Supporting Information

Access to 5*H*-benzo[*a*]carbazol-6-ols and Benzo[6,7]cyclohepta[1,2-*b*]indol-6-ols via Rhodium-Catalyzed C-H Activation/Carbenoid Insertion/Aldol-Type Cyclization

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Contents:

1. Single Crystal X-ray Structure Determination. Data collection and structural analysis of crystal were collected on an Agilent Technologies SuperNova Single Crystal Diffractometer equipped with graphite monochromatic Cu/Mo Kα radiation (λ = 1.54184 Å). The crystal was kept at 293 (10) K during data collection. Using Olex2[1], the structure was solved with the Superflip structure solution program using Charge Flipping and refined with the ShelXL refinement package using Least Squares minimisation. The hydrogen atoms on the ligands were placed in idealized positions and refined using a riding model. The detailed crystallographic data and structure refinement parameters for these compounds are summarized in **Table S1 (3k) and Table S2 (5e).** CCDC 1985868 and 1985869 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

(1) Single crystal structure of **3k**

Table S1. Crystal data and structure refinement for **3k**

Identification code	hqf-gxm-ii-154
Empirical formula	$C_{20}H_{16}ClNO_5$
Formula weight	385.79
Temperature/K	294.59(10)
Crystal system	monoclicnic
Space group	$P2_1/c$
a/Å	11.4022(2)
b/Å	8.74662(16)
c/Å	17.8884(4)
α/°	90
β/°	104.315(2)
γ/°	90
Volume/Å^3	1728.63(6)
Z	4
ρ_{calc}g/cm^3	1.482
μ/mm^{-1}	2.254
F(000)	800.0
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.002 to 147.564
Index ranges	$-14 \le h \le 13$, $-10 \le k \le 7$, $-22 \le l \le 21$
Reflections collected	10033

Independent reflections	3424 [R_{int} = 0.0185, R_{sigma} = 0.0168]
Data/restraints/parameters	3424/0/254
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	R_1 = 0.0390, wR_2 = 0.1013
Final R indexes [all data]	R_1 = 0.0439, wR_2 = 0.1062
Largest diff. peak/hole / e $Å^{-3}$	0.24/-0.40

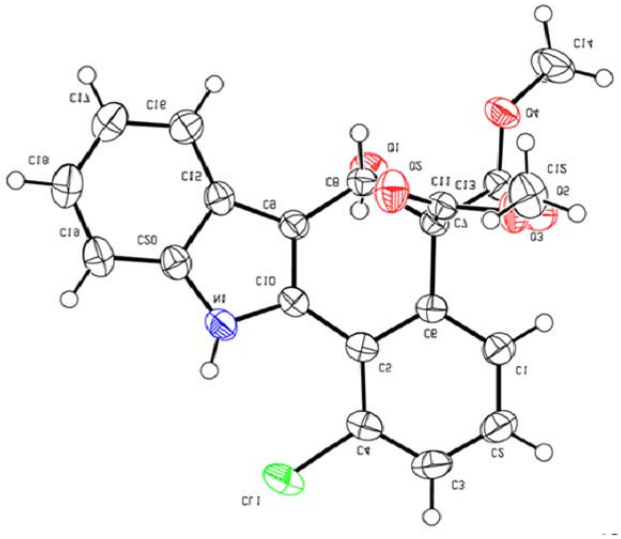


Figure S1 X-Ray structure of **3k** with 50% probability ellipsoids

(2) Single crystal structure of **5e**

Table S2. Crystal data and structure refinement for **5e**

Identification code	GXM-II-246
Empirical formula	$C_{24}H_{25}NO_5$
Formula weight	407.45
Temperature/K	289.46(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	11. 8560(3)
b/Å	14.5868(4)
c/Å	23.9797(6)
α/°	90
β/°	90
γ/°	90
Volume/$Å^3$	4147.08(18)
Z	8
ρ_{calc}g/cm^3	1.305
μ/mm^{-1}	0.746
F(000)	1728.0
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.374 to 147.892

Index ranges	$-14 \leq h \leq 10$, $-12 \leq k \leq 17$, $-29 \leq l \leq 28$
Reflections collected	16243
Independent reflections	4152 [R_{int} = 0.0434, R_{sigma} = 0.0300]
Data/restraints/parameters	4152/0/360
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0470, wR_2 = 0.1117
Final R indexes [all data]	R_1 = 0.0690, wR_2 = 0.1295
Largest diff. peak/hole / e $Å^{-3}$	0.25/-0.25

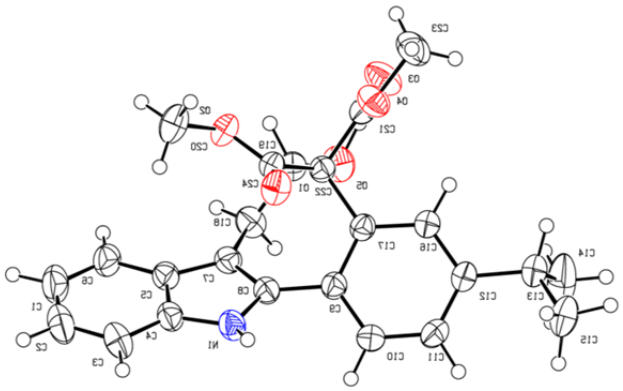
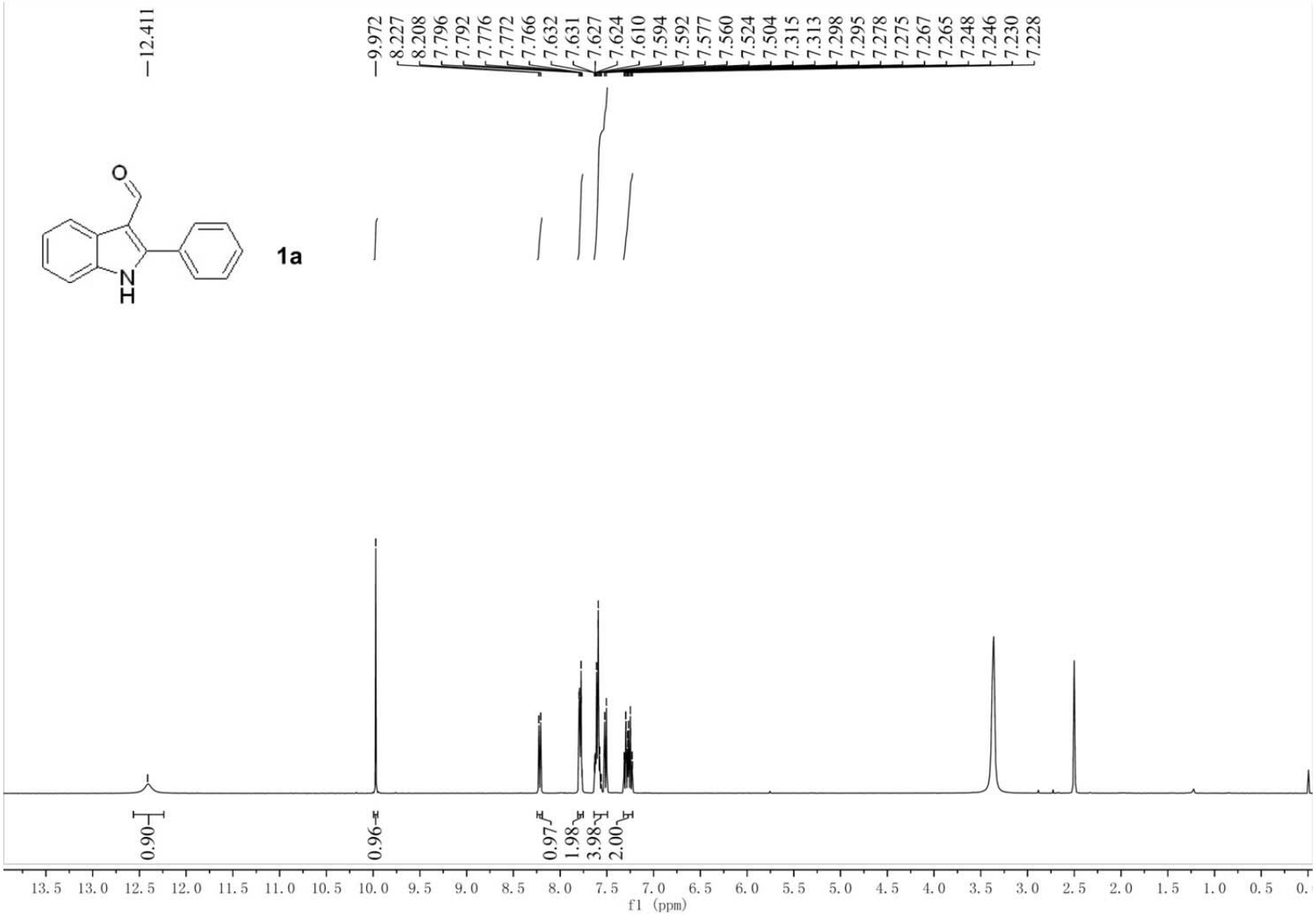
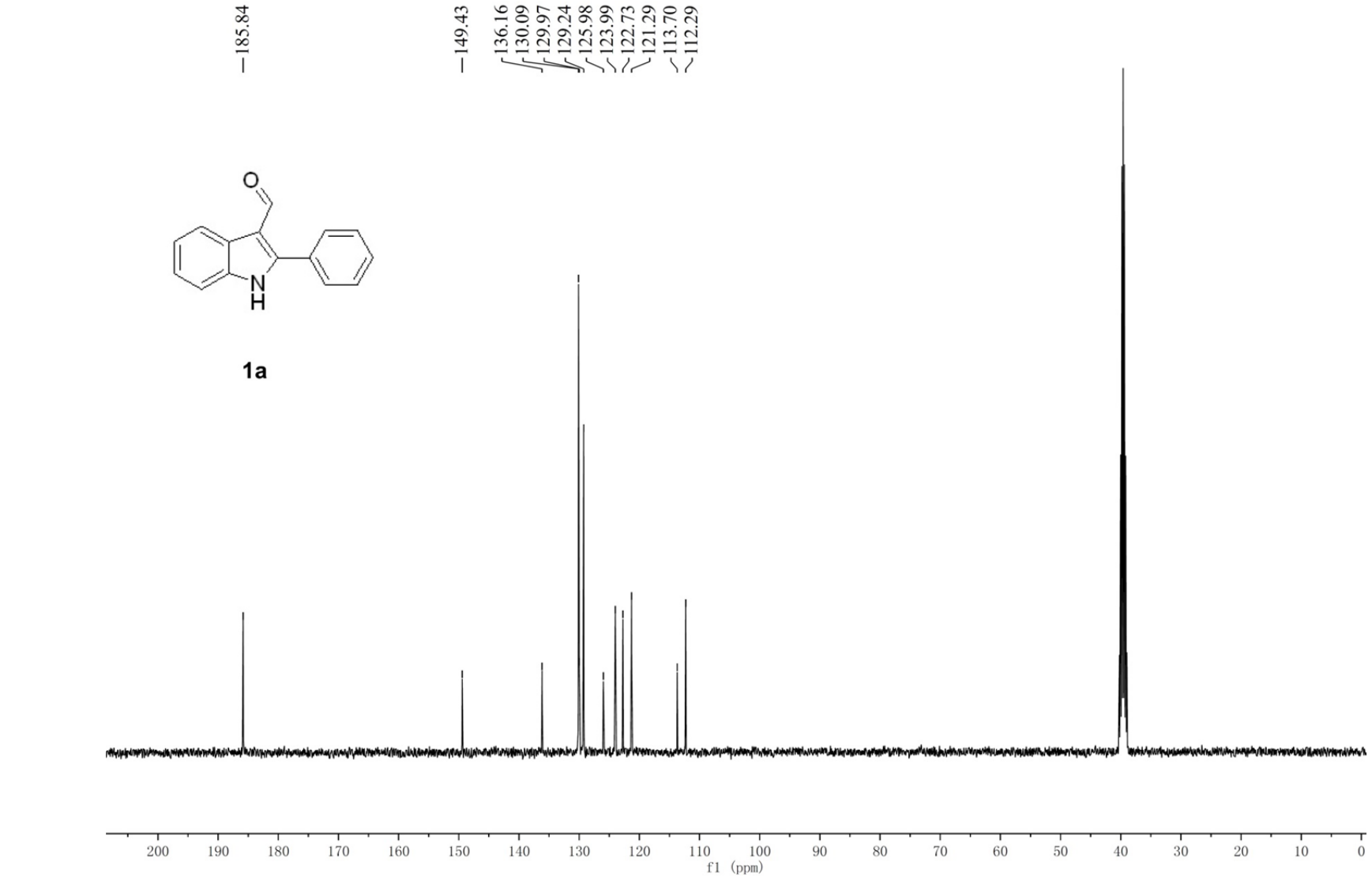


Figure S1 X-Ray structure of **5e** with 50% probability ellipsoids

References:
1 (a) G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.*, 2008, **64**, 112-122. A. V. Dolomanov; L. J. Bourhis; (b) R. J. Gildea; J. A. K. Howard; H. Puschman, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.

