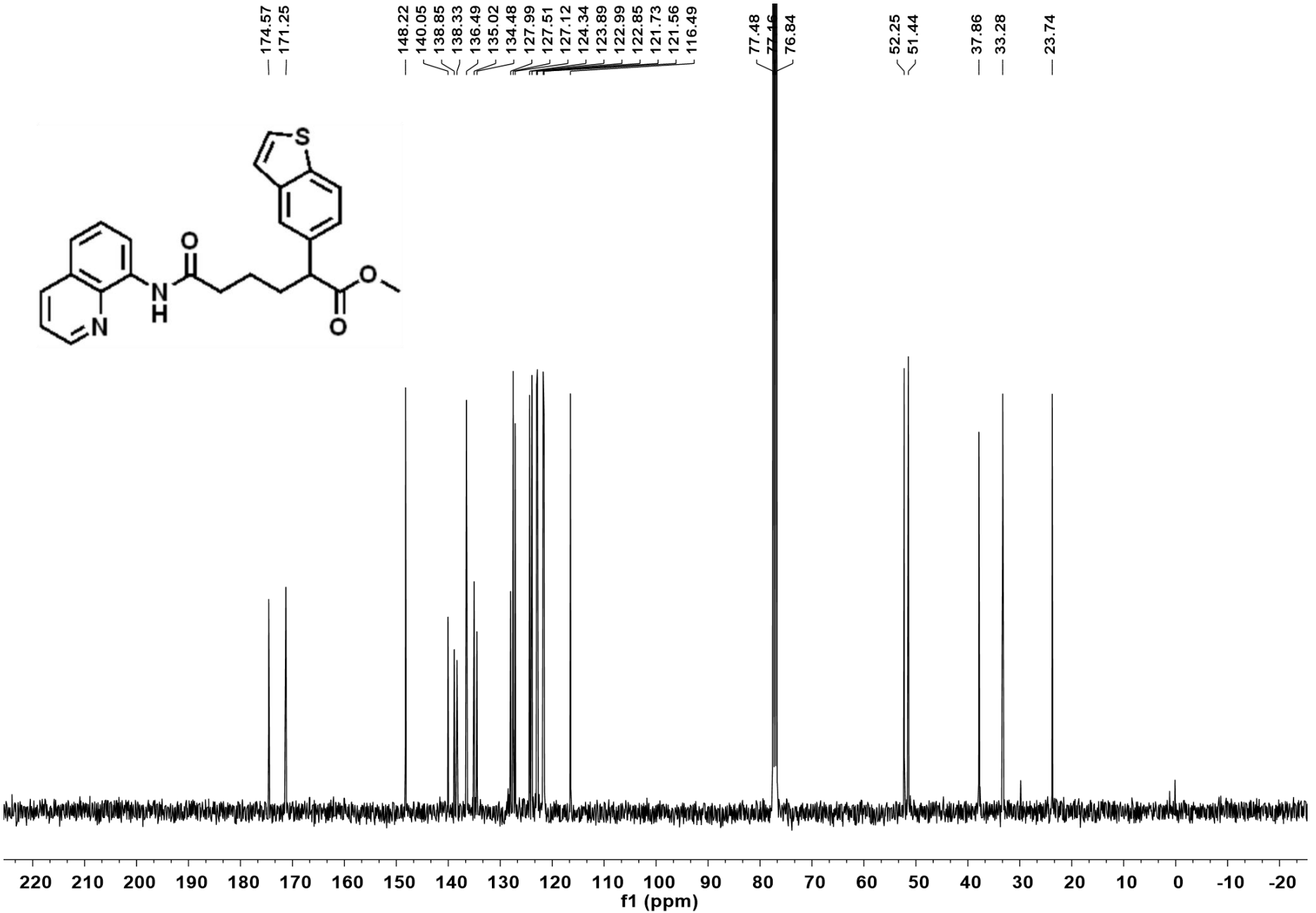
138.37
136.49
135.10
134.51
128.02
127.52
126.68
124.48
123.88
123.63
121.81
121.72
121.56
116.52
77.48
77.16
76.84
52.25
51.56
37.85
33.30
23.76
S
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


9.77 8.78 8.78 8.77 8.76 8.76 8.75 8.74 8.74 8.16 8.16 8.14 8.14 7.83 7.81 7.78 7.77 7.54 7.52 7.50 7.50 7.49 7.48 7.47 7.46 7.45 7.44 7.43 7.43 7.42 7.33 7.32 7.31 7.30 7.29 7.28 7.26 3.77 3.75 3.73 3.66 2.63 2.62 2.59 2.58 2.57 2.56 2.54 2.32 2.30 2.30 2.29 2.28 2.28 2.27 2.26 2.26 2.25 2.24 2.24 2.22 2.04 2.03 2.02 2.02 2.01 2.00 2.00 1.99 1.98 1.98 1.97 1.96 1.95 1.87 1.87 1.85 1.84 1.82 1.81 1.79 1.78 1.76 1.76 1.75 1.75 1.73 1.72 0.00
S
O
N
H
N
O
O
0.91
1.00
0.97
1.00
2.00
4.01
2.00
1.00
3.00
2.05
1.00
1.02
2.09
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
f1 (ppm)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135.02
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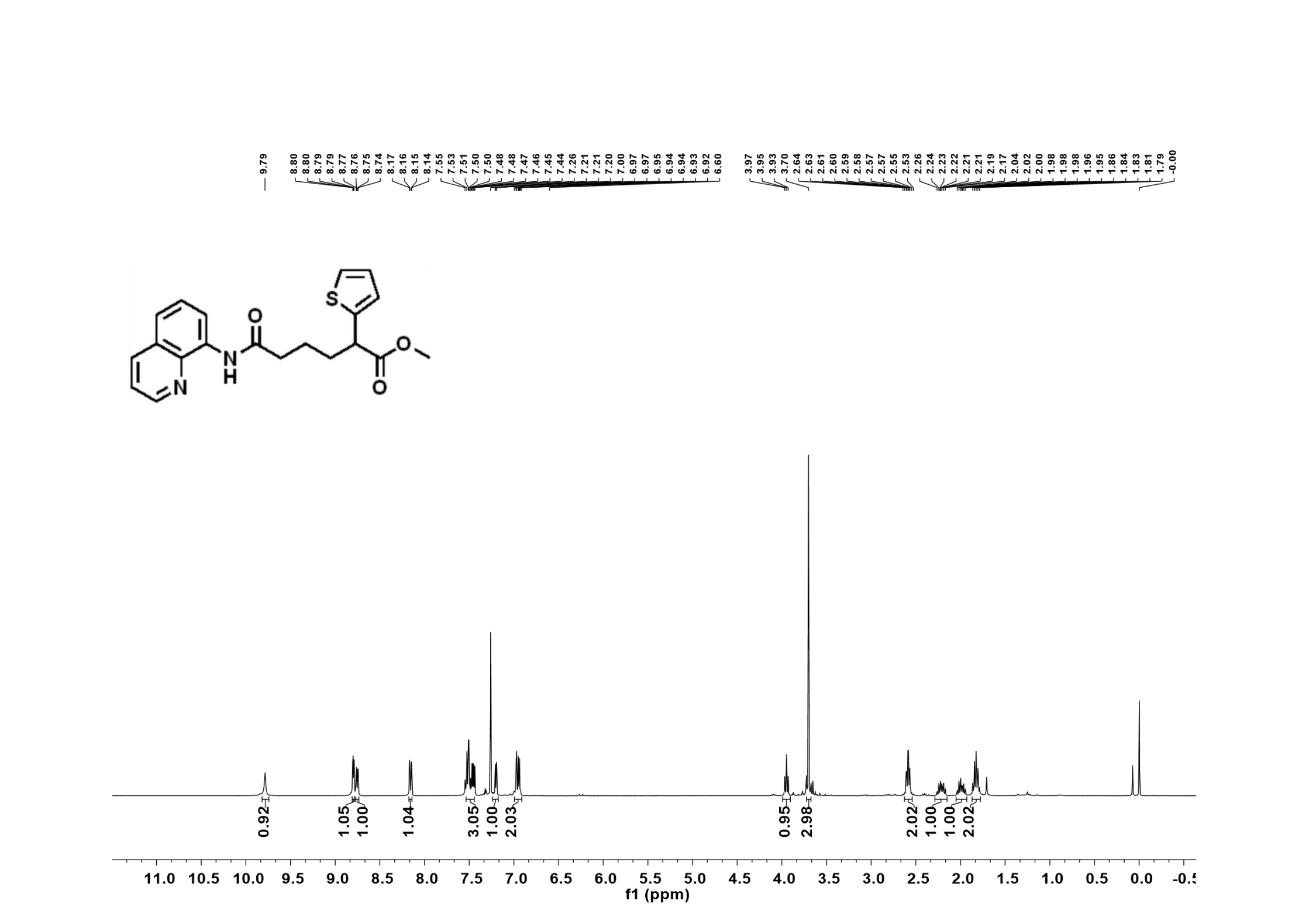
127.51
127.12
124.34
123.89
122.99
122.85
121.73
121.56
116.49
77.48
77.16
76.84
52.25
51.44
37.86
33.28
23.74
S
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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8.80
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8.77
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8.75
8.74
8.17
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8.15
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7.55
7.53
7.51
7.50
7.50
7.48
7.48
7.47
7.46
7.45
7.44
7.26
7.21
7.21
7.20
7.00
6.97
6.97
6.95
6.94
6.94
6.93
6.92
6.60
3.97
3.95
3.93
3.70
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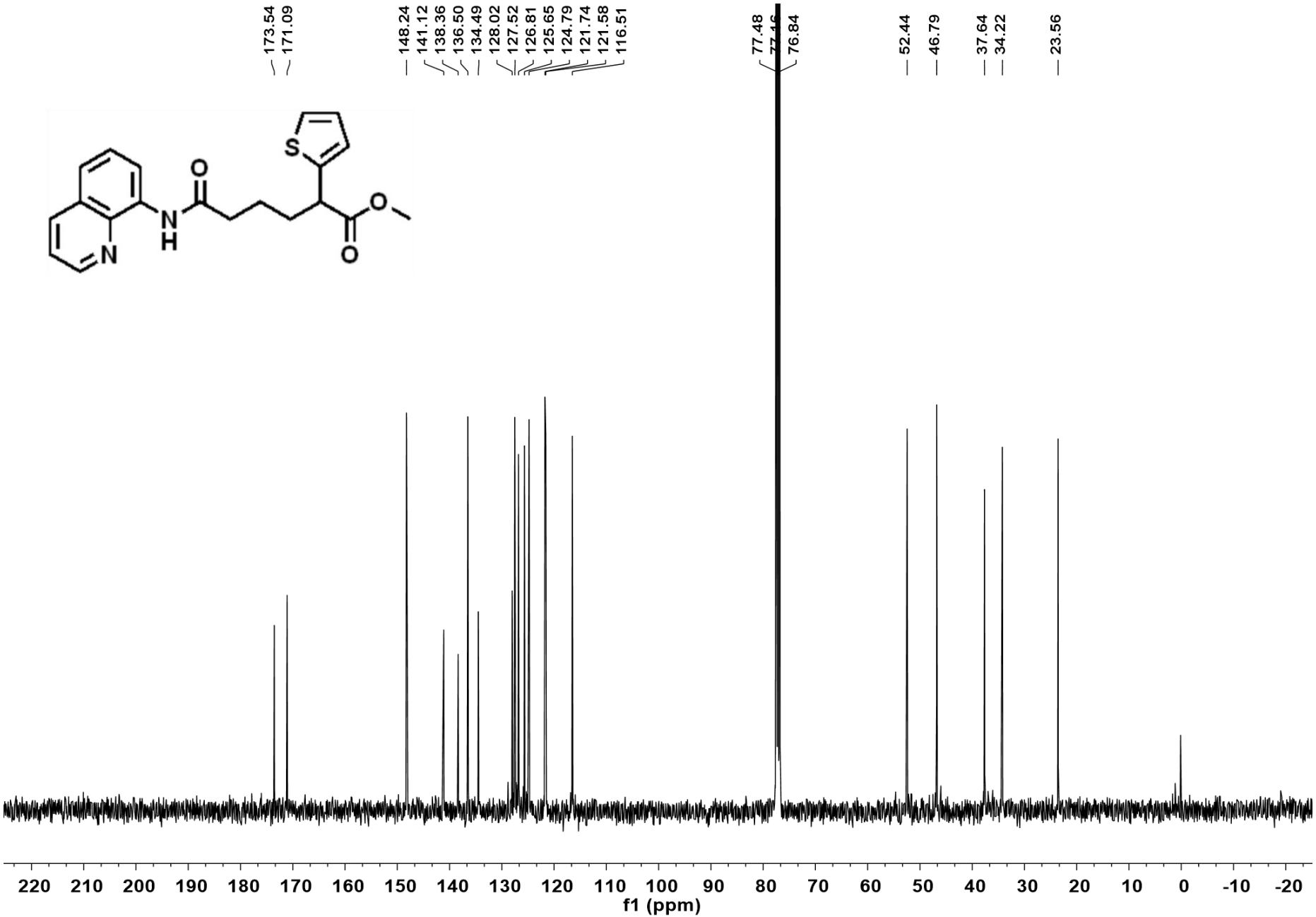
2.63
2.61
2.60
2.59
2.58
2.57
2.57
2.55
2.53
2.26
2.24
2.23
2.22
2.21
2.21
2.19
2.17
2.04
2.02
2.00
1.98
1.98
1.98
1.96
1.95
1.86
1.84
1.83
1.81
1.79
-0.00
S
O
N
H
N
O
O
0.92
1.05
1.00
1.04
3.05
1.00
2.03
0.95
2.98
2.02
1.00
1.00
2.02
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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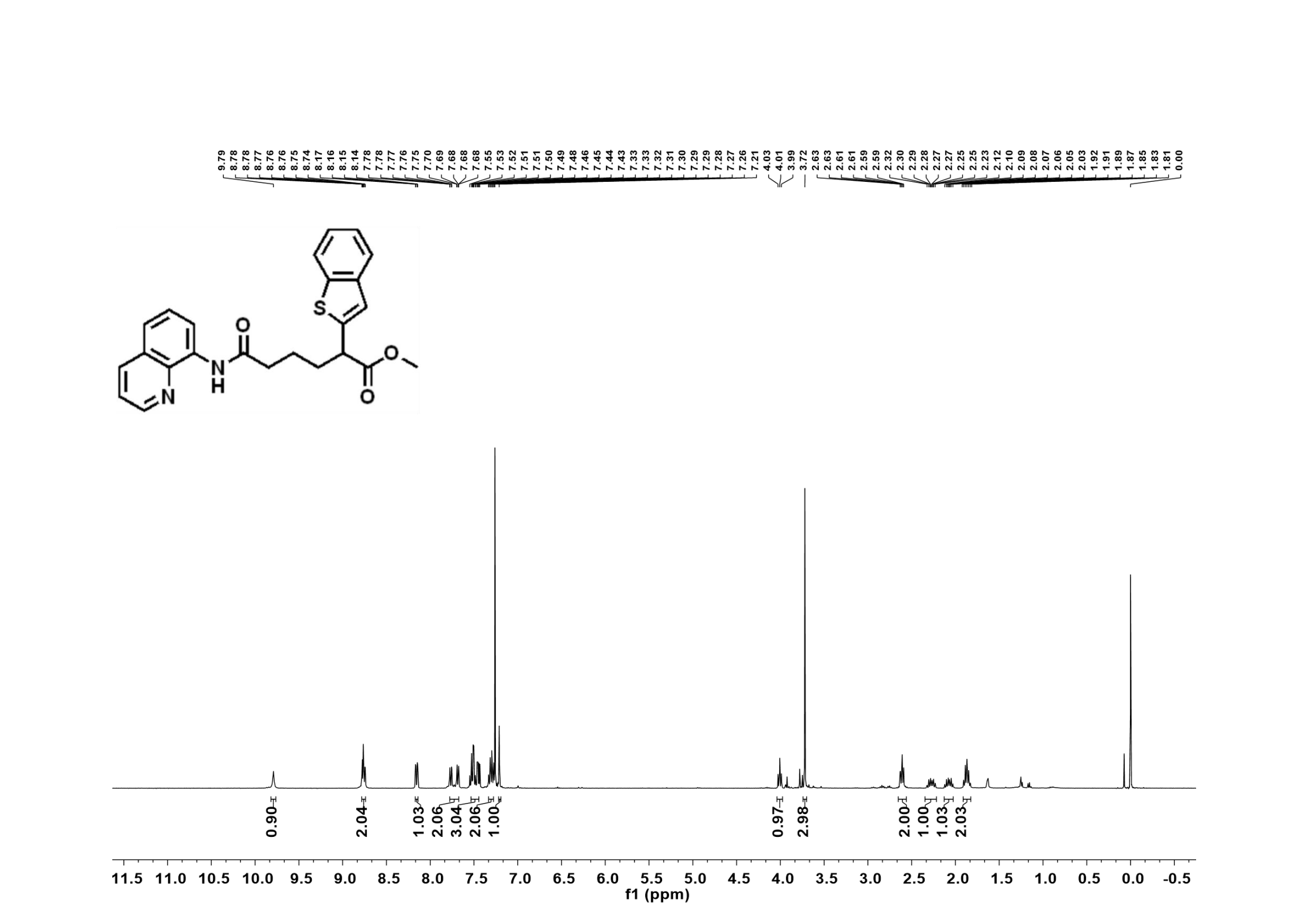
125.65
124.79
121.74
121.58
116.51
77.48
77.16
76.84
52.44
46.79
37.64
34.22
23.56
S
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


9.79 8.78 8.78 8.77 8.76 8.76 8.75 8.74 8.17 8.16 8.15 8.14 7.78 7.78 7.77 7.76 7.75 7.70 7.69 7.68 7.68 7.68 7.55 7.53 7.52 7.51 7.51 7.50 7.49 7.48 7.46 7.45 7.44 7.43 7.33 7.33 7.32 7.31 7.30 7.29 7.29 7.28 7.27 7.26 7.21 4.03 4.01 3.99 3.72 2.63 2.63 2.61 2.61 2.59 2.59 2.32 2.30 2.29 2.28 2.27 2.27 2.25 2.25 2.23 2.12 2.10 2.09 2.08 2.07 2.06 2.05 2.03 1.92 1.91 1.89 1.87 1.85 1.83 1.81 0.00
O
N
H
O
O
S
N
0.90 2.04 1.03 2.06 3.04 2.06 1.00 0.97 2.98 2.00 1.00 1.03 2.03
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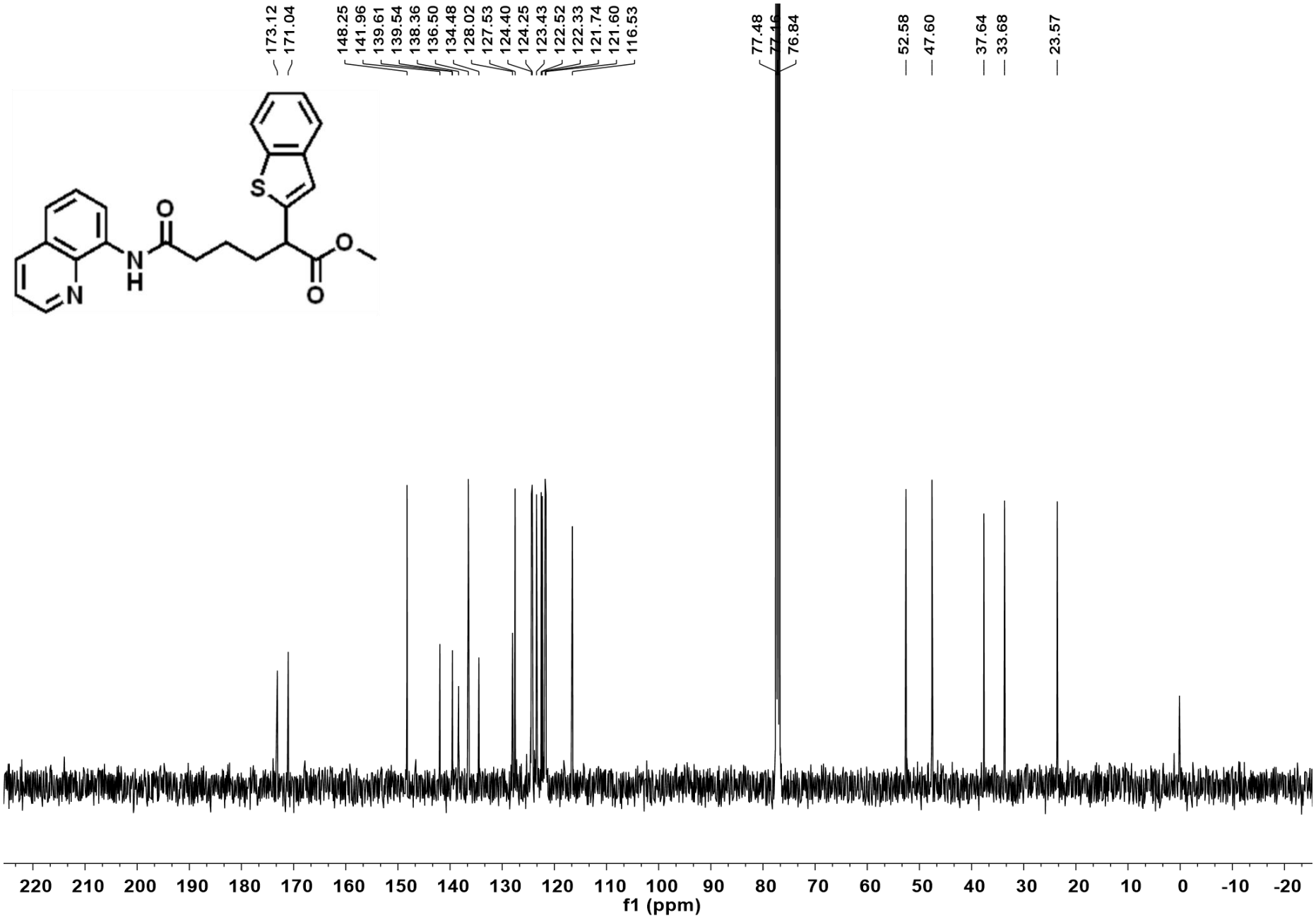
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122.33
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121.60
116.53
77.48
77.16
76.84
52.58
47.60
37.64
33.68
23.57
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S
O
O
N
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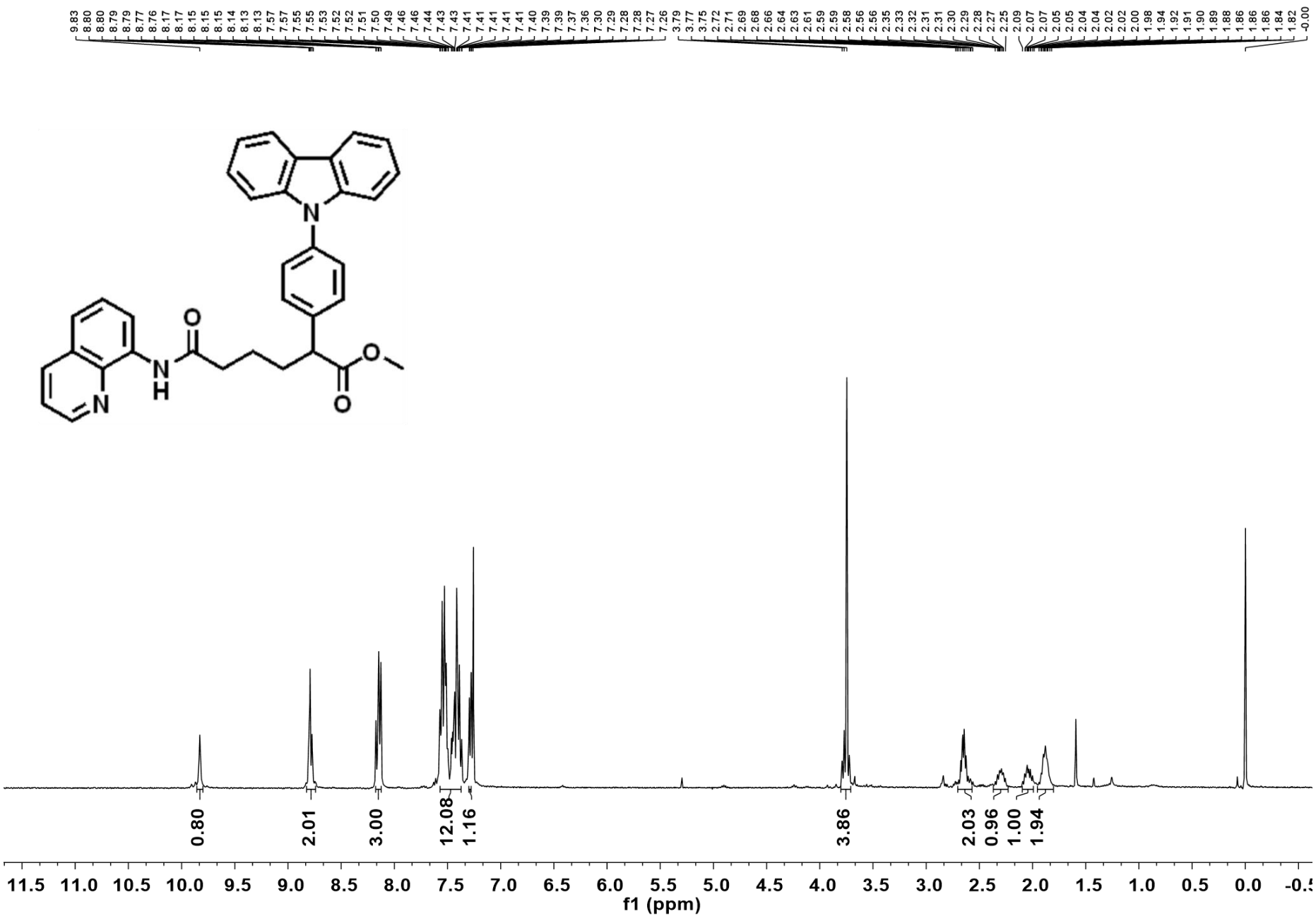
f1 (ppm)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3.79 3.77 3.75 2.72 2.71 2.69 2.68 2.66 2.64 2.63 2.61 2.59 2.59 2.58 2.56 2.56 2.35 2.33 2.32 2.31 2.31 2.30 2.29 2.28 2.27 2.25 2.09 2.07 2.07 2.05 2.05 2.04 2.04 2.02 2.02 2.00 1.98 1.94 1.92 1.91 1.90 1.89 1.88 1.86 1.86 1.86 1.84 1.82 -0.00
N
O
N
H
O
O
0.80
2.01
3.00
12.08
1.16
3.86
2.03
0.96
1.00
1.94
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
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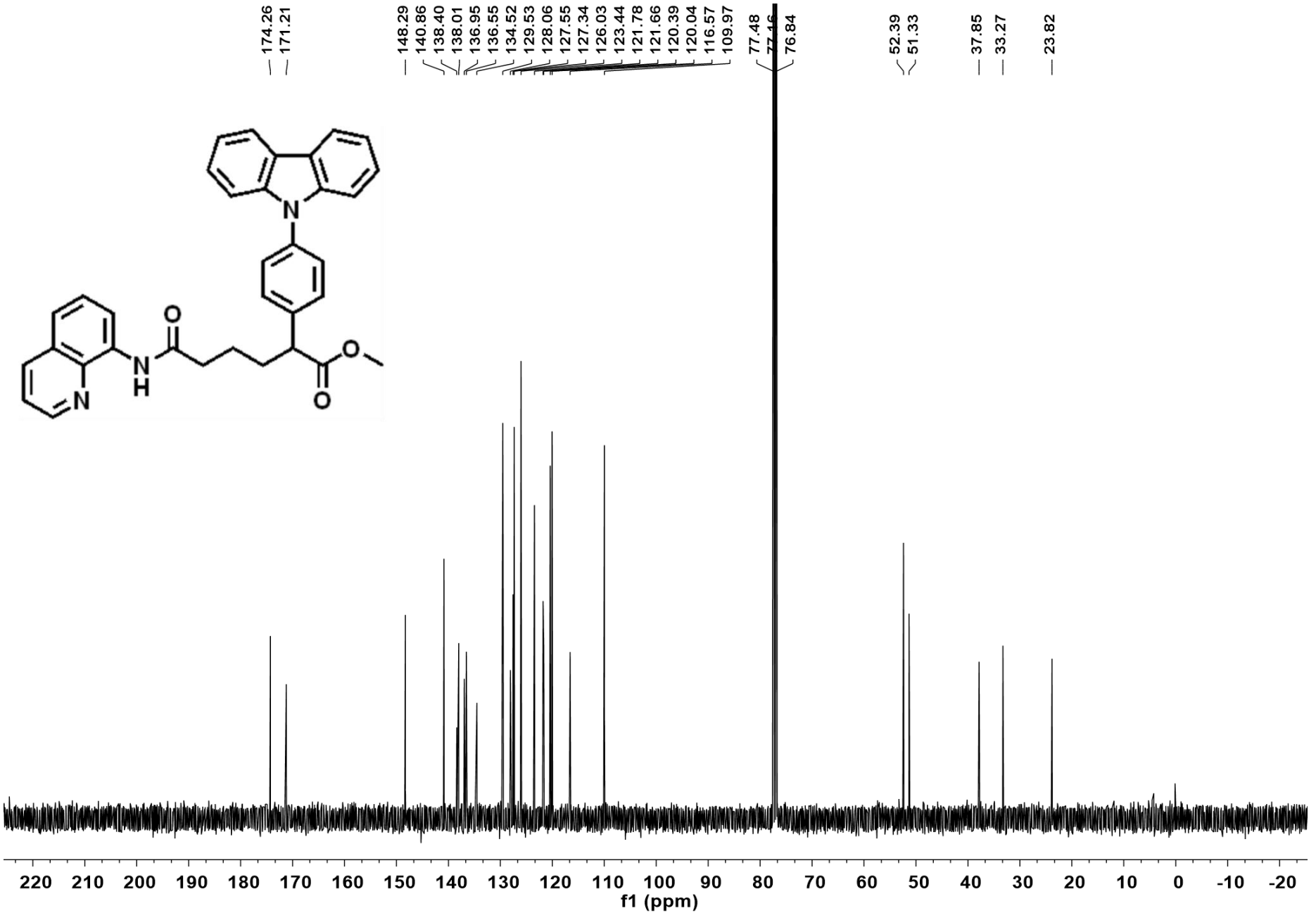
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120.04
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77.16
76.84
52.39
51.33
37.85
33.27
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O
O
N
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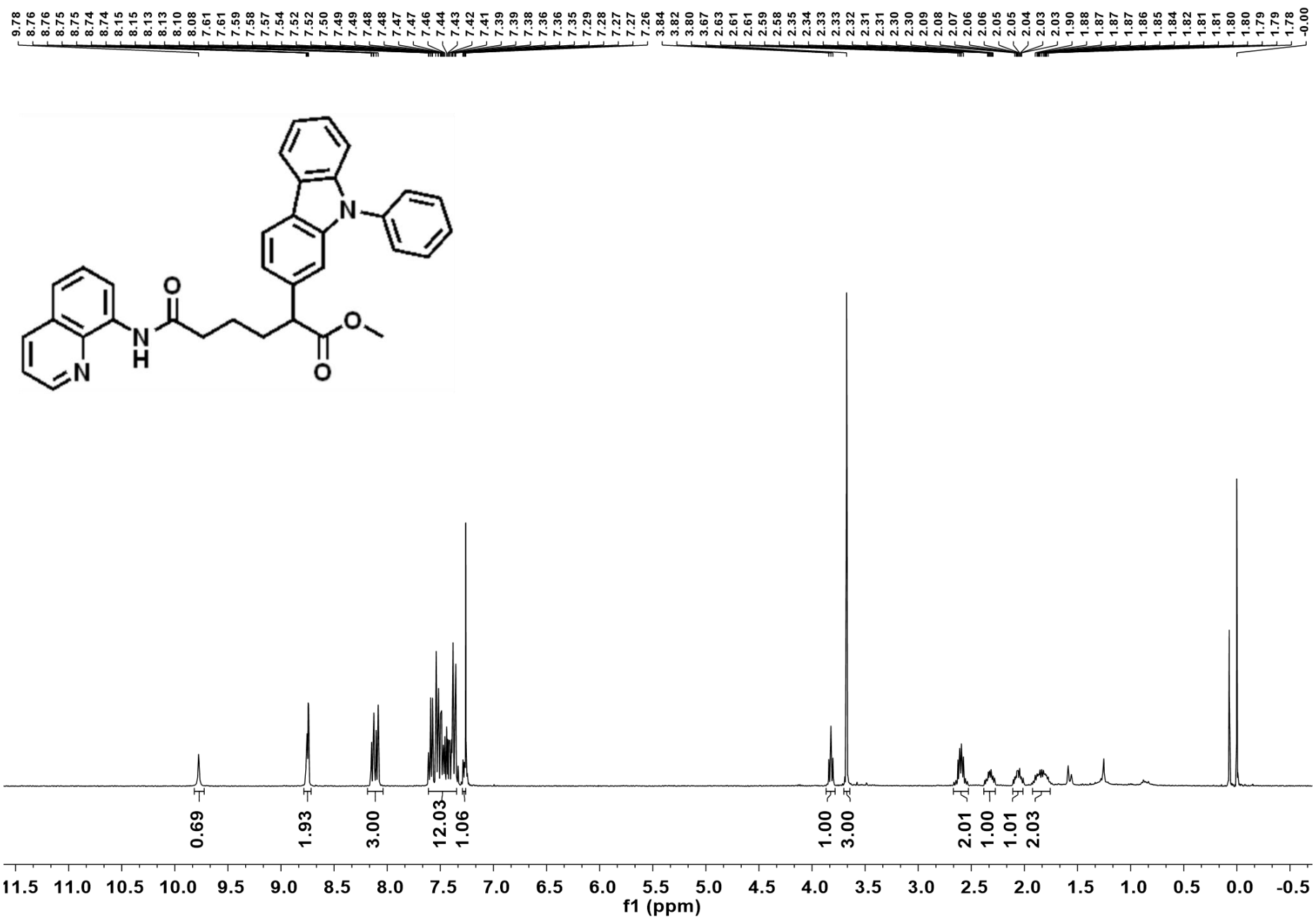