2. Copies of ^{1}H and ^{13}C-NMR charts of materials

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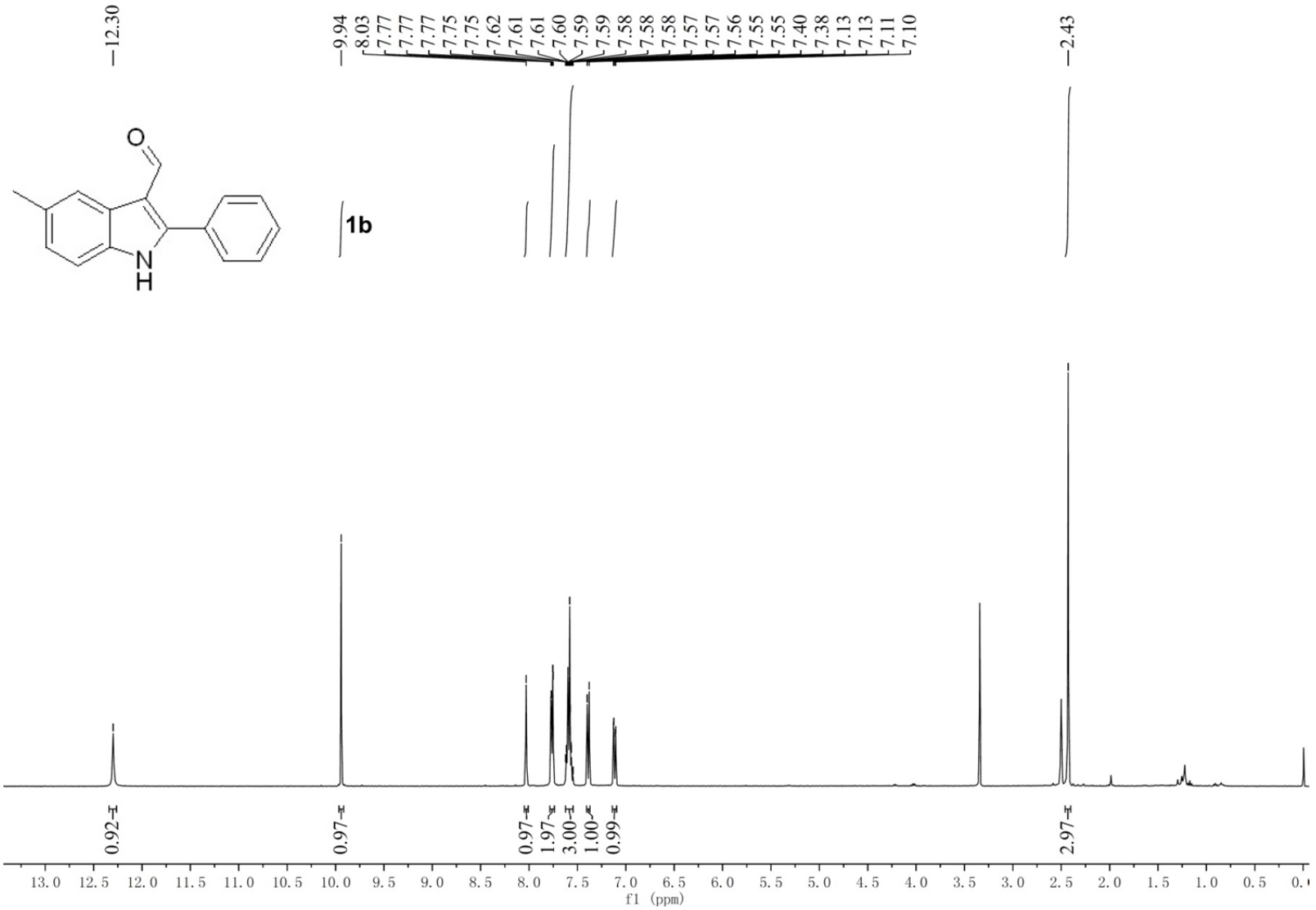
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7.10
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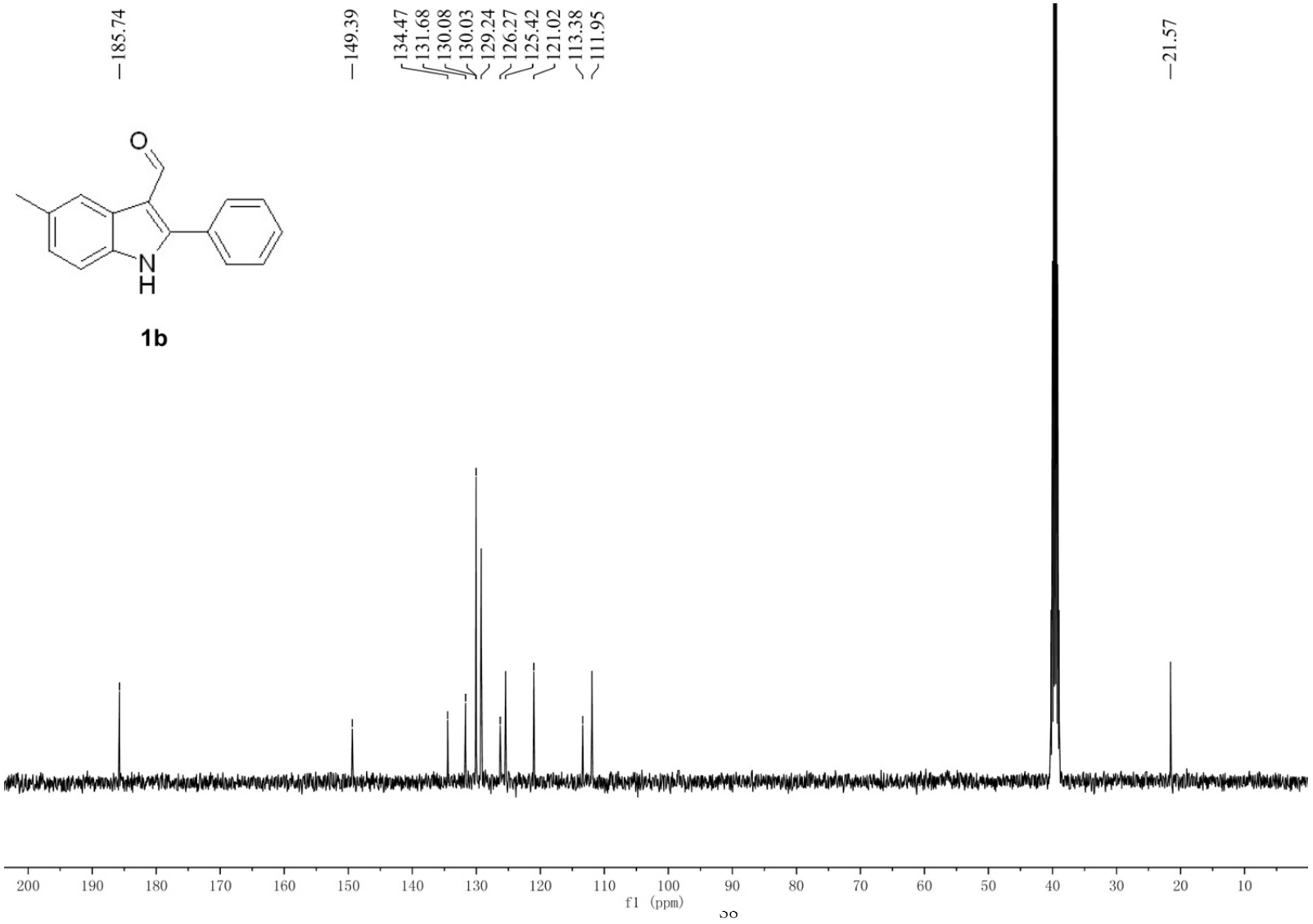
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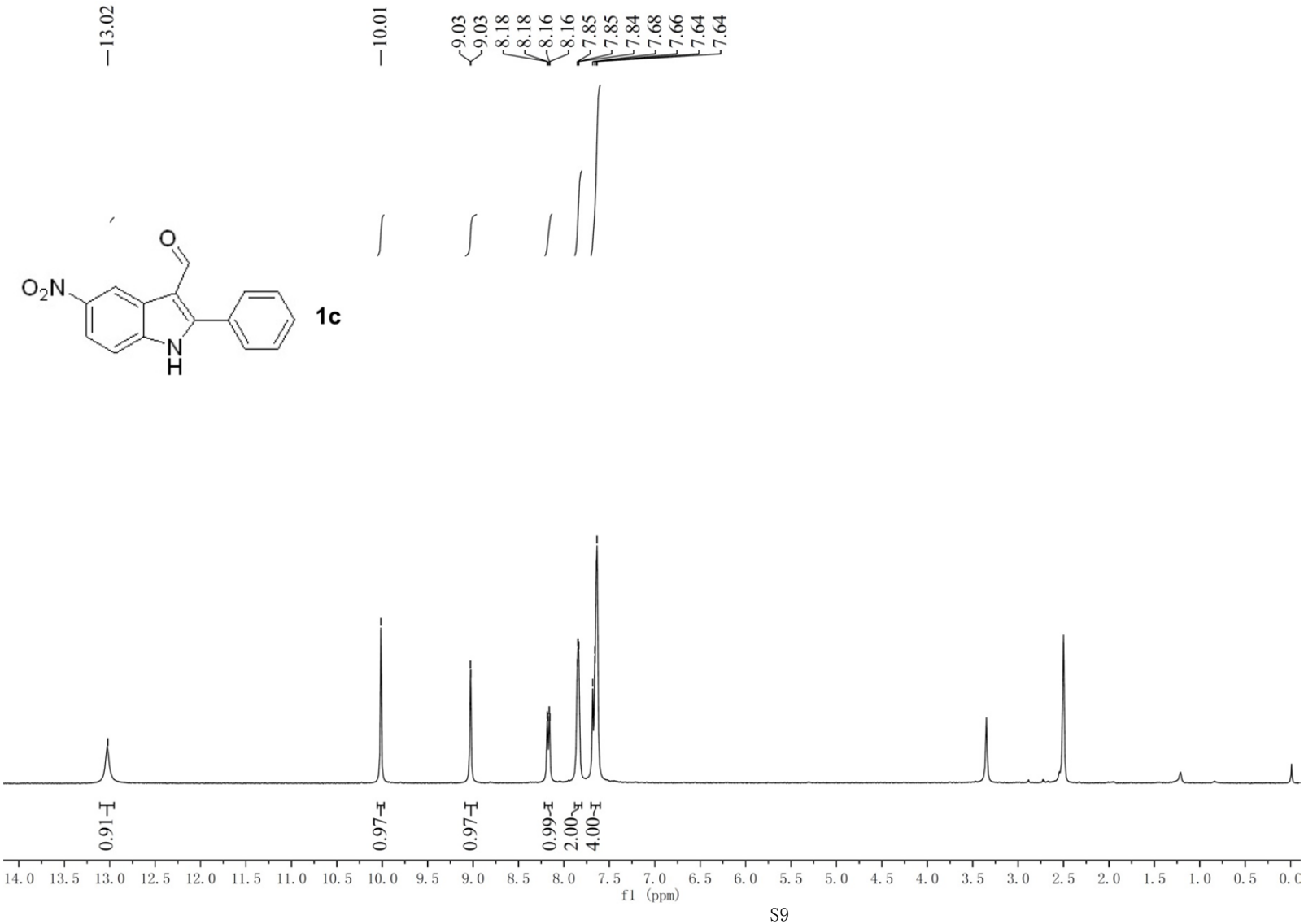
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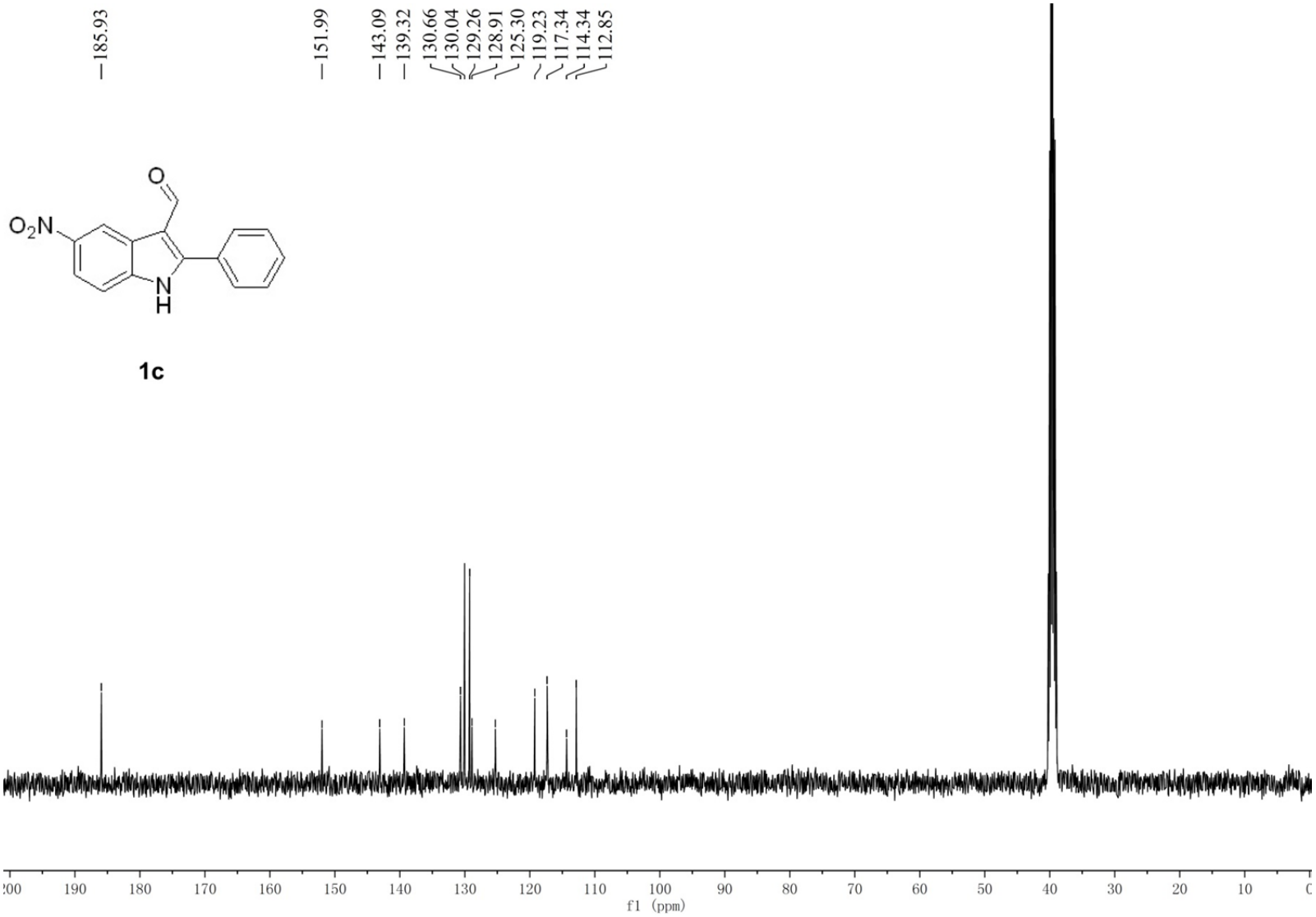
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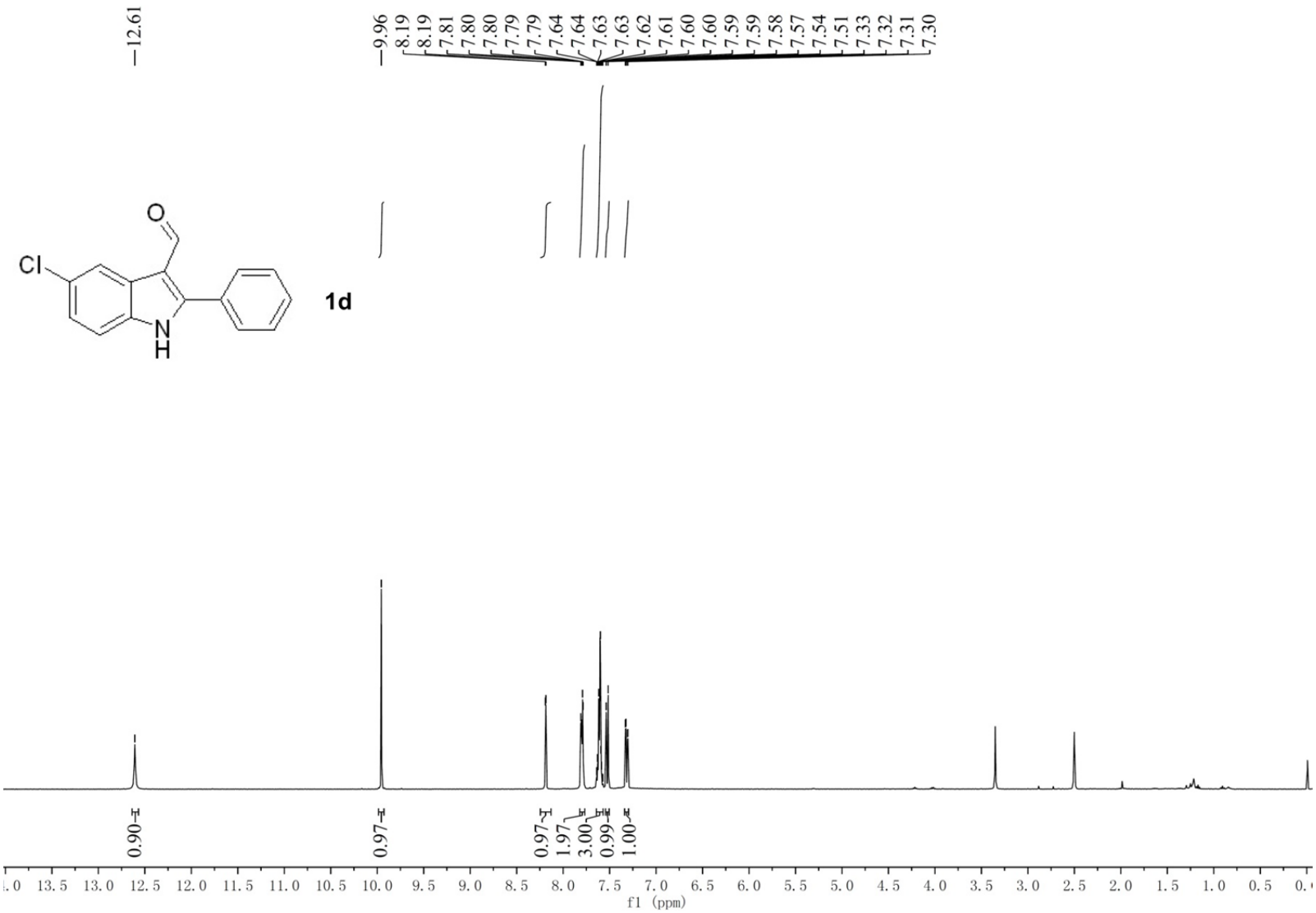
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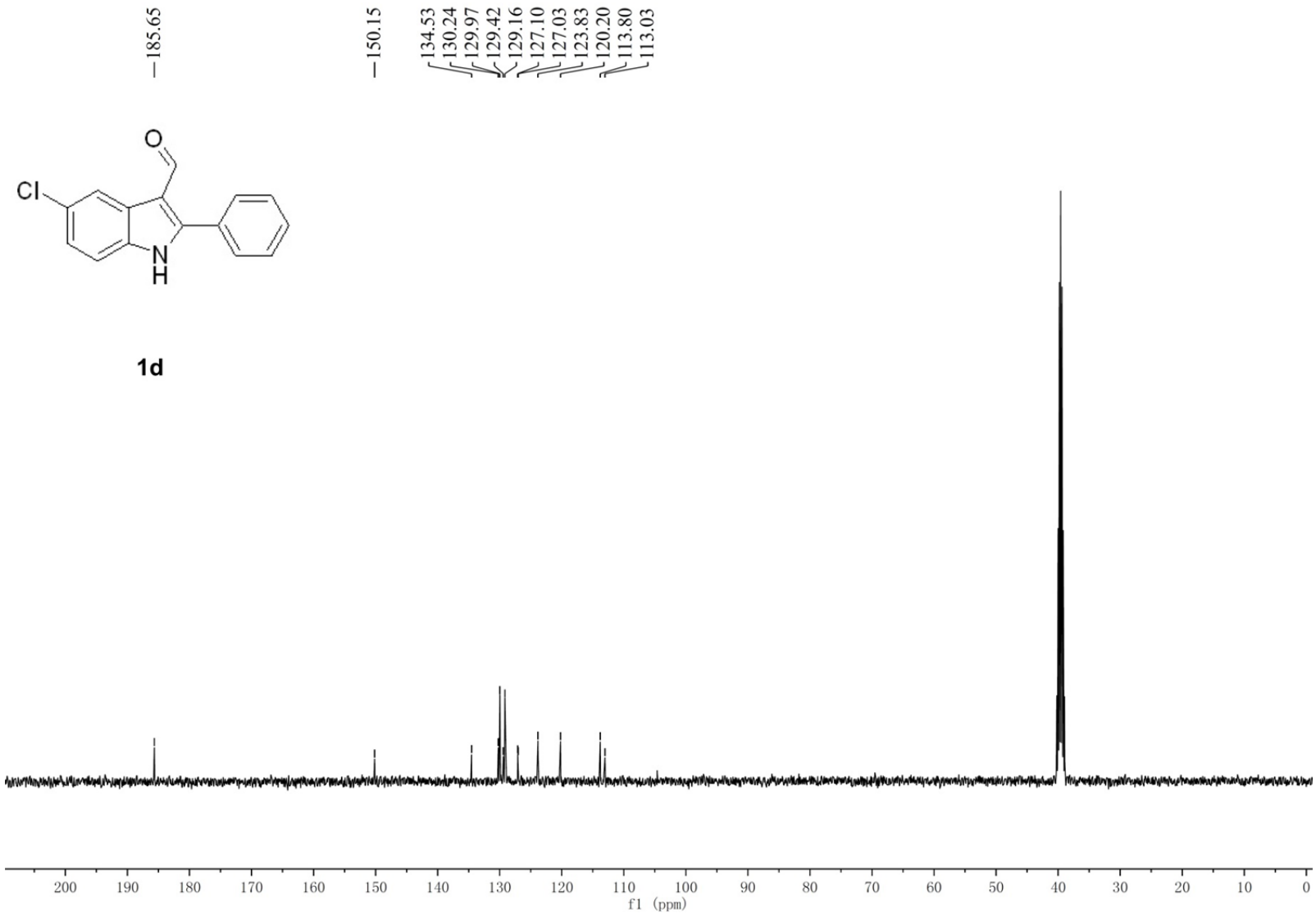
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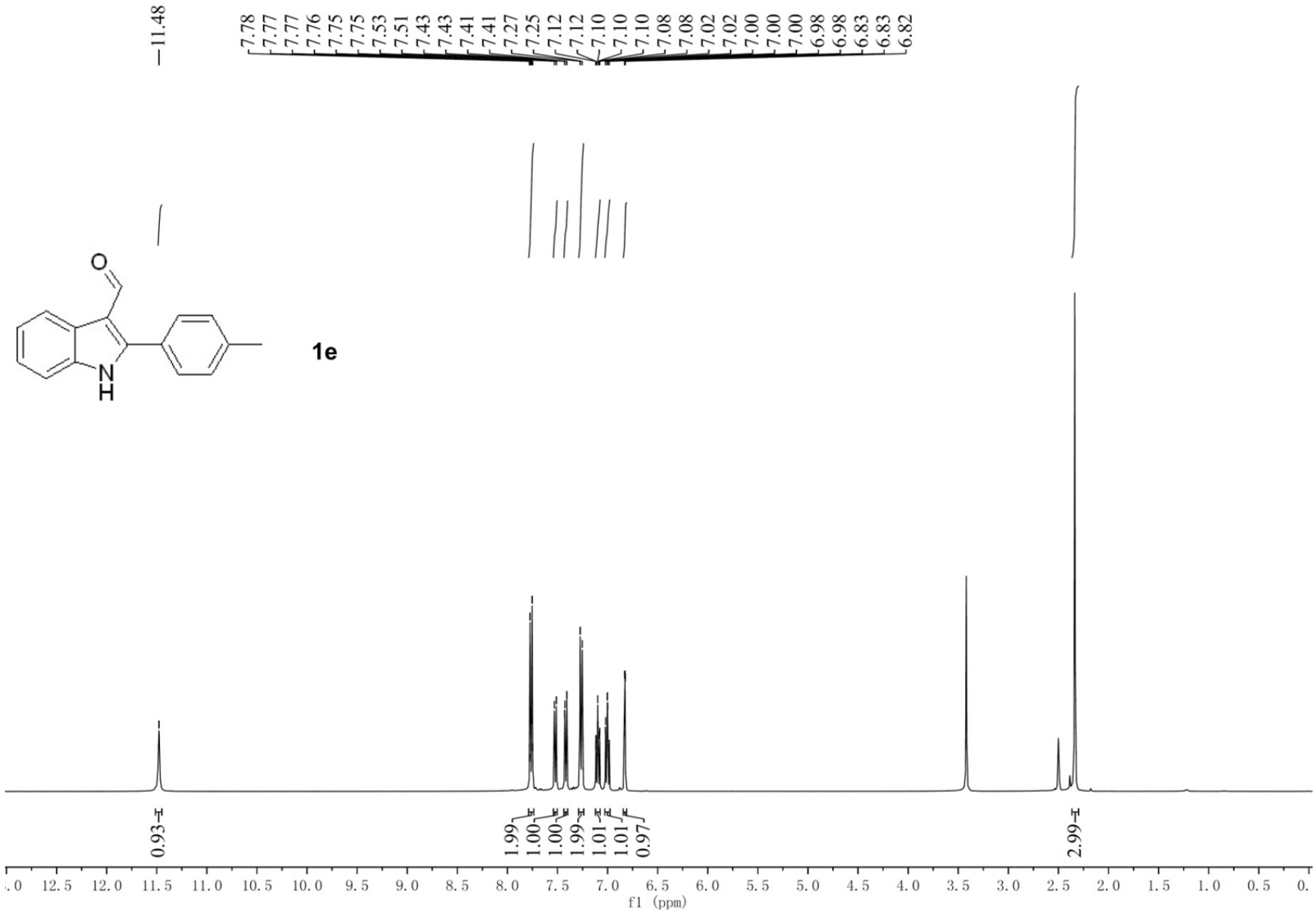
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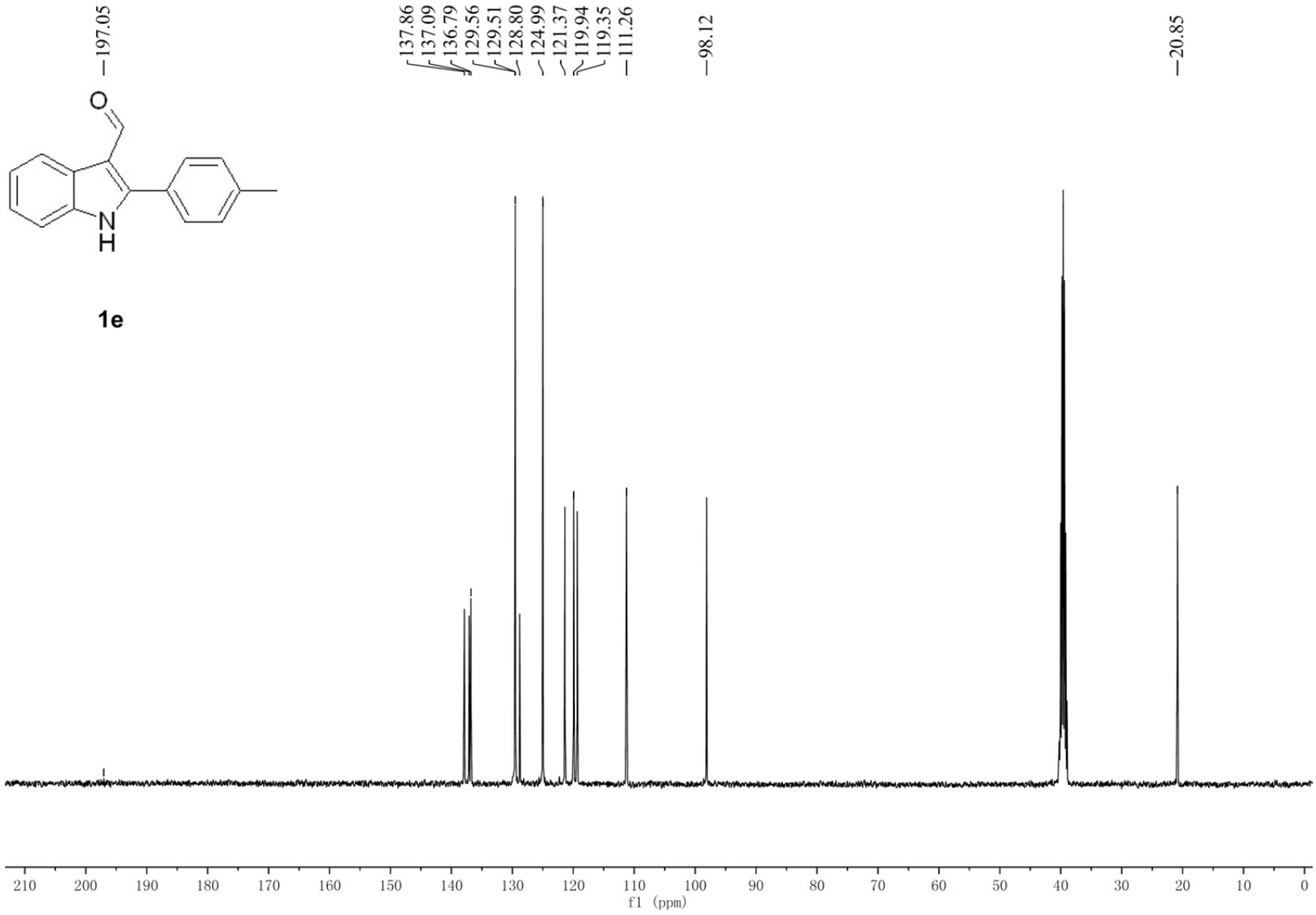
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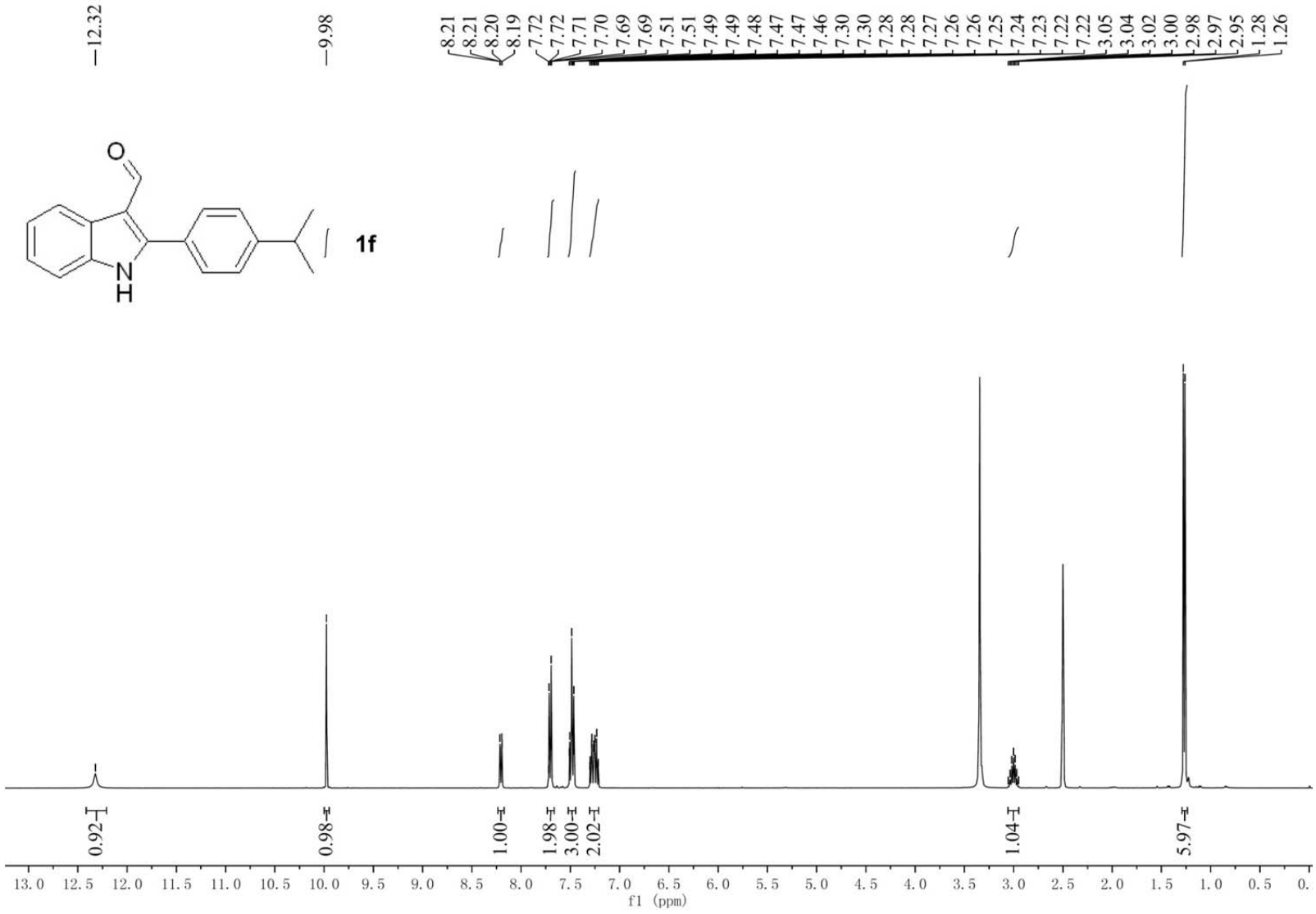
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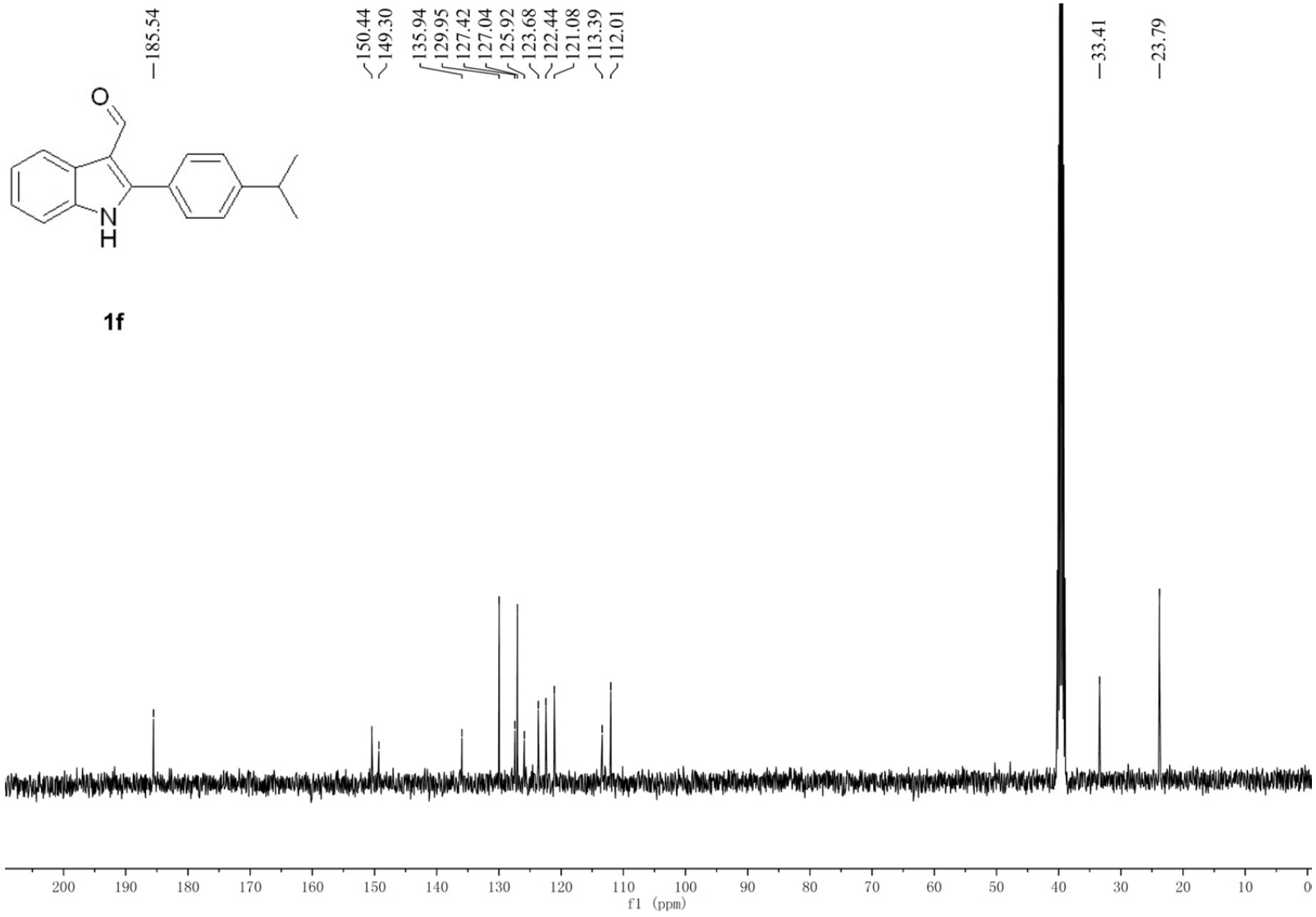
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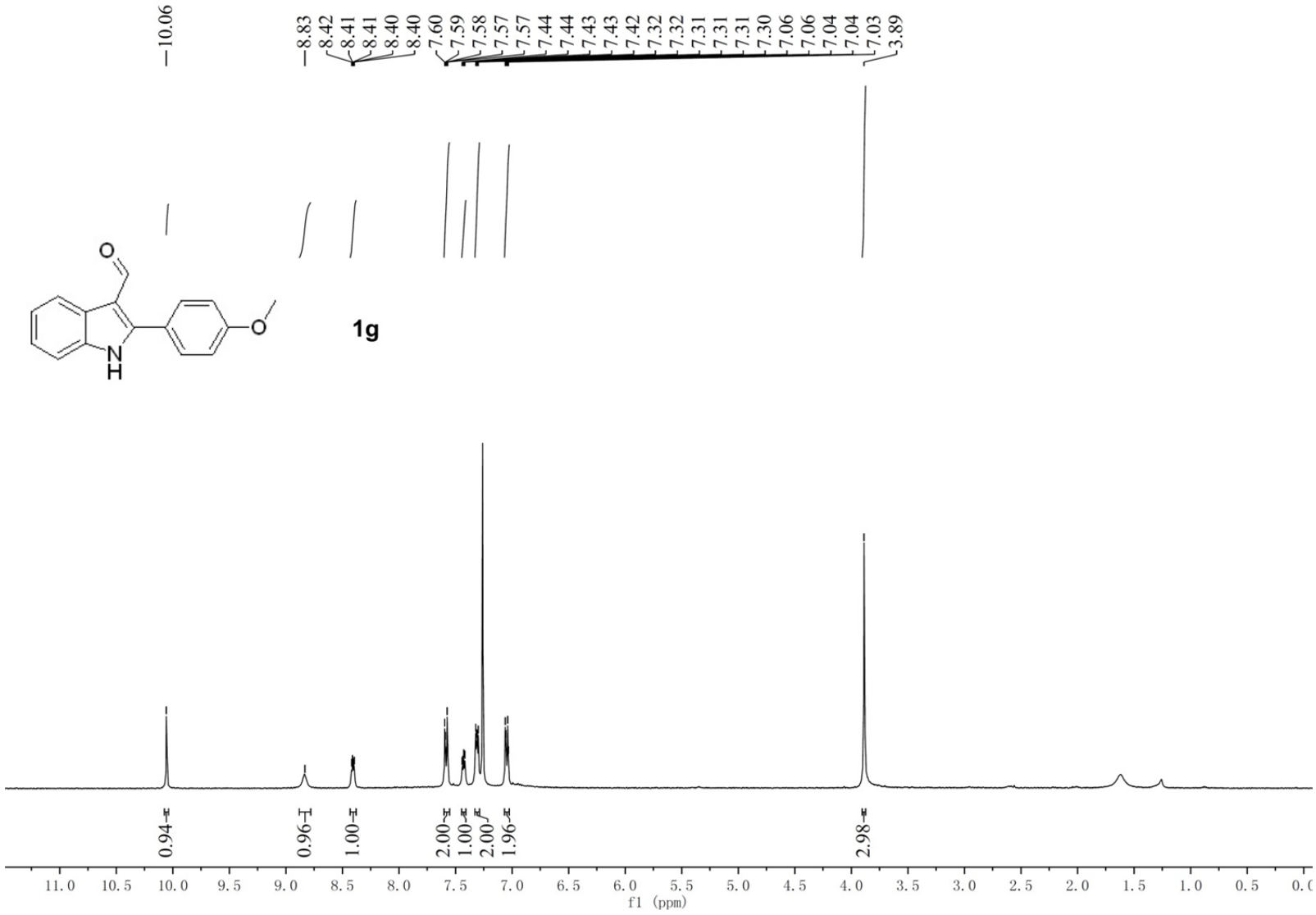
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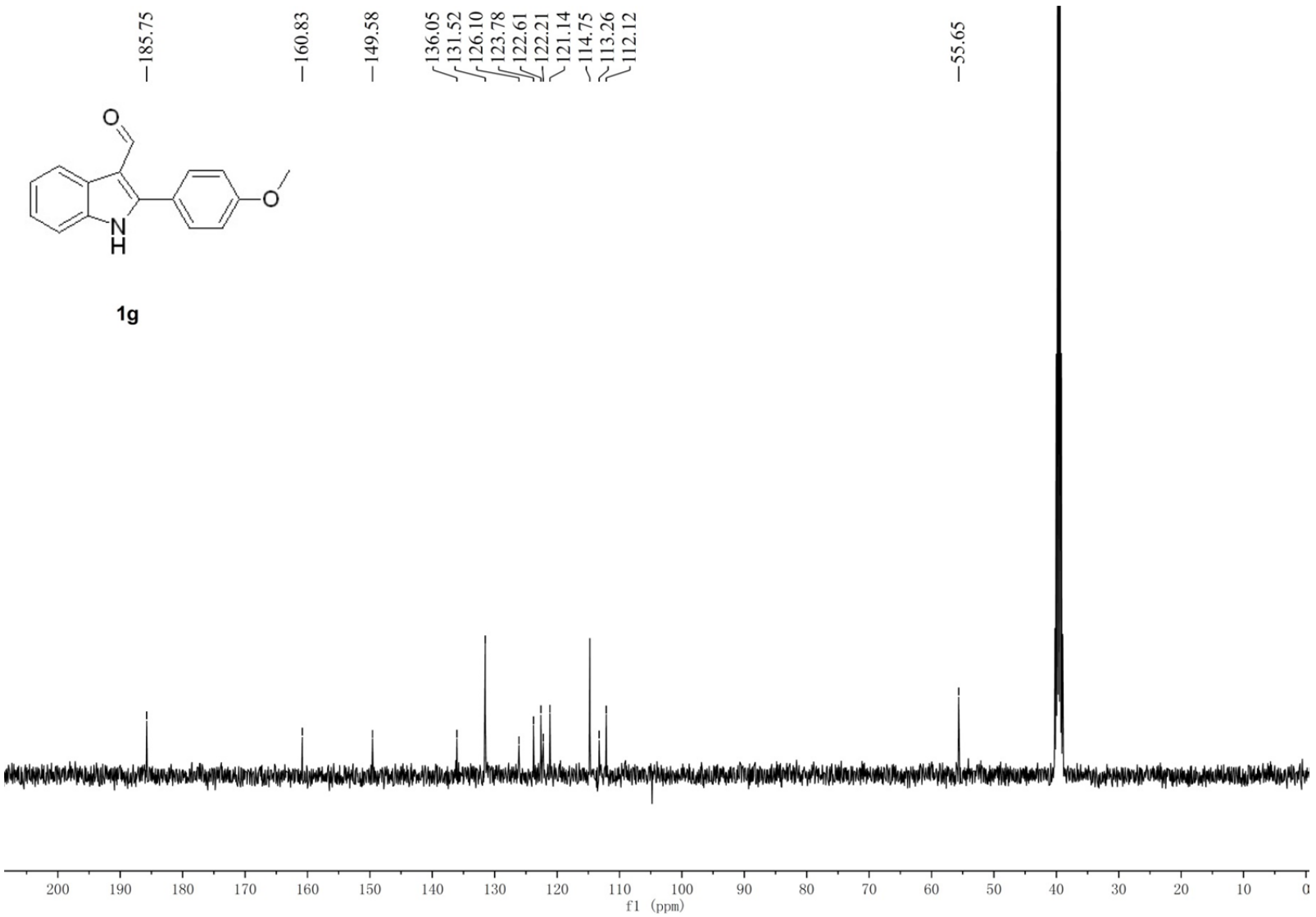