f1 (ppm)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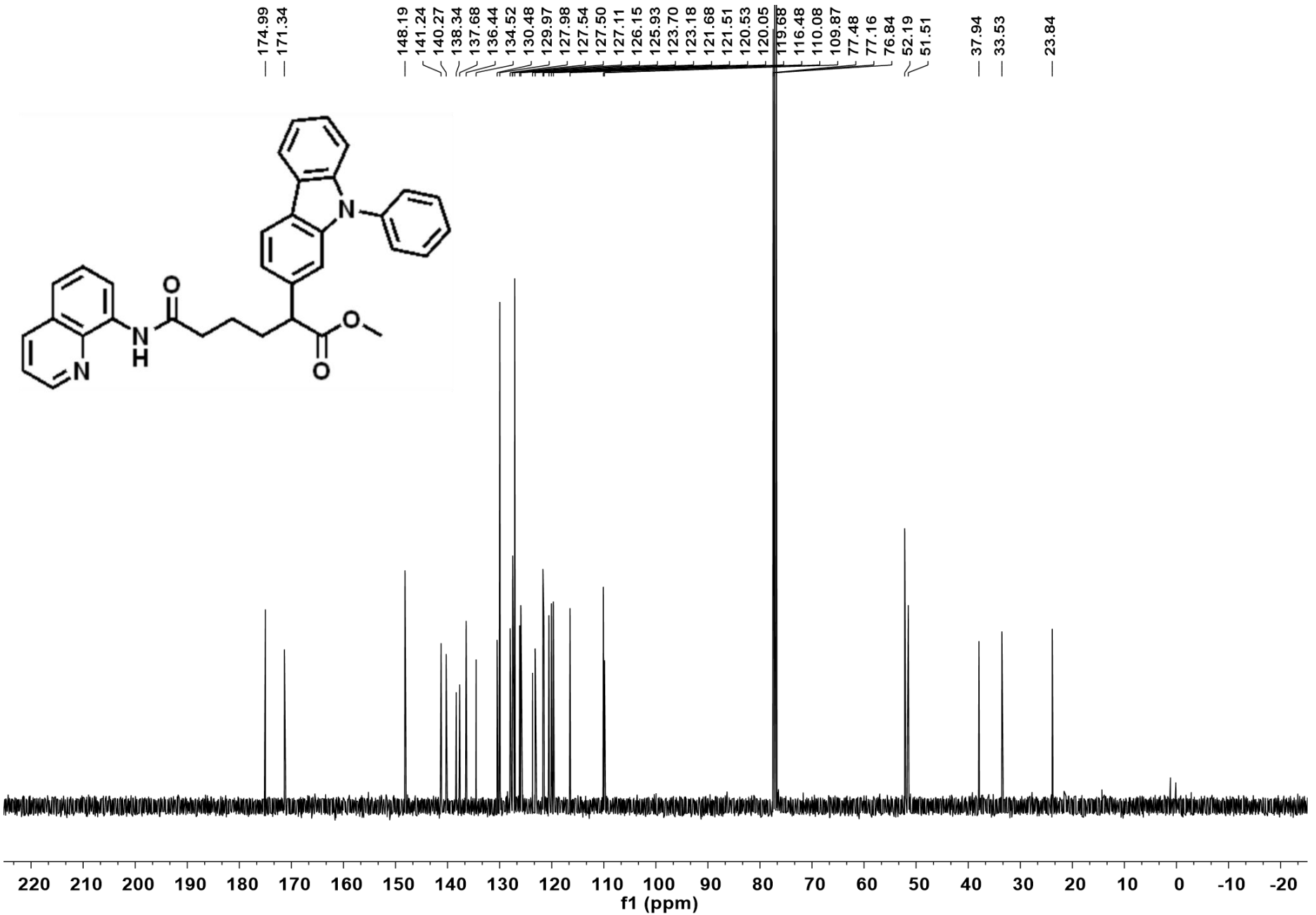
3.84 3.82 3.80 3.67 2.63 2.61 2.61 2.59 2.58 2.35 2.34 2.33 2.33 2.32 2.31 2.31 2.30 2.30 2.09 2.08 2.07 2.06 2.06 2.05 2.05 2.04 2.03 2.03 1.90 1.88 1.87 1.87 1.87 1.86 1.85 1.84 1.82 1.81 1.81 1.80 1.80 1.79 1.79 1.78 -0.00
O
N
H
N
O
O
0.69
1.93
3.00
12.03
1.06
1.00
3.00
2.01
1.00
1.01
2.03
11.5 11.0 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
f1 (ppm)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127.54
127.50
127.11
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123.70
123.18
121.68
121.51
120.53
120.05
119.68
116.48
110.08
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77.48
77.16
76.84
52.19
51.51
37.94
33.53
23.84
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H
N
O
O
N
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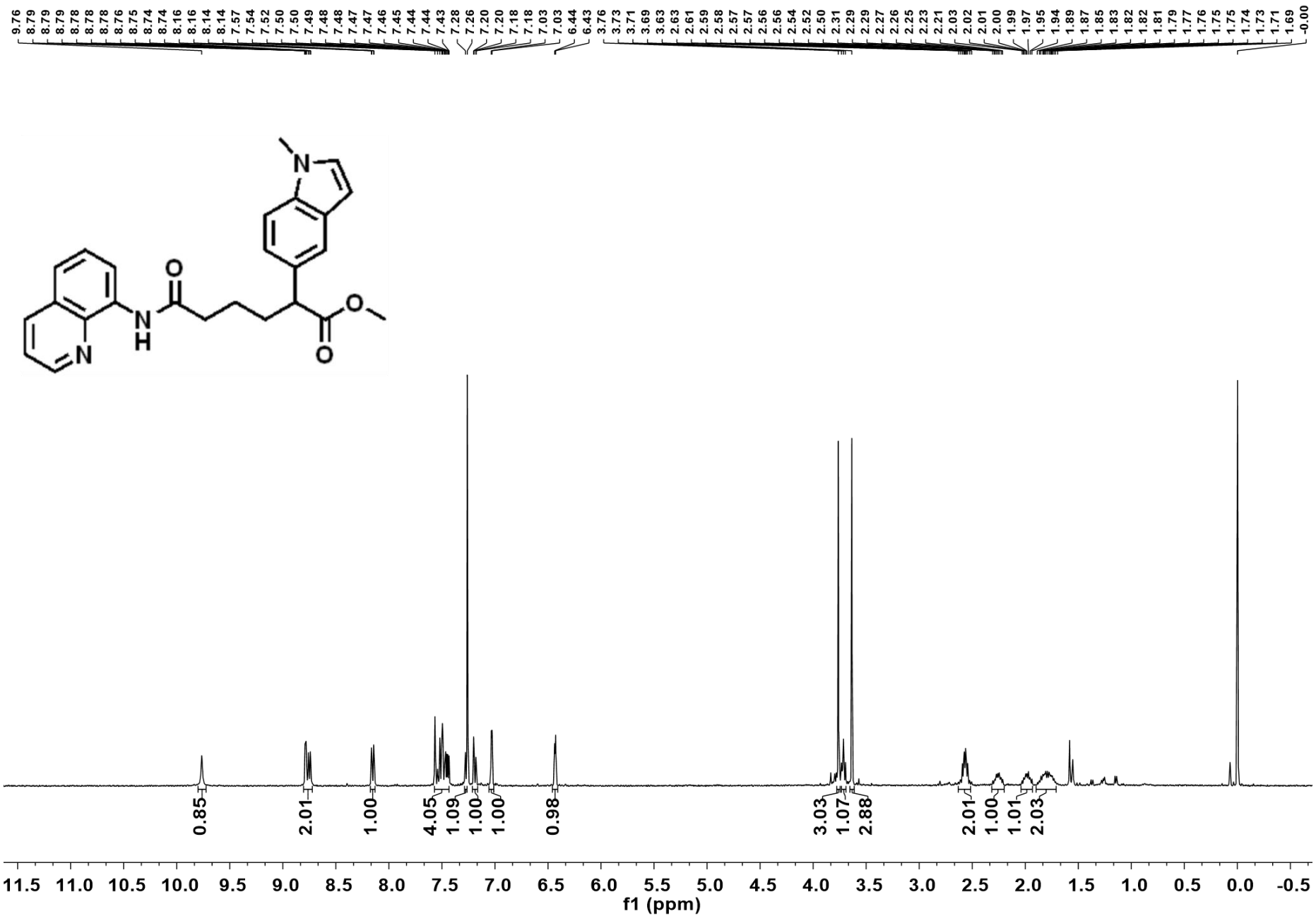
f1 (ppm)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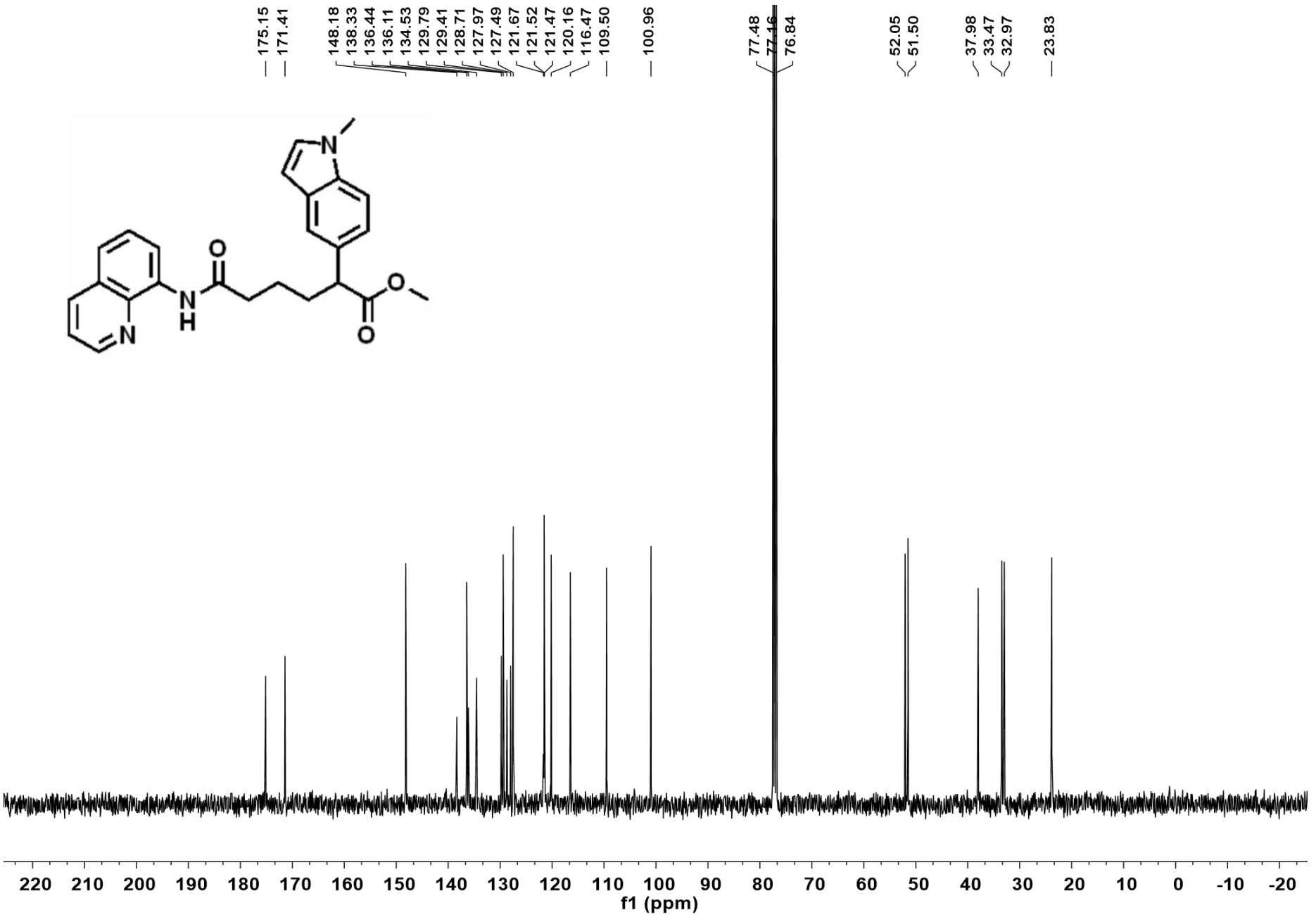
N
O
N
H
N
O
O
0.85
2.01
1.00
4.05
1.09
1.00
1.00
0.98
3.03
1.07
2.88
2.01
1.00
1.01
2.03
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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121.52
121.47
120.16
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109.50
100.96
77.48
77.16
76.84
52.05
51.50
37.98
33.47
32.97
23.83
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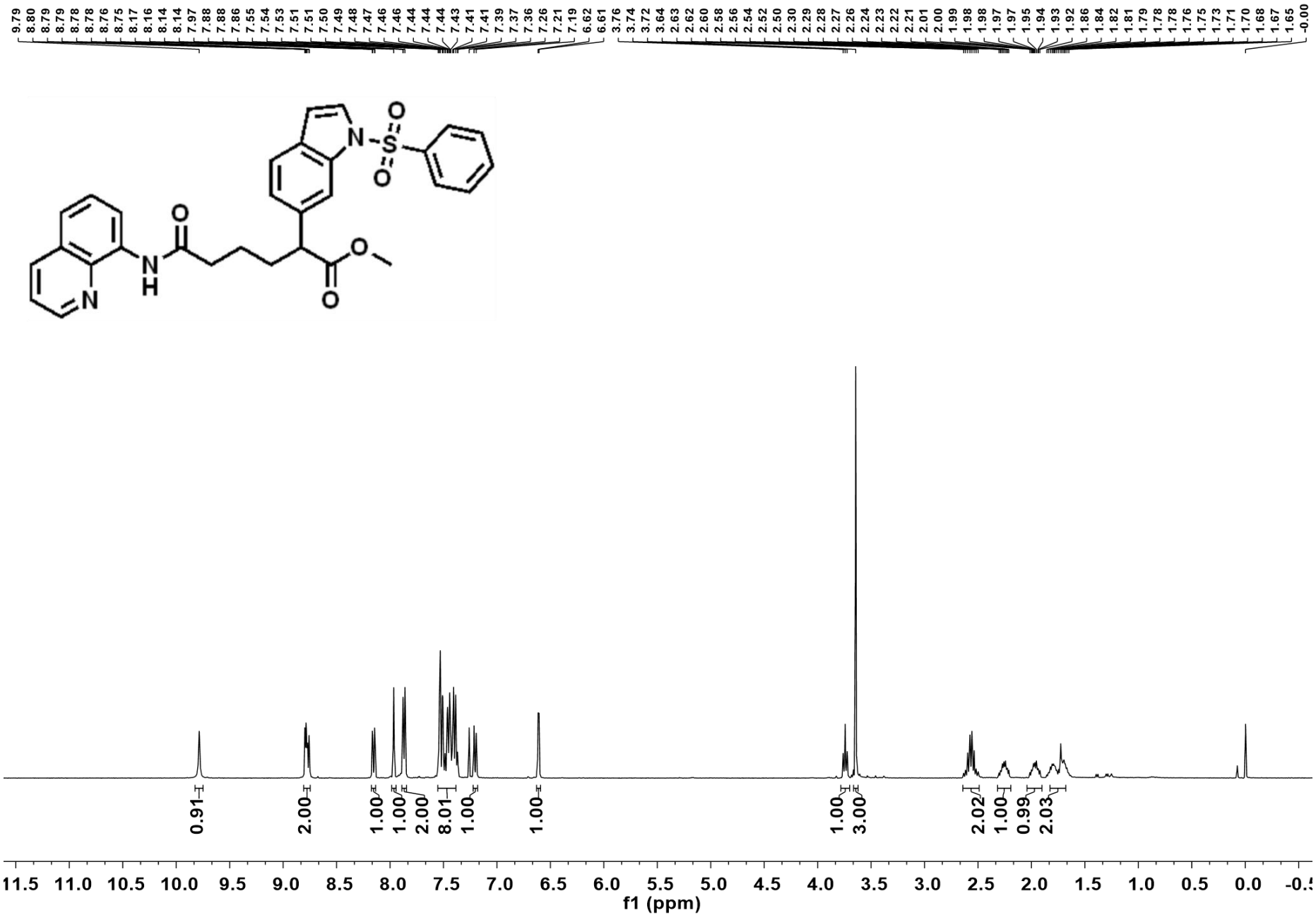
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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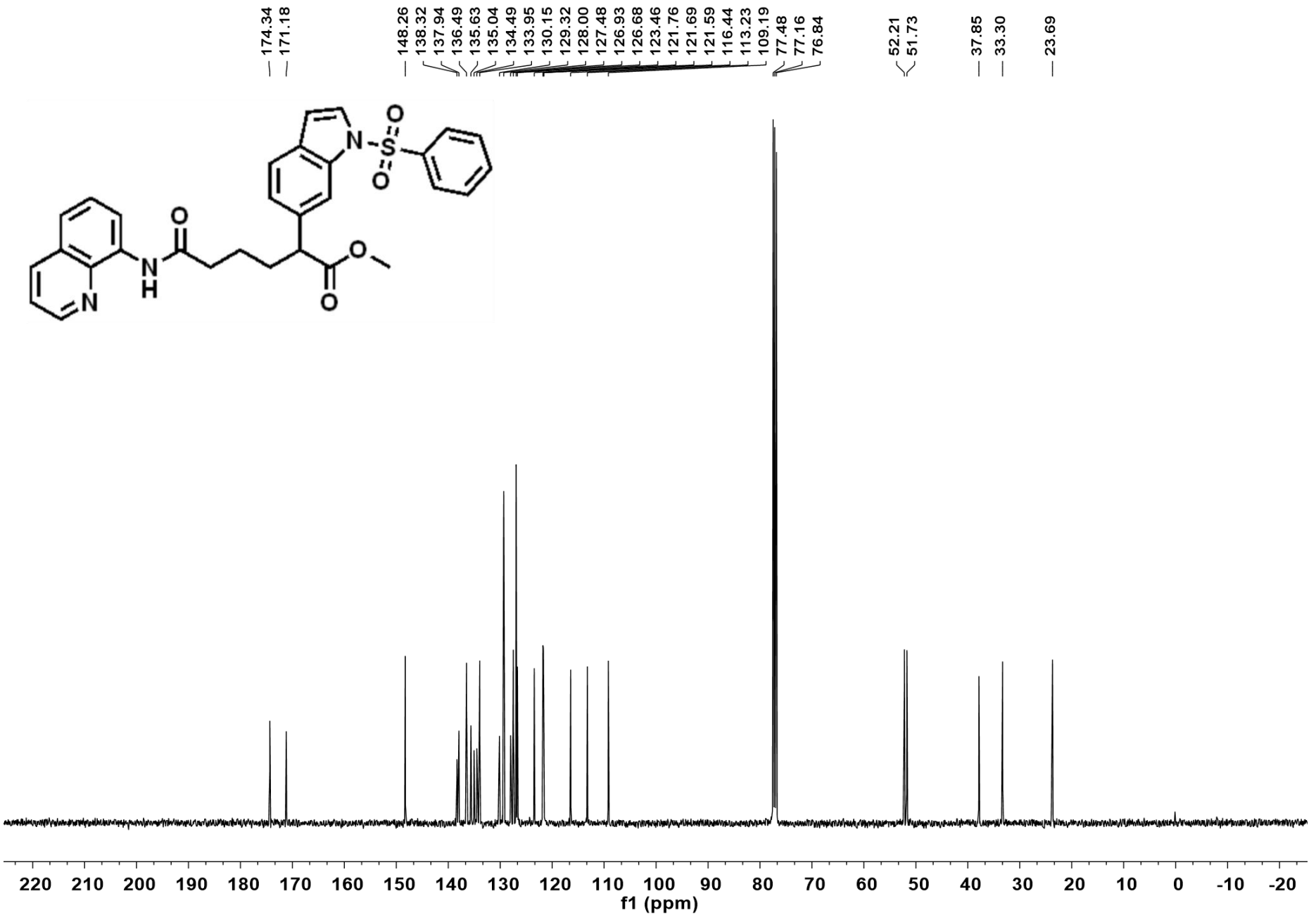
3.76 3.74 3.72 3.64 2.63 2.62 2.60 2.58 2.56 2.54 2.52 2.50 2.30 2.29 2.28 2.27 2.26 2.24 2.23 2.22 2.21 2.01 2.00 1.99 1.98 1.98 1.97 1.97 1.95 1.94 1.93 1.92 1.86 1.84 1.82 1.81 1.79 1.78 1.78 1.76 1.75 1.73 1.71 1.70 1.68 1.67 1.65 -0.00
O
N
S
O
O
N
H
O
O
O
N
0.91
2.00
1.00
1.00
2.00
8.01
1.00
1.00
1.00
3.00
2.02
1.00
0.99
2.03
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
f1 (ppm)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121.69
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113.23
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77.48
77.16
76.84
52.21
51.73
37.85
33.30
23.69
O
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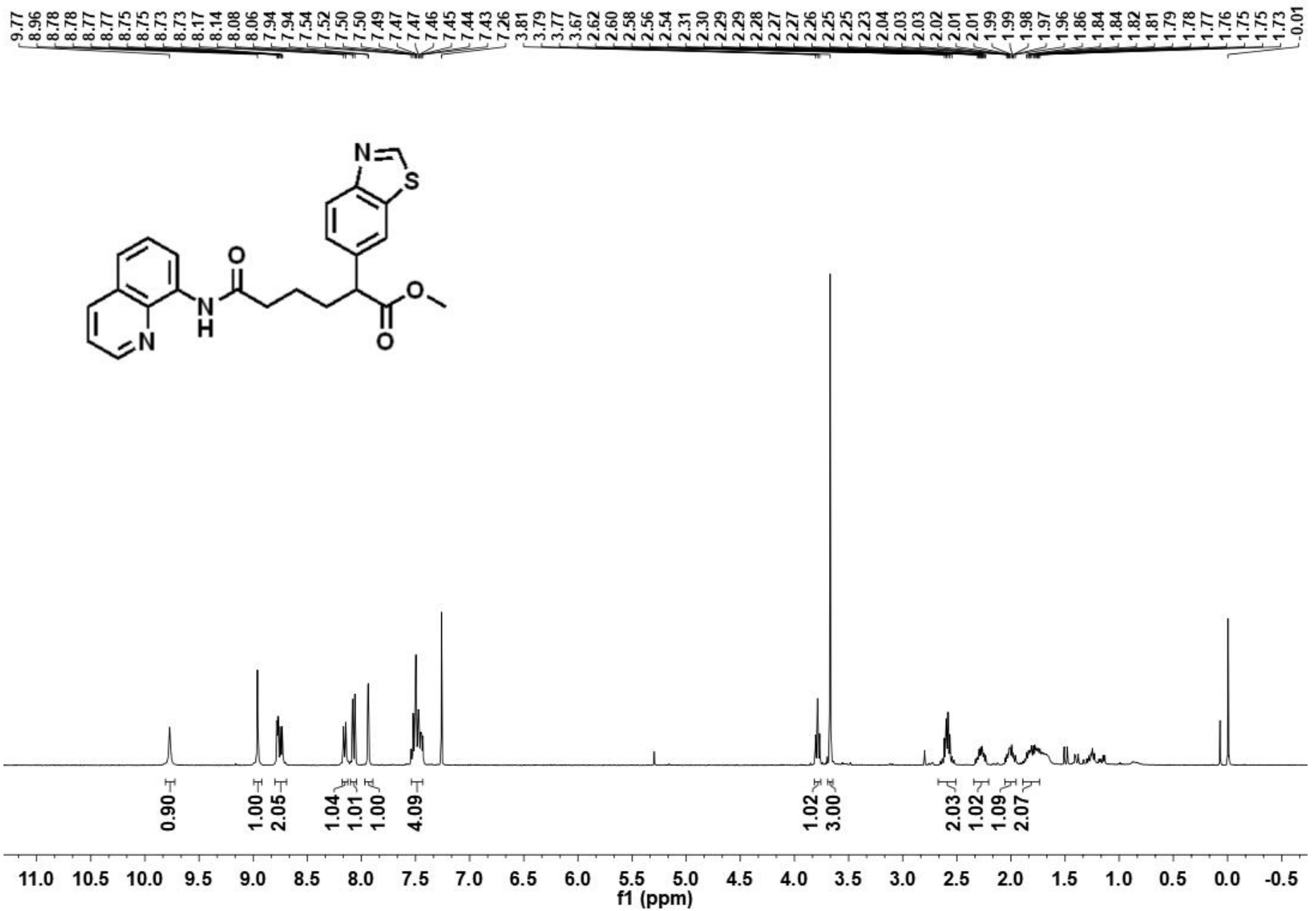
N
H
O
O
N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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2.31
2.30
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2.27
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2.01
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1.99
1.98
1.97
1.96
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1.82
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1.77
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1.75
1.75
1.73
-0.01
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O
N
H
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O
O
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1.04
1.01
1.00
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9.0
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6.0
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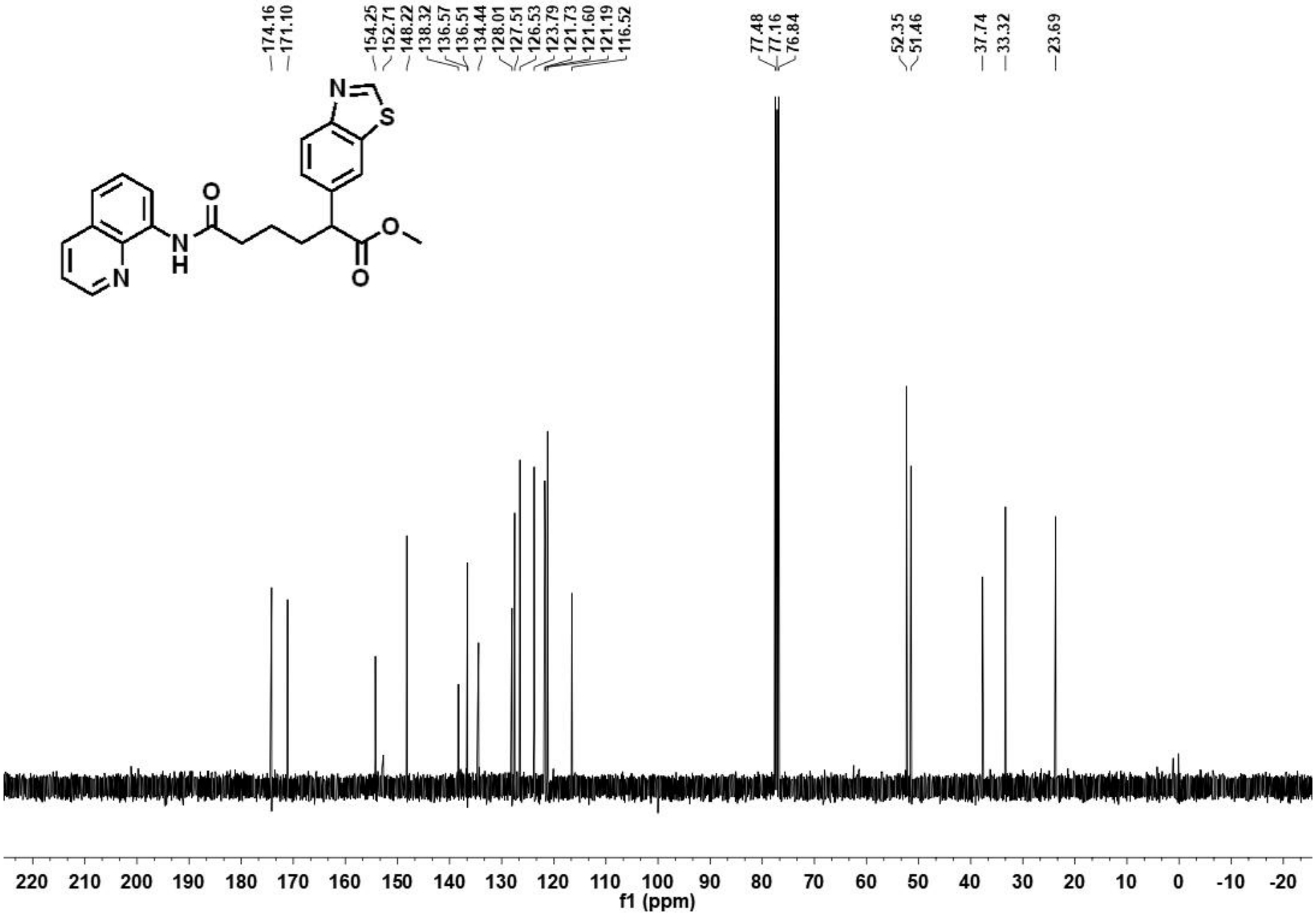
-0.5
f1 (ppm)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77.16
76.84
52.35
51.46
37.74
33.32
23.69
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H
O
O
N
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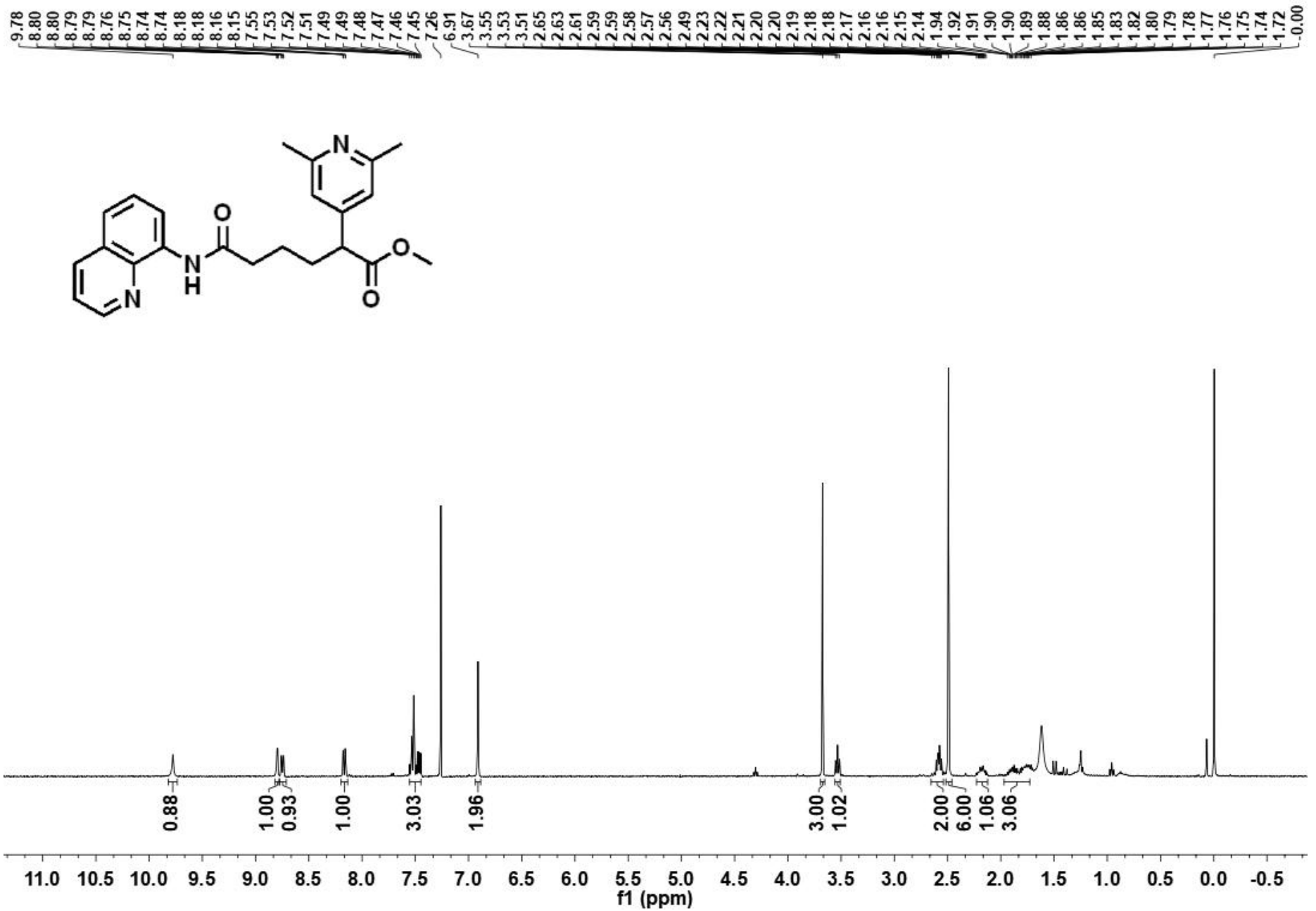
f1 (ppm)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7.52
7.51
7.49
7.49
7.48
7.47
7.46
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7.26
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2.56
2.49
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2.16
2.16
2.15
2.14
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1.91
1.90
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1.79
1.78
1.77