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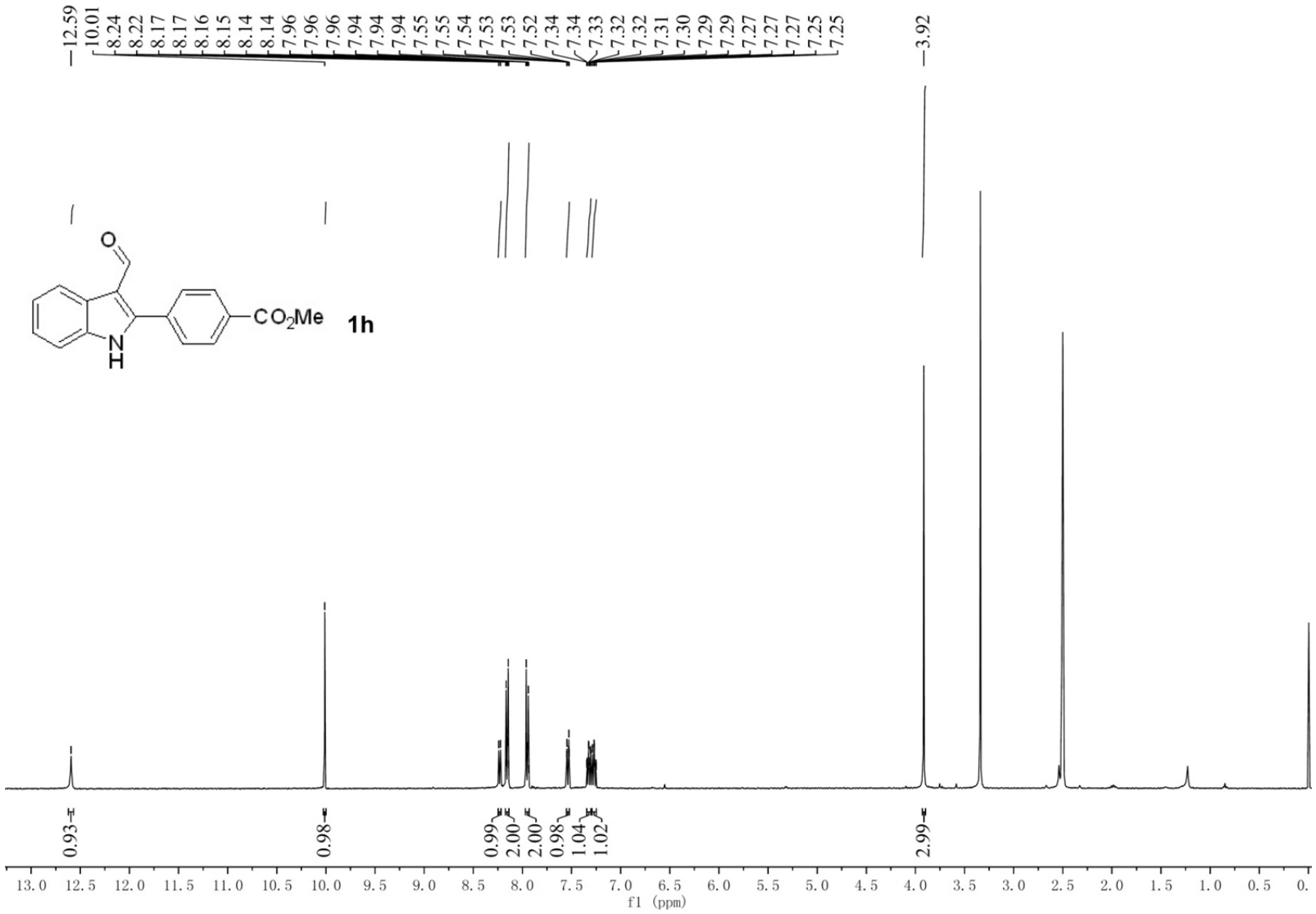
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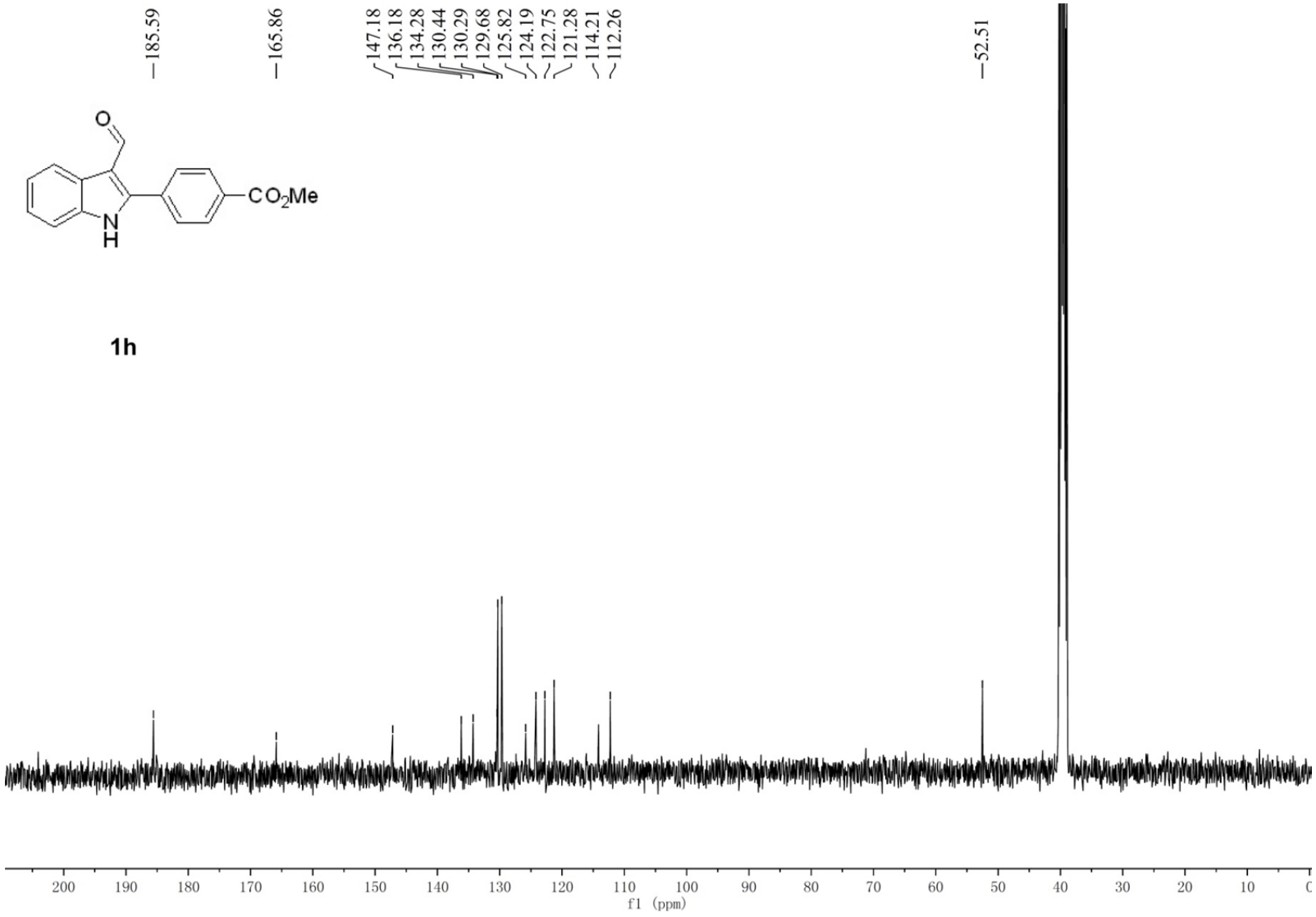
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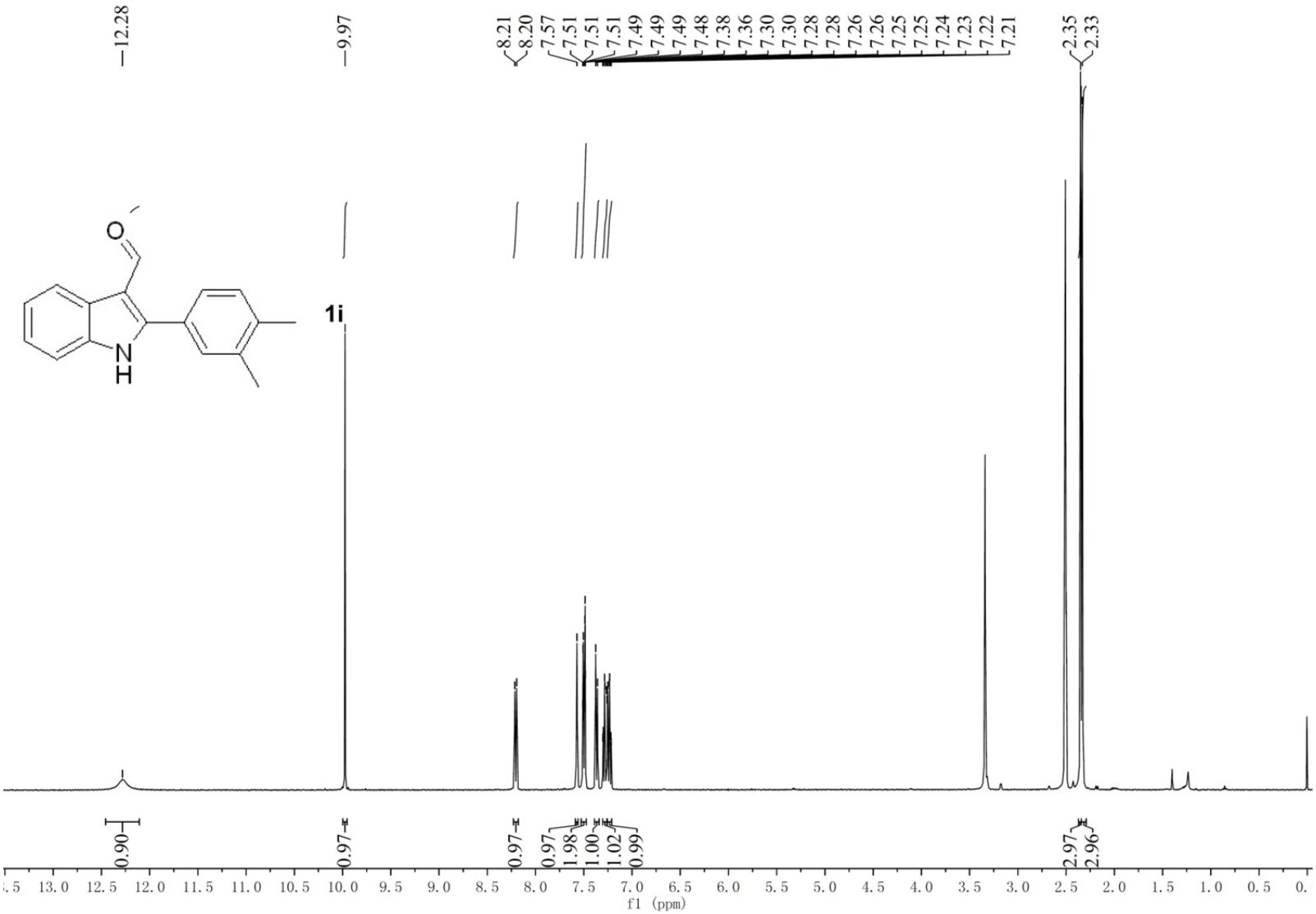
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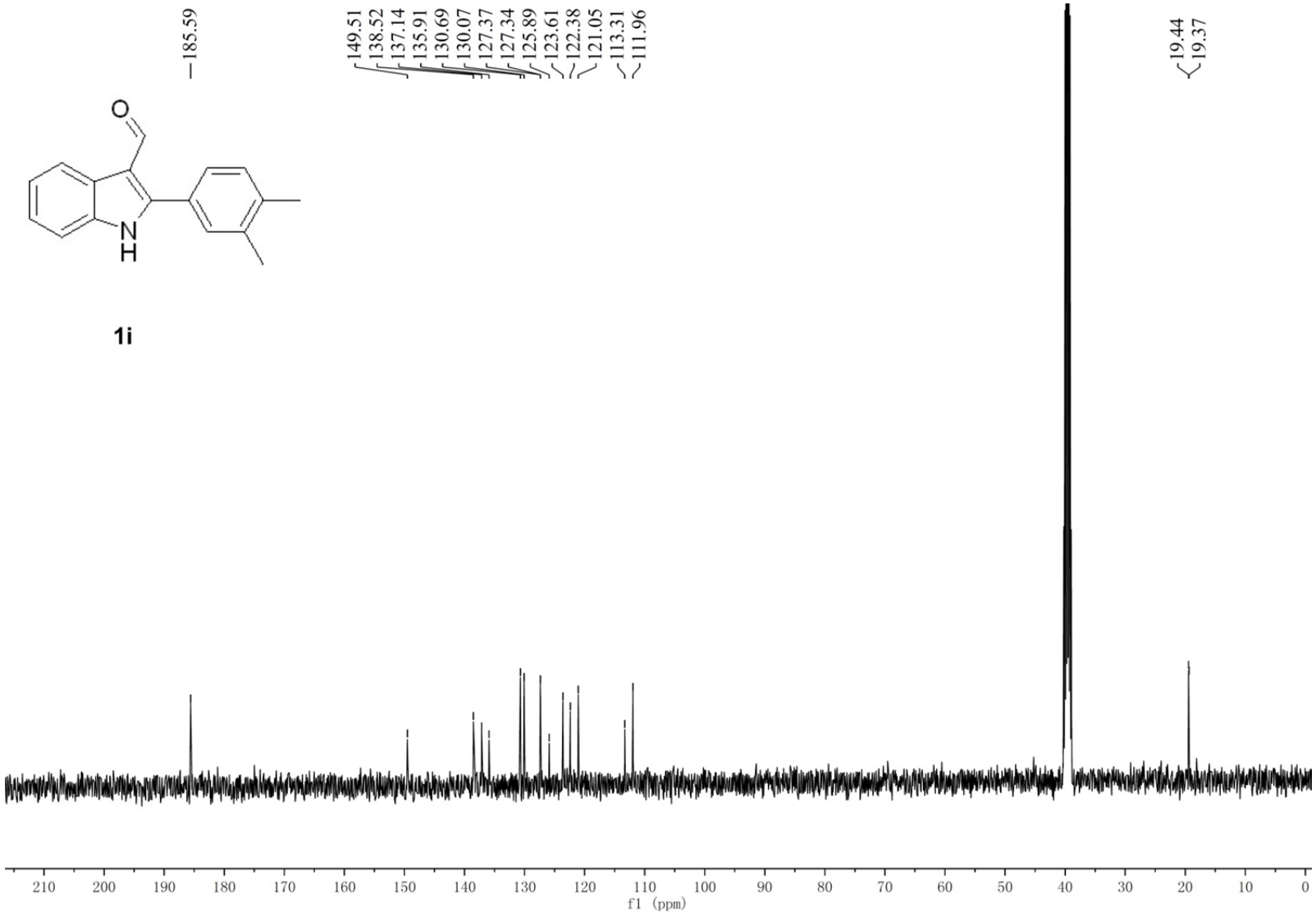
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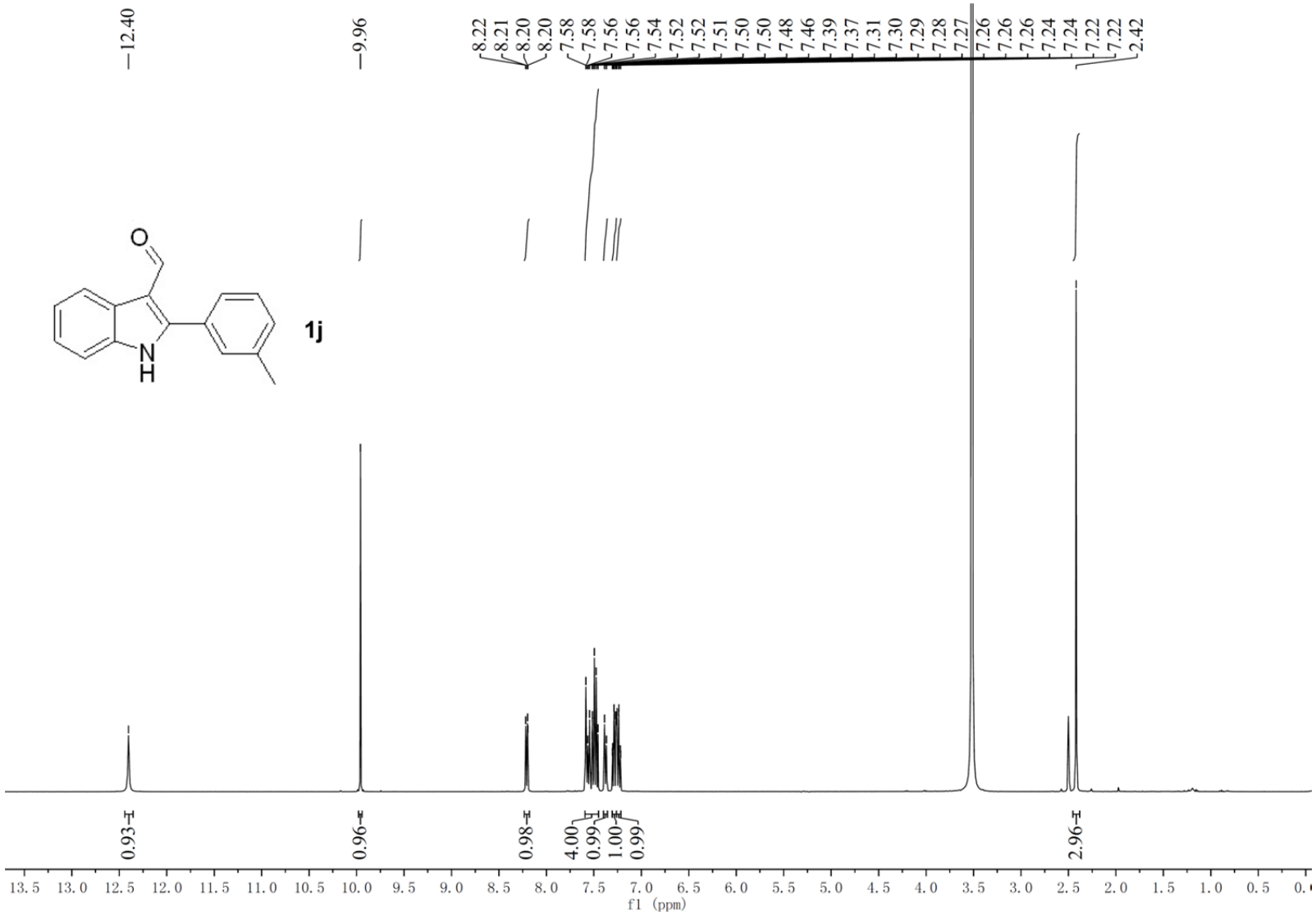
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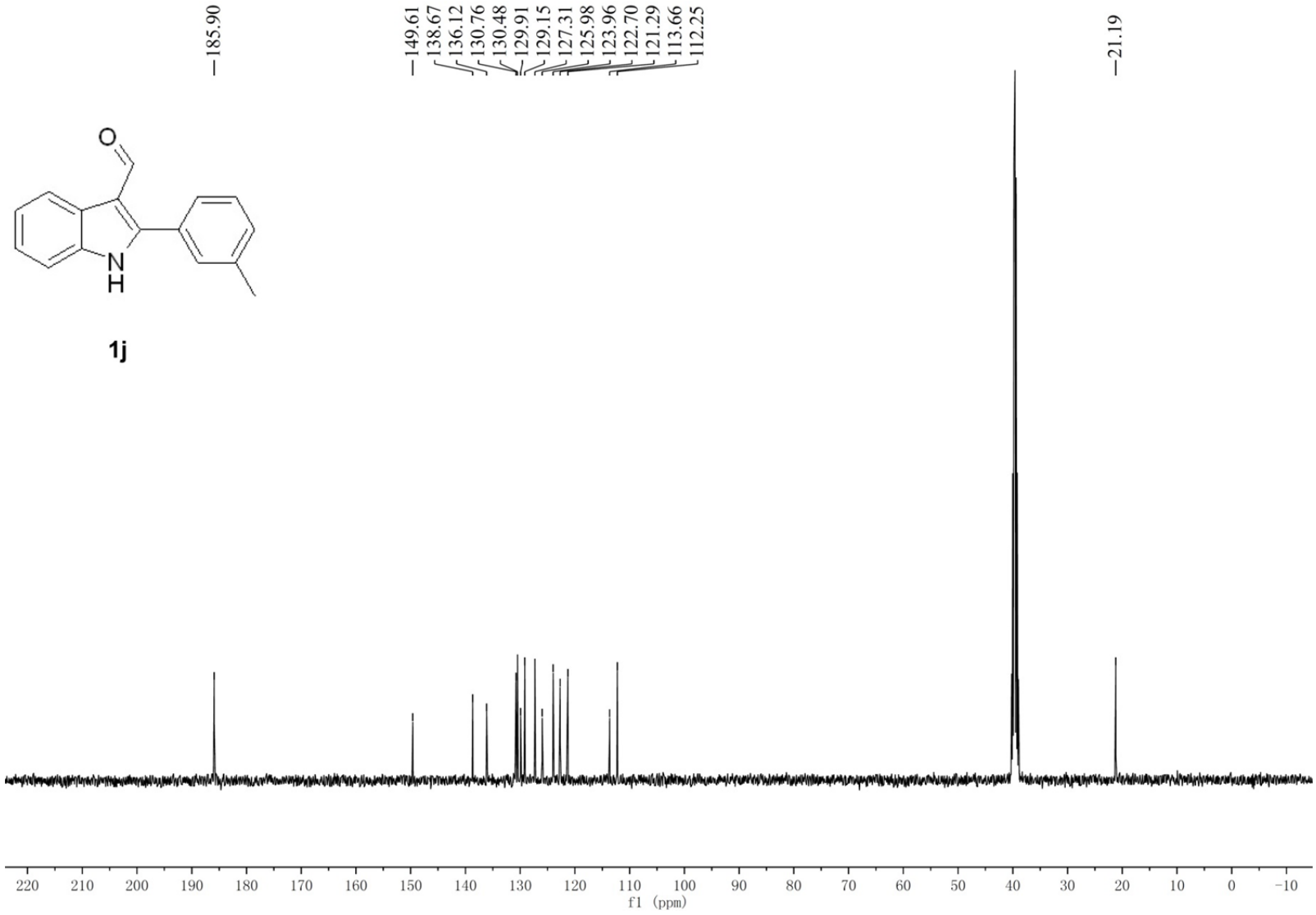
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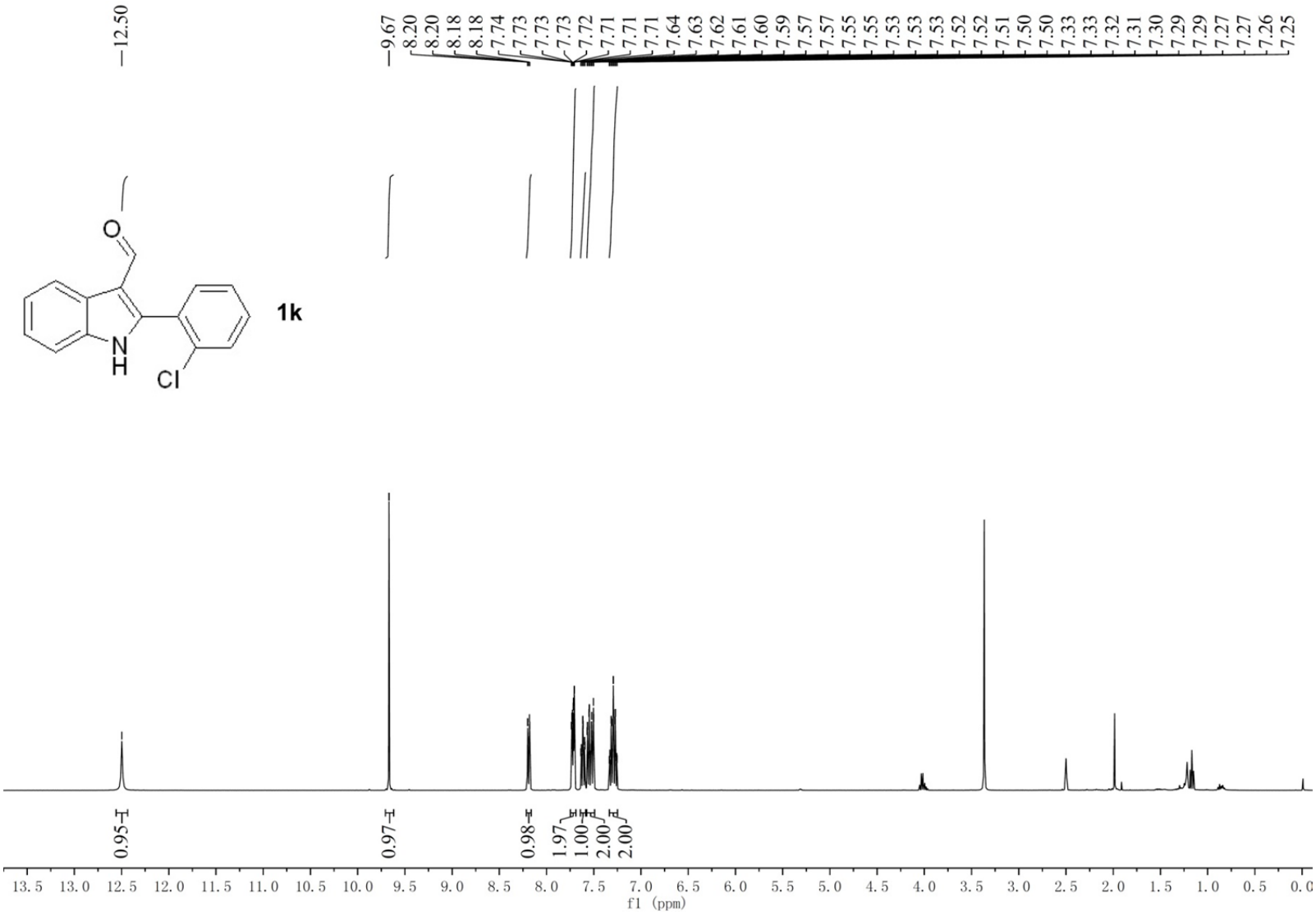