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1.75
1.74
1.72
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H
O
O
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0.93
1.00
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1.96
3.00
1.02
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3.06
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6.0
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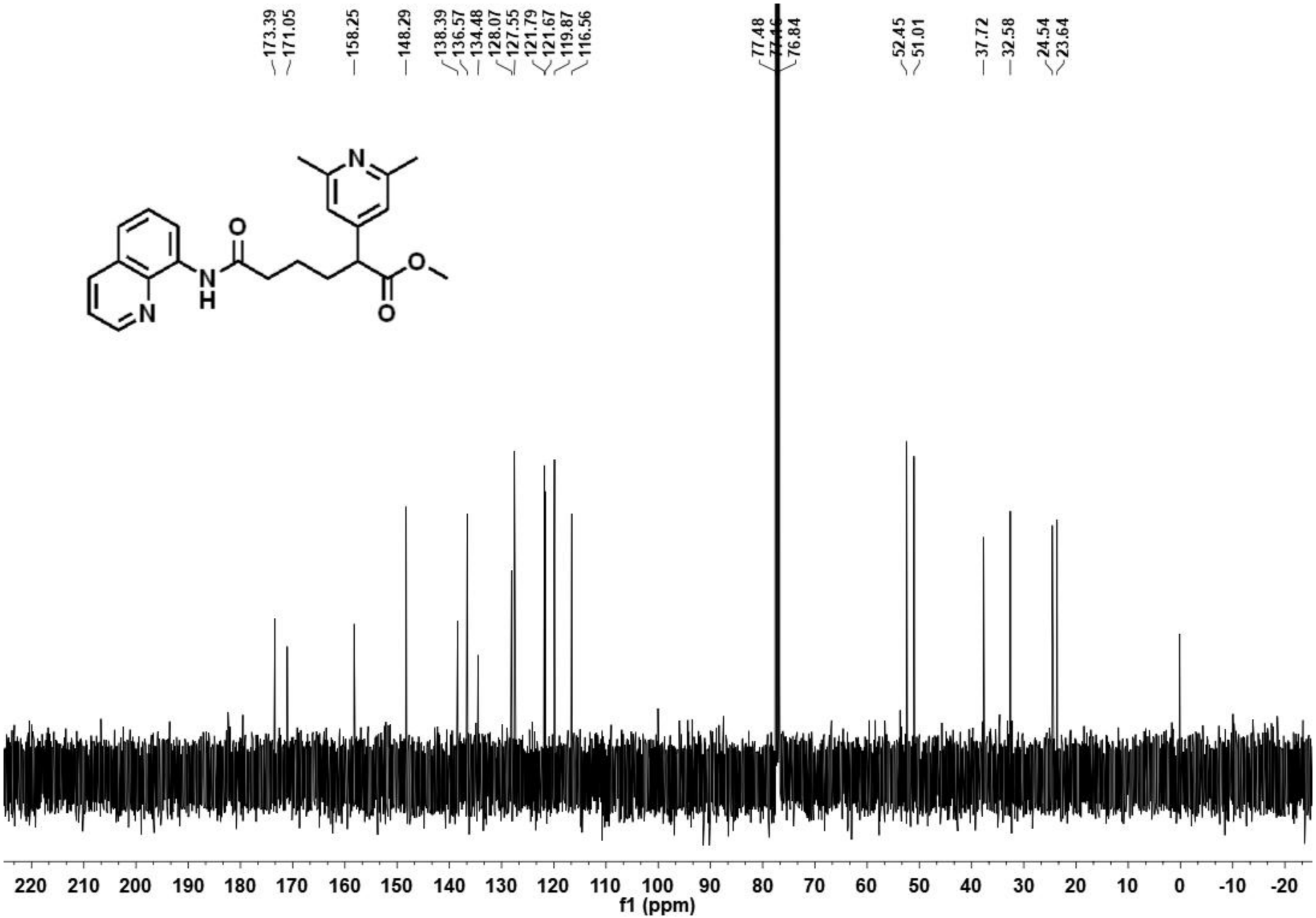
f1 (ppm)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32.58
24.54
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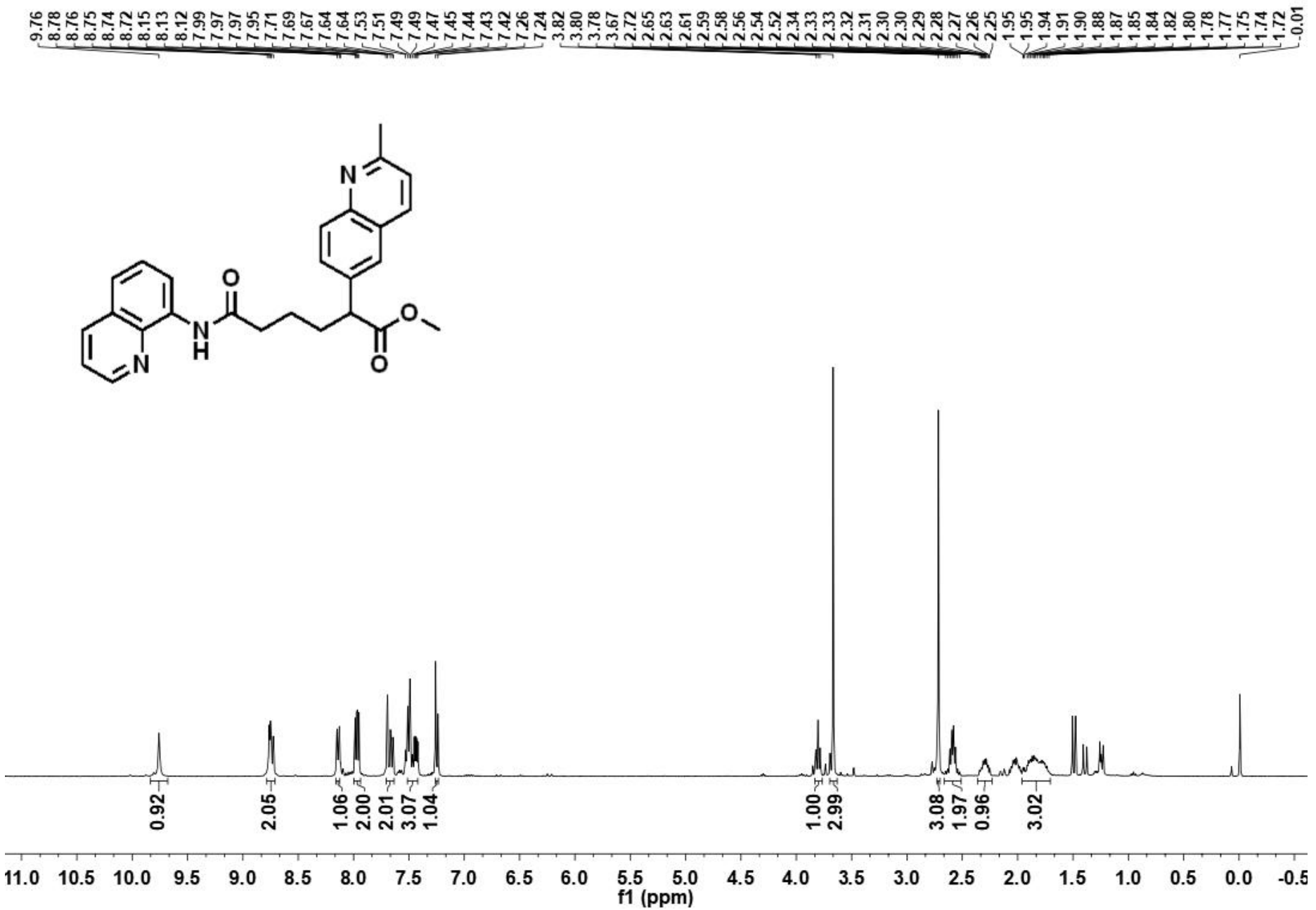
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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3.78
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1.82
1.80
1.78
1.77
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1.74
1.72
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N
H
O
O
0.92
2.05
1.06
2.00
2.01
3.07
1.04
1.00
2.99
3.08
1.97
0.96
3.02
11.0
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
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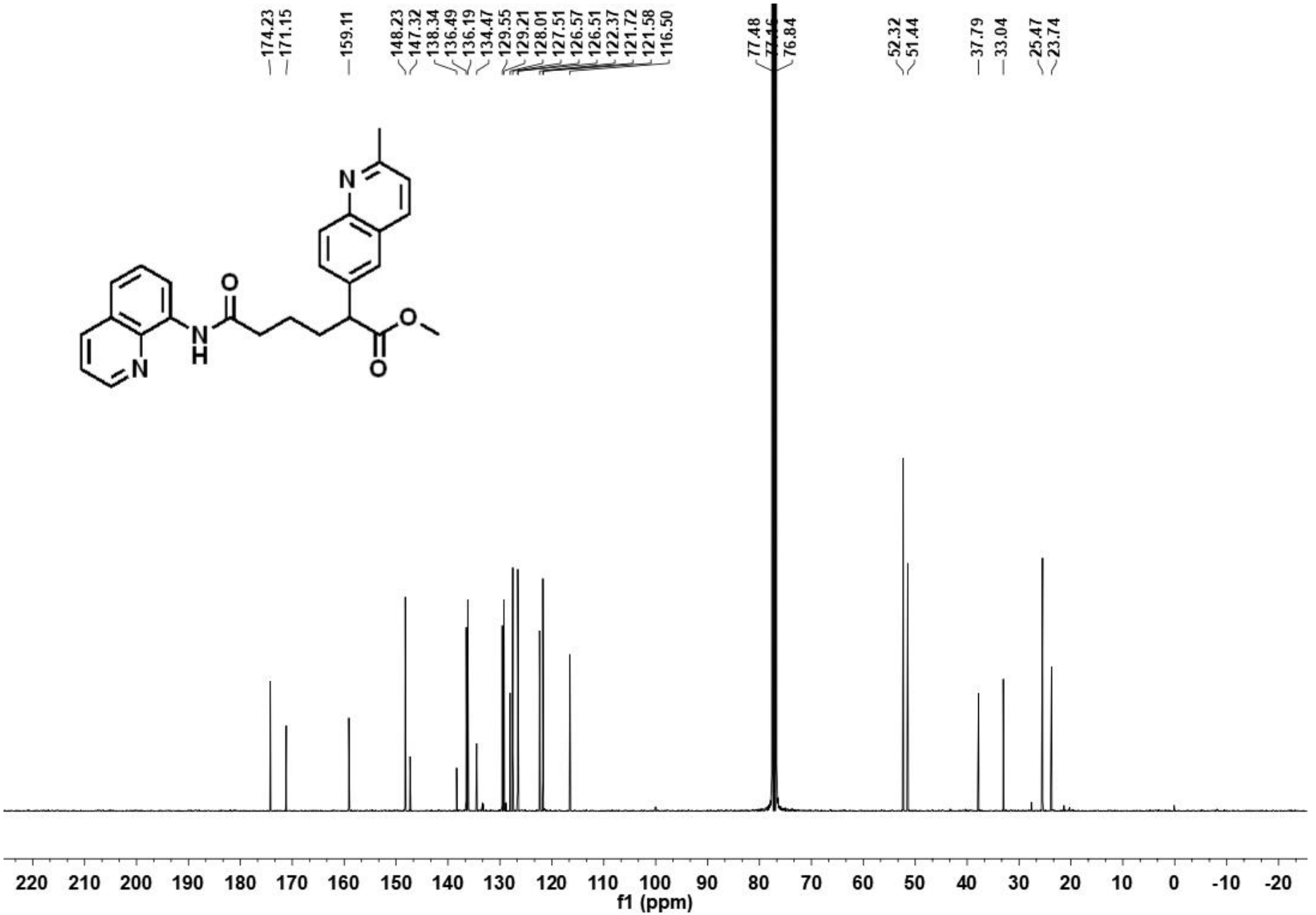
1.0
0.5
0.0
-0.5
f1 (ppm)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126.57
126.51
122.37
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121.58
116.50
77.48
76.84
52.32
51.44
37.79
33.04
25.47
23.74
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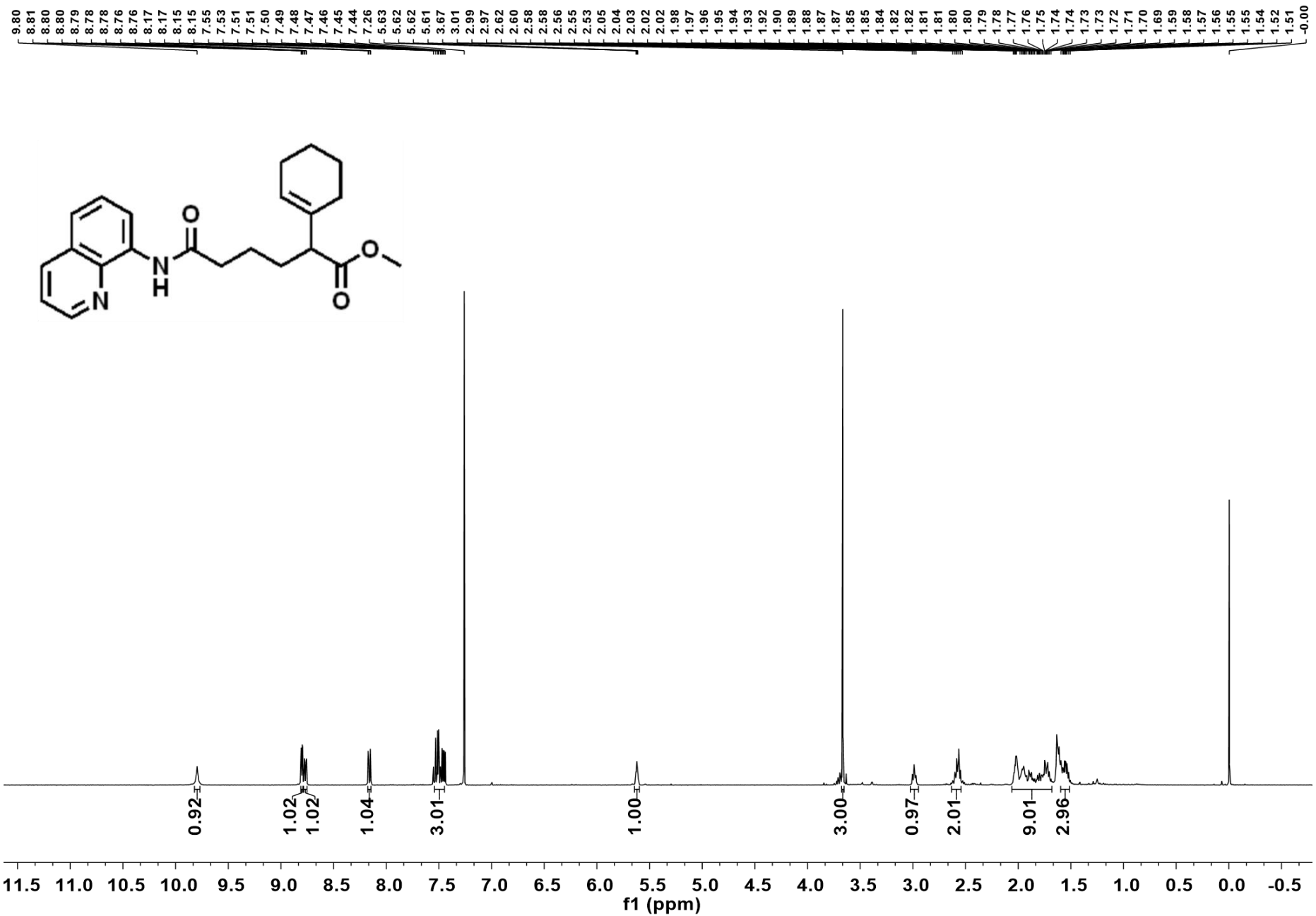
N
H
O
O
N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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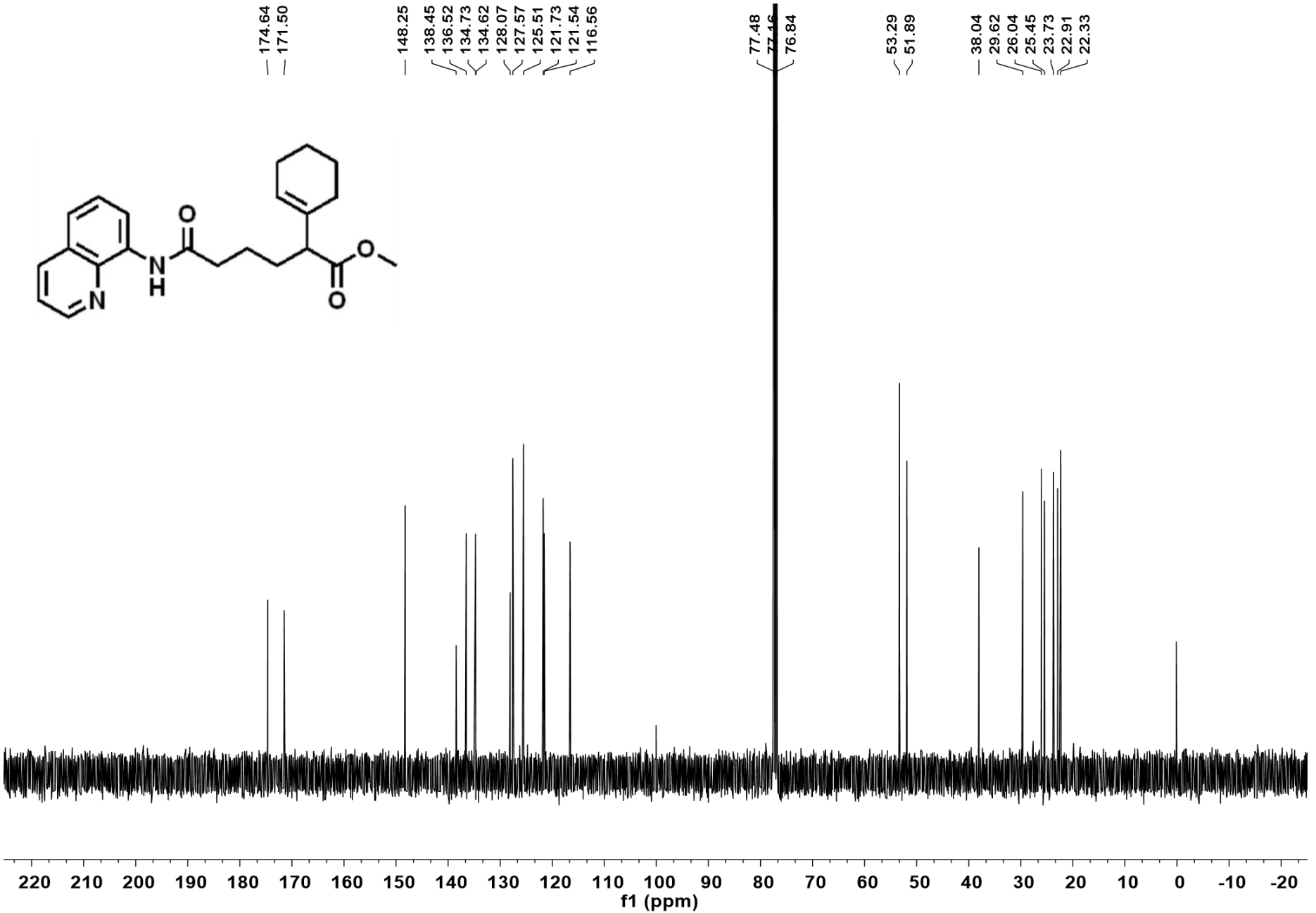
O
N
H
N
O
O
0.92
1.02
1.02
1.04
3.01
1.00
3.00
0.97
2.01
9.01
2.96
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.07
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125.51
121.73
121.54
116.56
77.48
77.16
76.84
53.29
51.89
38.04
29.62
26.04
25.45
23.73
22.91
22.33
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N
H
N
O
O
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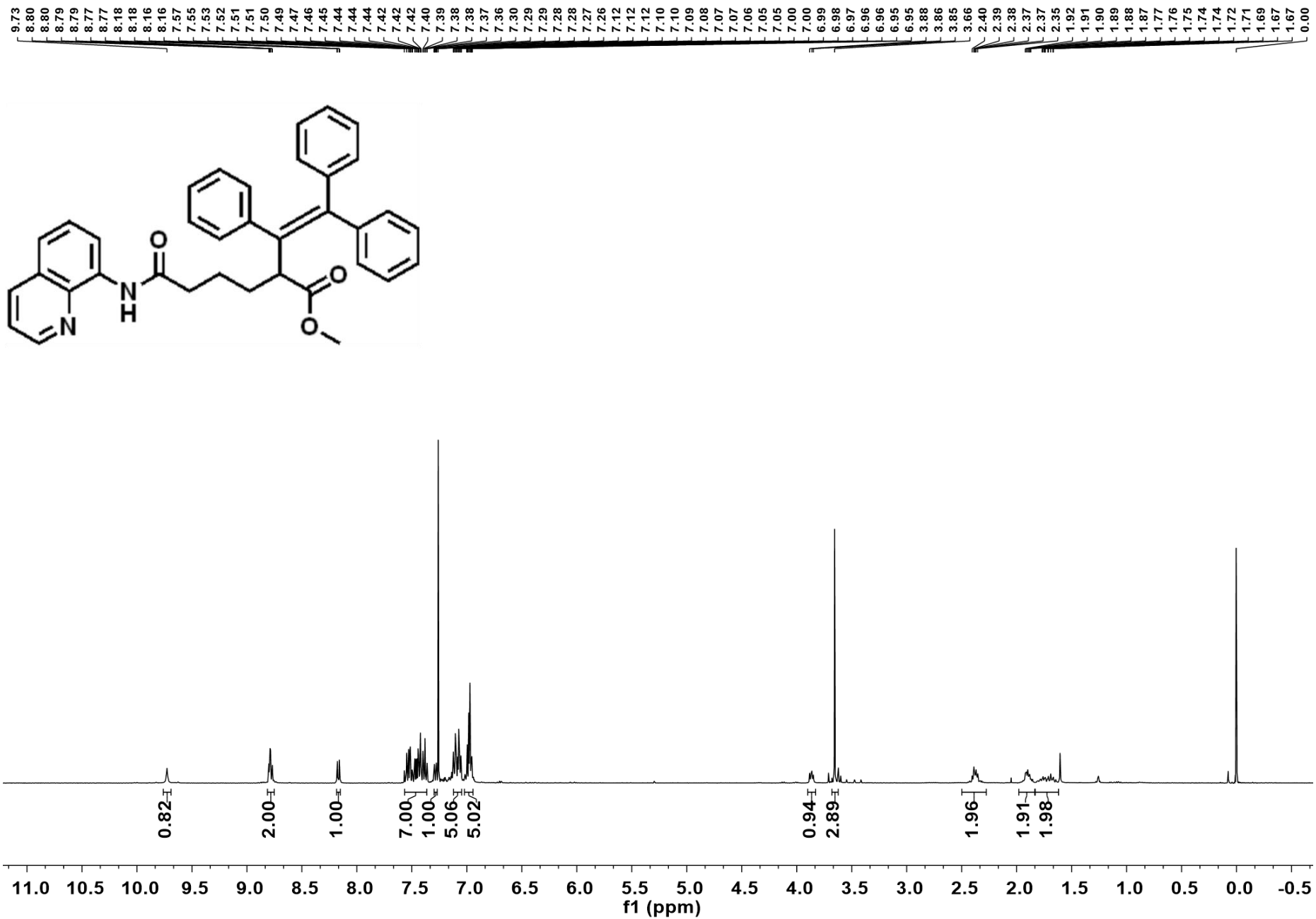
f1 (ppm)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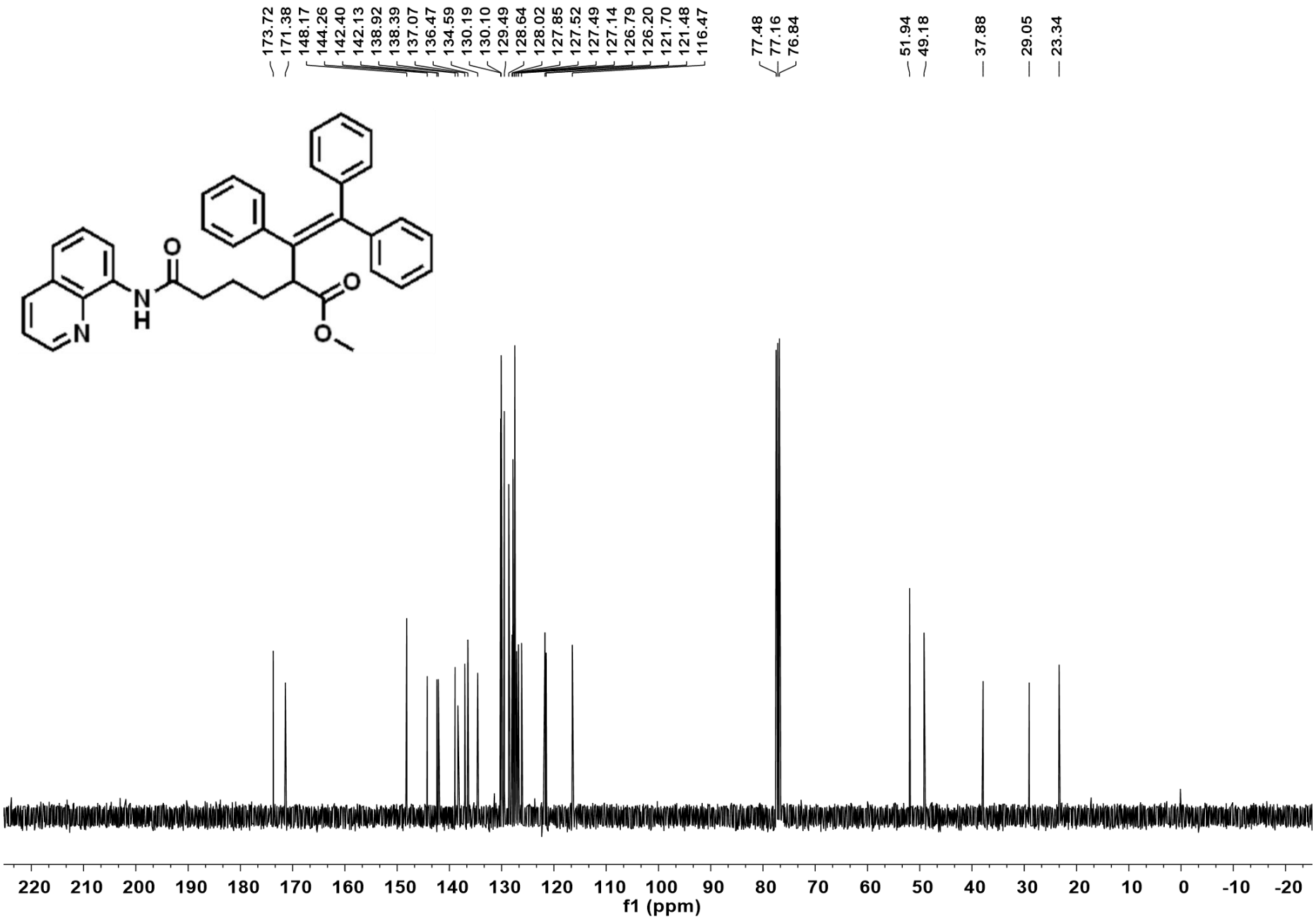
O
N
H
N
O
O
0.82
2.00
1.00
7.00
1.00
5.06
5.02
0.94
2.89
1.96
1.91
1.98
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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130.10
129.49
128.64
128.02
127.85
127.52
127.49
127.14
126.79
126.20
121.70
121.48
116.47
77.48
77.16
76.84
51.94
49.18
37.88
29.05
23.34
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H
N
O
O
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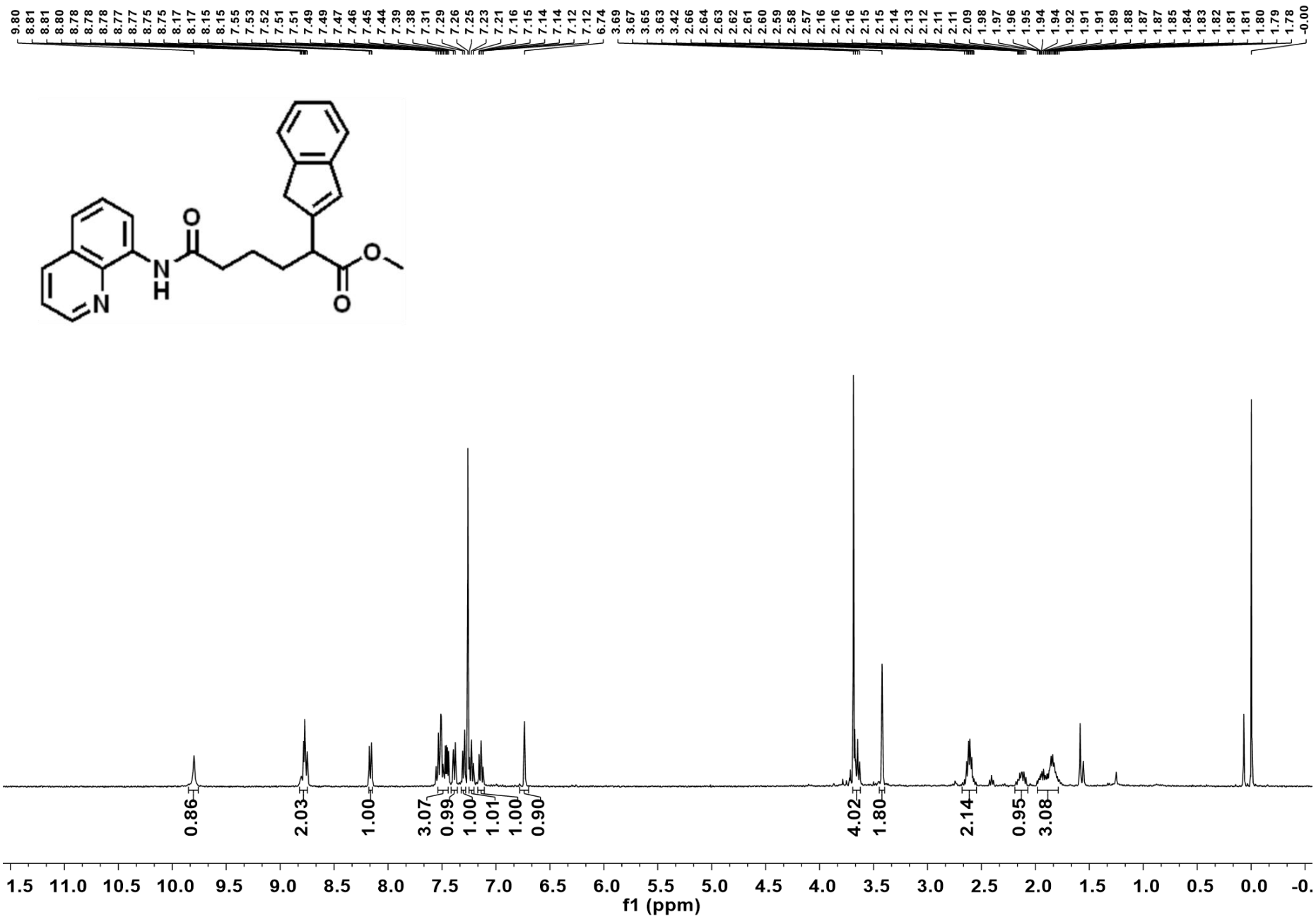
f1 (ppm)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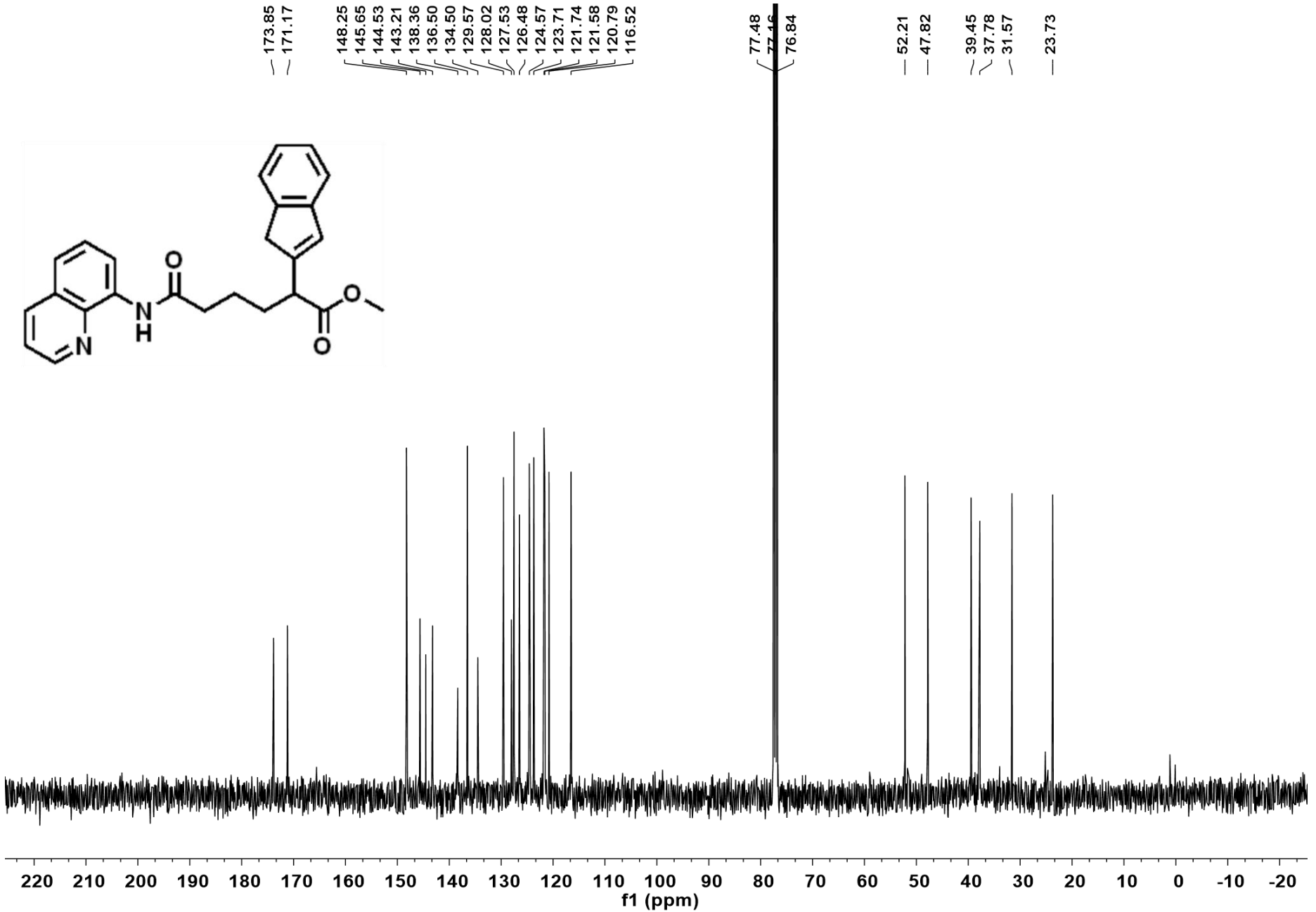
3.69 3.67 3.65 3.63 3.42 2.66 2.64 2.63 2.62 2.61 2.60 2.59 2.58 2.57 2.16 2.16 2.16 2.15 2.15 2.14 2.13 2.12 2.11 2.11 2.09 1.98 1.97 1.96 1.95 1.94 1.94 1.92 1.91 1.91 1.89 1.88 1.87 1.87 1.85 1.84 1.83 1.82 1.81 1.81 1.80 1.79 1.78 -0.00
O
N
H
N
O
O
0.86
2.03
1.00
3.07
0.99
1.00
1.01
1.00
0.90
4.02
1.80
2.14
0.95
3.08
1.5 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.
f1 (ppm)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136.50
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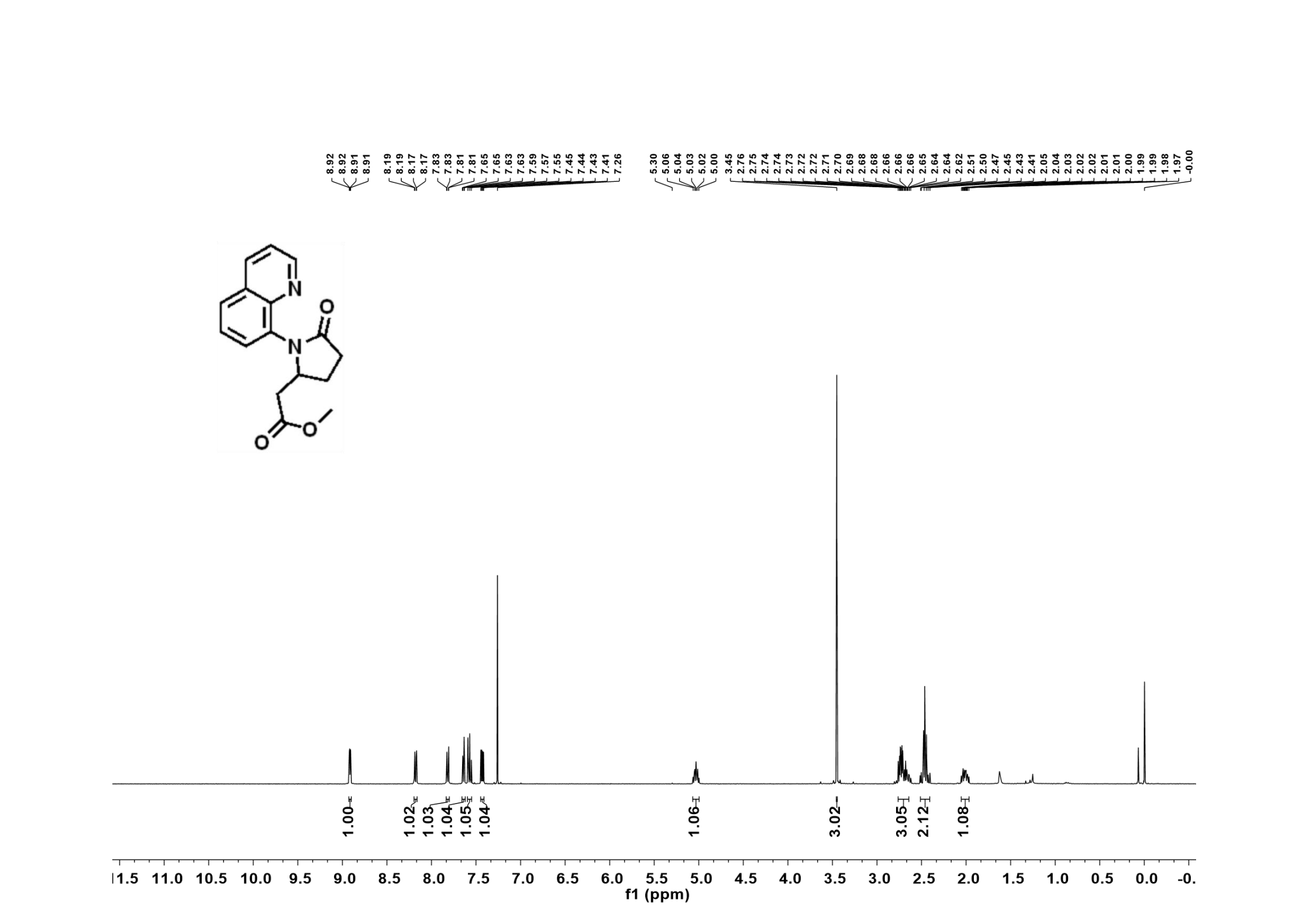
129.57
128.02
127.53
126.48
124.57
123.71
121.74
121.58
120.79
116.52
77.48
77.16
76.84
52.21
47.82
39.45
37.78
31.57
23.73
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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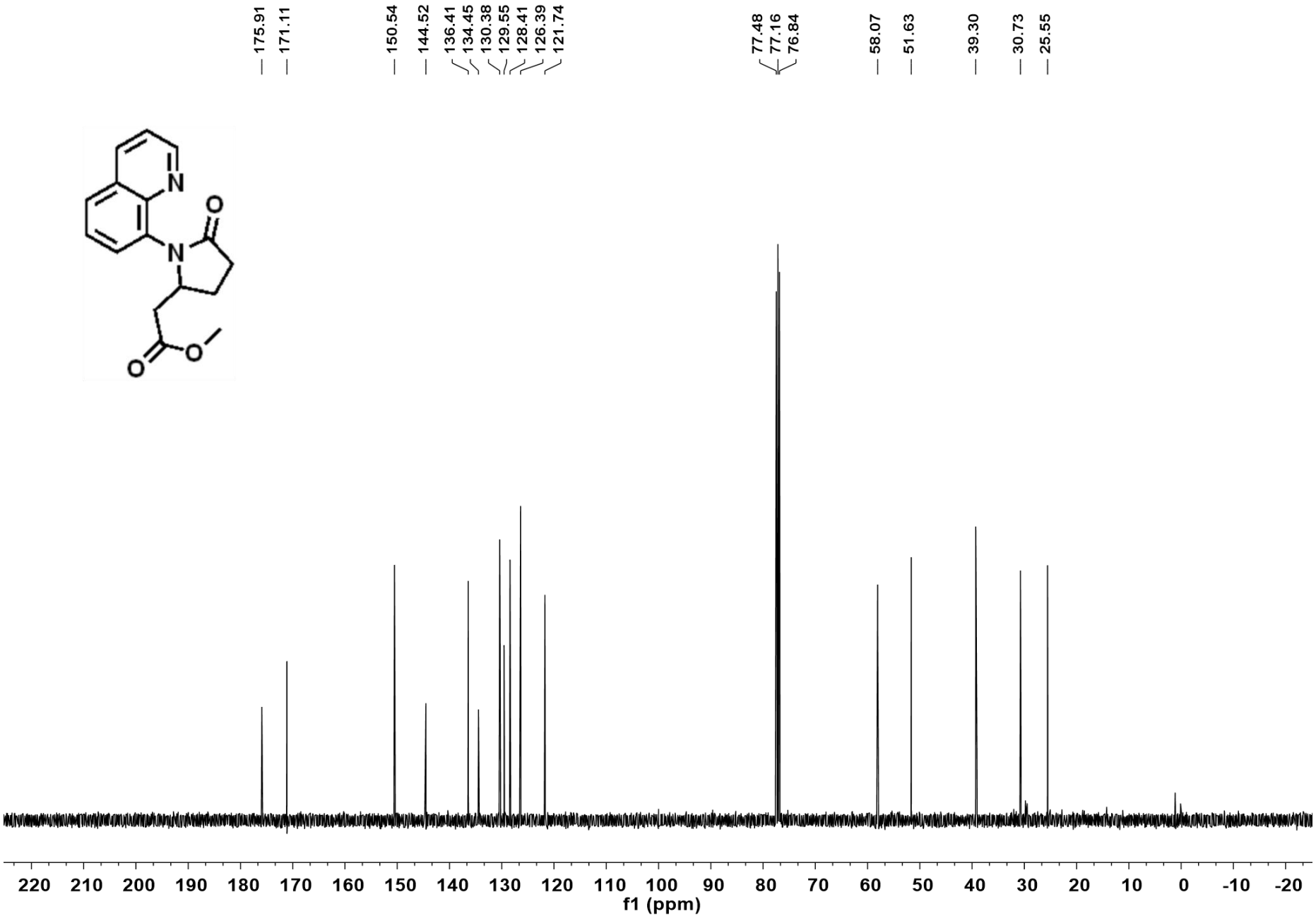
5.30 5.06 5.04 5.03 5.02 5.00 3.45 2.76 2.75 2.74 2.74 2.73 2.72 2.72 2.71 2.70 2.69 2.68 2.68 2.66 2.66 2.66 2.65 2.64 2.64 2.62 2.51 2.50 2.47 2.45 2.43 2.41 2.05 2.04 2.03 2.02 2.02 2.01 2.01 2.00 1.99 1.99 1.98 1.97 -0.00
N
O
N
O
O
O
1.00 1.02 1.03 1.04 1.05 1.04 1.06 3.02 3.05 2.12 1.08
11.5 11.0 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.
f1 (ppm)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129.55
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126.39
121.74
77.48
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76.84
58.07
51.63
39.30
30.73
25.55
N
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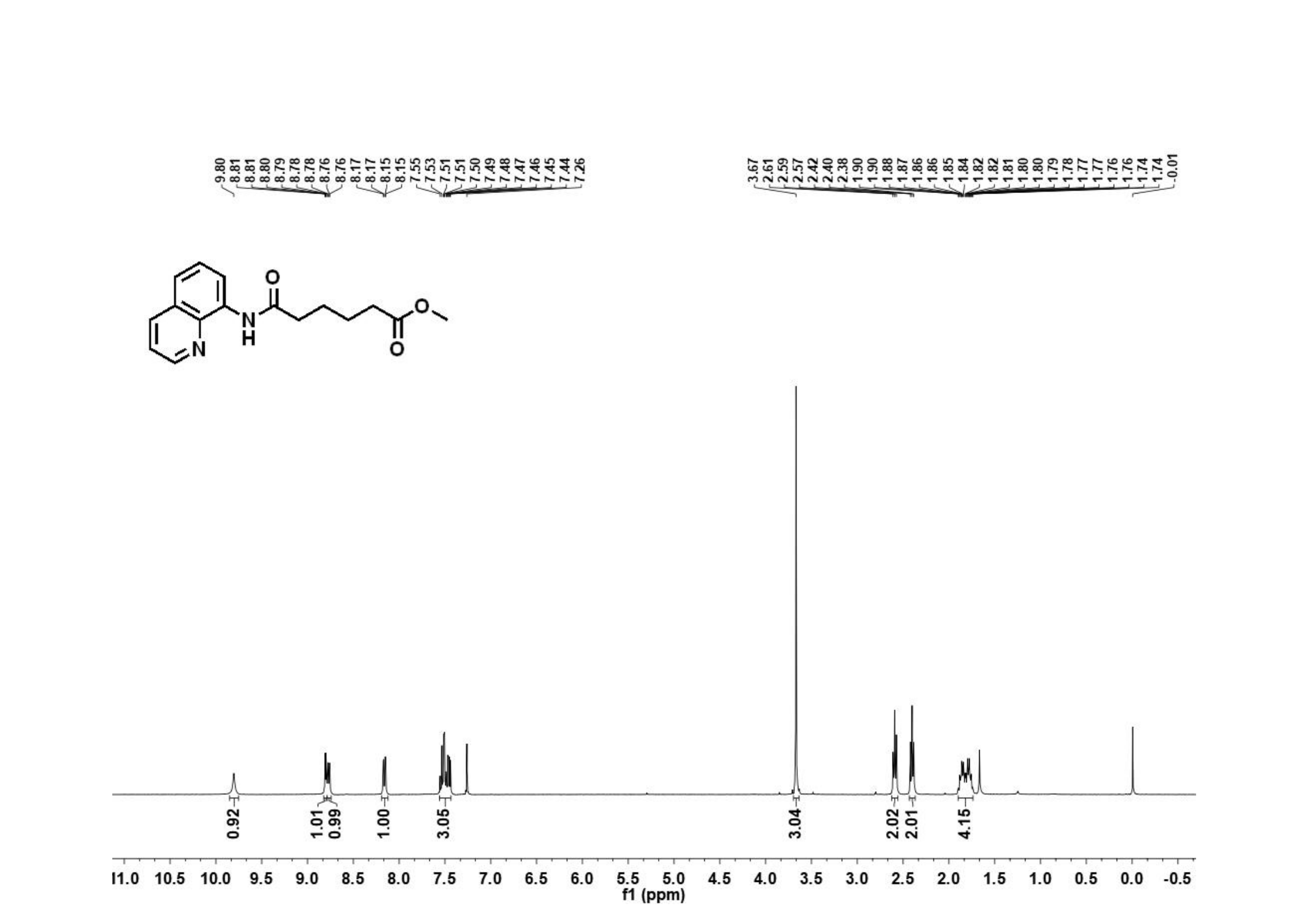
N
O
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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8.81
8.81
8.80
8.79
8.78
8.78
8.76
8.76
8.17
8.17
8.15
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7.55
7.53
7.51
7.51
7.50
7.49
7.48
7.47
7.46
7.45
7.44
7.26
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2.57
2.42
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2.38
1.90
1.90
1.88
1.87
1.86
1.86
1.85
1.84
1.82
1.82
1.81
1.80
1.80
1.79
1.78
1.77
1.77
1.76
1.76
1.74
1.74
-0.01
O
N
H
O
O
O
N
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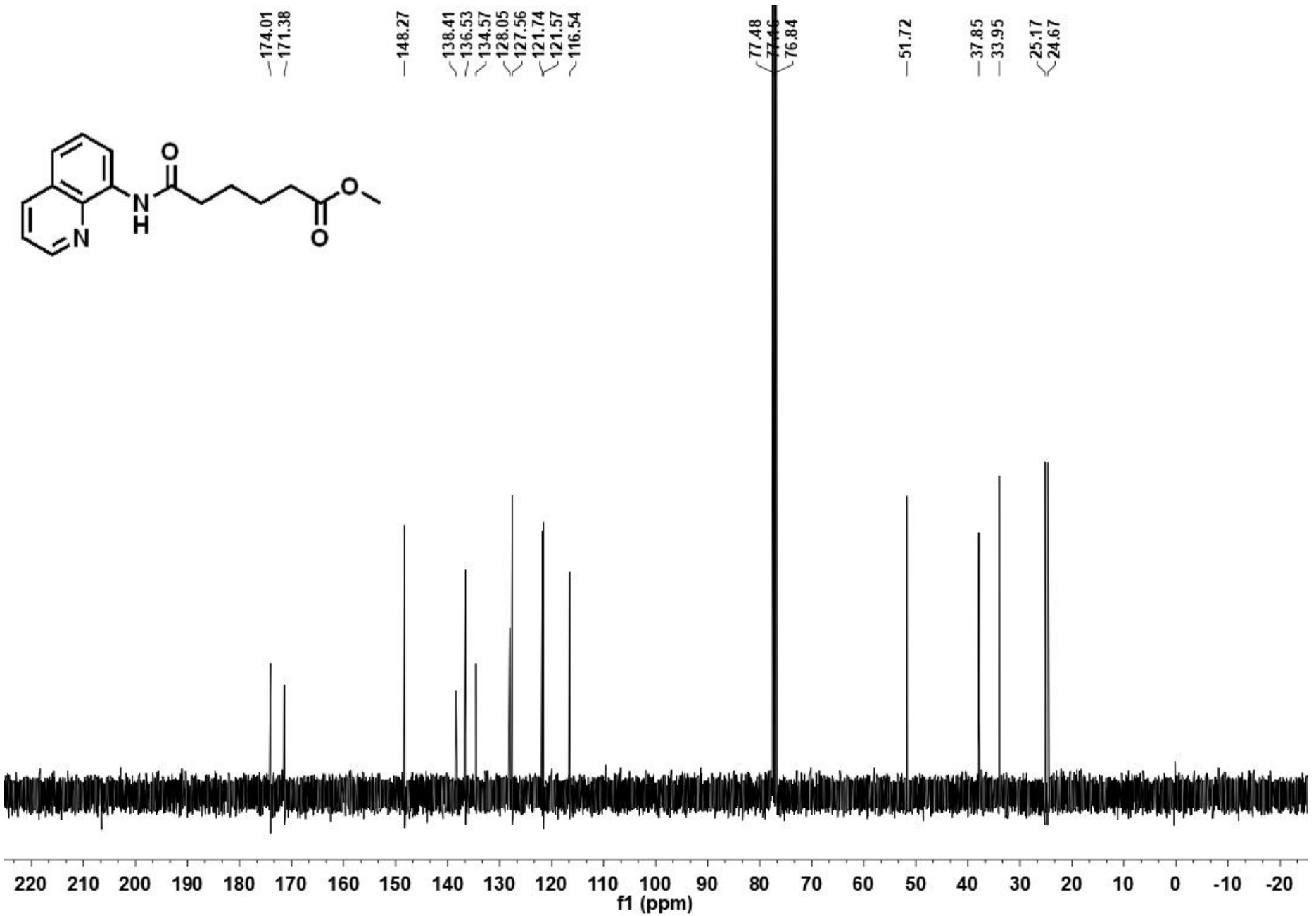
1.01
0.99
1.00
3.05
3.04
2.02
2.01
4.15
f1 (ppm)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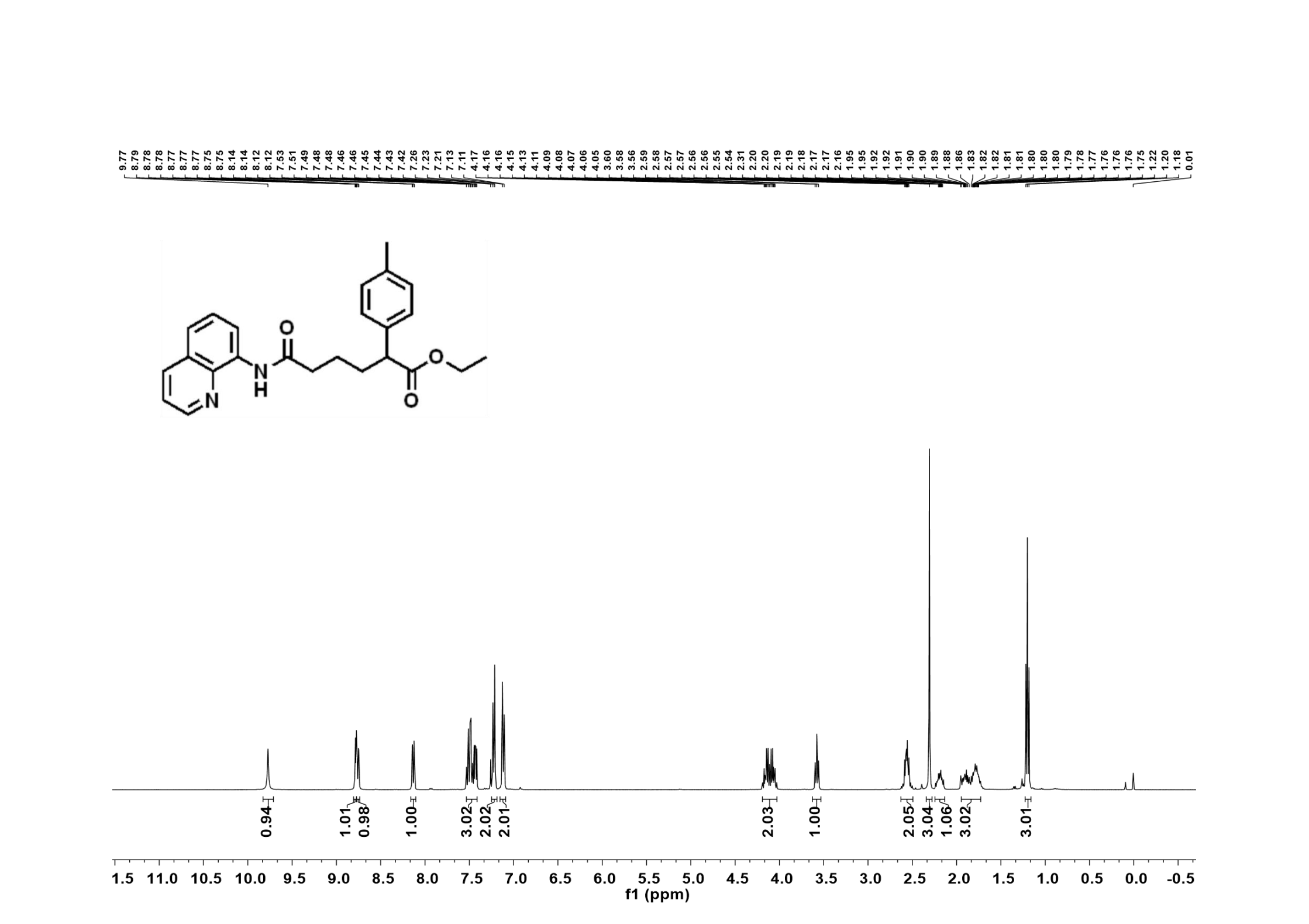
171.38
148.27
138.41
136.53
134.57
128.05
127.56
121.74
121.57
116.54
77.48
76.84
51.72
37.85
33.95
25.17
24.67
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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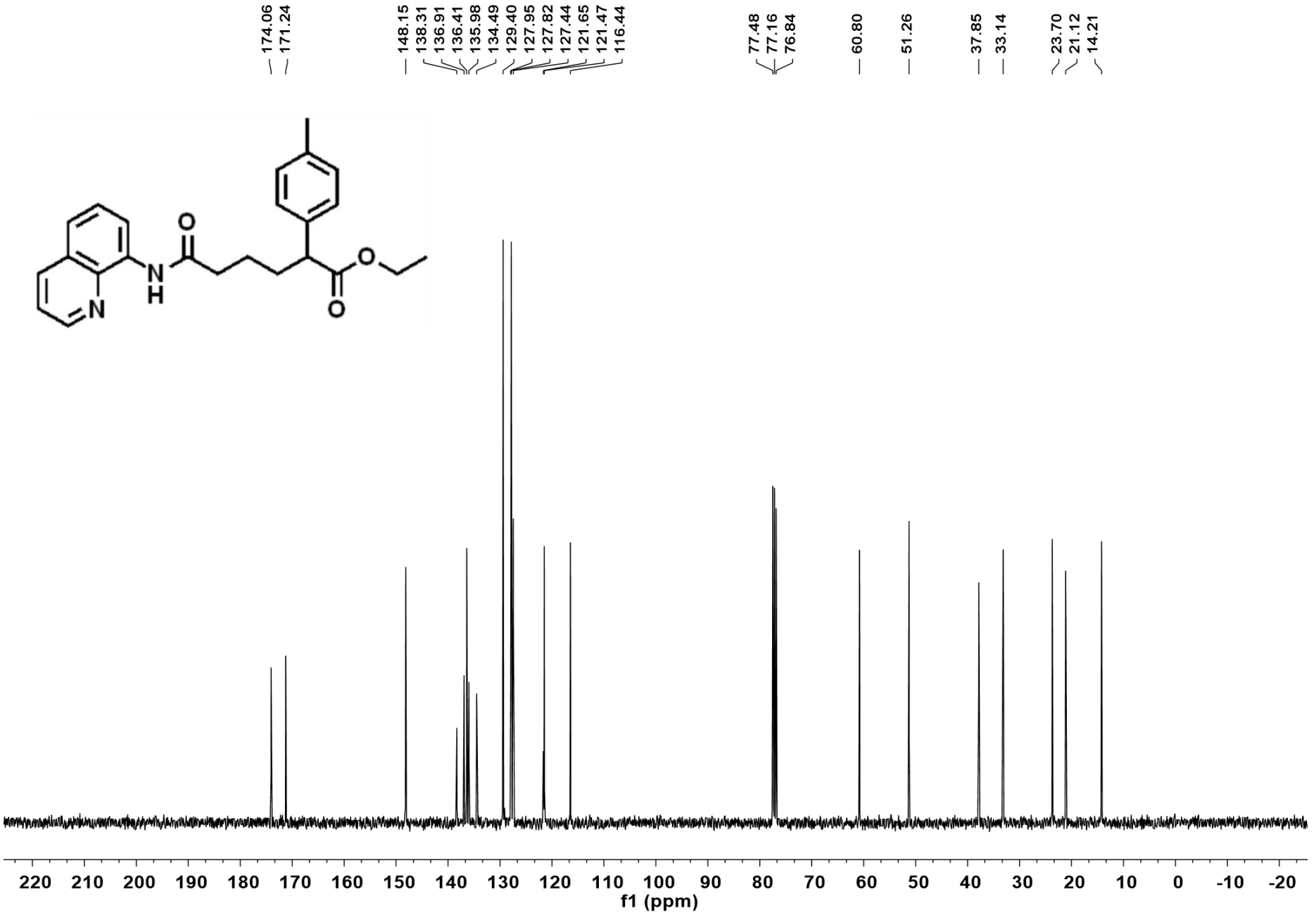
O
N
H
N
O
O
0.94
1.01
0.98
1.00
3.02
2.02
2.01
2.03
1.00
2.05
3.04
1.06
3.02
3.01
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.40
127.95
127.82
127.44
121.65
121.47
116.44
77.48
77.16
76.84
60.80
51.26
37.85
33.14
23.70
21.12
14.21
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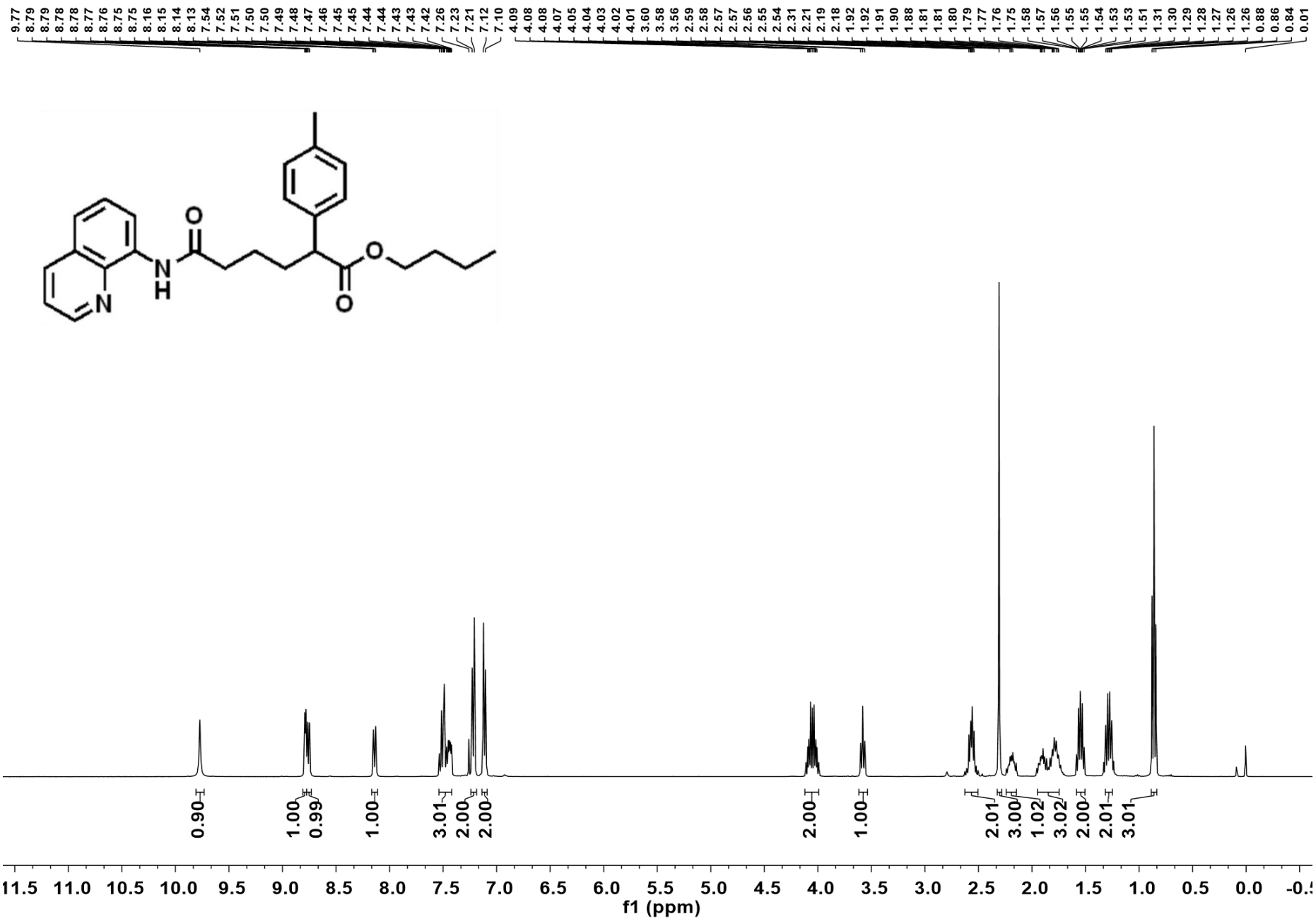
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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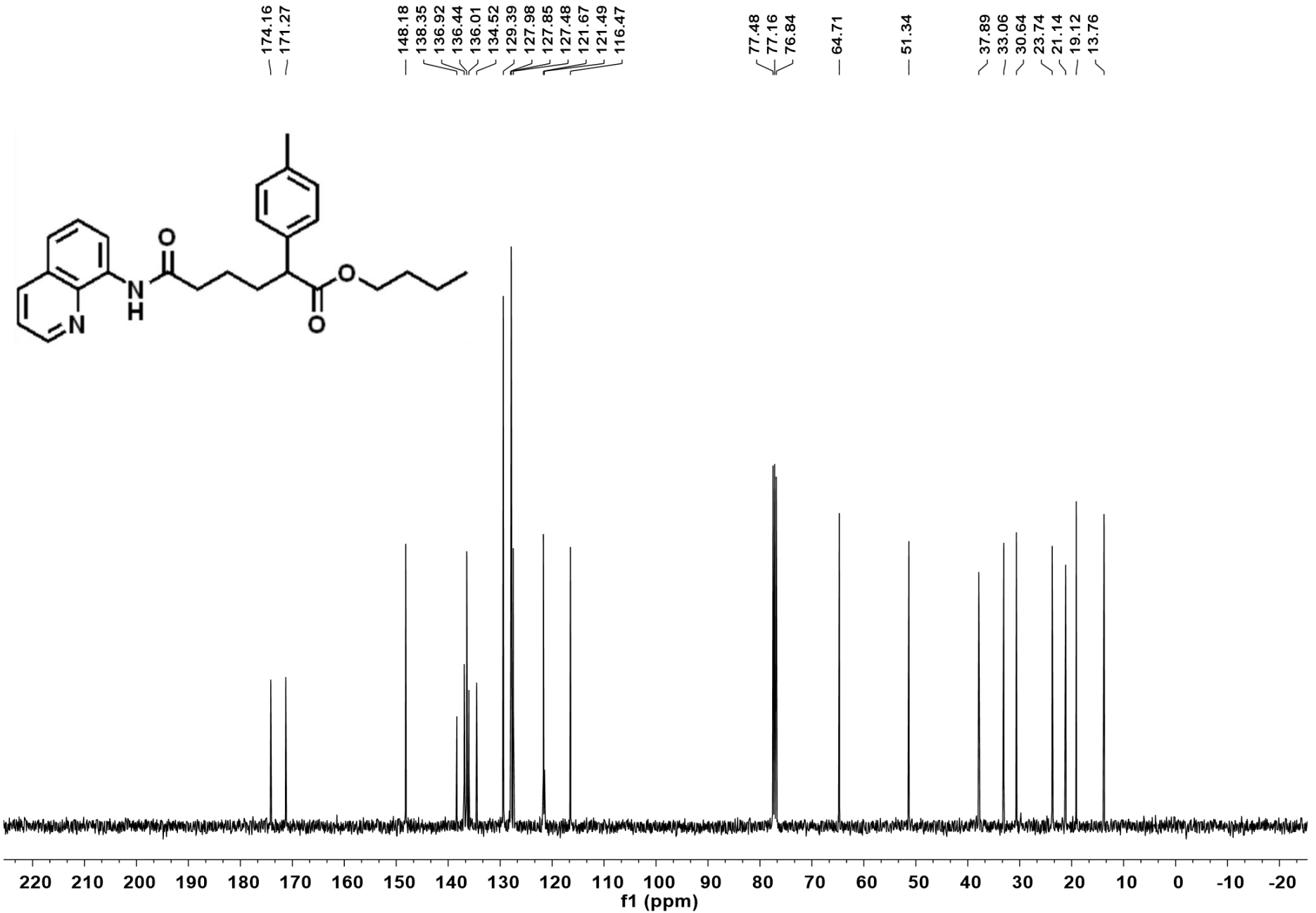
4.09 4.08 4.08 4.07 4.05 4.04 4.03 4.02 4.01 3.60 3.58 3.56 2.59 2.58 2.57 2.57 2.56 2.55 2.54 2.31 2.21 2.19 2.18 1.92 1.92 1.91 1.90 1.88 1.81 1.81 1.80 1.79 1.77 1.76 1.75 1.58 1.57 1.56 1.55 1.55 1.54 1.53 1.53 1.51 1.31 1.30 1.29 1.28 1.27 1.26 1.26 0.88 0.86 0.84 0.01
O
N
H
N
O
O
0.90
1.00
0.99
1.00
3.01
2.00
2.00
2.00
1.00
2.01
3.00
1.02
3.02
2.00
2.01
3.01
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
f1 (ppm)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127.85
127.48
121.67
121.49
116.47
77.48
77.16
76.84
64.71
51.34
37.89
33.06
30.64
23.74
21.14
19.12
13.76
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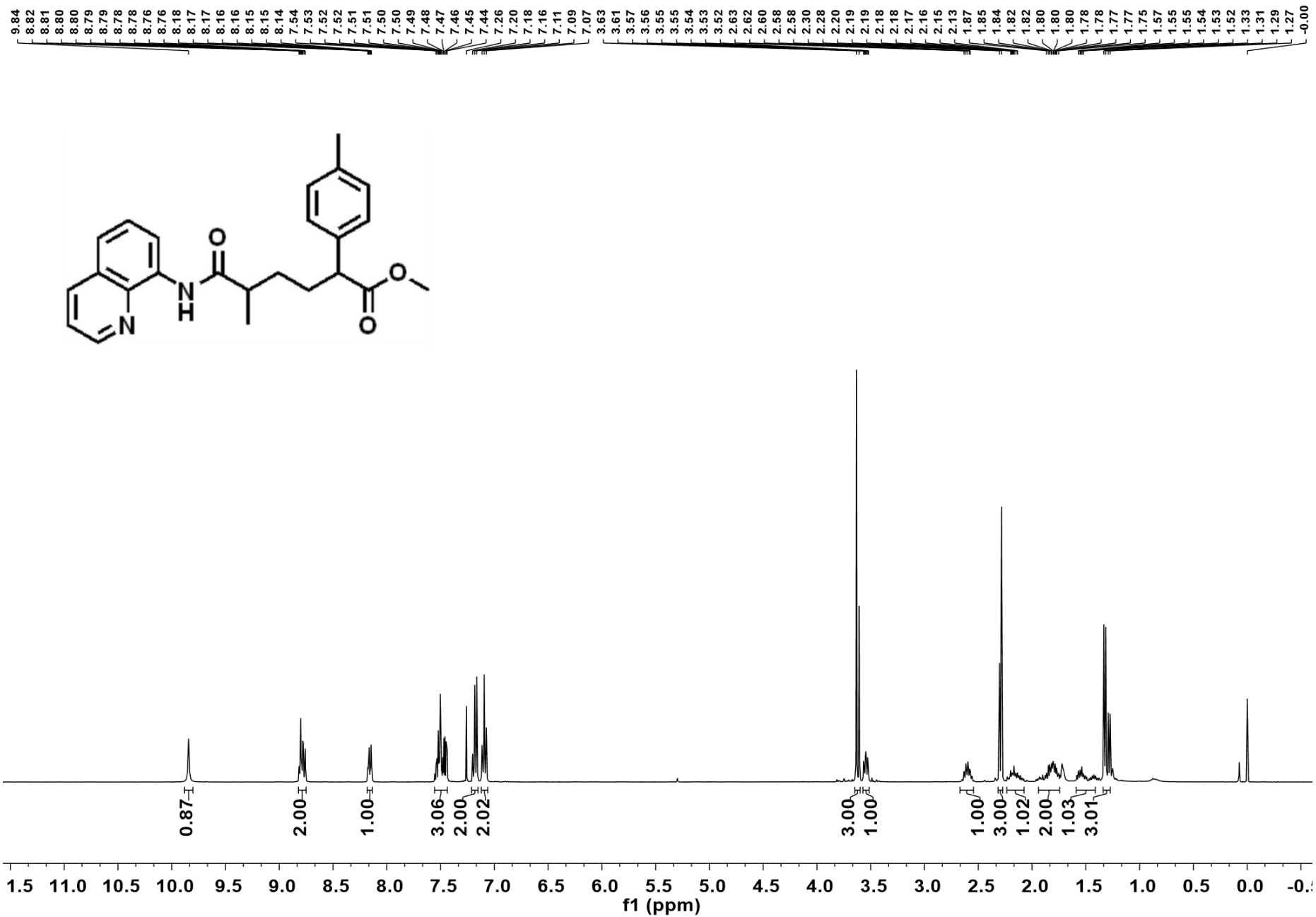
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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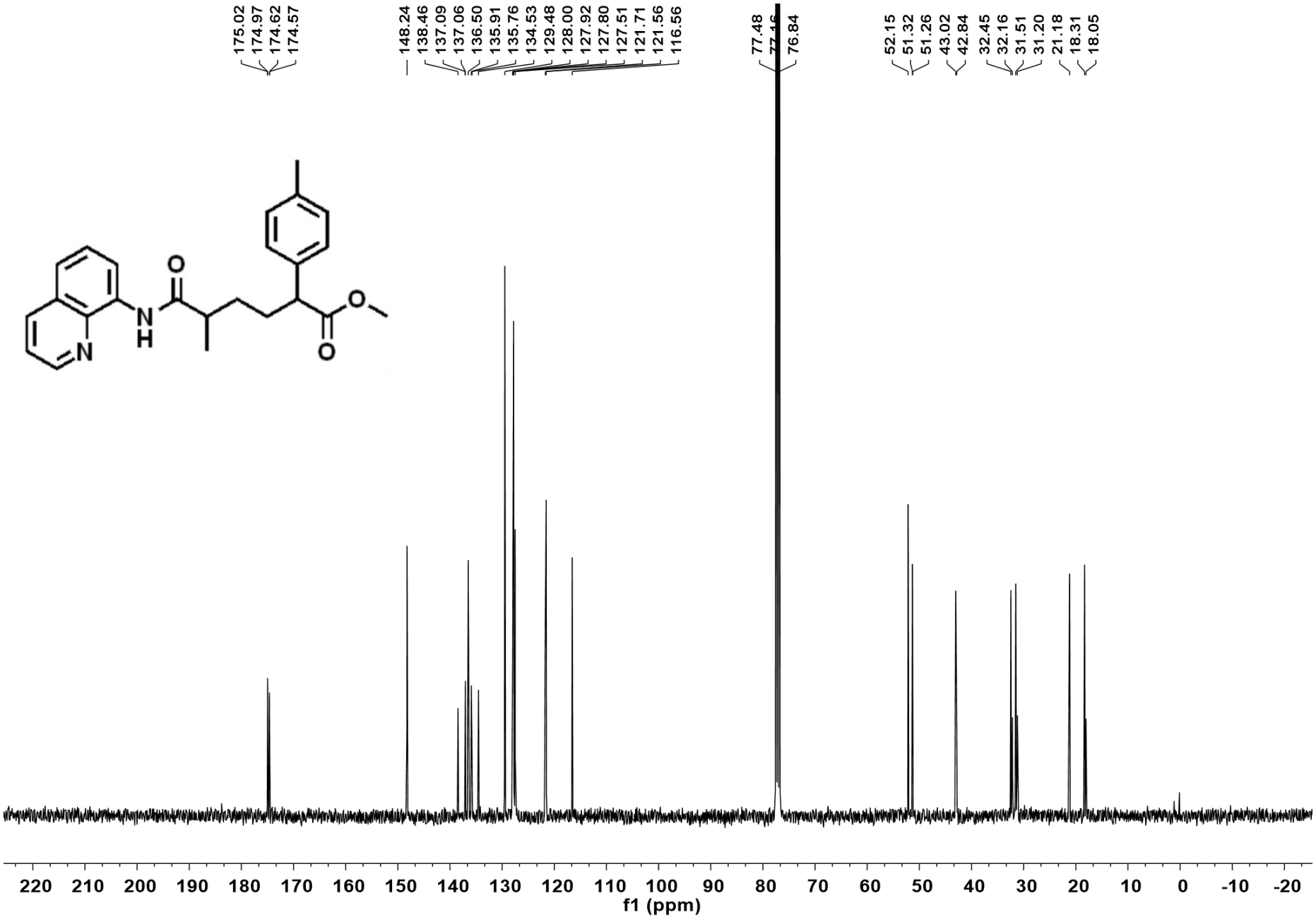
O
N
H
N
O
O
0.87
2.00
1.00
3.06
2.00
2.02
3.00
1.00
1.00
3.00
1.02
2.00
1.03
3.01
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.76
134.53
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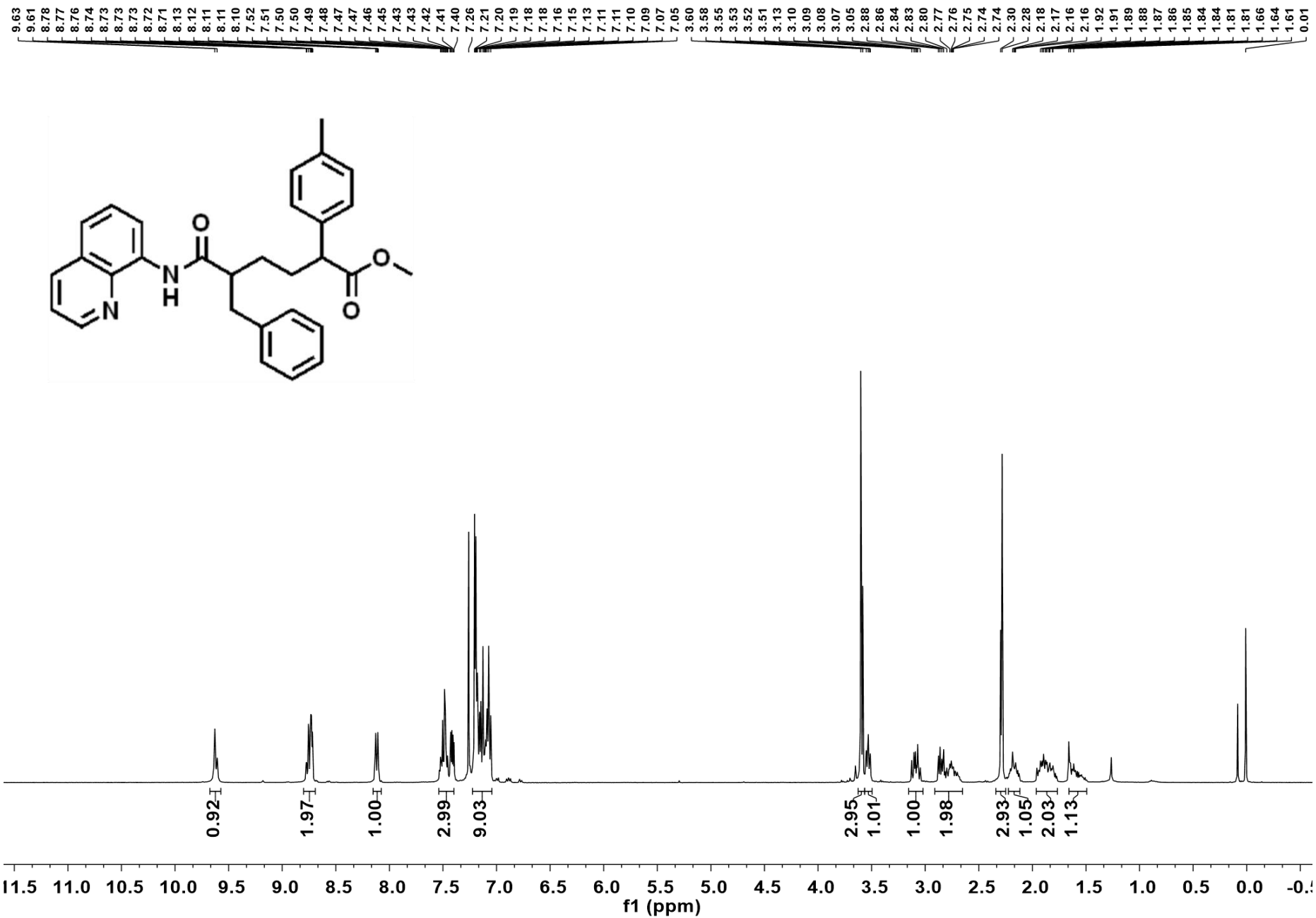
128.00
127.92
127.80
127.51
121.71
121.56
116.56
77.48
77.16
76.84
52.15
51.32
51.26
43.02
42.84
32.45
32.16
31.51
31.20
21.18
18.31
18.05
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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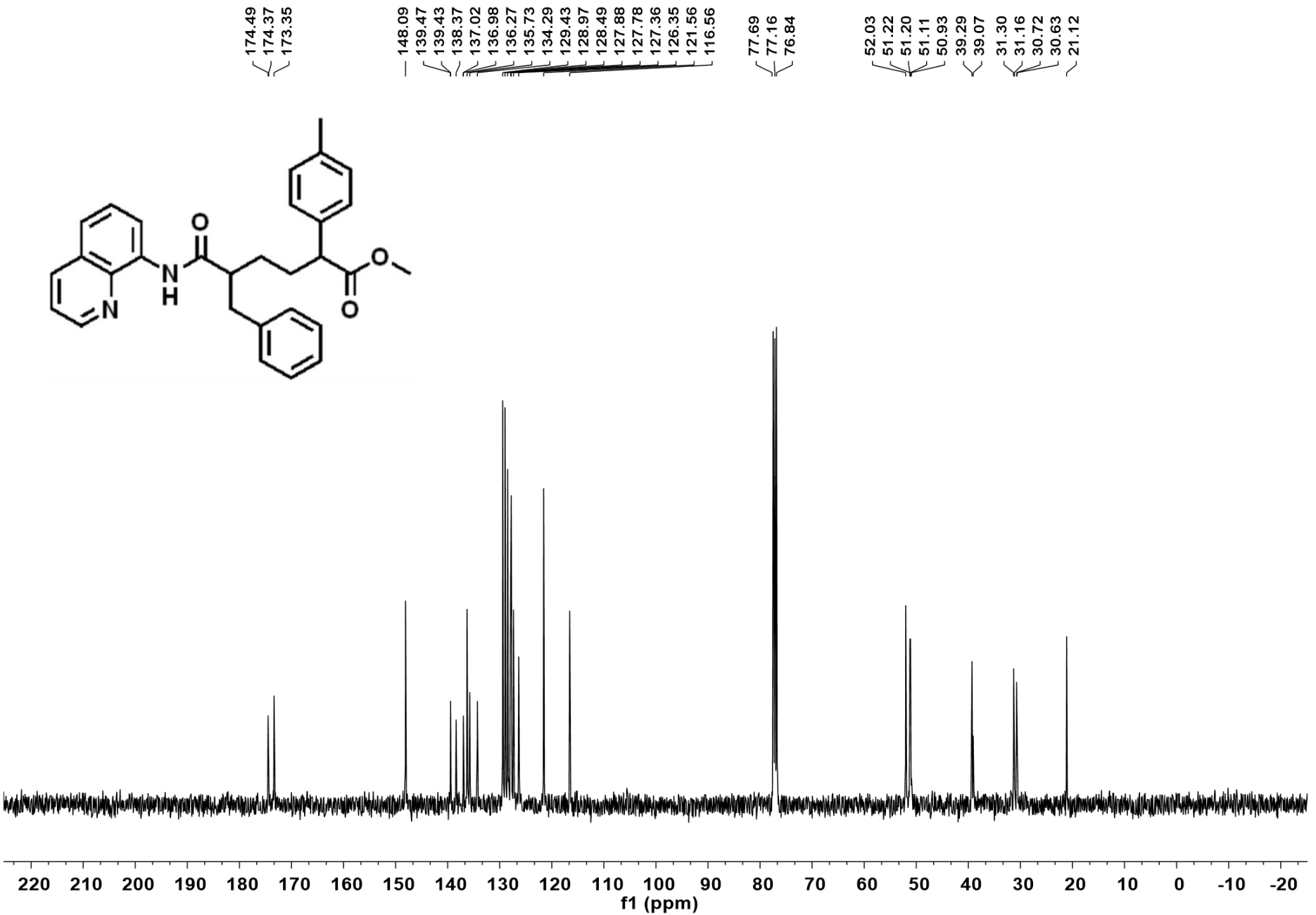
O
N
H
N
O
O
0.92 1.97 1.00 2.99 9.03 2.95 1.01 1.00 1.98 2.93 1.05 2.03 1.13
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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173.35
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137.02
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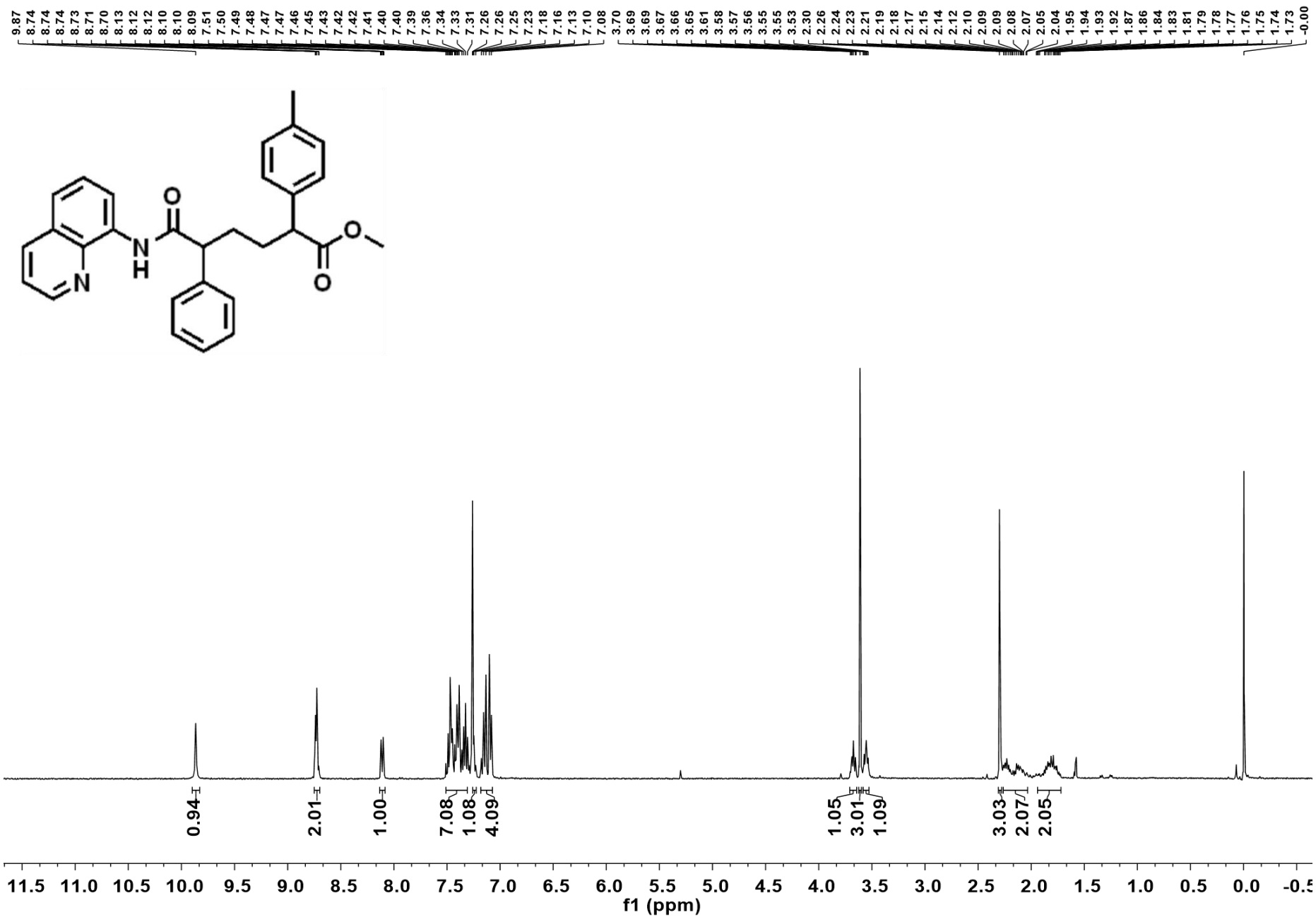
135.73
134.29
129.43
128.97
128.49
127.88
127.78
127.36
126.35
121.56
116.56
77.69
77.16
76.84
52.03
51.22
51.20
51.11
50.93
39.29
39.07
31.30
31.16
30.72
30.63
21.12