112.25
21.19
O
N
H
1j
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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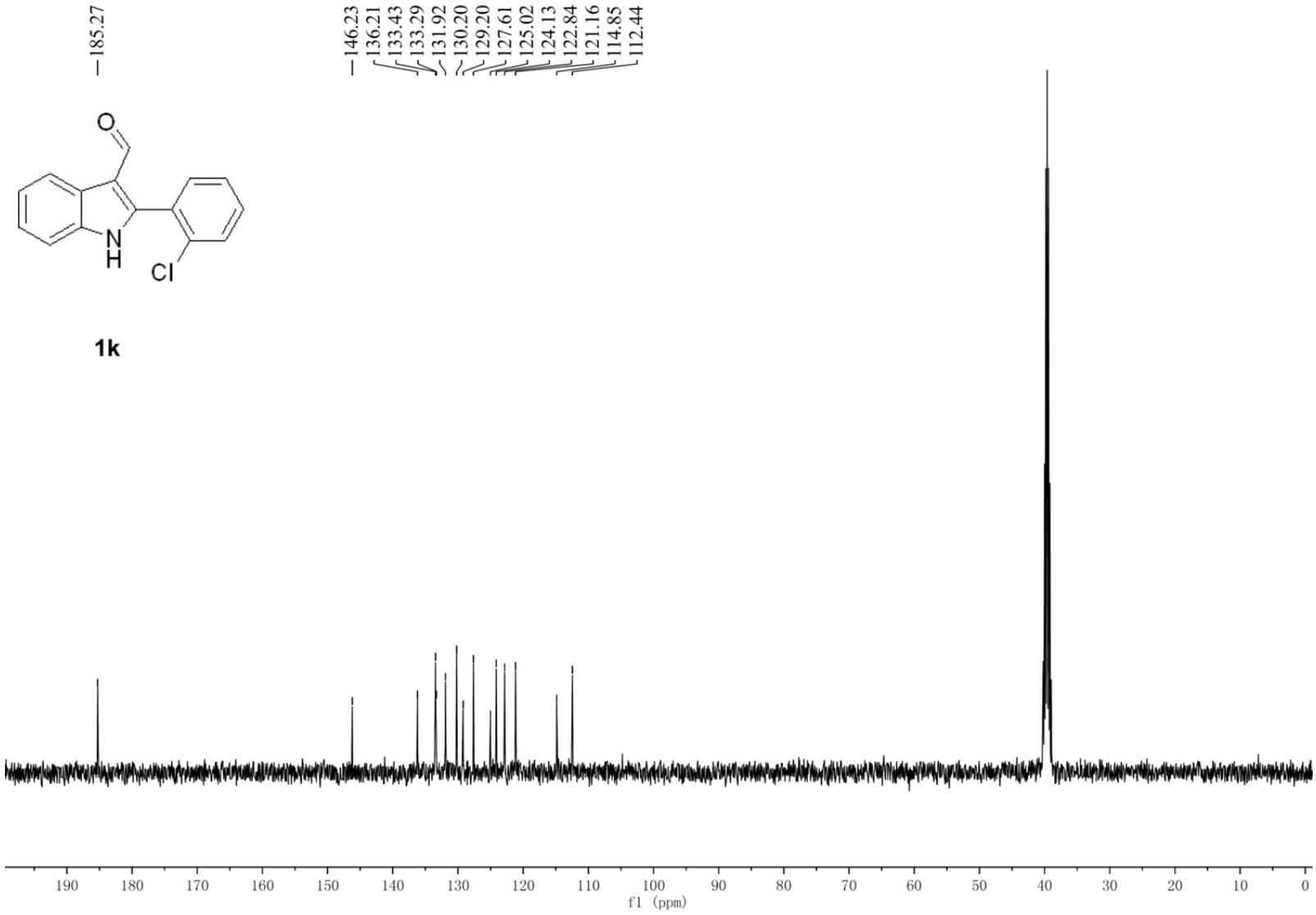
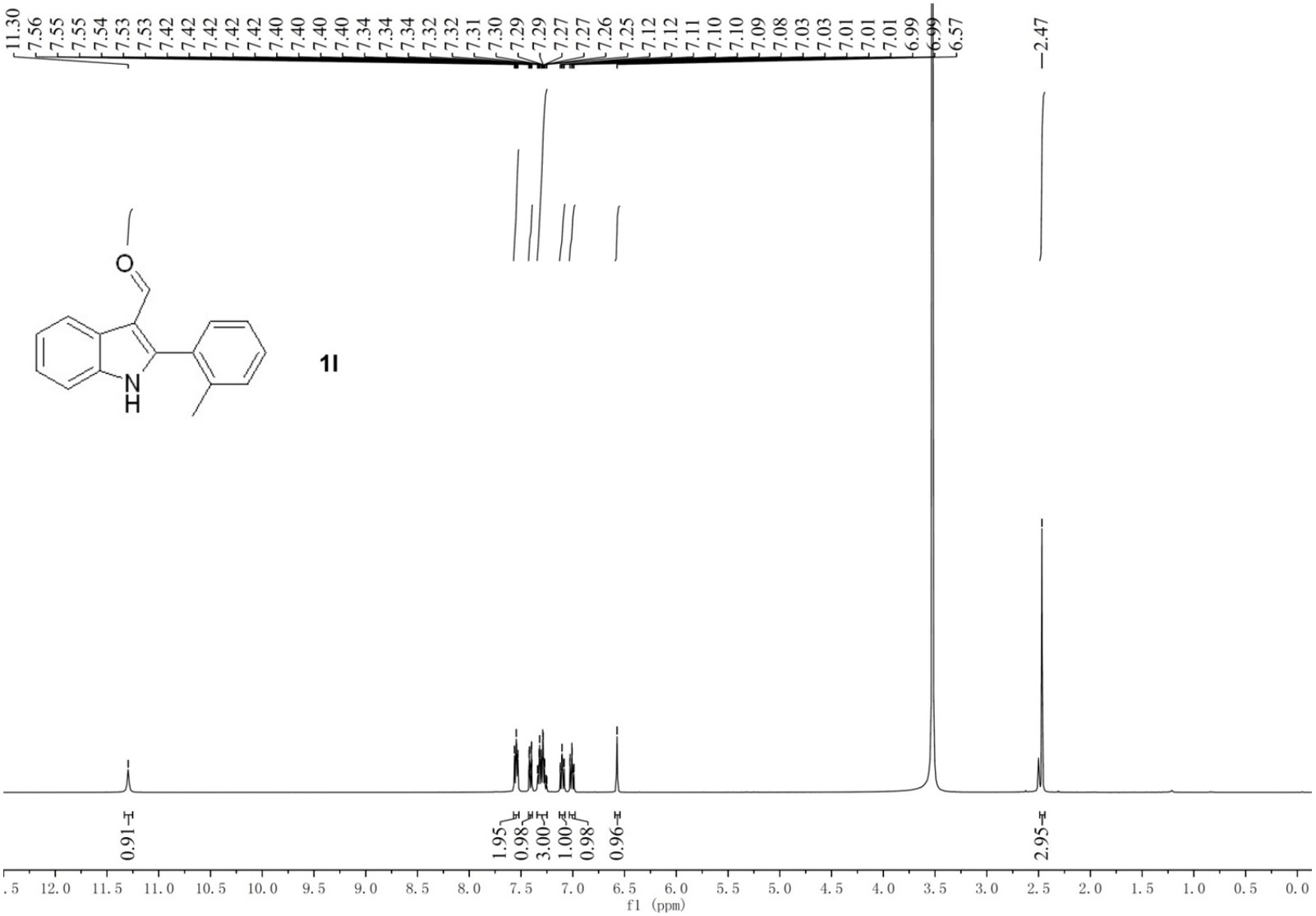
8.20
8.20
8.18
8.18
7.74
7.73
7.73
7.73
7.72
7.71
7.71
7.71
7.64
7.63
7.62
7.61
7.60
7.59
7.57
7.57
7.55
7.55
7.53
7.53
7.53
7.52
7.52
7.51
7.50
7.50
7.33
7.33
7.32
7.31
7.30
7.29
7.29
7.27
7.27
7.26
7.25
O
N
H
Cl
1k
0.95
0.97
0.98
1.97
1.00
2.00
2.00
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 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
f1 (ppm)