O
N
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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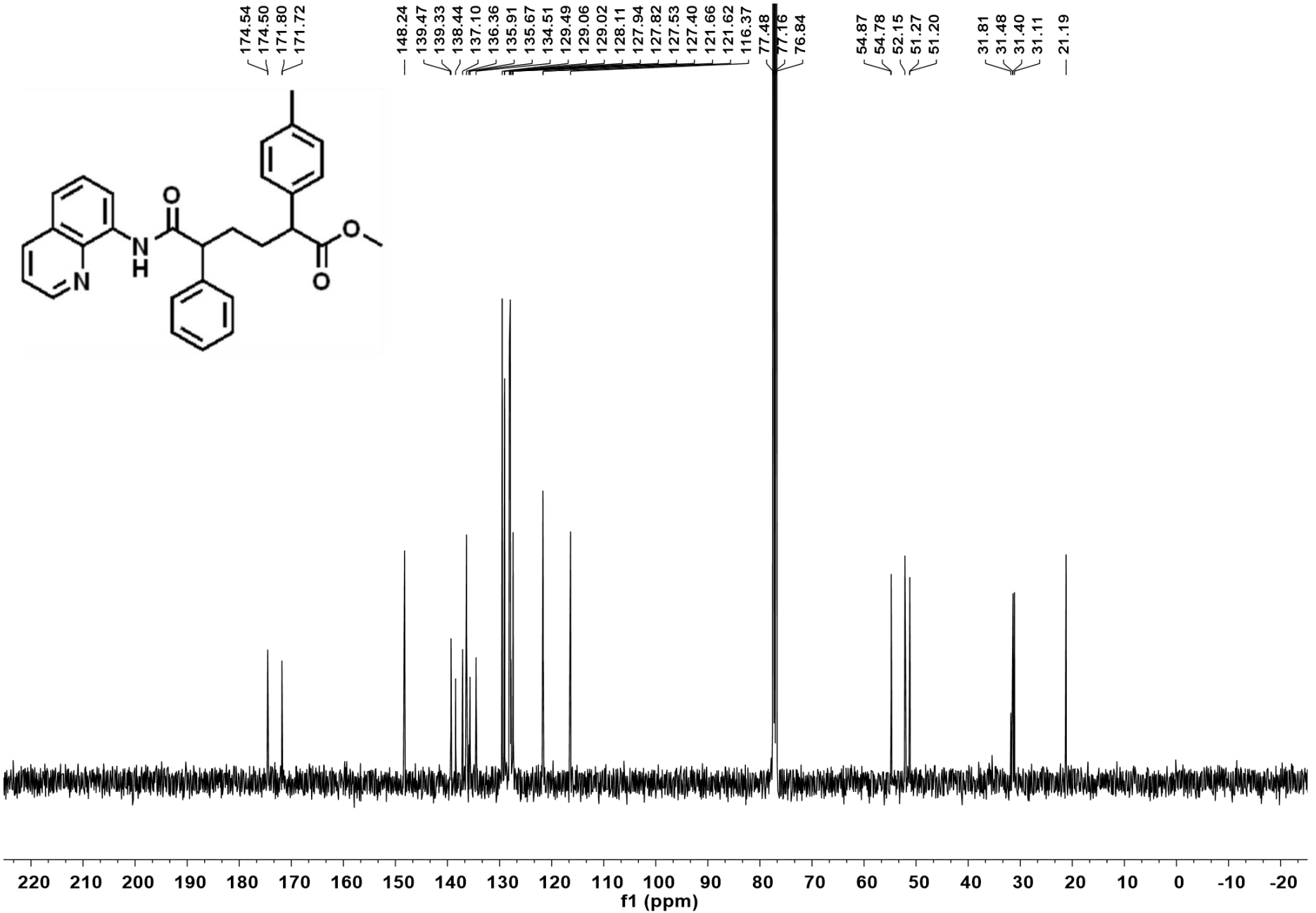
O
N
H
N
O
O
0.94
2.01
1.00
7.08
1.08
4.09
1.05
3.01
1.09
3.03
2.07
2.05
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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127.82
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127.40
121.66
121.62
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77.48
77.16
76.84
54.87
54.78
52.15
51.27
51.20
31.81
31.48
31.40
31.11
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O
O
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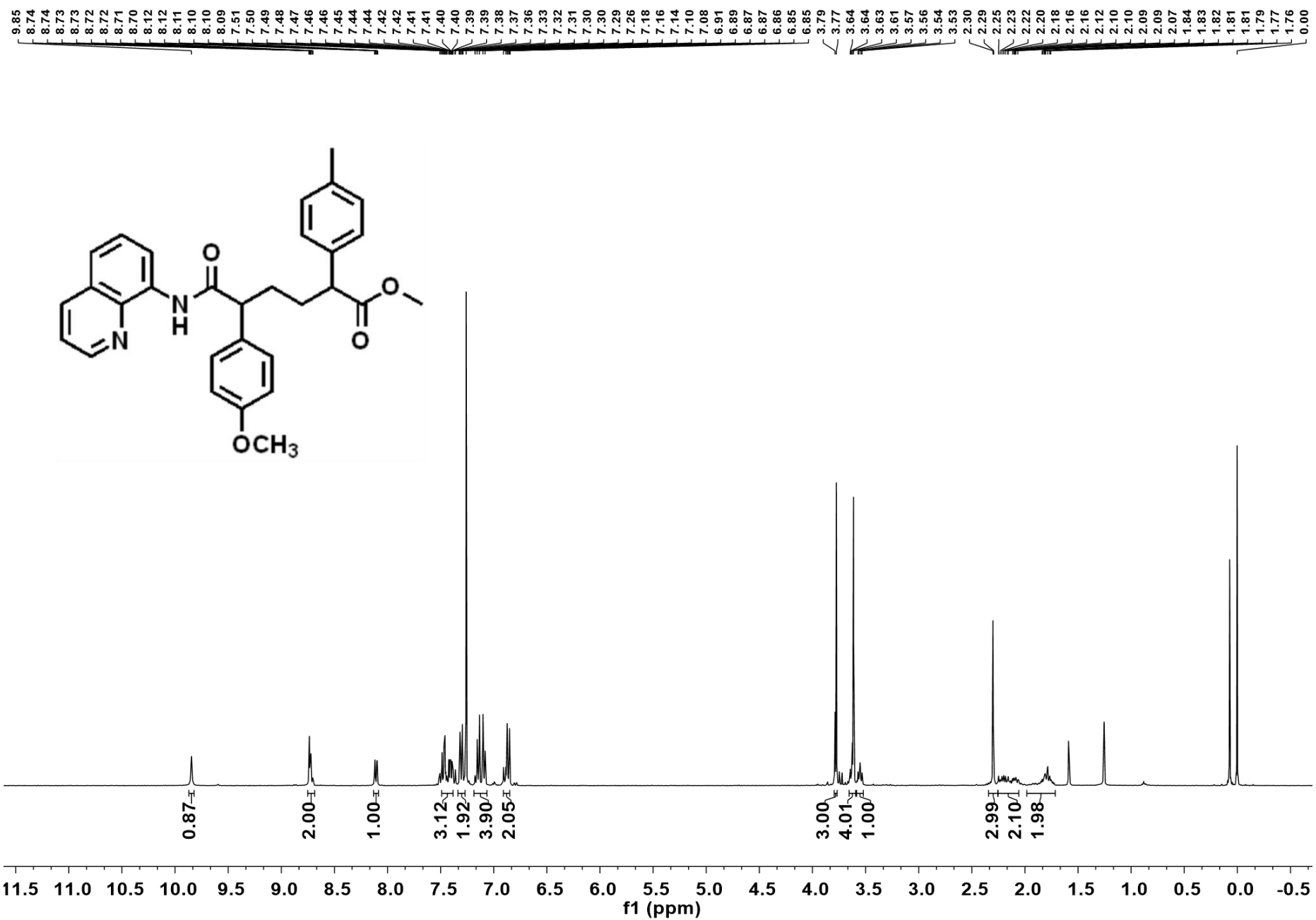
f1 (ppm)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O
N
H
N
O
O
OCH3
0.87
2.00
1.00
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1.92
3.90
2.05
3.00
4.01
1.00
2.99
2.10
1.98
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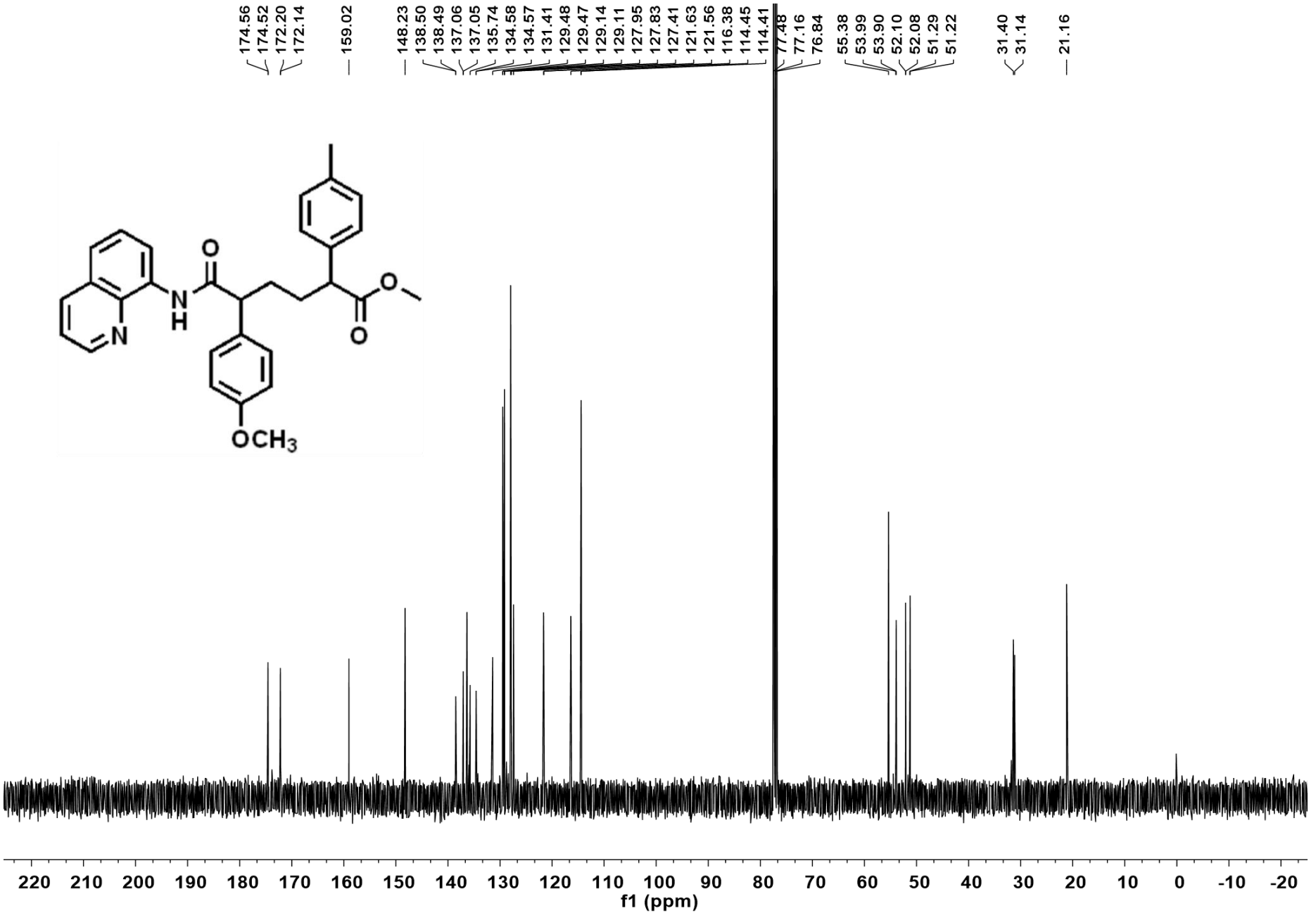
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53.99
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52.10
52.08
51.29
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31.40
31.14
21.16
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O
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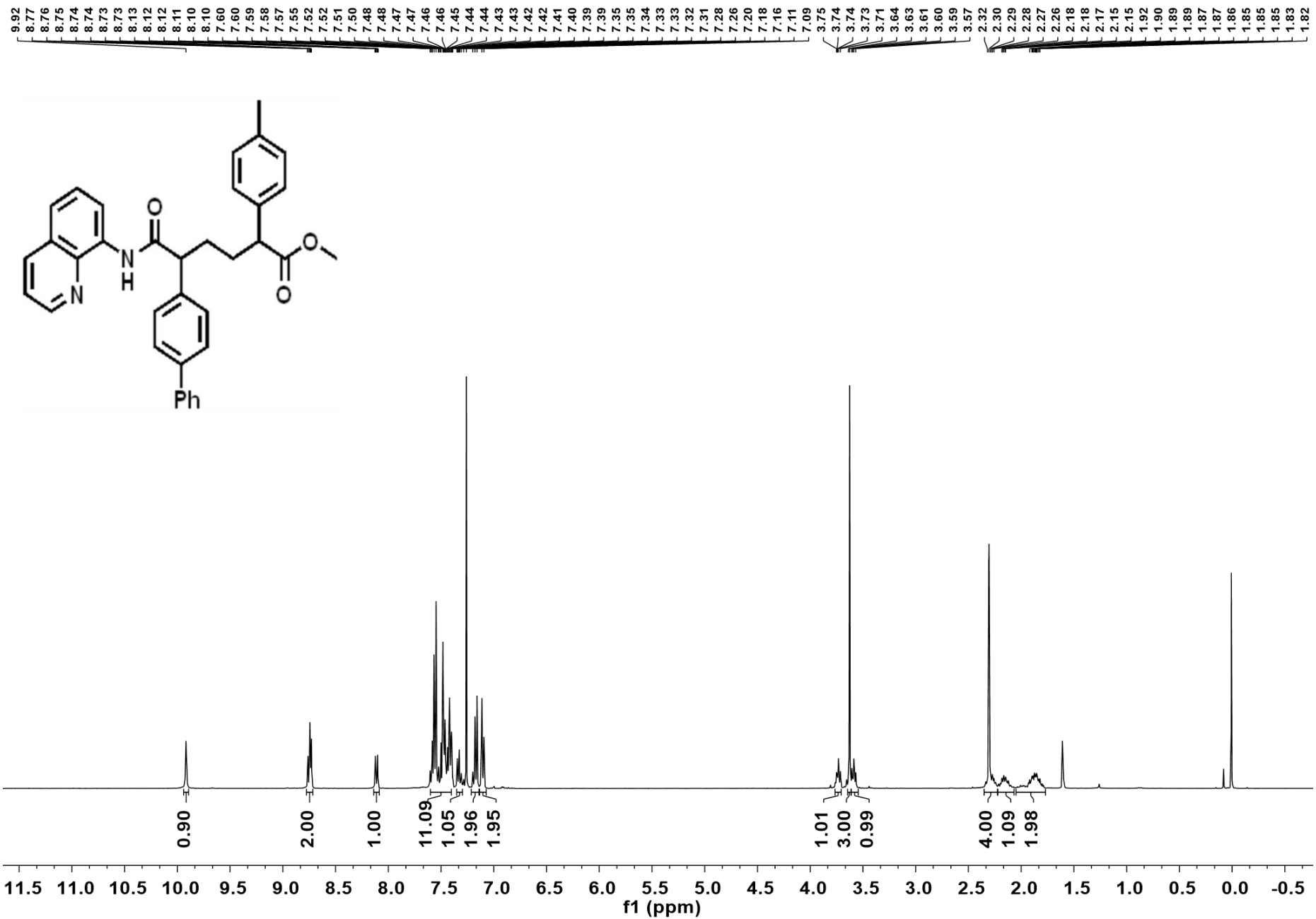
f1 (ppm)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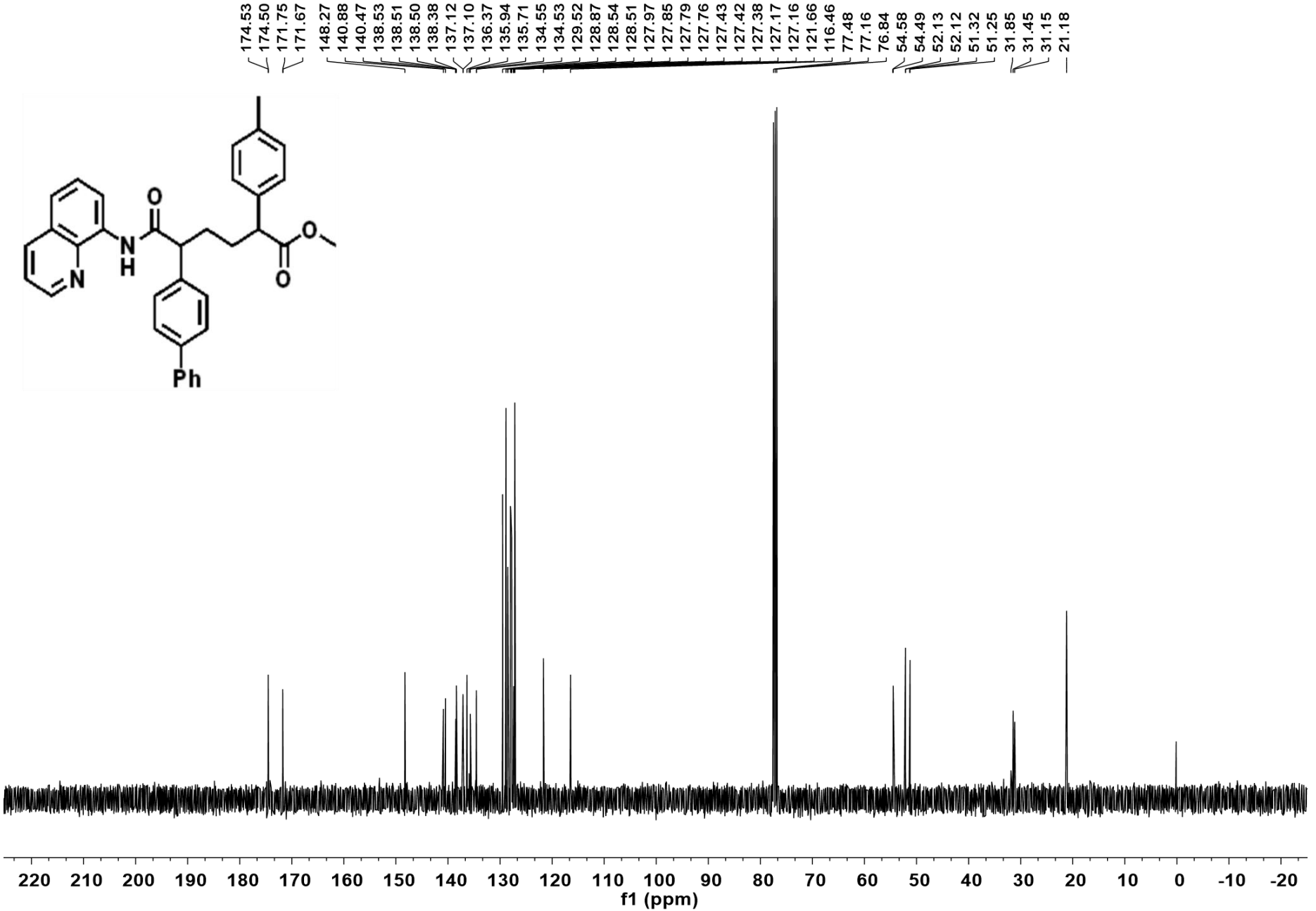
O
N
H
N
O
O
Ph
0.90
2.00
1.00
11.09
1.05
1.96
1.95
1.01
3.00
0.99
4.00
1.09
1.98
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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137.10
136.37
135.94
135.71
134.55
134.53
129.52
128.87
128.54
128.51
127.97
127.85
127.79
127.76
127.43
127.42
127.38
127.17
127.16
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54.49
52.13
52.12
51.32
51.25
31.85
31.45
31.15
21.18
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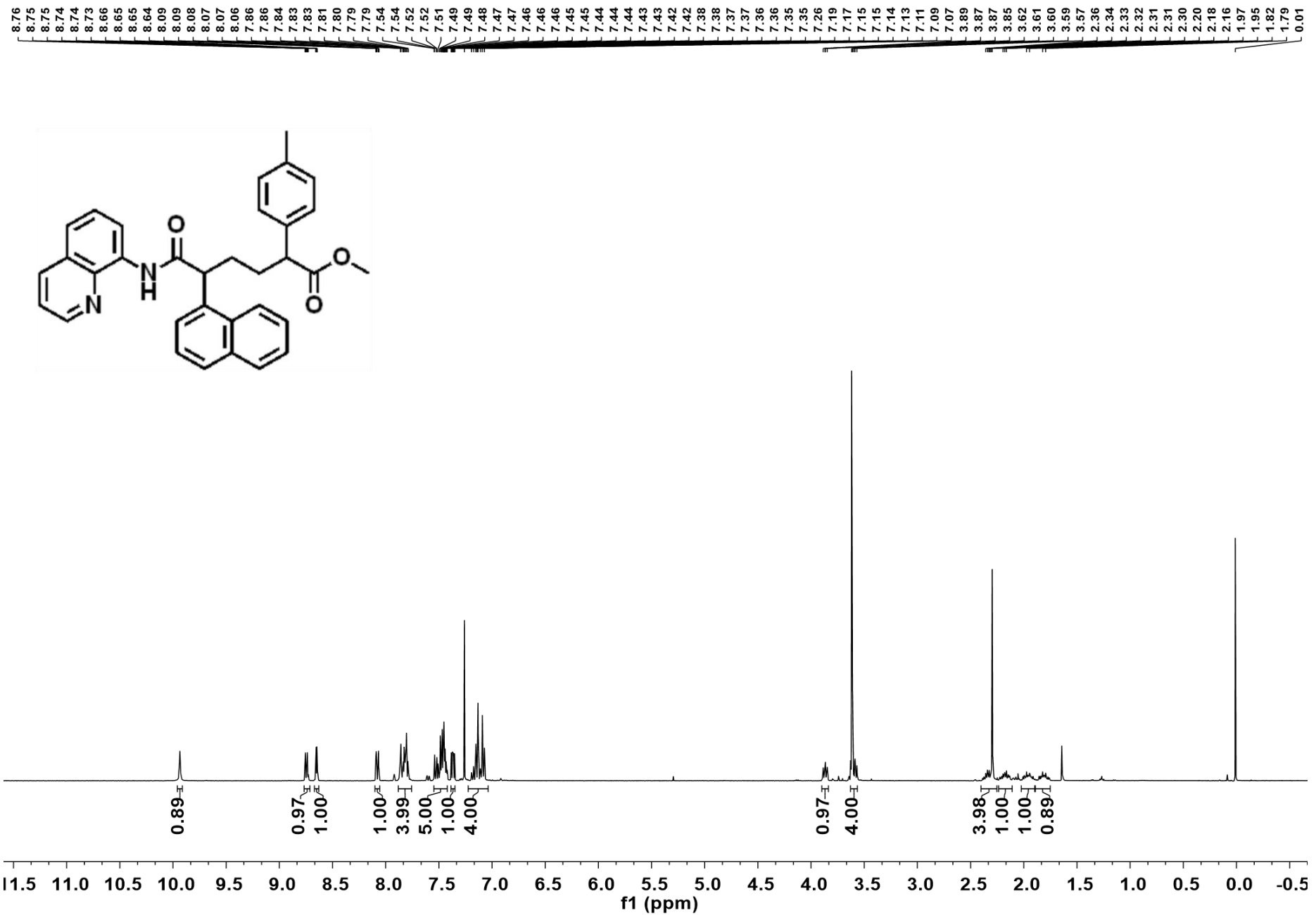
H
N
O
O
Ph
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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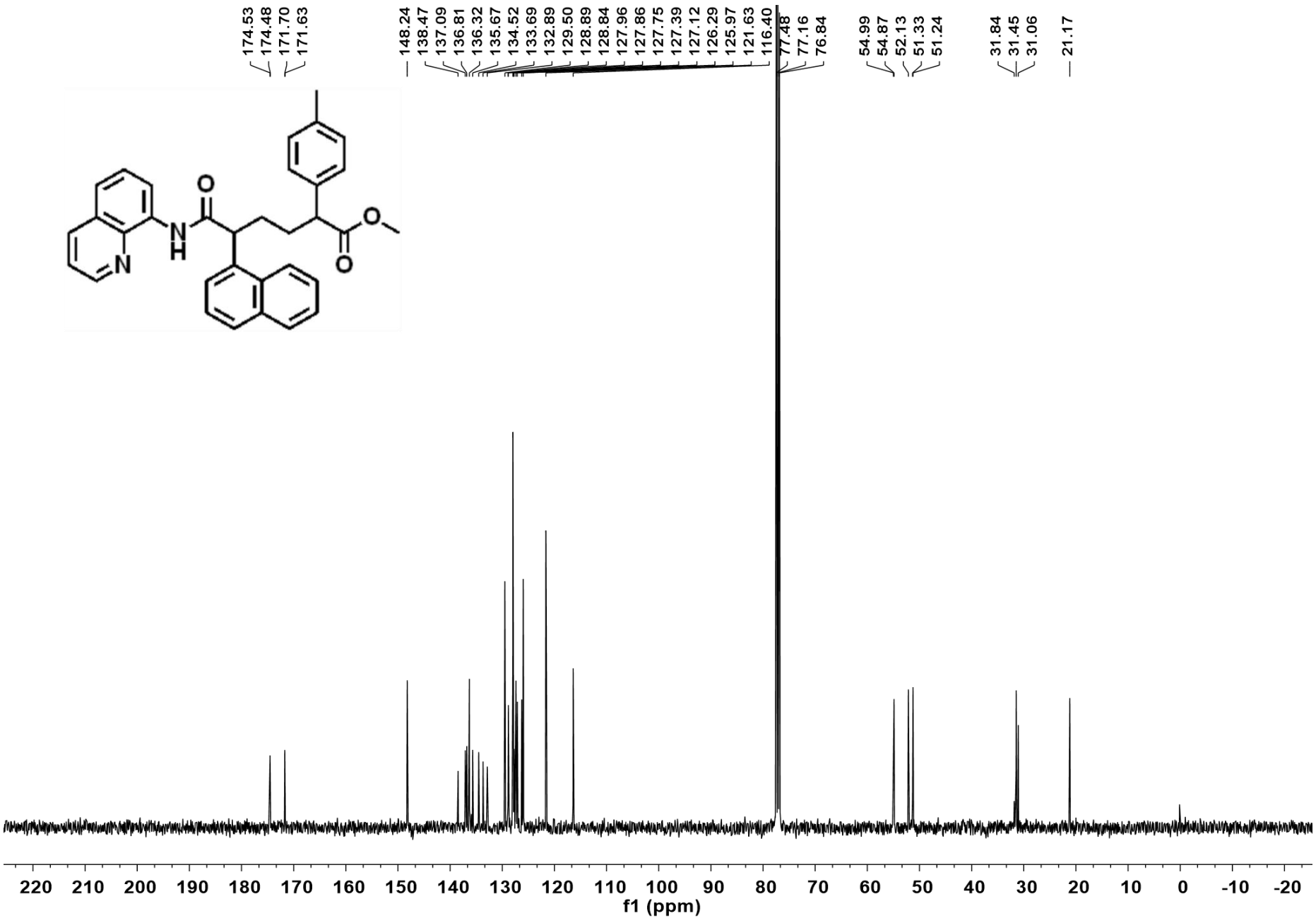
O
N
H
N
O
O
0.89
0.97
1.00
1.00
3.99
5.00
1.00
4.00
0.97
4.00
3.98
1.00
1.00
0.89
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.52
133.69
132.89
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128.89
128.84
127.96
127.86
127.75
127.39
127.12
126.29
125.97
121.63
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77.48
77.16
76.84
54.99
54.87
52.13
51.33
51.24
31.84
31.45
31.06
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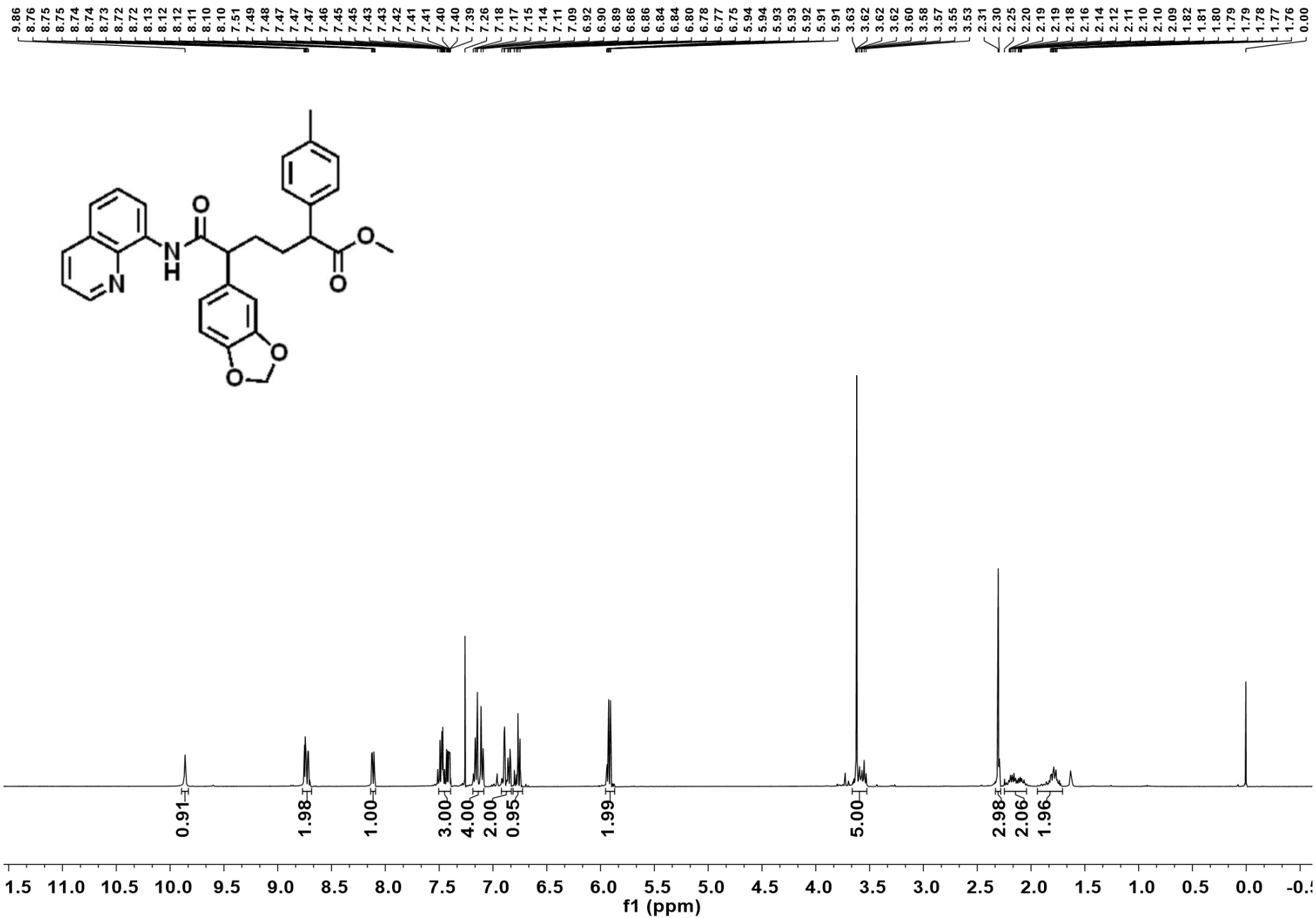
H
N
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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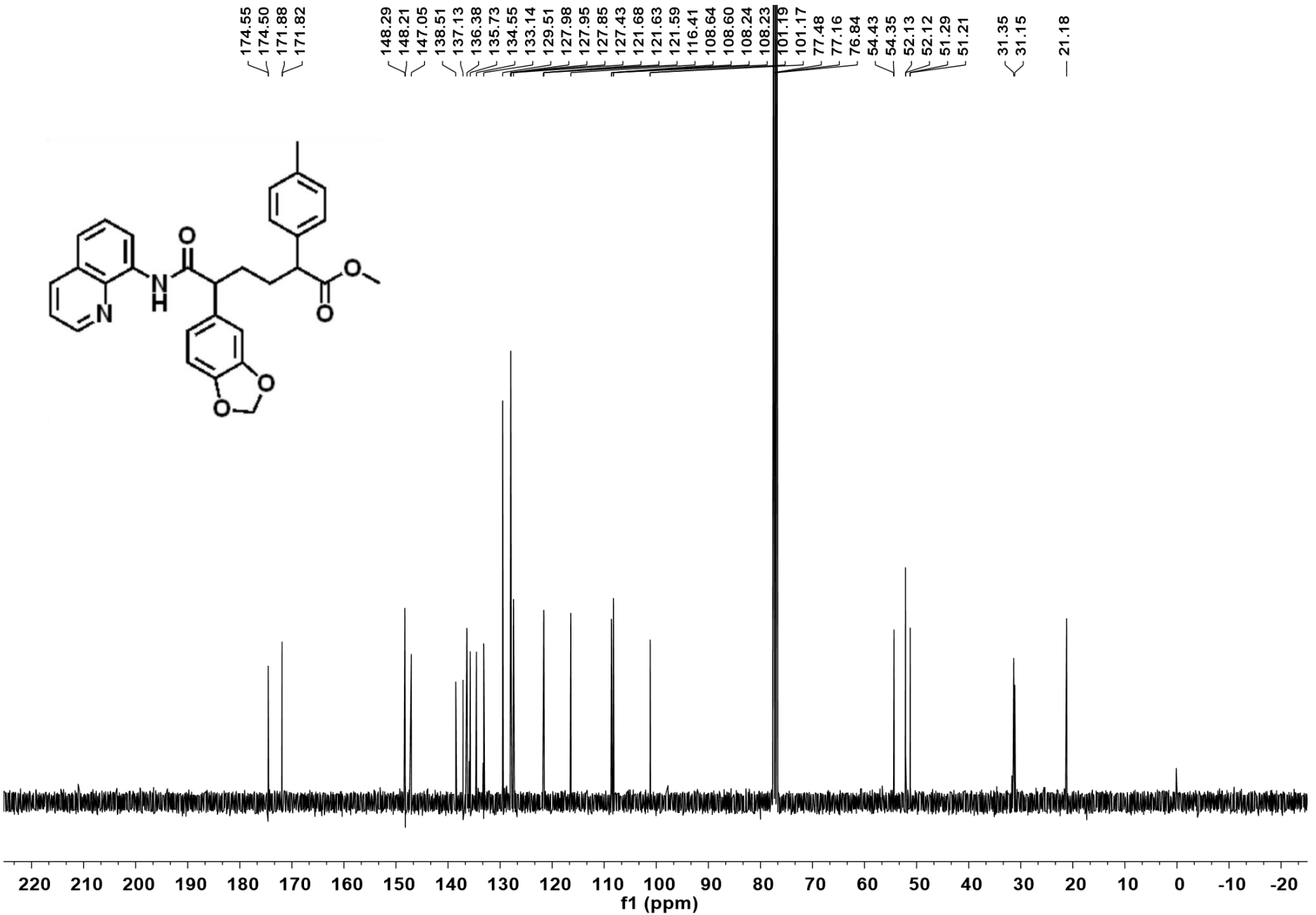
N
H
O
O
O
O
O
N
0.91
1.98
1.00
3.00
4.00
2.00
0.95
1.99
5.00
2.98
2.06
1.96
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.95
127.85
127.43
121.68
121.63
121.59
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108.60
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108.23
101.19
101.17
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77.16
76.84
54.43
54.35
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52.12
51.29
51.21
31.35
31.15
21.18
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O
O
O
O
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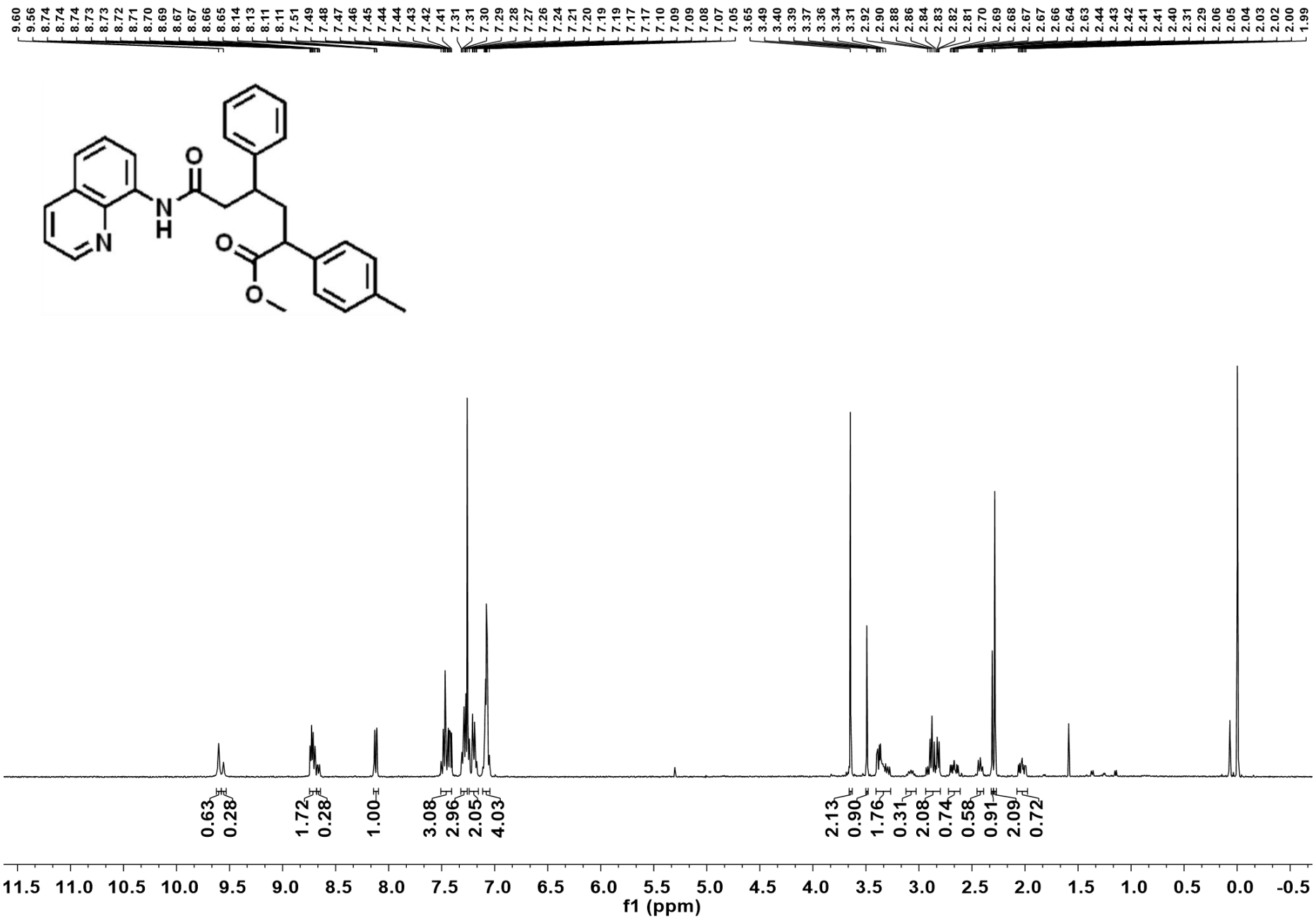
f1 (ppm)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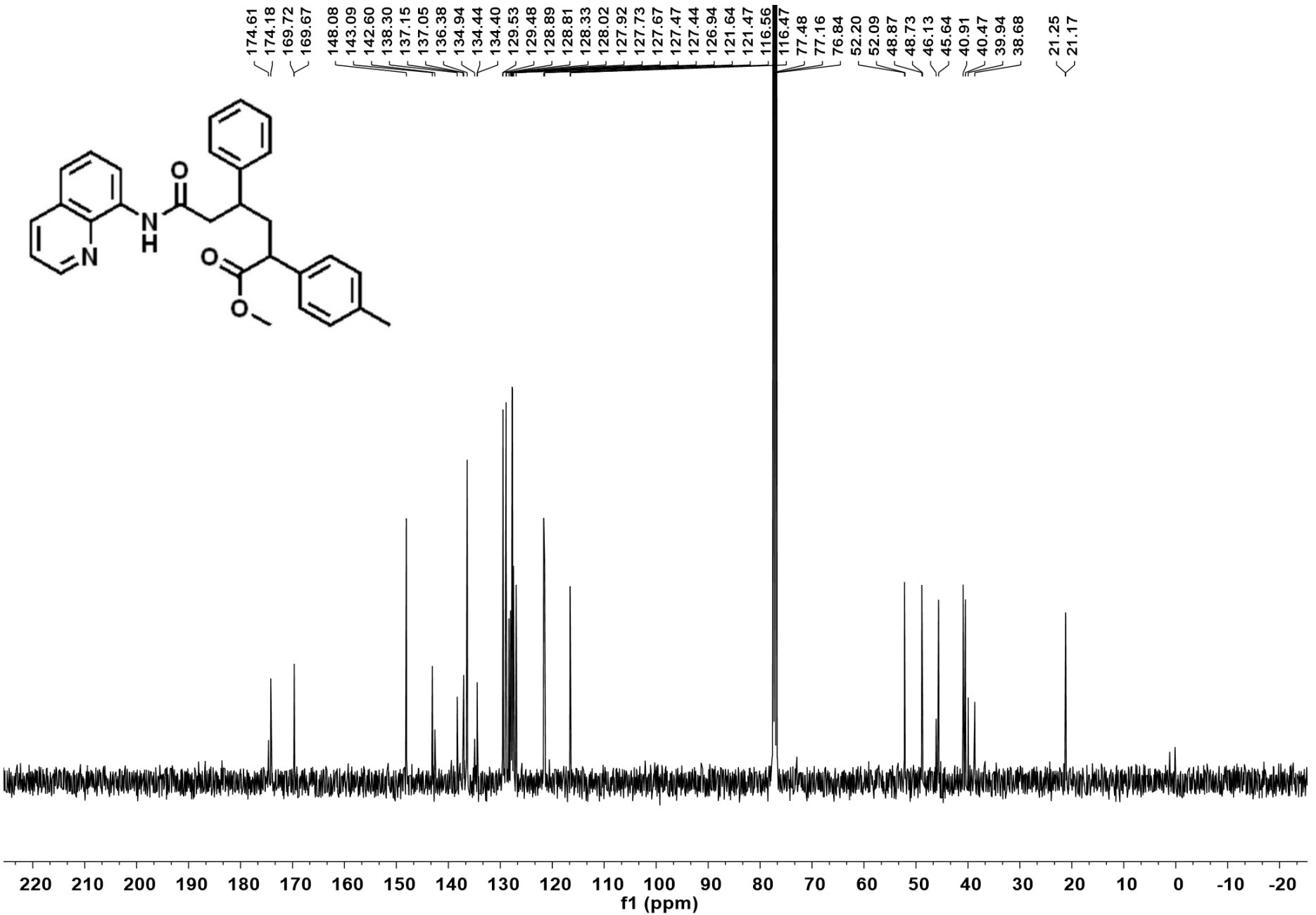
O
N
H
N
O
O
0.63 0.28 1.72 0.28 1.00 3.08 2.96 2.05 4.03 2.13 0.90 1.76 0.31 2.08 0.74 0.58 0.91 2.09 0.72
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.48
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128.33
128.02
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127.73
127.67
127.47
127.44
126.94
121.64
121.47
116.56
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77.48
77.16
76.84
52.20
52.09
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48.73
46.13
45.64
40.91
40.47
39.94
38.68
21.25
21.17
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H
N
O
O
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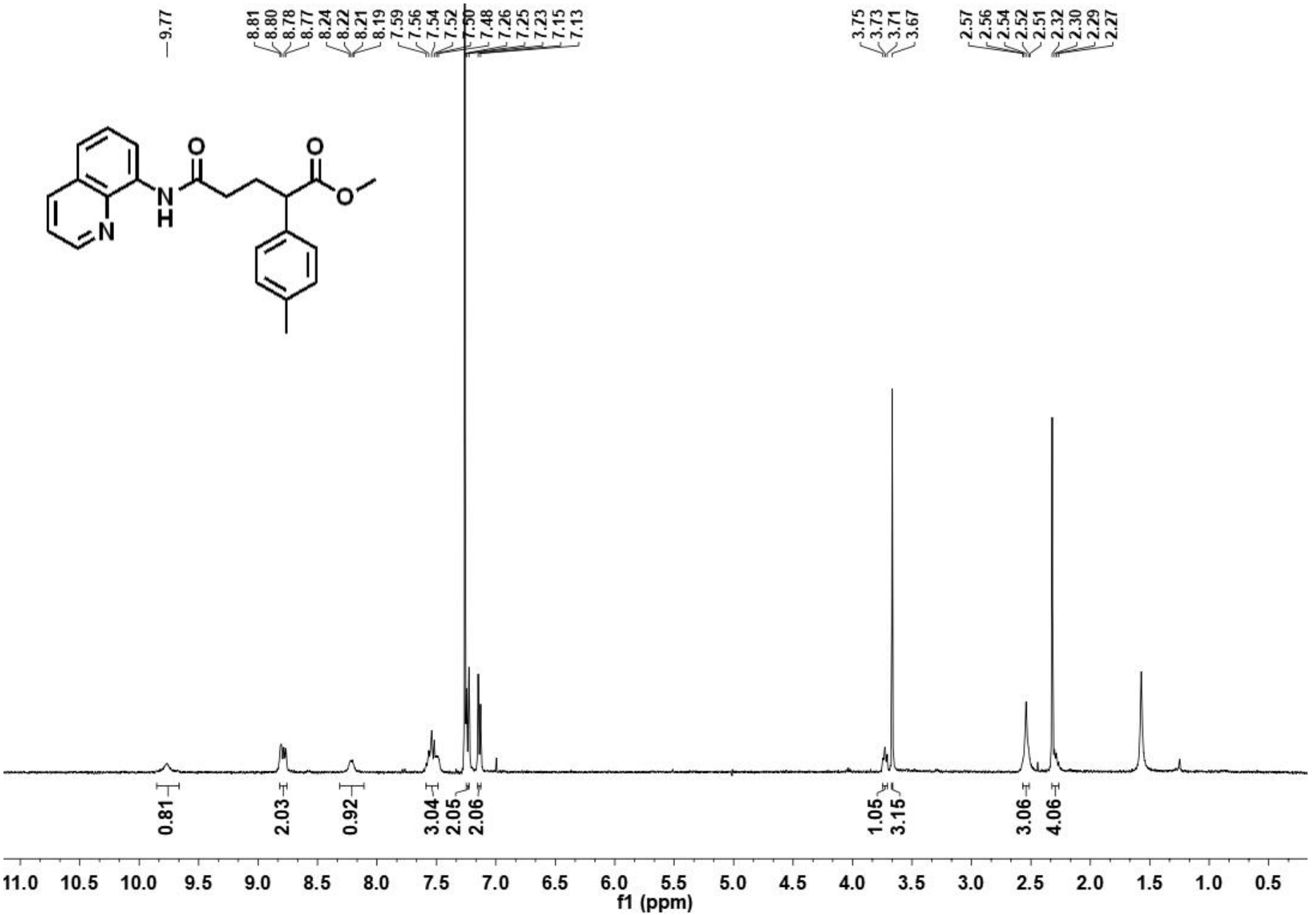
f1 (ppm)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7.50
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7.23
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7.13
3.75
3.73
3.71
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2.54
2.52
2.51
2.32
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2.29
2.27
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O
N
H
O
N
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2.03
0.92
3.04
2.05
2.06
1.05
3.15
3.06
4.06
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10.0
9.5
9.0
8.5
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6.5
6.0
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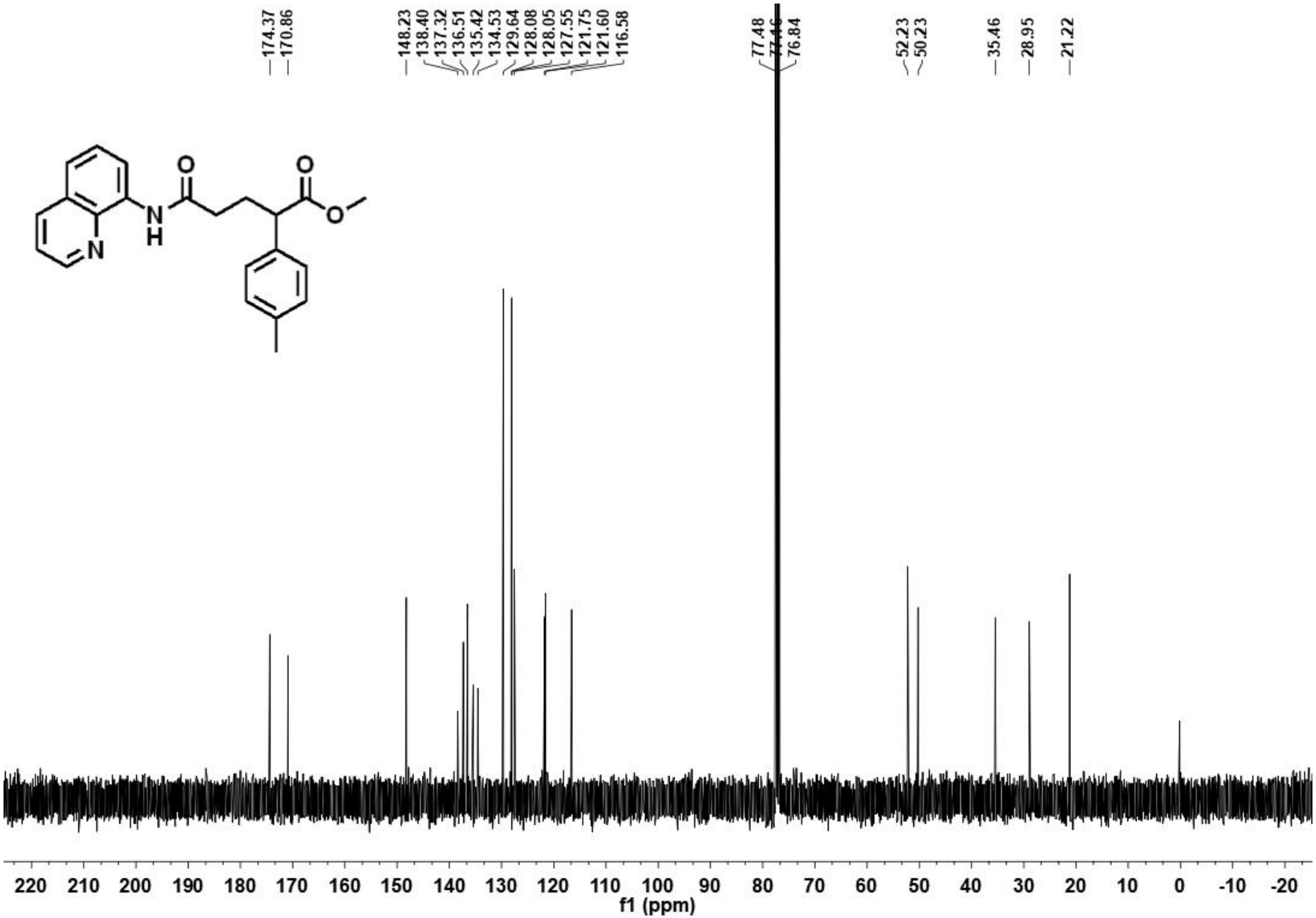
0.5
f1 (ppm)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121.60
116.58
77.48
76.84
52.23
50.23
35.46
28.95
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N
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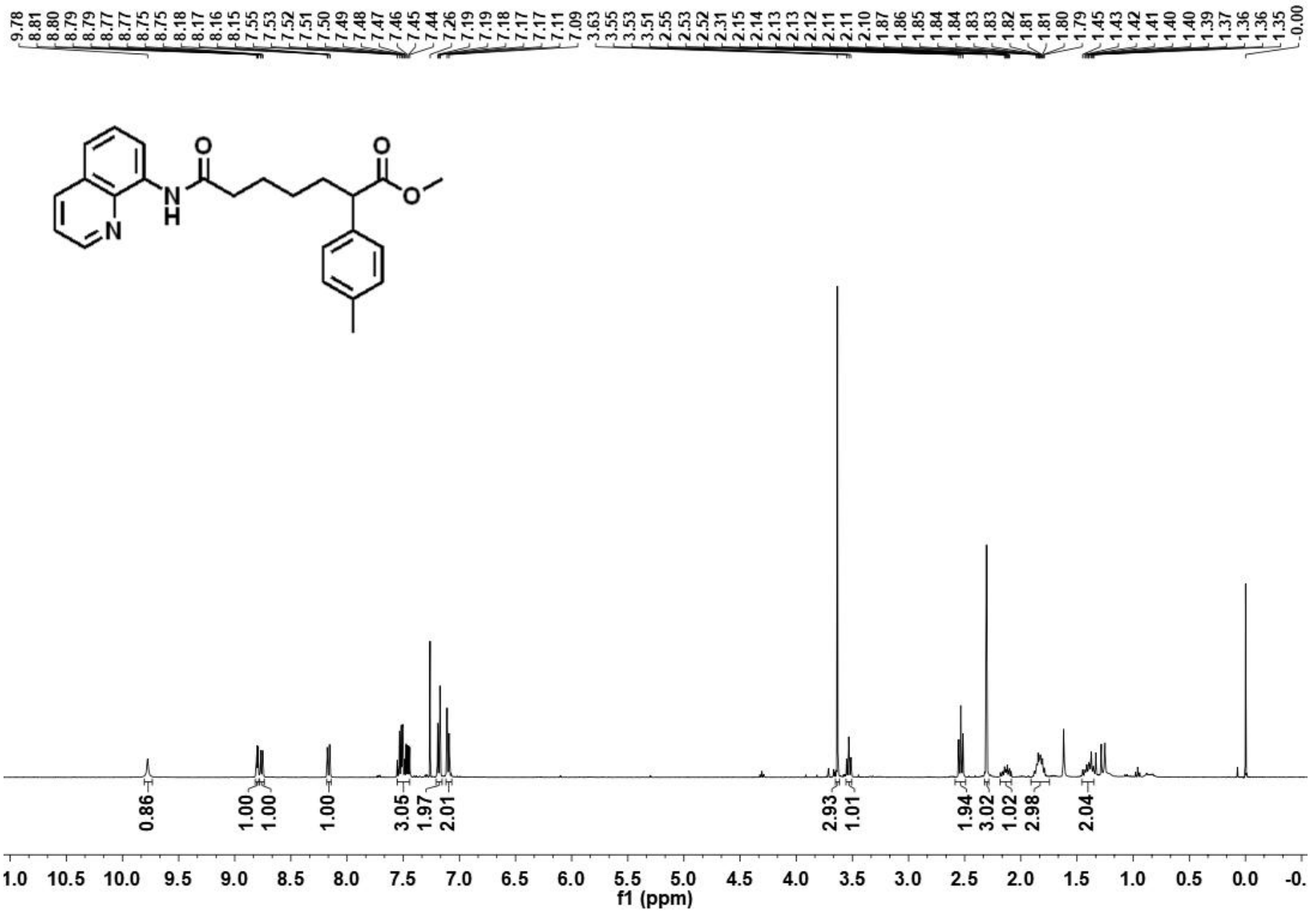
N
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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1.80
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1.43
1.42
1.41
1.40
1.40
1.39
1.37
1.36
1.36
1.35
-0.00
O
O
N
H
N
O
0.86
1.00
1.00
1.00
3.05
1.97
2.01
2.93
1.01
1.94
3.02
1.02
2.98
2.04
1.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
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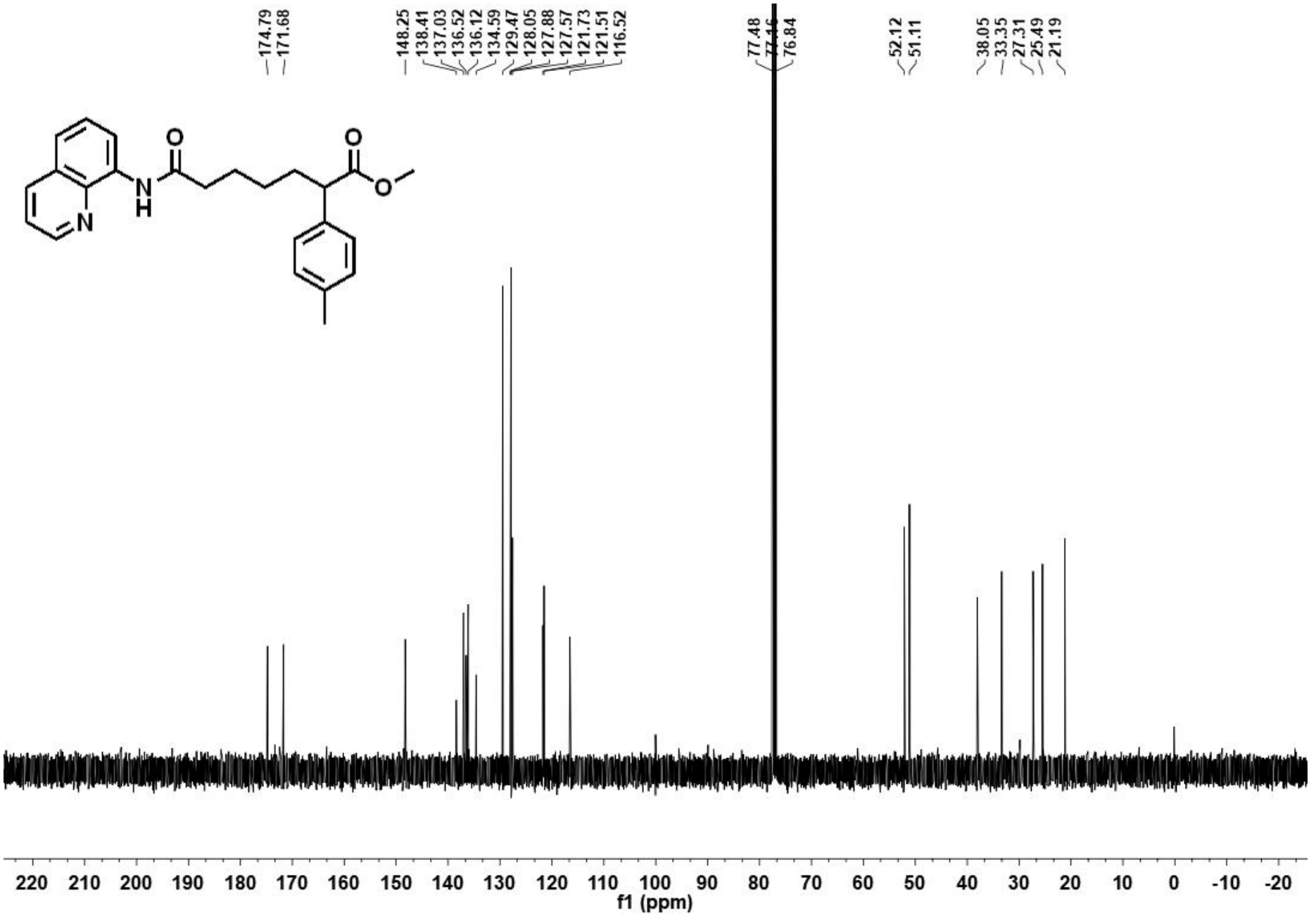
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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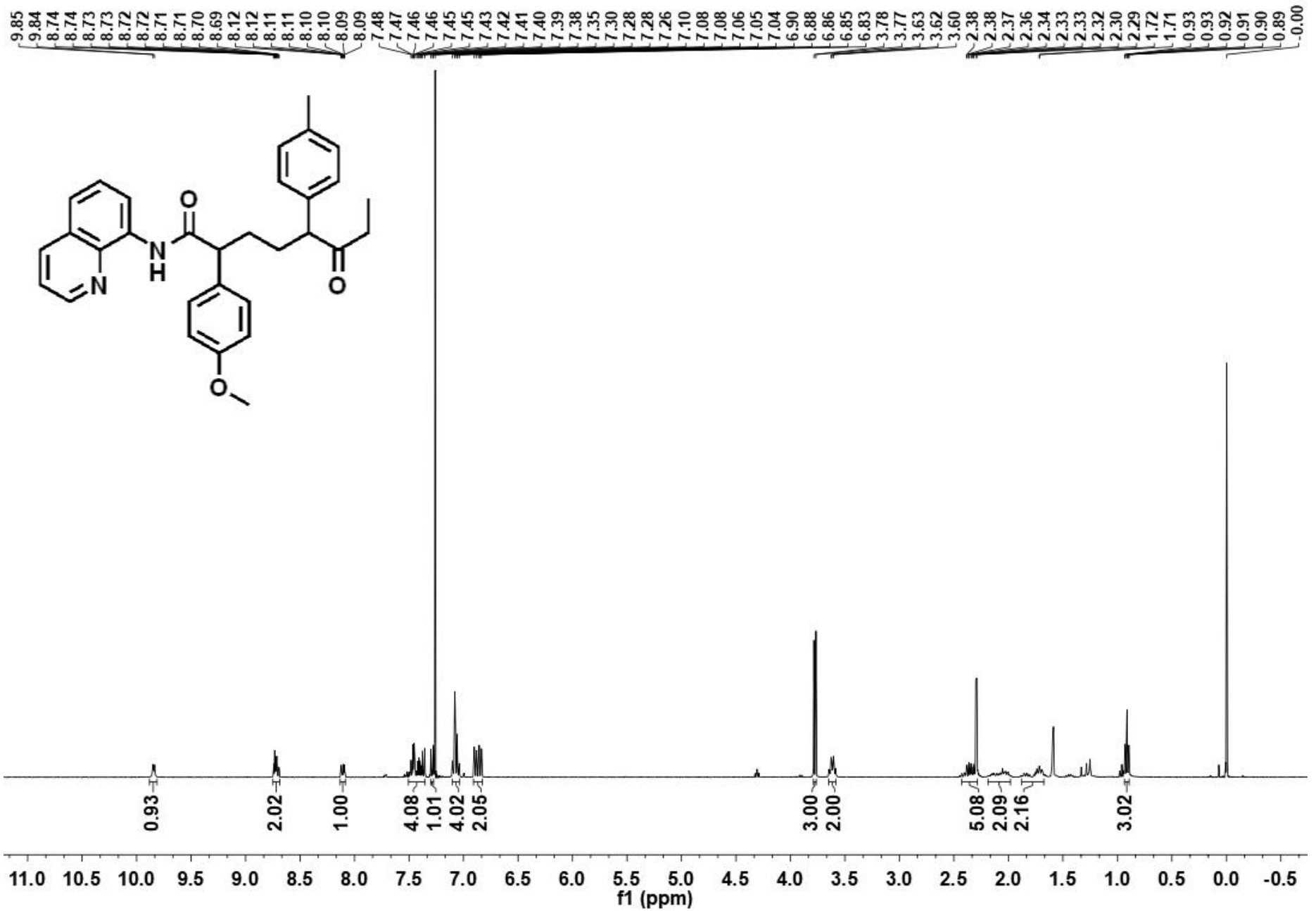
116.52
77.48
77.16
76.84
52.12
51.11
38.05
33.35
27.31
25.49
21.19
O
O
N
H
N
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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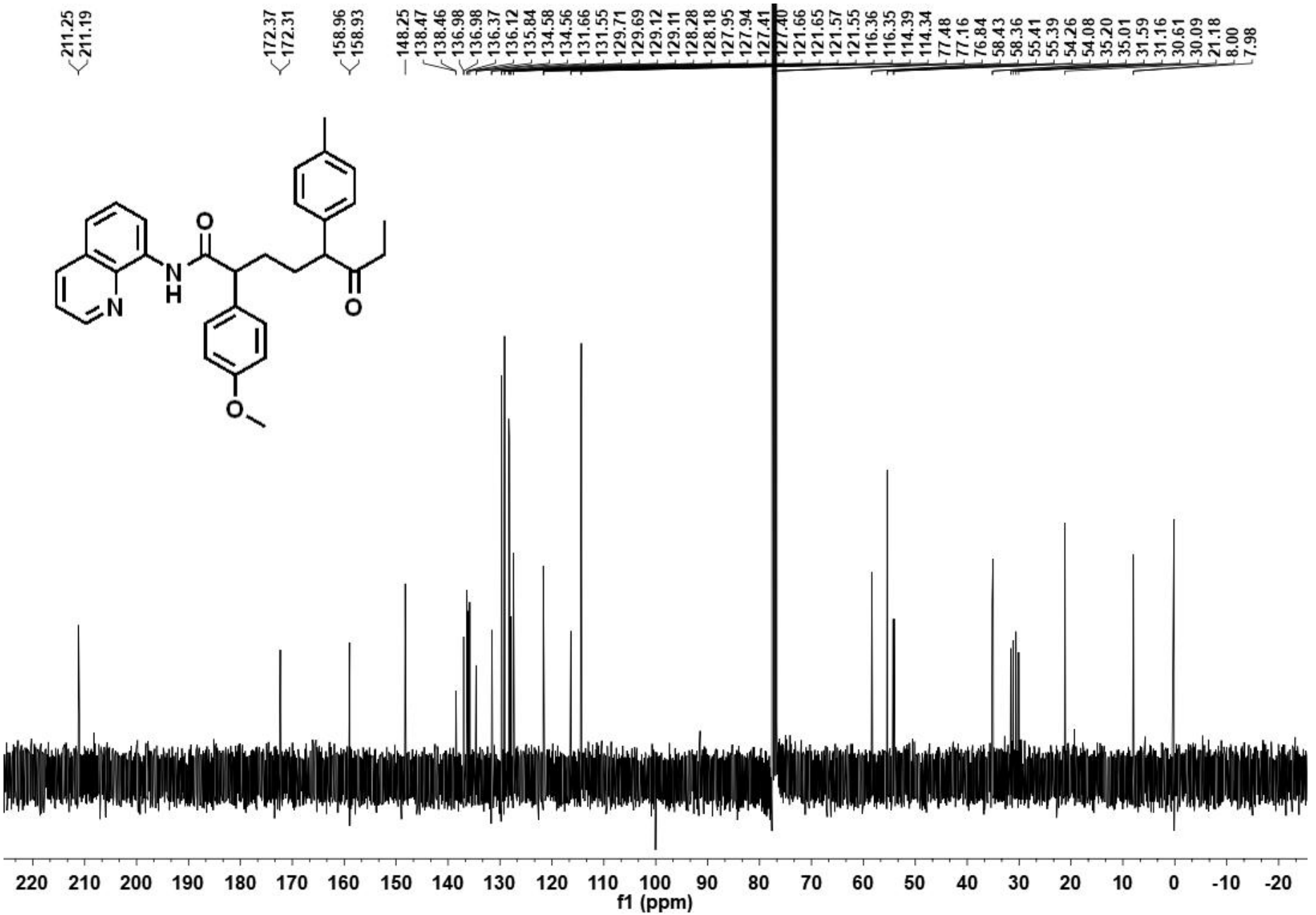
7.48 7.47 7.46 7.46 7.45 7.45 7.43 7.42 7.41 7.40 7.39 7.38 7.35 7.30 7.28 7.28 7.26 7.10 7.08 7.08 7.06 7.05 7.04 6.90 6.88 6.86 6.85 6.83 3.78 3.77 3.63 3.62 3.60
2.38 2.38 2.37 2.36 2.34 2.33 2.33 2.32 2.30 2.29 1.72 1.71 0.93 0.93 0.92 0.91 0.90 0.89 -0.00
O
N
H
N
O
O
0.93
2.02
1.00
4.08
1.01
4.02
2.05
3.00
2.00
5.08
2.09
2.16
3.02
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)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30.09
21.18
8.00
7.98
O
N
H
N
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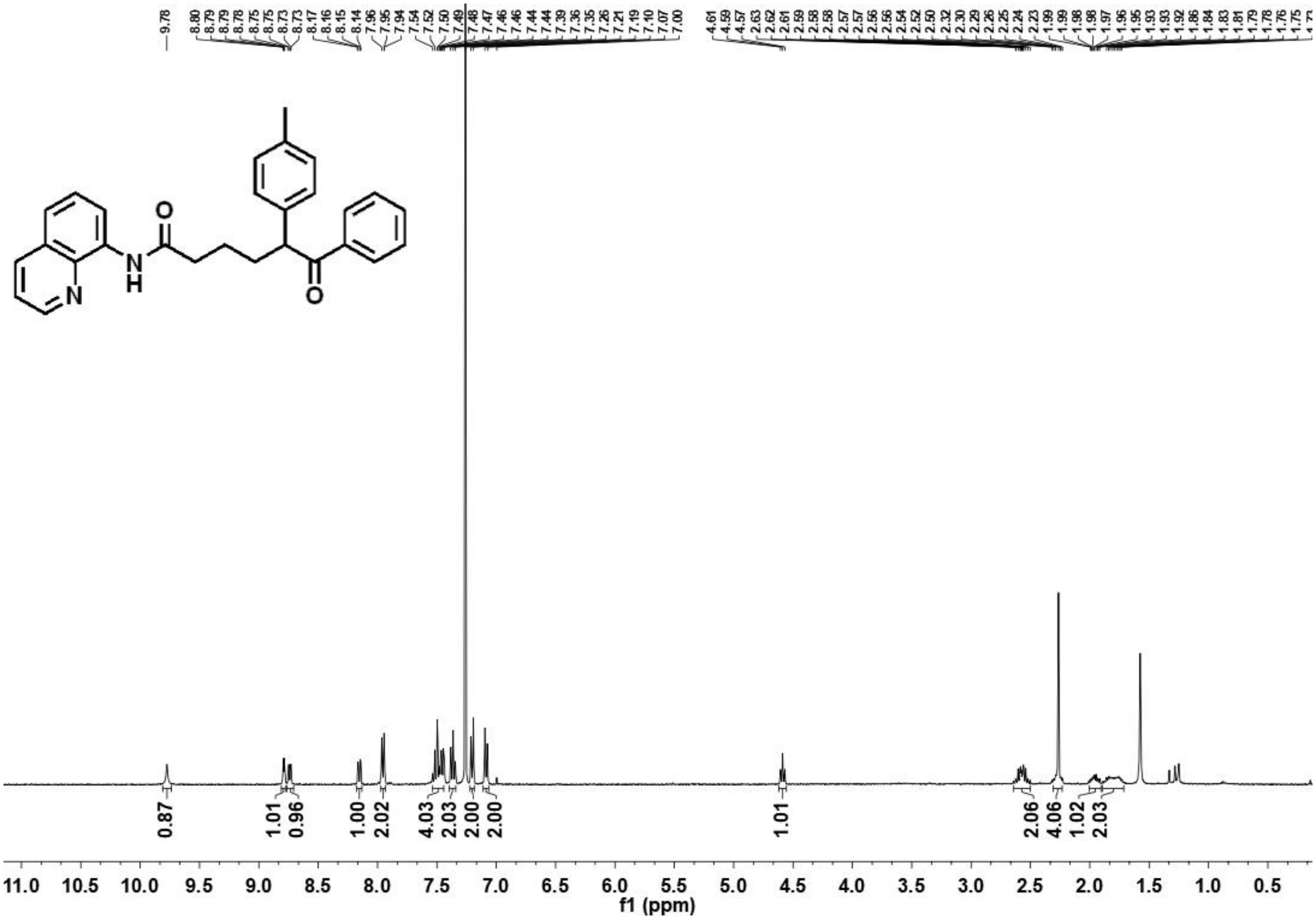
f1 (ppm)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7.44
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7.35
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7.10
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2.24
2.23
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1.99
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1.98
1.97
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1.95
1.93
1.93
1.92
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1.81
1.79
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1.75
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H
N
O
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0.96
1.00
2.02
4.03
2.03
2.00
2.00
1.01
2.06
4.06
1.02
2.03
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10.5
10.0
9.5
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8.5
8.0