185.27
146.23
136.21
133.43
133.29
131.92
130.20
129.20
127.61
125.02
124.13
122.84
121.16
114.85
112.44
O
N
H
Cl
1k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.56
7.55
7.55
7.54
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7.42
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7.42
7.42
7.40
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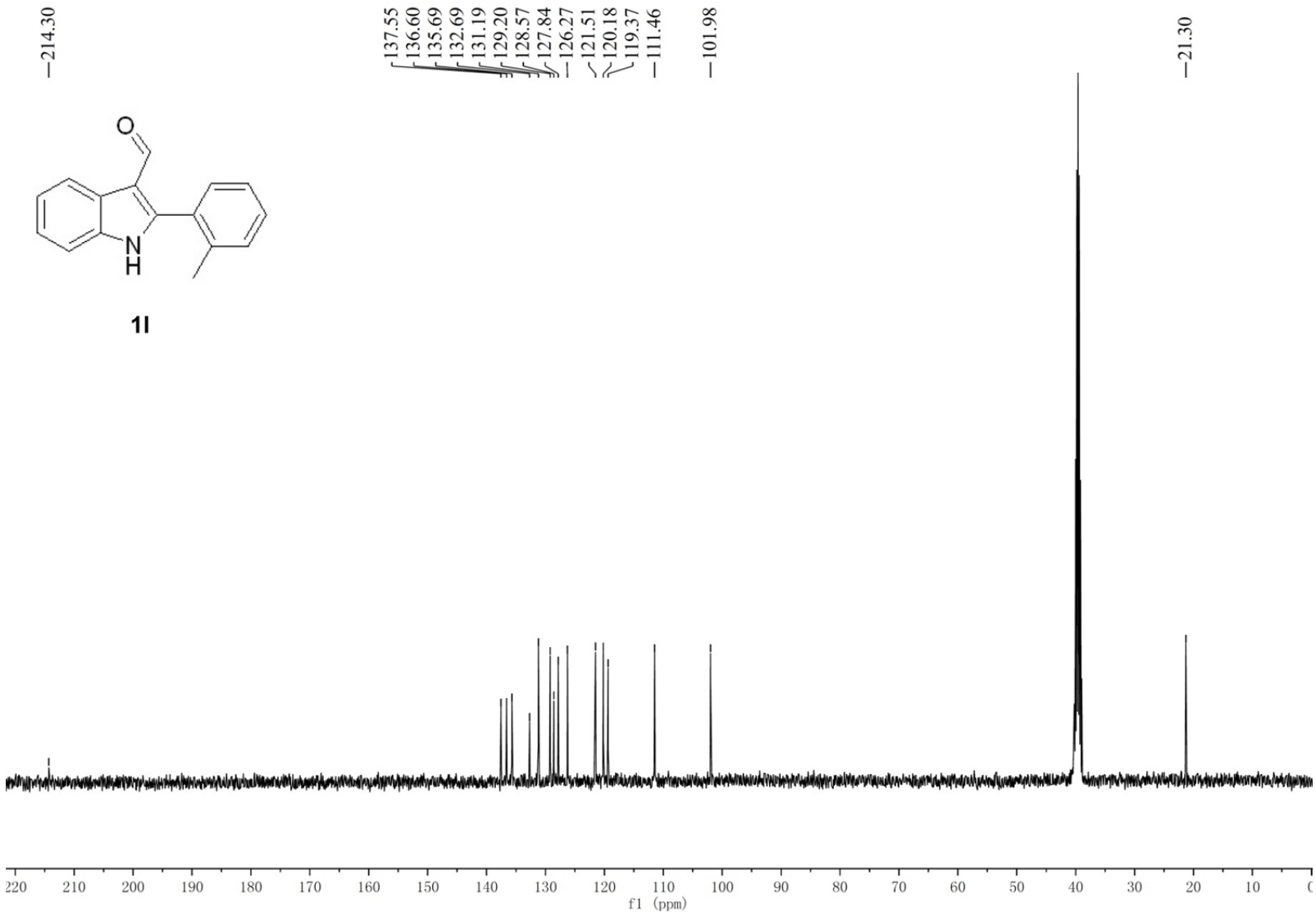
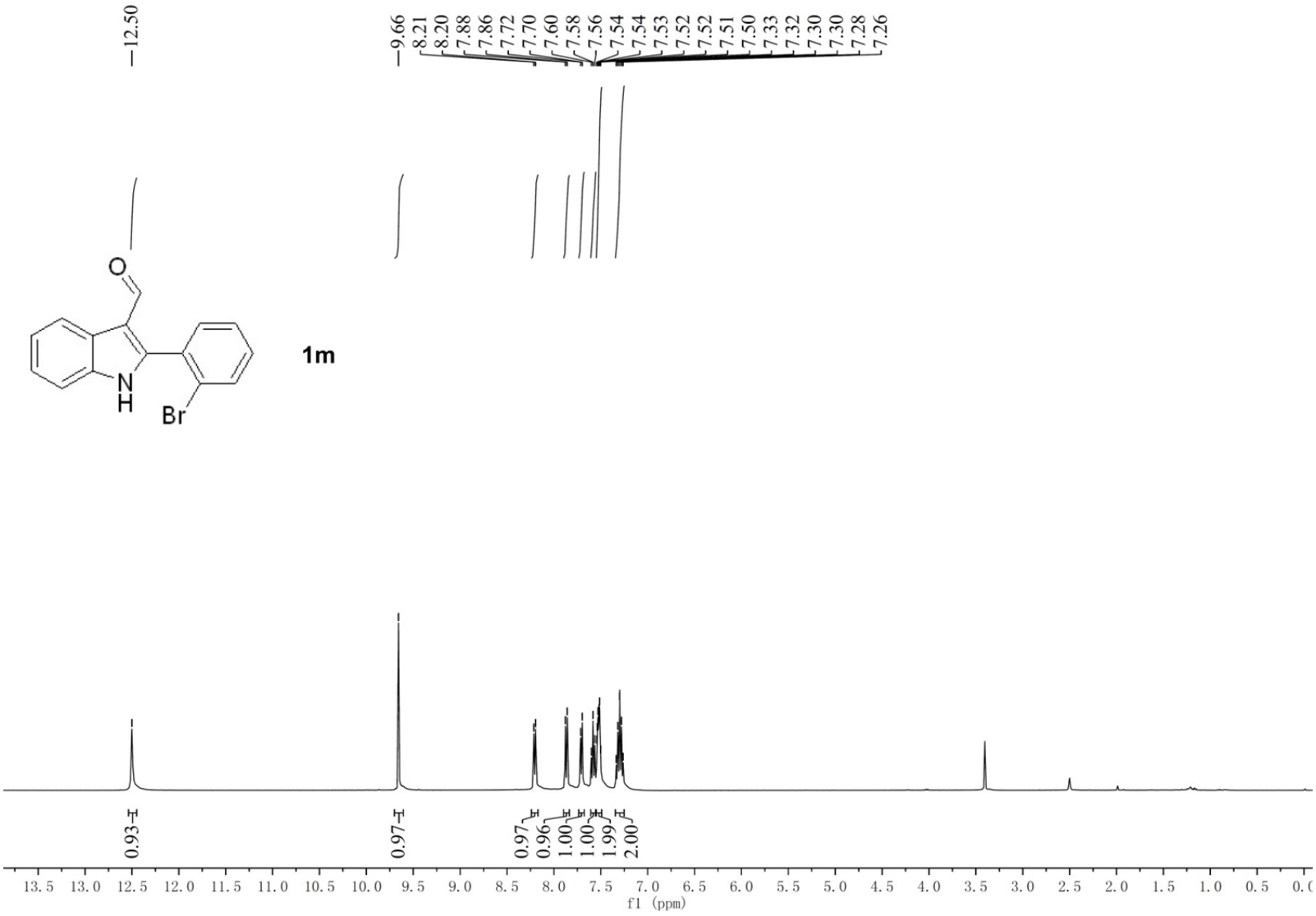
7.40
7.40
7.34
7.34
7.34
7.32
7.32
7.31
7.30
7.29
7.29
7.27
7.27
7.26
7.25
7.12
7.12
7.11
7.10
7.10
7.09
7.08
7.03
7.03
7.01
7.01
7.01
6.99
6.99
6.57
2.47
O
N
H
1l
0.91
1.95
0.98
3.00
1.00
0.98
0.96
2.95
f1 (ppm)