7.5
7.0
6.5
6.0
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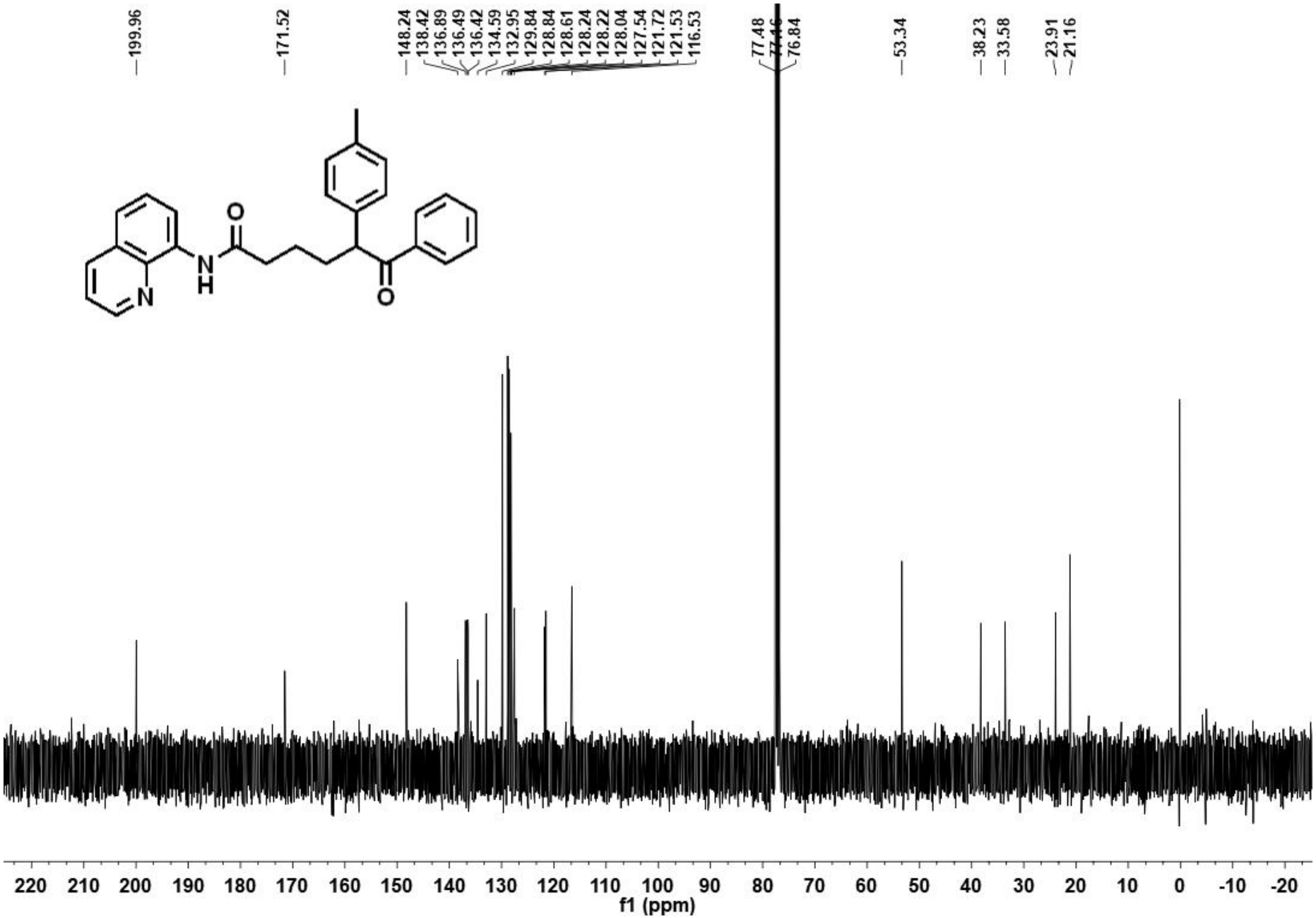
f1 (ppm)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76.84
53.34
38.23
33.58
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H
N
O
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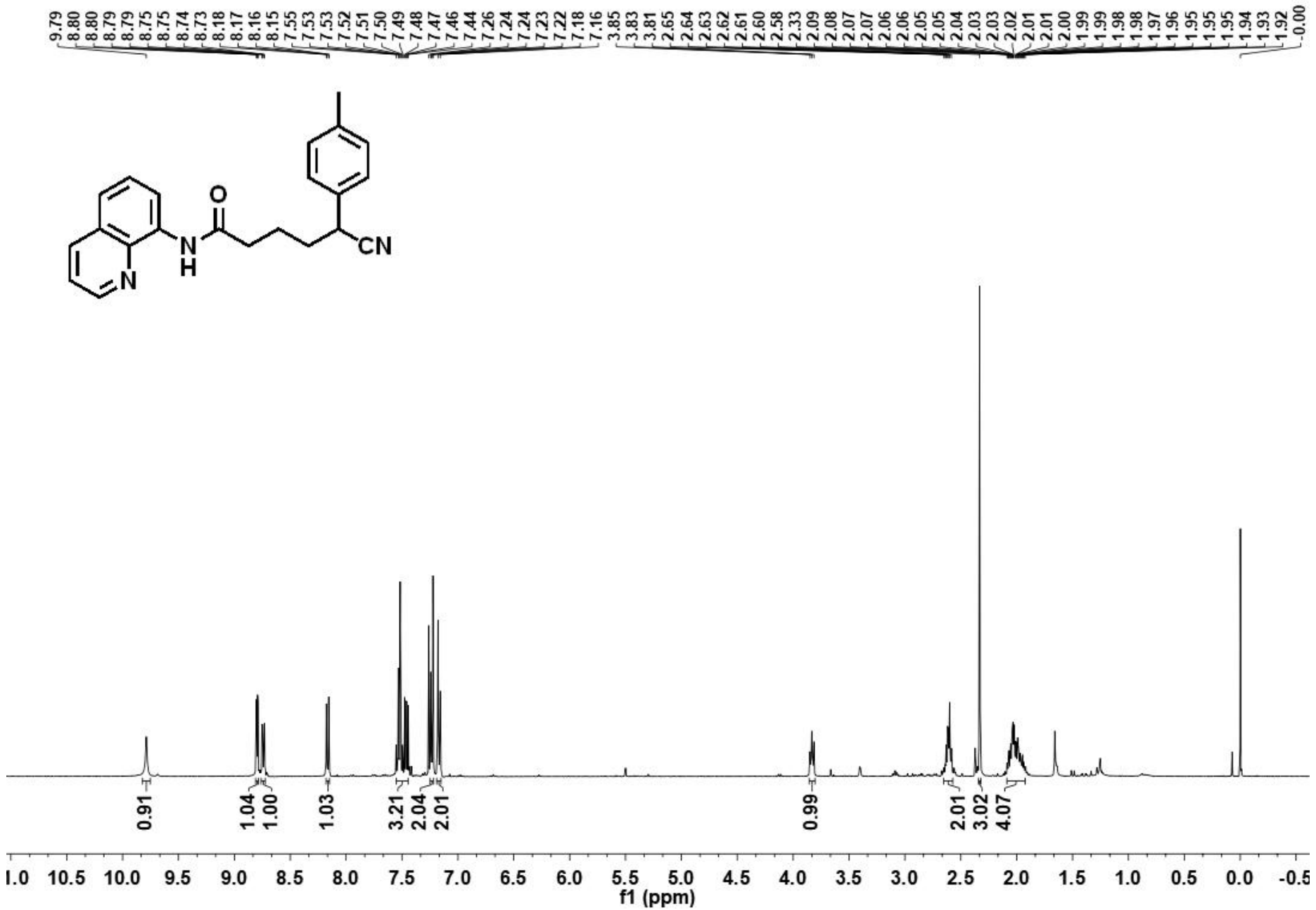
f1 (ppm)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7.48
7.47
7.46
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7.24
7.24
7.23
7.22
7.18
7.16
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2.60
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2.08
2.07
2.07
2.06
2.06
2.05
2.05
2.04
2.03
2.03
2.02
2.01
2.01
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1.97
1.96
1.95
1.95
1.95
1.94
1.93
1.92
-0.00
O
N
H
N
CN
0.91
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1.00
1.03
3.21
2.04
2.01
0.99
2.01
3.02
4.07
1.0
10.5
10.0
9.5
9.0
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7.0
6.5
6.0
5.5
5.0
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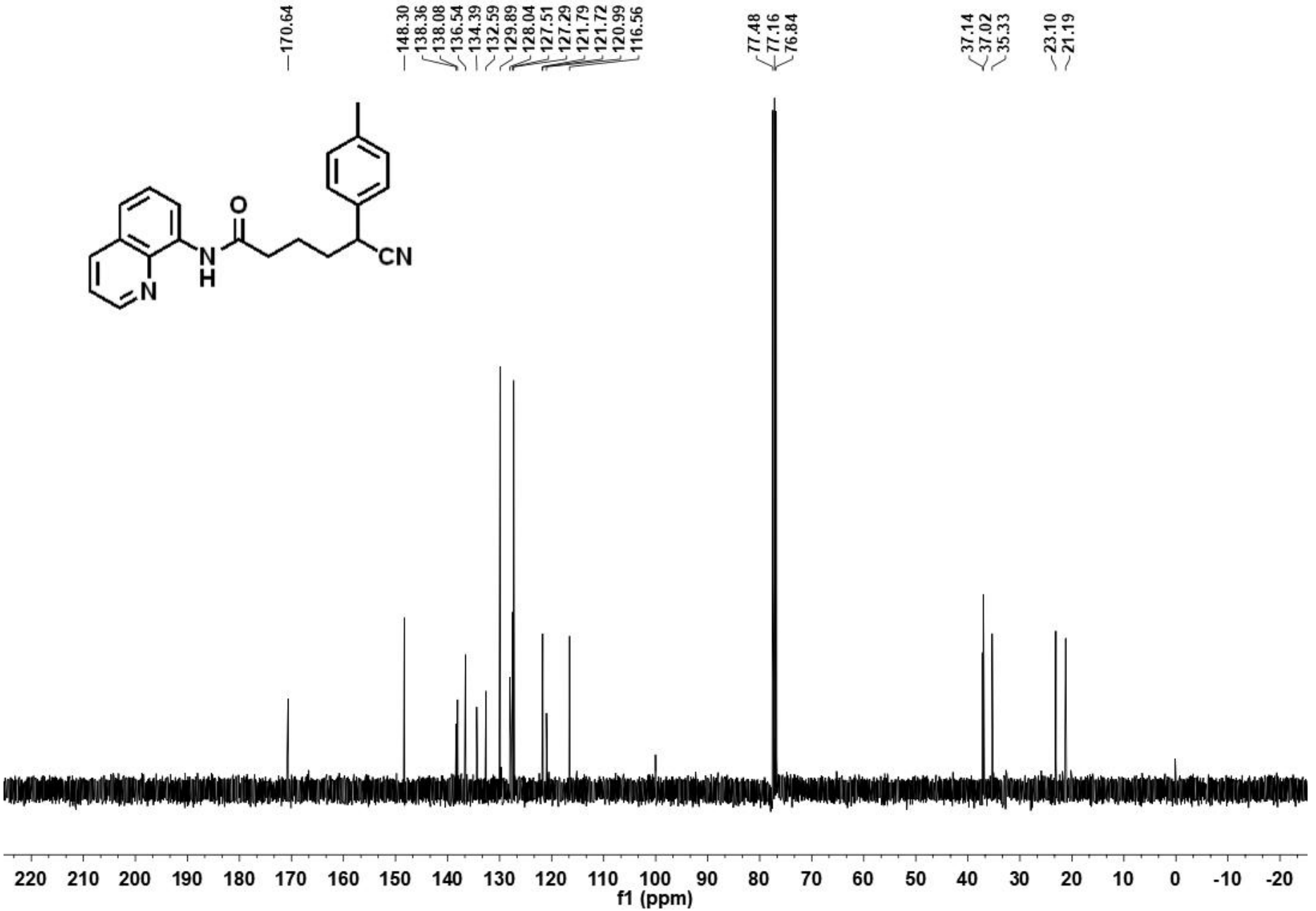
-0.5
f1 (ppm)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127.29
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76.84
37.14
37.02
35.33
23.10
21.19
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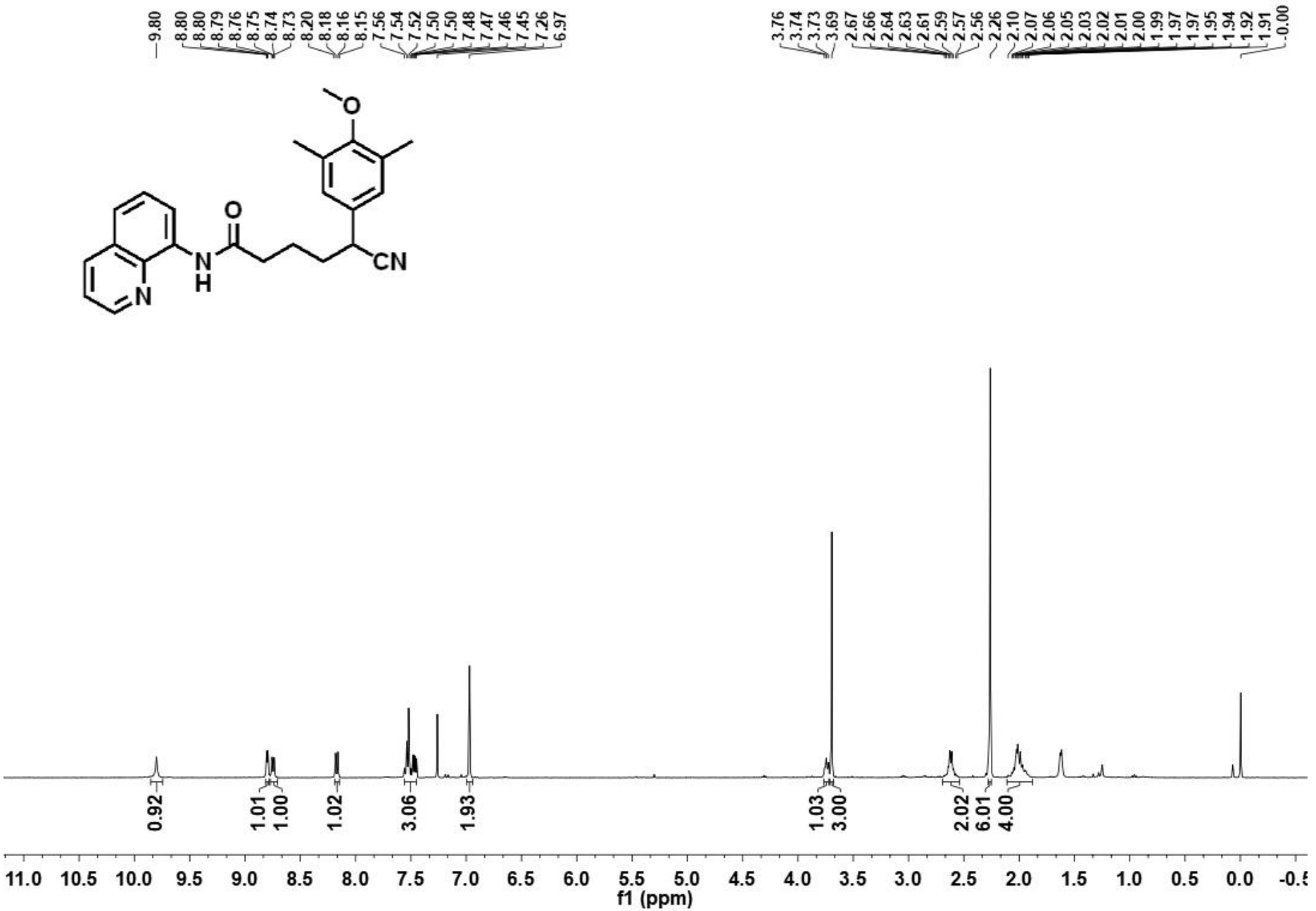
N
H
N
CN
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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8.18
8.16
8.15
7.56
7.54
7.52
7.50
7.50
7.48
7.47
7.46
7.45
7.26
6.97
3.76
3.74
3.73
3.69
2.67
2.66
2.64
2.63
2.61
2.59
2.57
2.56
2.26
2.10
2.07
2.06
2.05
2.03
2.02
2.01
2.00
1.99
1.97
1.97
1.95
1.94
1.92
1.91
0.00
O
O
N
H
N
CN
0.92
1.01
1.00
1.02
3.06
1.93
1.03
3.00
2.02
6.01
4.00
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
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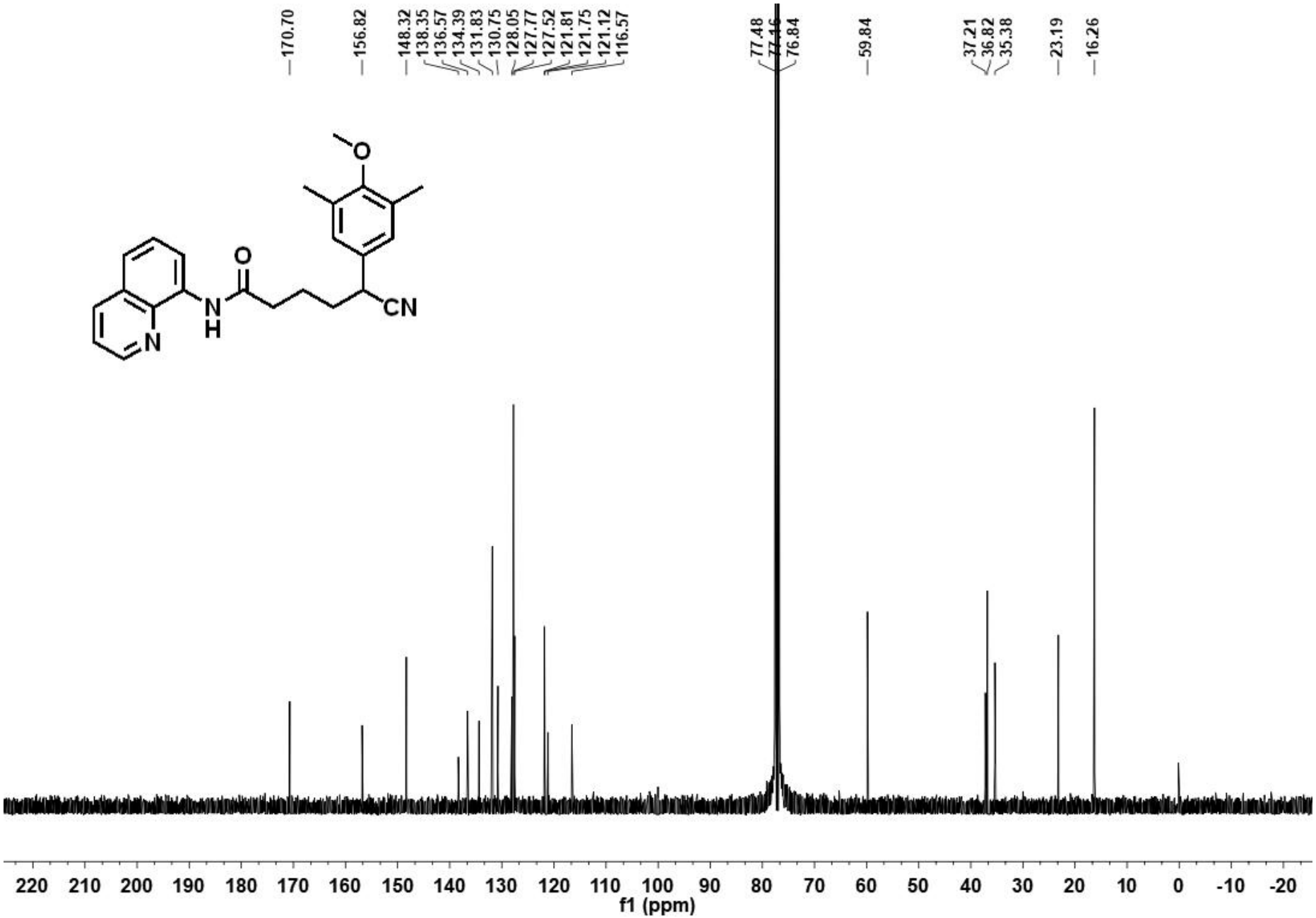
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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134.39
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130.75
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127.77
127.52
121.81
121.75
121.12
116.57
77.48
77.16
76.84
59.84
37.21
36.82
35.38
23.19
16.26
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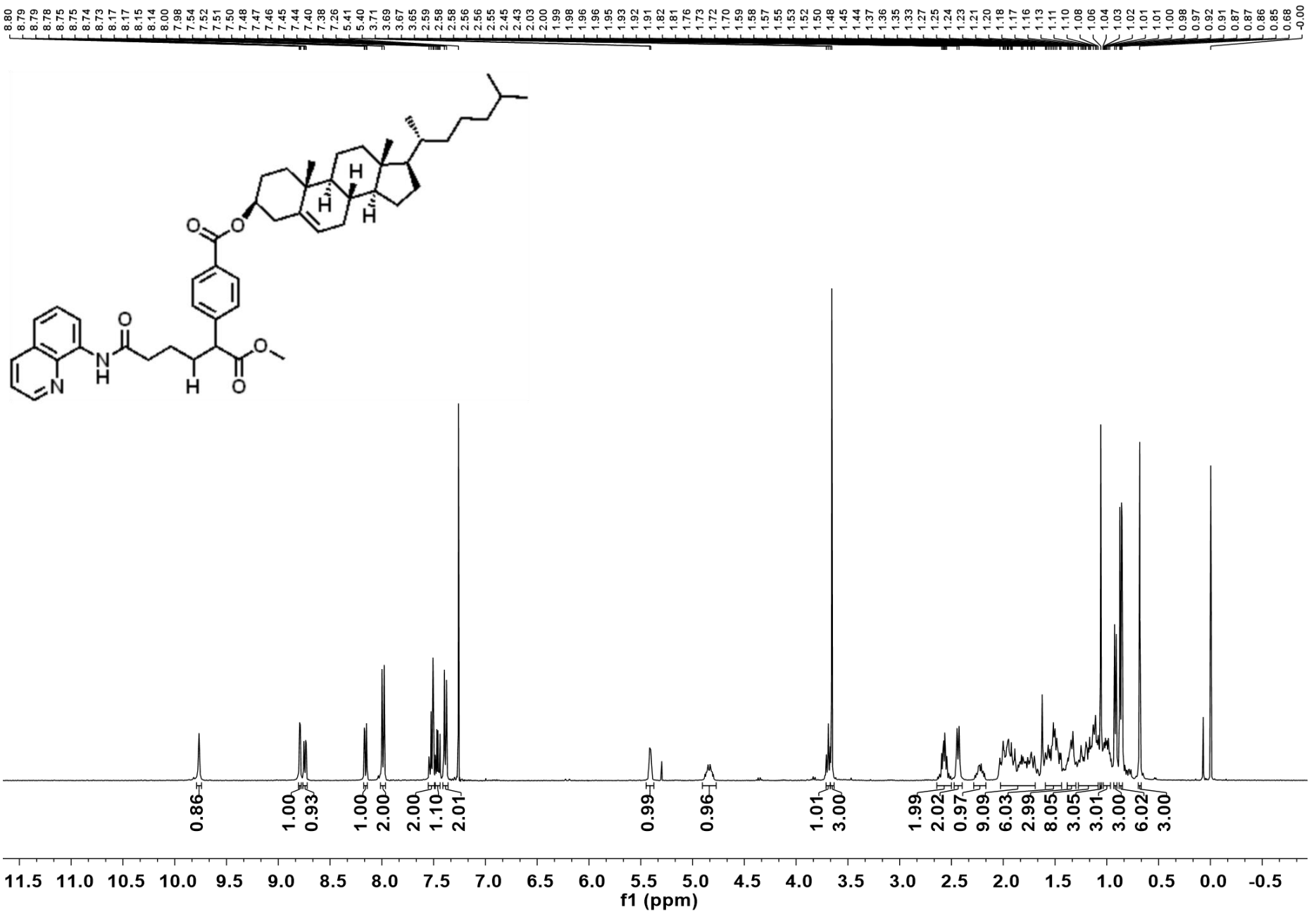
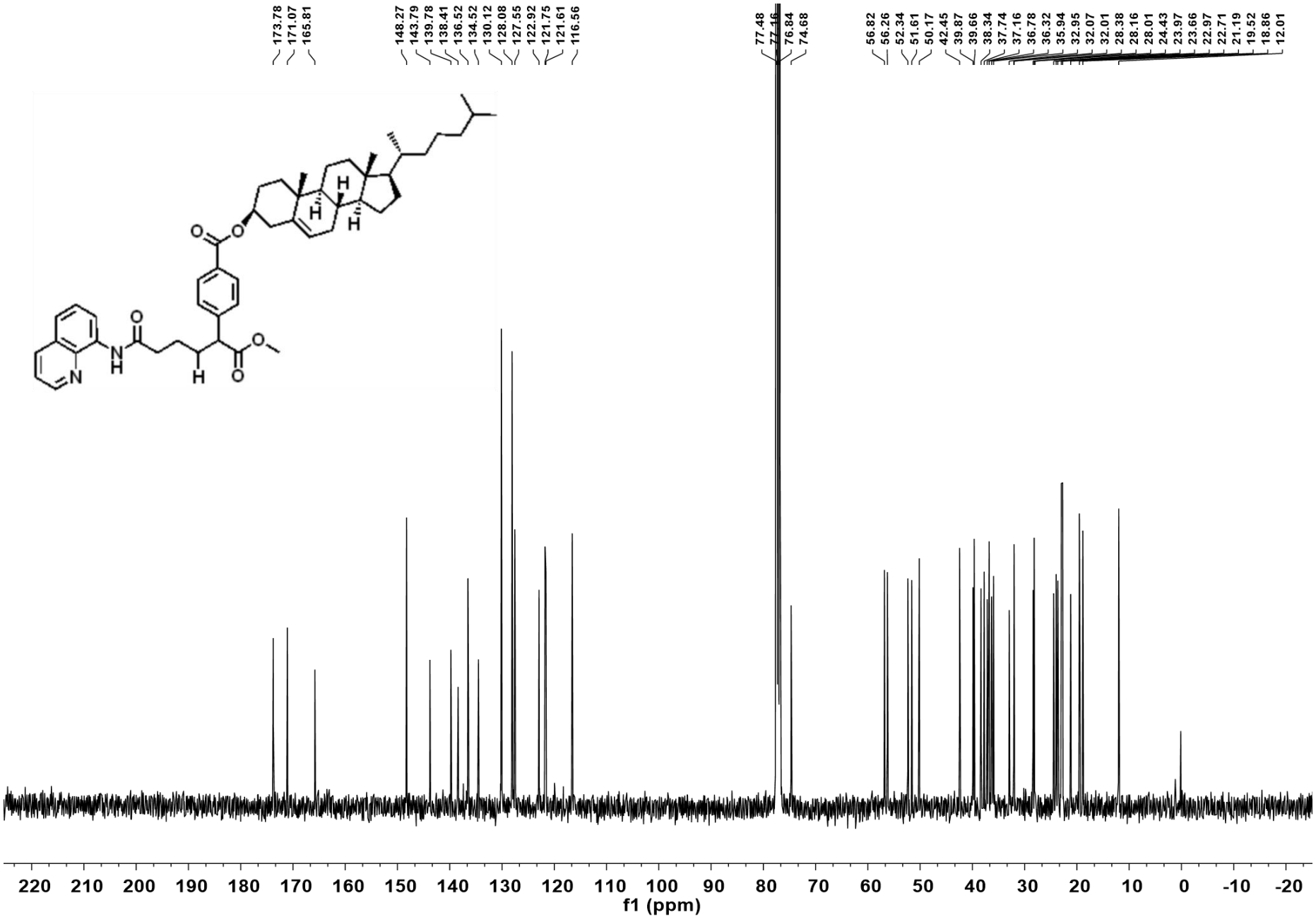
O
N
H
N
CN
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)



8.80 8.79 8.79 8.78 8.75 8.75 8.74 8.73 8.17 8.17 8.15 8.14 8.00 7.98 7.54 7.52 7.51 7.50 7.48 7.47 7.46 7.45 7.44 7.40 7.38 7.26 5.41 5.40 3.71 3.69 3.67 3.65 2.59 2.58 2.58 2.56 2.56 2.55 2.45 2.43 2.03 2.00 1.99 1.98 1.96 1.96 1.95 1.93 1.92 1.91 1.82 1.81 1.76 1.73 1.72 1.70 1.59 1.58 1.57 1.55 1.53 1.52 1.50 1.48 1.45 1.44 1.37 1.36 1.35 1.33 1.27 1.25 1.24 1.23 1.21 1.20 1.18 1.17 1.16 1.13 1.11 1.10 1.08 1.06 1.04 1.03 1.02 1.01 1.01 1.00 0.98 0.97 0.92 0.91 0.87 0.87 0.86 0.85 0.68 -0.00
0.86 1.00 0.93 1.00 2.00 2.00 1.10 2.01 0.99 0.96 1.01 3.00 1.99 2.02 0.97 9.09 6.03 2.99 8.05 3.05 3.01 3.00 6.02 3.00
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
f1 (ppm)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130.12
128.08
127.55
122.92
121.75
121.61
116.56
77.48
77.16
76.84
74.68
56.82
56.26
52.34
51.61
50.17
42.45
39.87
39.66
38.34
37.74
37.16
36.78
36.32
35.94
32.95
32.07
32.01
28.38
28.16
28.01
24.43
23.97
23.66
22.97
22.71
21.19
19.52
18.86
12.01
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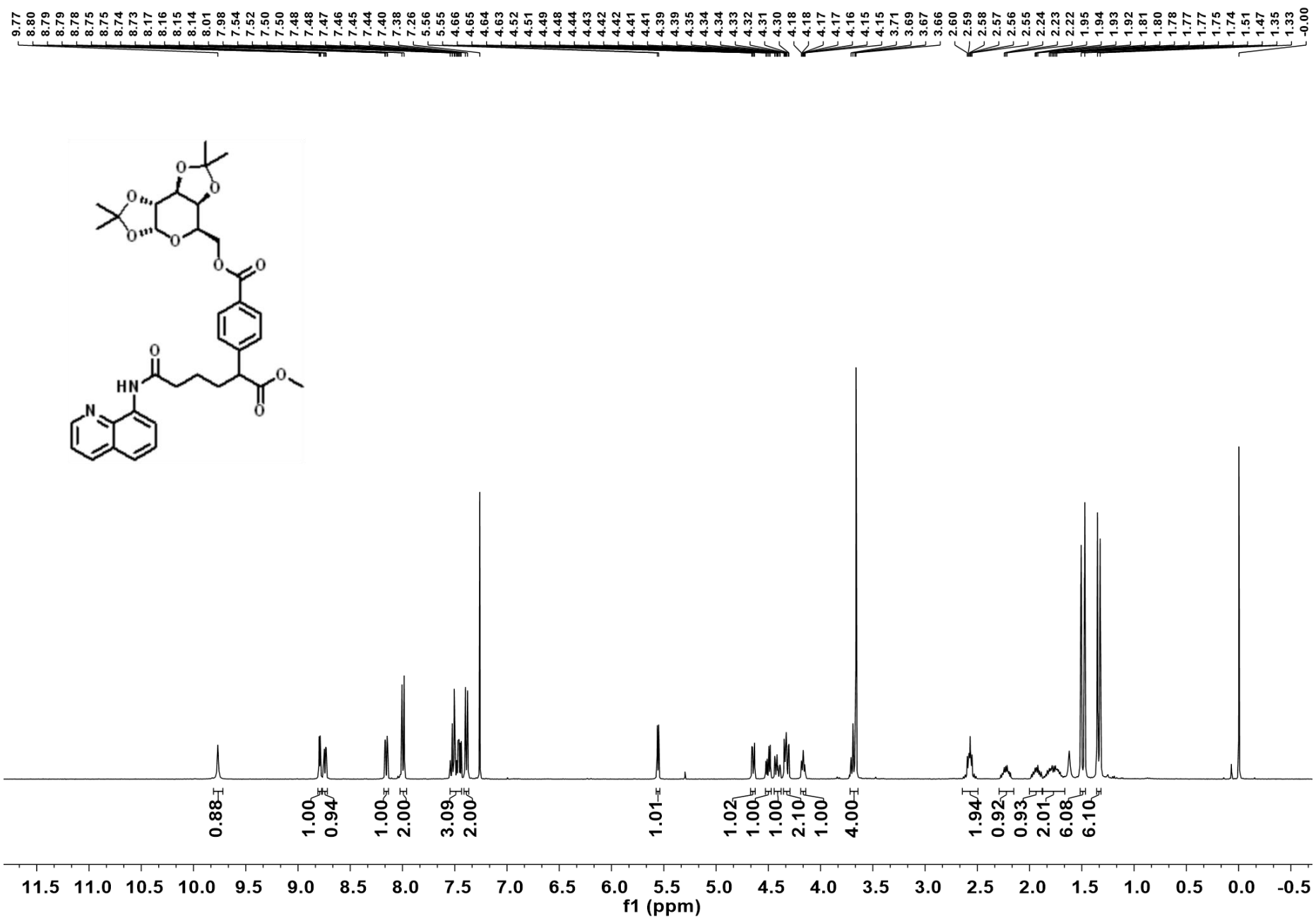
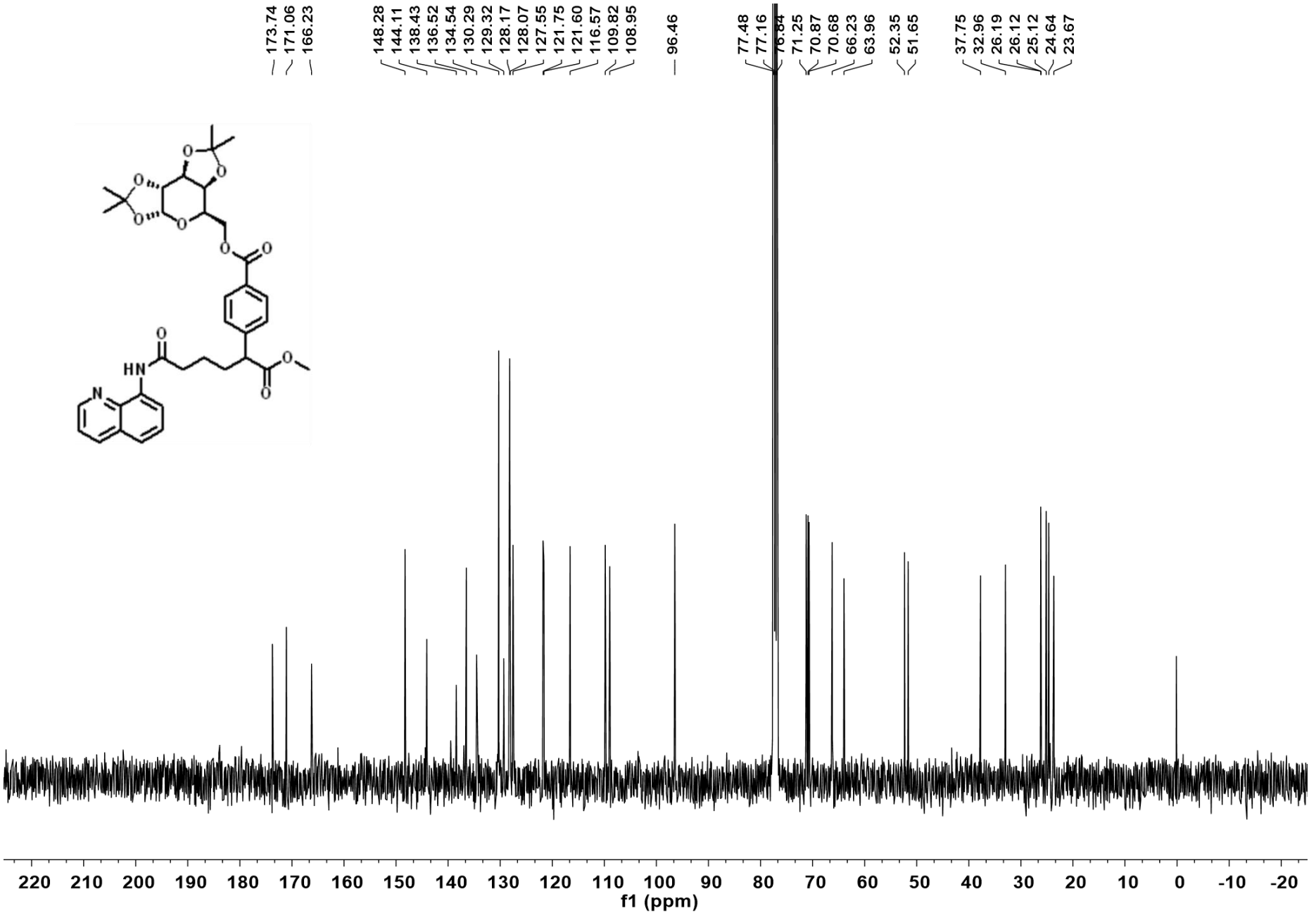
f1 (ppm)