214.30
137.55
136.60
135.69
132.69
131.19
129.20
128.57
127.84
126.27
121.51
120.18
119.37
111.46
101.98
21.30
O
N
H
1l
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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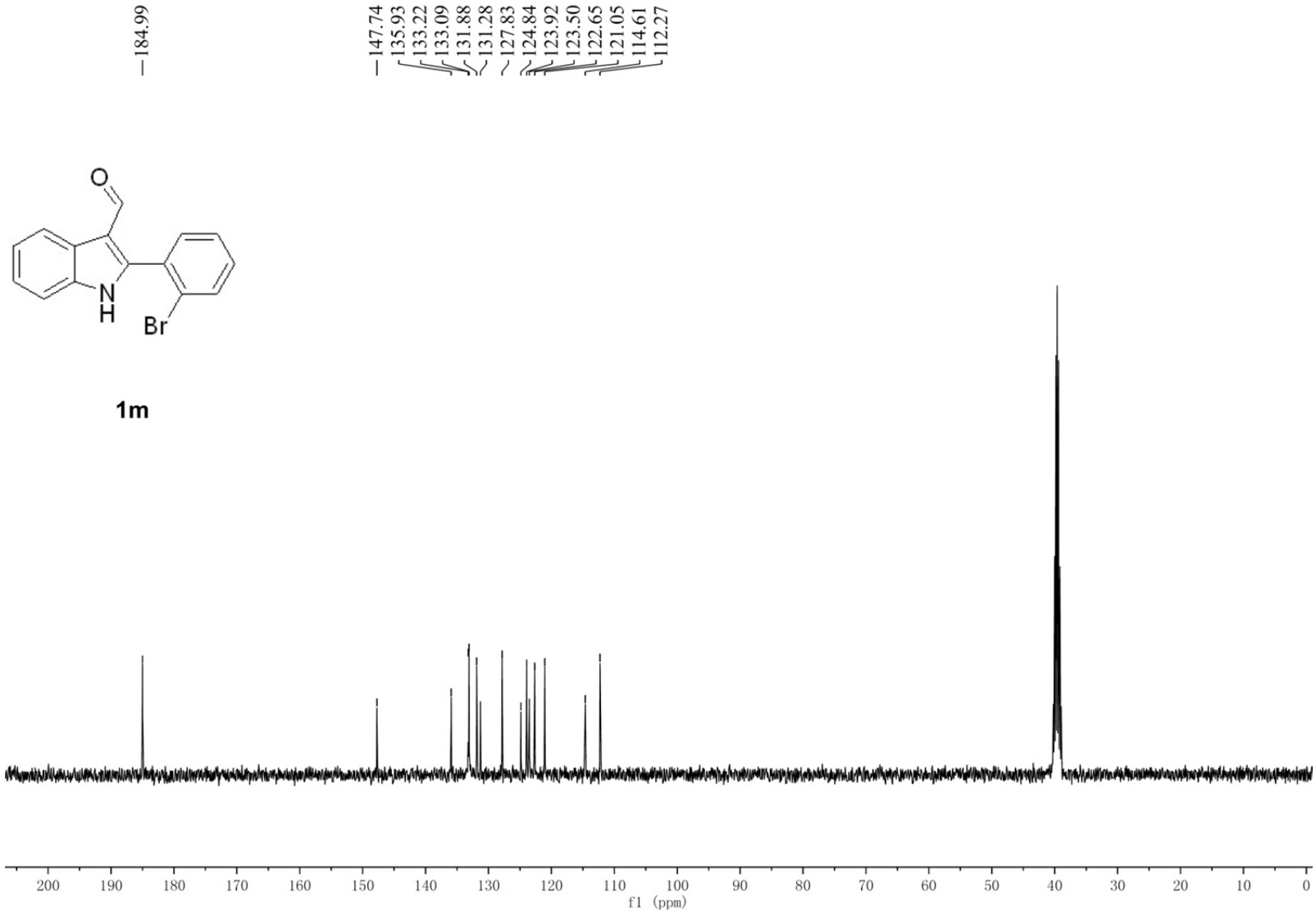
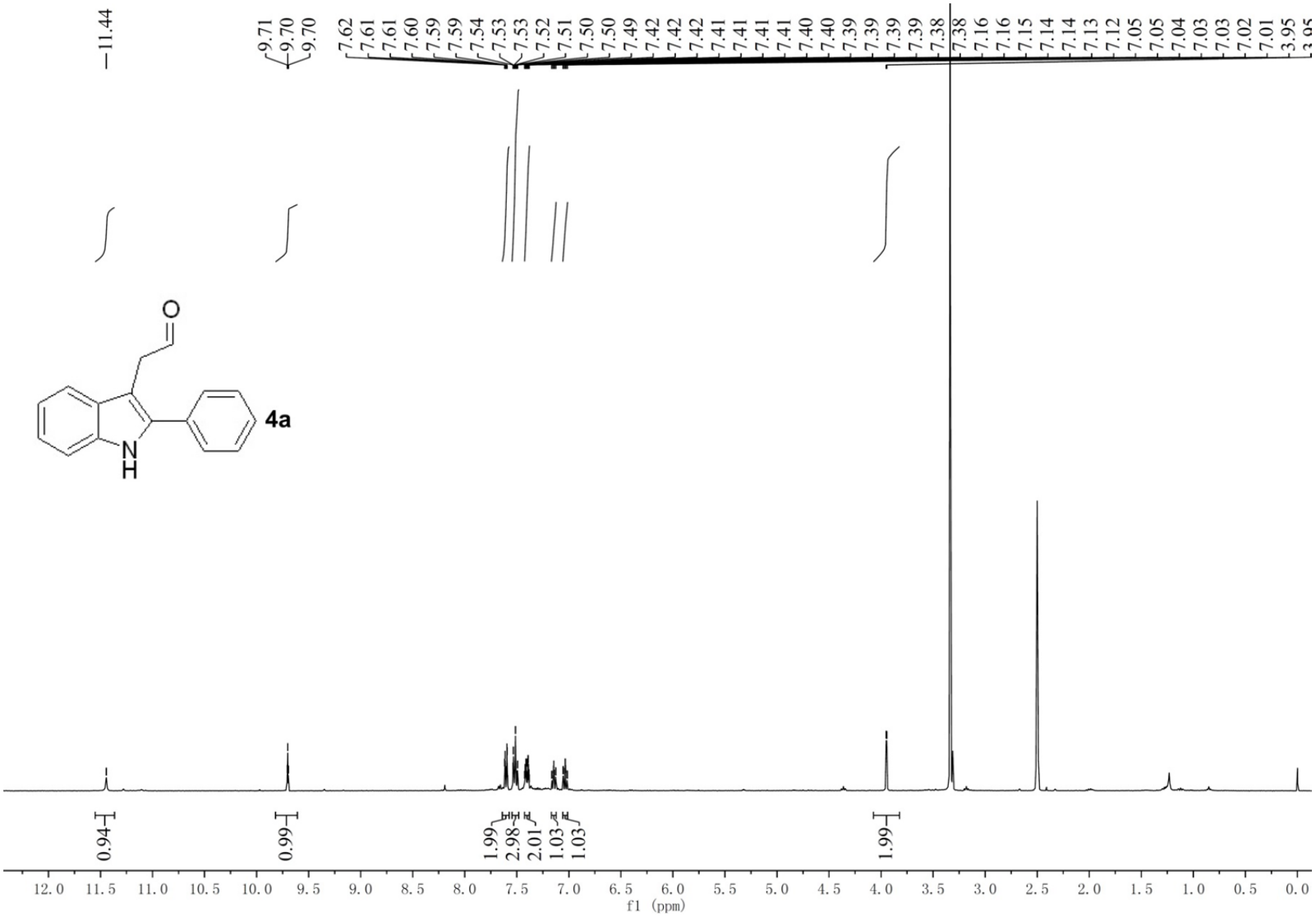
8.21
8.20
7.88
7.86
7.72
7.70
7.60
7.58
7.56
7.54
7.54
7.53
7.52
7.52
7.51
7.50
7.33
7.32
7.30
7.30
7.28
7.26
O
N
H
Br
1m
0.93
0.97
0.97
0.96
1.00
1.00
1.99
2.00
f1 (ppm)