9.77 8.80 8.79 8.79 8.78 8.75 8.75 8.74 8.73 8.17 8.16 8.15 8.14 8.01 7.98 7.54 7.52 7.50 7.50 7.48 7.48 7.47 7.46 7.45 7.44 7.40 7.38 7.26 5.56 5.55 4.66 4.65 4.64 4.63 4.52 4.51 4.49 4.48 4.44 4.43 4.42 4.42 4.41 4.41 4.39 4.39 4.35 4.34 4.34 4.33 4.32 4.31 4.30 4.18 4.18 4.17 4.17 4.16 4.15 4.15 3.71 3.69 3.67 3.66 2.60 2.59 2.58 2.57 2.56 2.55 2.24 2.23 2.22 1.95 1.94 1.93 1.92 1.81 1.80 1.78 1.77 1.77 1.75 1.74 1.51 1.47 1.35 1.33 -0.00
HN
N
0.88 1.00 0.94 1.00 2.00 3.09 2.00 1.01 1.02 1.00 1.00 2.10 1.00 4.00 1.94 0.92 0.93 2.01 6.08 6.10
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
f1 (ppm)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129.32
128.17
128.07
127.55
121.75
121.60
116.57
109.82
108.95
96.46
77.48
77.16
76.84
71.25
70.87
70.68
66.23
63.96
52.35
51.65
37.75
32.96
26.19
26.12
25.12
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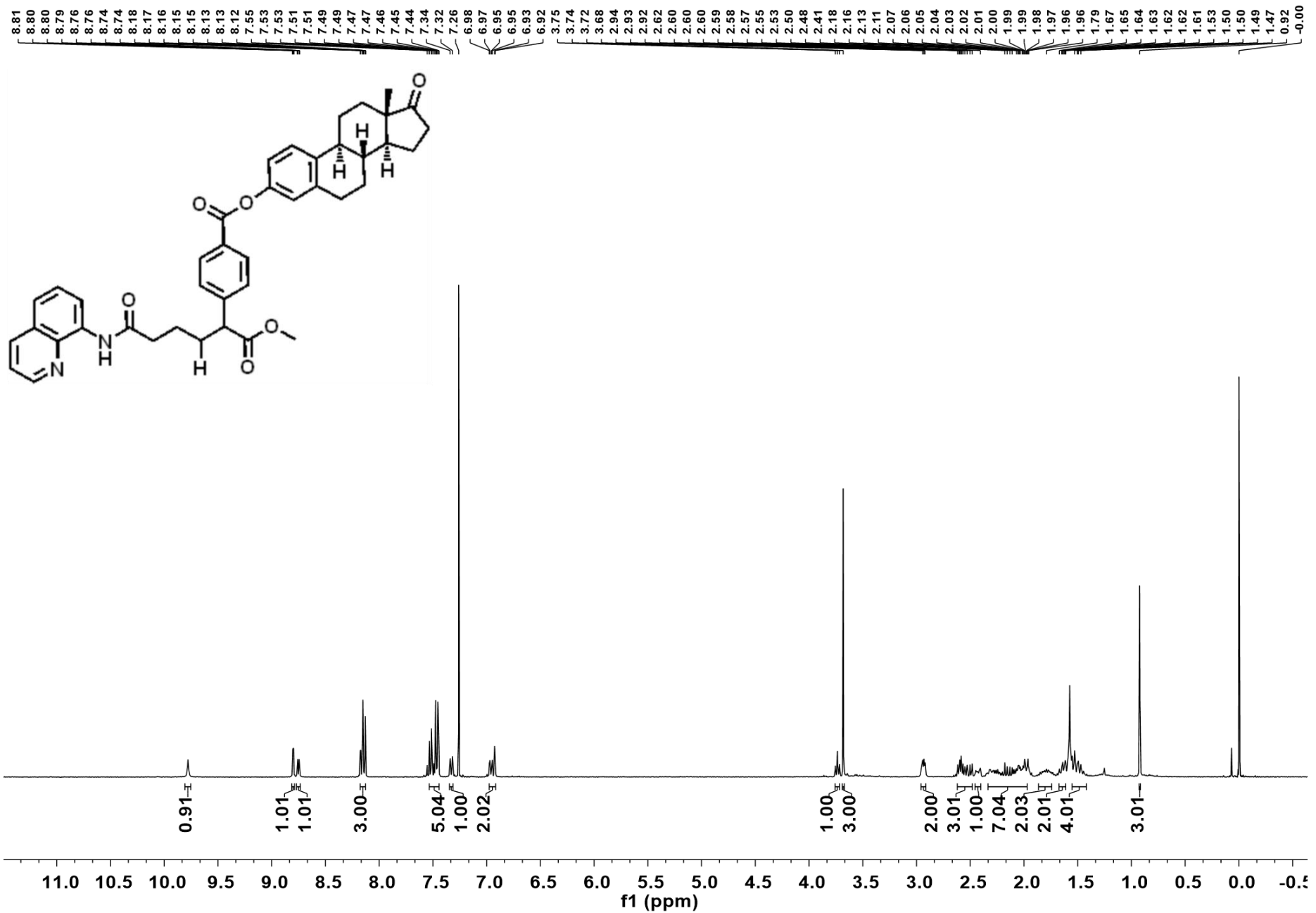
23.67
HN
N
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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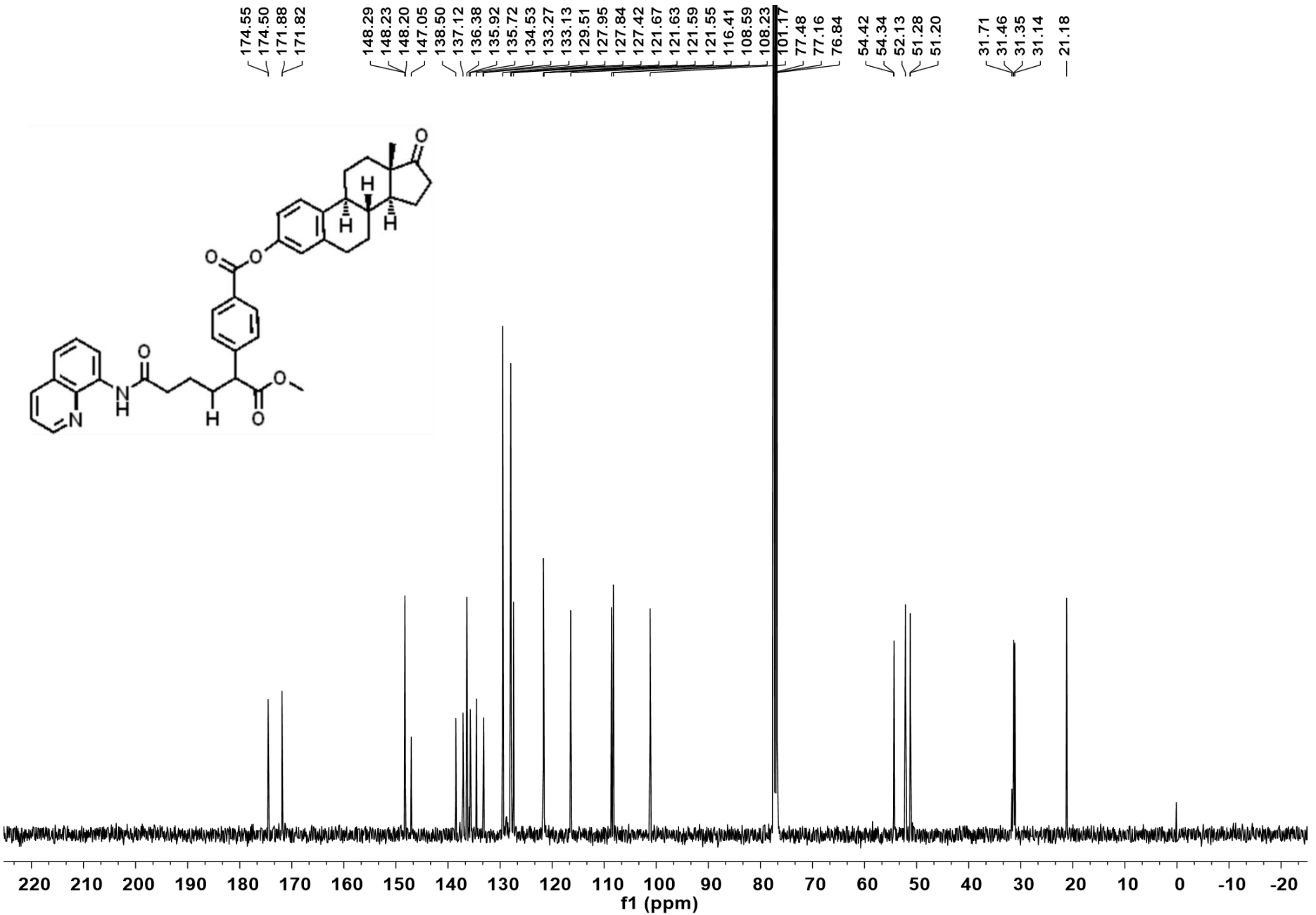
O
H
H
H
O
O
O
N
H
N
H
O
O
0.91
1.01
1.01
3.00
5.04
1.00
2.02
1.00
3.00
2.00
3.01
1.00
7.04
2.03
2.01
4.01
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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171.82
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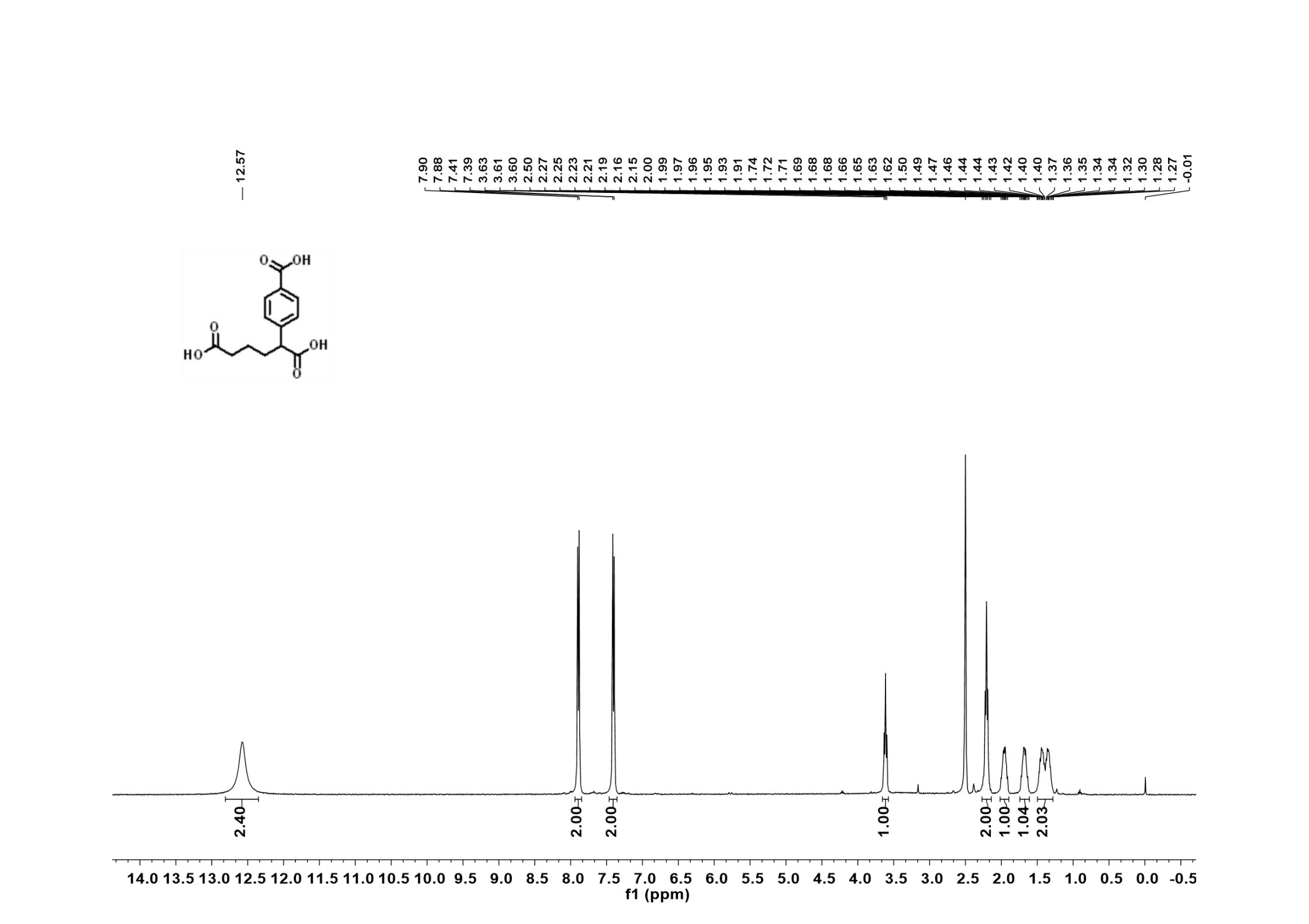
148.20
147.05
138.50
137.12
136.38
135.92
135.72
134.53
133.27
133.13
129.51
127.95
127.84
127.42
121.67
121.63
121.59
121.55
116.41
108.59
108.23
101.17
77.48
77.16
76.84
54.42
54.34
52.13
51.28
51.20
31.71
31.46
31.35
31.14
21.18
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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2.27
2.25
2.23
2.21
2.19
2.16
2.15
2.00
1.99
1.97
1.96
1.95
1.93
1.91
1.74
1.72
1.71
1.69
1.68
1.68
1.66
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1.63
1.62
1.50
1.49
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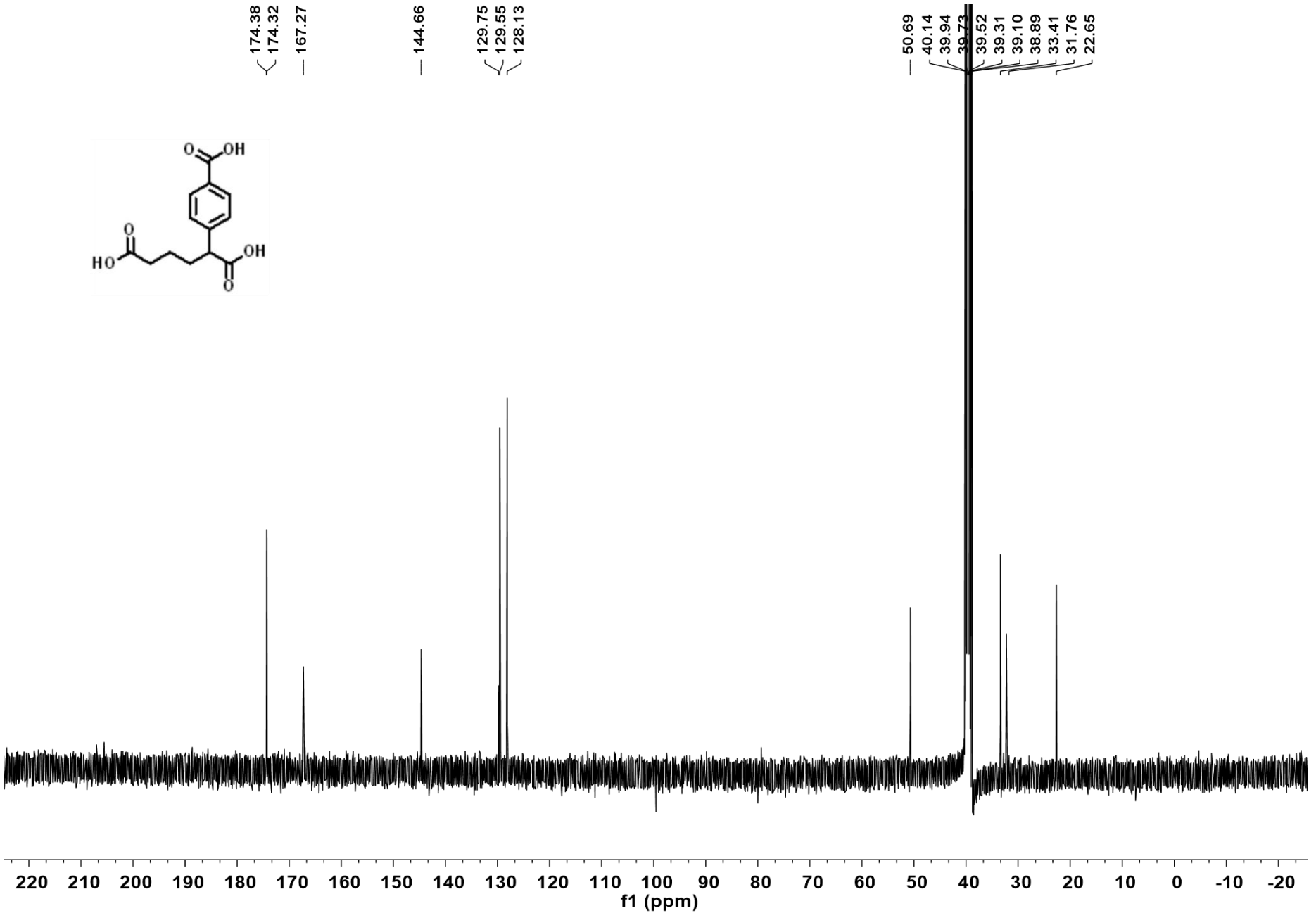
1.46
1.44
1.44
1.43
1.42
1.40
1.40
1.37
1.36
1.35
1.34
1.34
1.32
1.30
1.28
1.27
-0.01
HO
OH
OH
2.40
2.00
2.00
1.00
2.00
1.00
1.04
2.03
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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39.73
39.52
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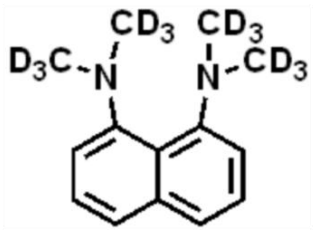
39.10
38.89
33.41
31.76
22.65
O
OH
HO
O
OH
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


CD3
CD3
D3C
N
N
CD3

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7.36
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7.33
7.33
7.32
7.32
7.31
7.30
7.30
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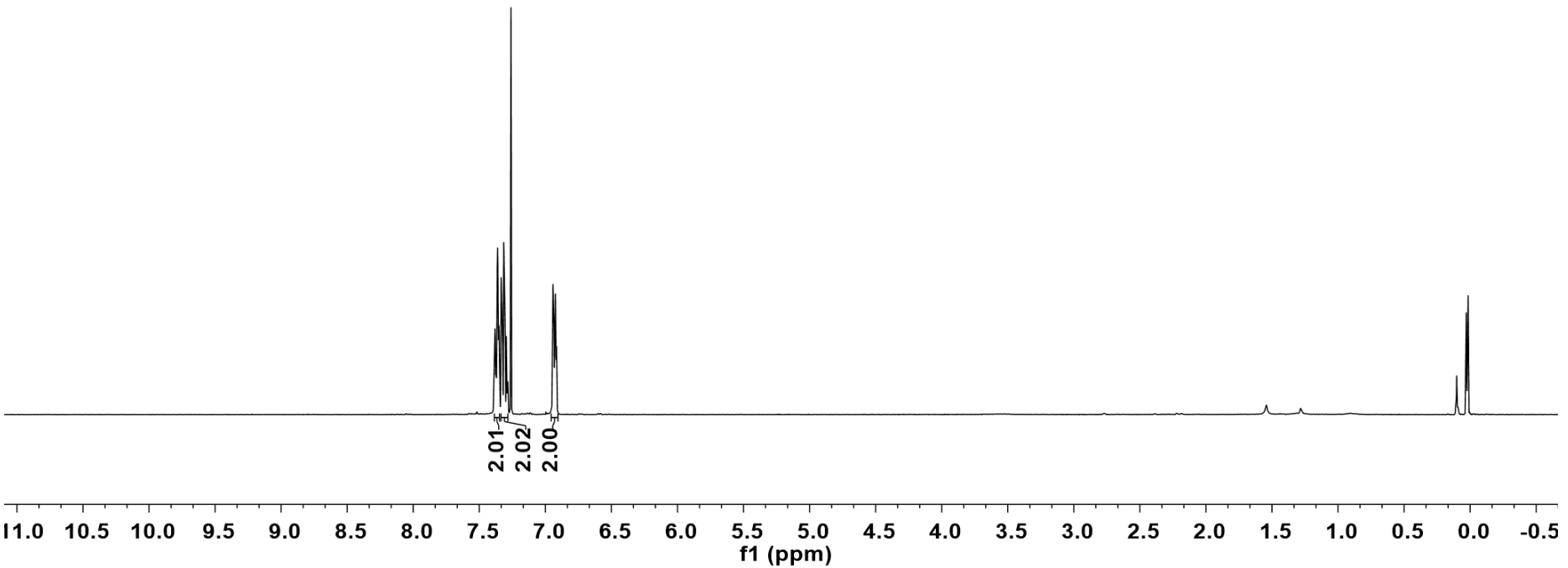
7.28
7.26
6.95
6.94
6.93
6.93
6.93
6.92
6.92
6.91

0.02


2.01
2.02
2.00
11.0
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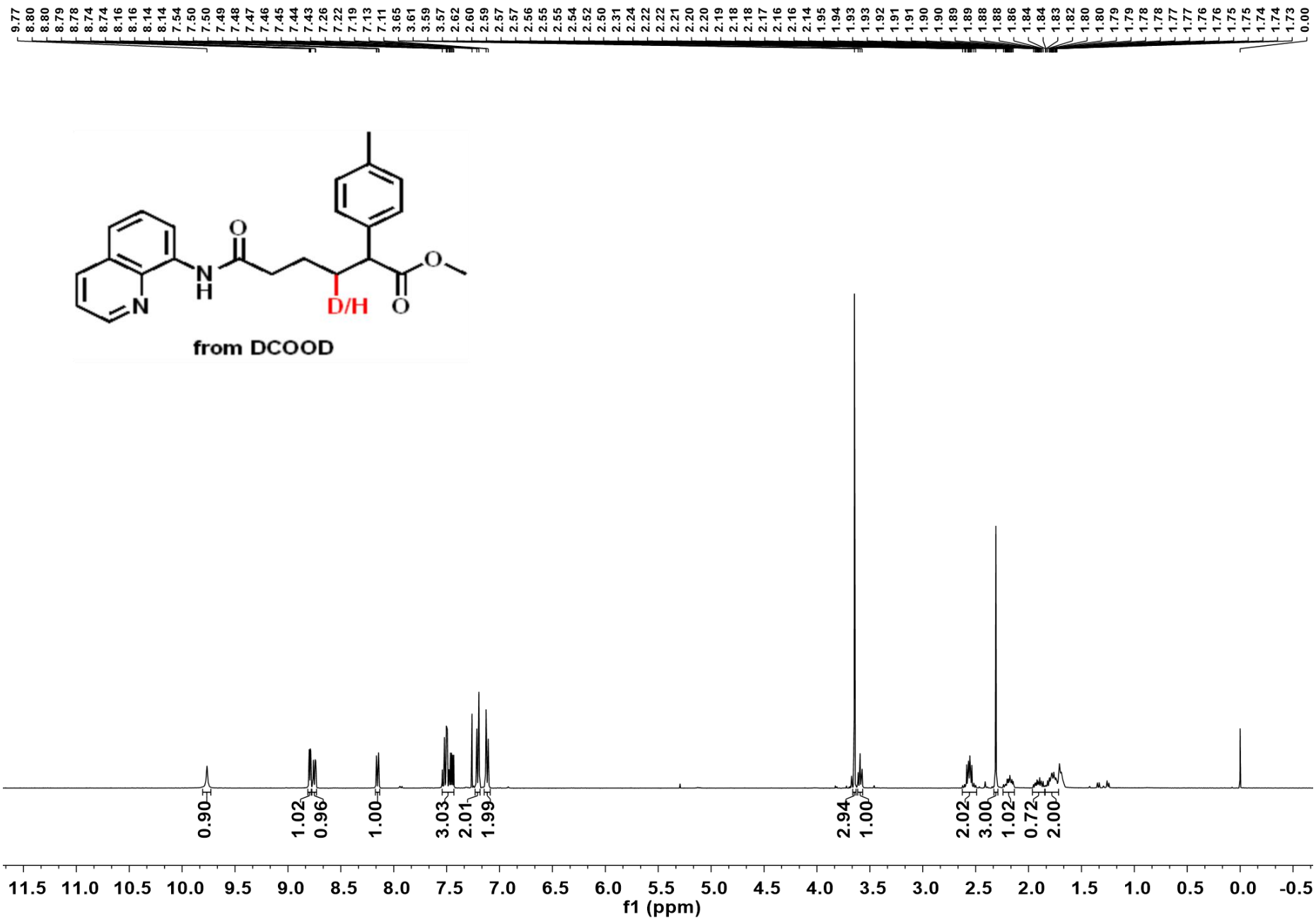
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


9.77 8.80 8.80 8.79 8.78 8.74 8.74 8.16 8.16 8.14 8.14 7.54 7.50 7.50 7.49 7.48 7.47 7.46 7.45 7.44 7.43 7.26 7.22 7.19 7.13 7.11 3.65 3.61 3.59 3.57 2.62 2.60 2.59 2.57 2.57 2.56 2.55 2.55 2.54 2.52 2.50 2.31 2.24 2.22 2.22 2.21 2.20 2.20 2.19 2.18 2.18 2.17 2.16 2.16 2.14 1.95 1.94 1.93 1.93 1.92 1.91 1.91 1.90 1.90 1.89 1.89 1.88 1.88 1.86 1.84 1.84 1.83 1.82 1.80 1.80 1.79 1.79 1.78 1.78 1.77 1.77 1.76 1.76 1.75 1.75 1.74 1.74 1.73 0.00
O
N
H
N
O
O
D/H
from DCOOD
0.90
1.02
0.96
1.00
3.03
2.01
1.99
2.94
1.00
2.02
3.00
1.02
0.72
2.00
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
f1 (ppm)

7.26
7.00
6.99
6.98
6.97
6.97
6.96
6.95
6.94
6.93
6.93
6.92
6.91
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1.69
1.68
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1.66
1.65
0.01
HO
O
O
O
+
HO
O
O
O
1.00
0.99
3.00
0.30
4.01
0.42
0.41
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)