184.99
147.74
135.93
133.22
133.09
131.88
131.28
127.83
124.84
123.92
123.50
122.65
121.05
114.61
112.27
O
N
H
Br
1m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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9.71
9.70
9.70
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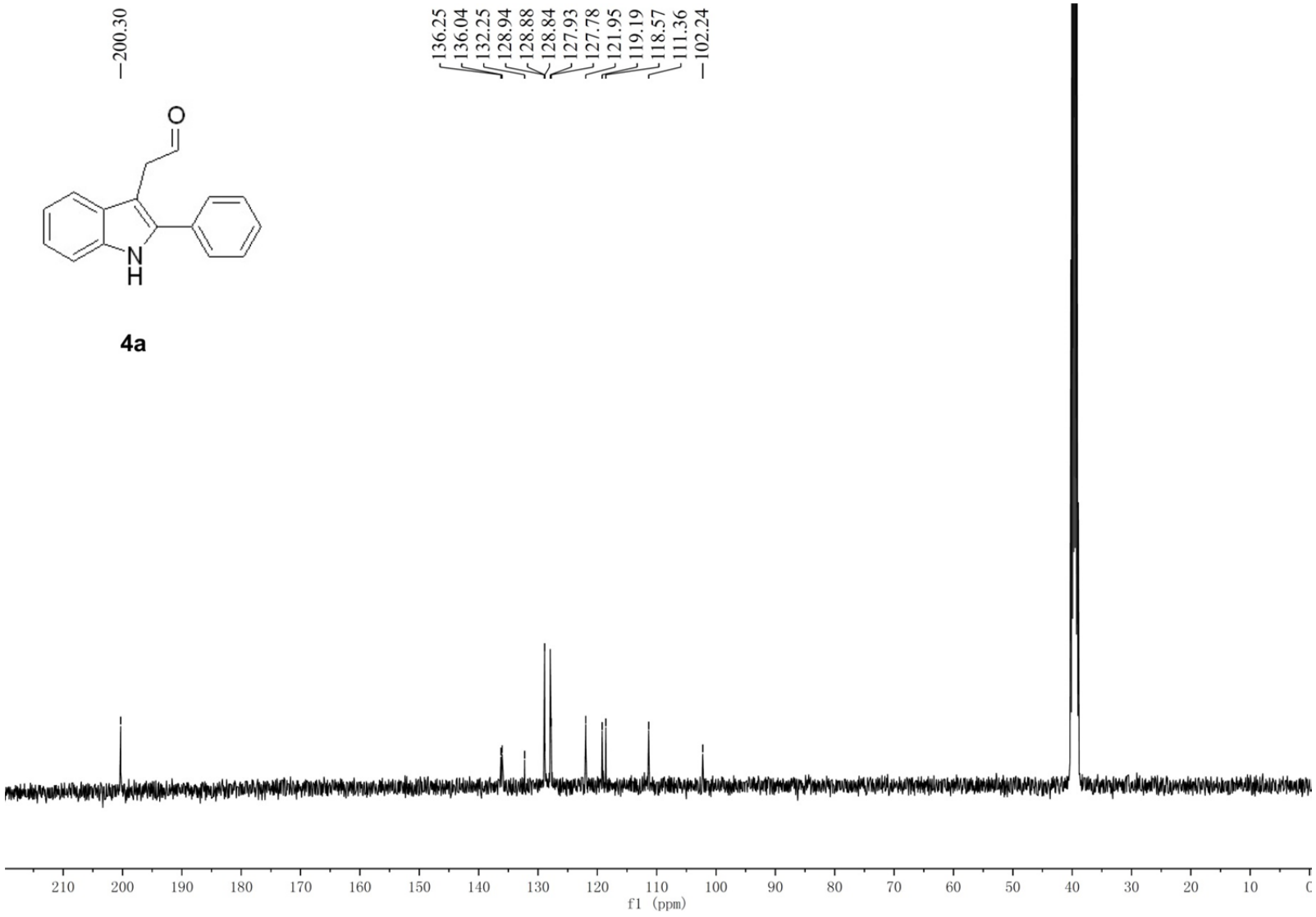
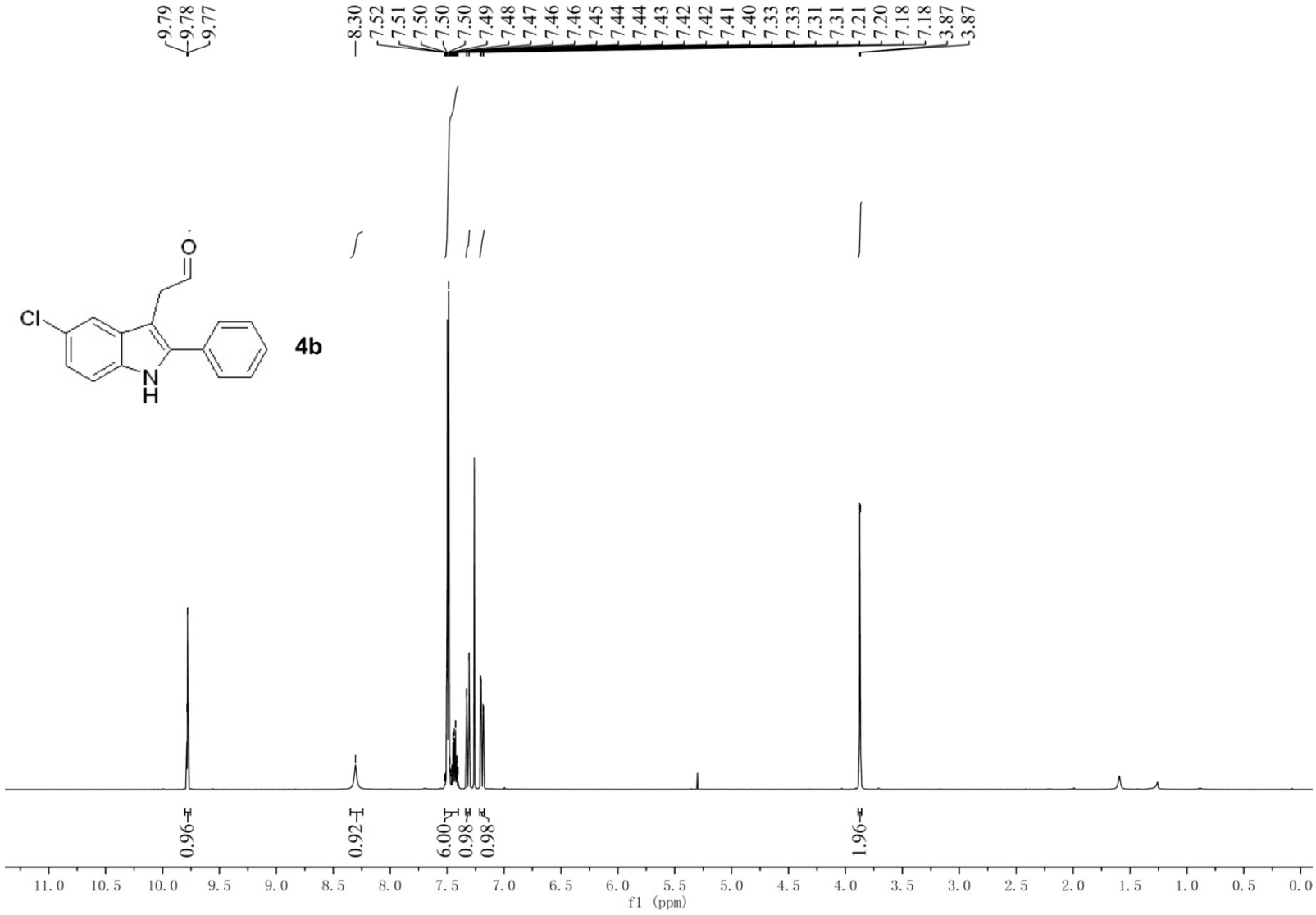
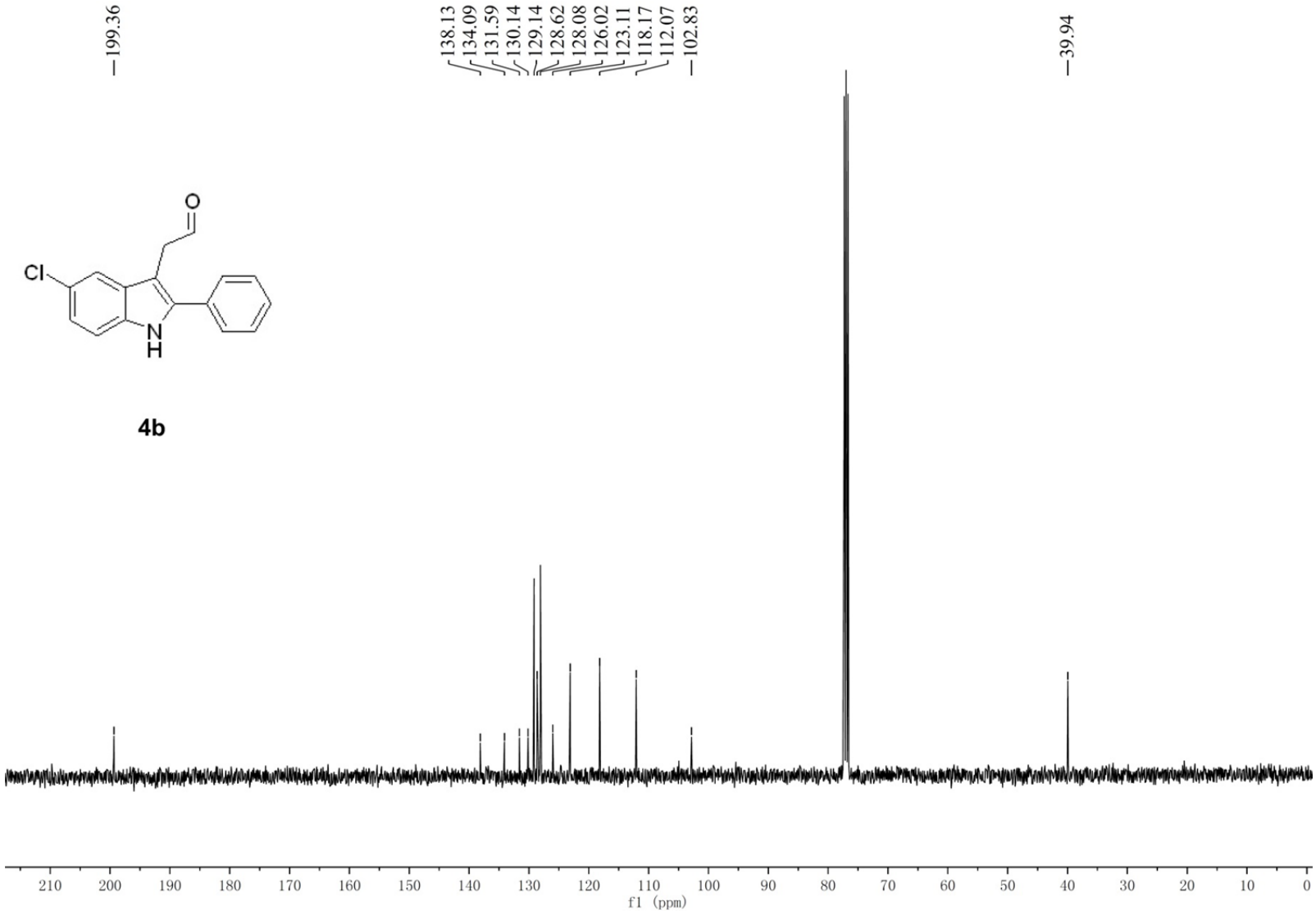
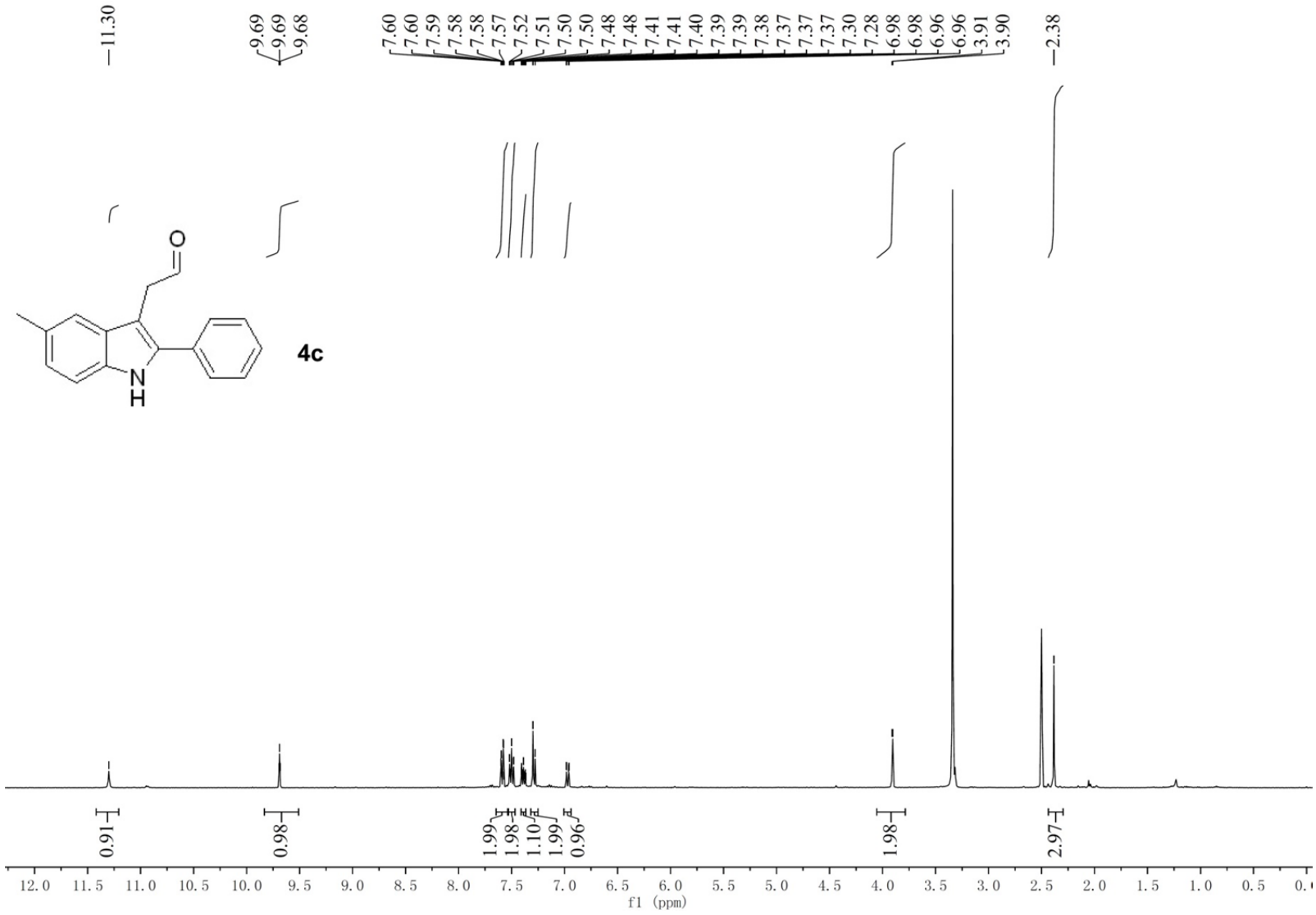
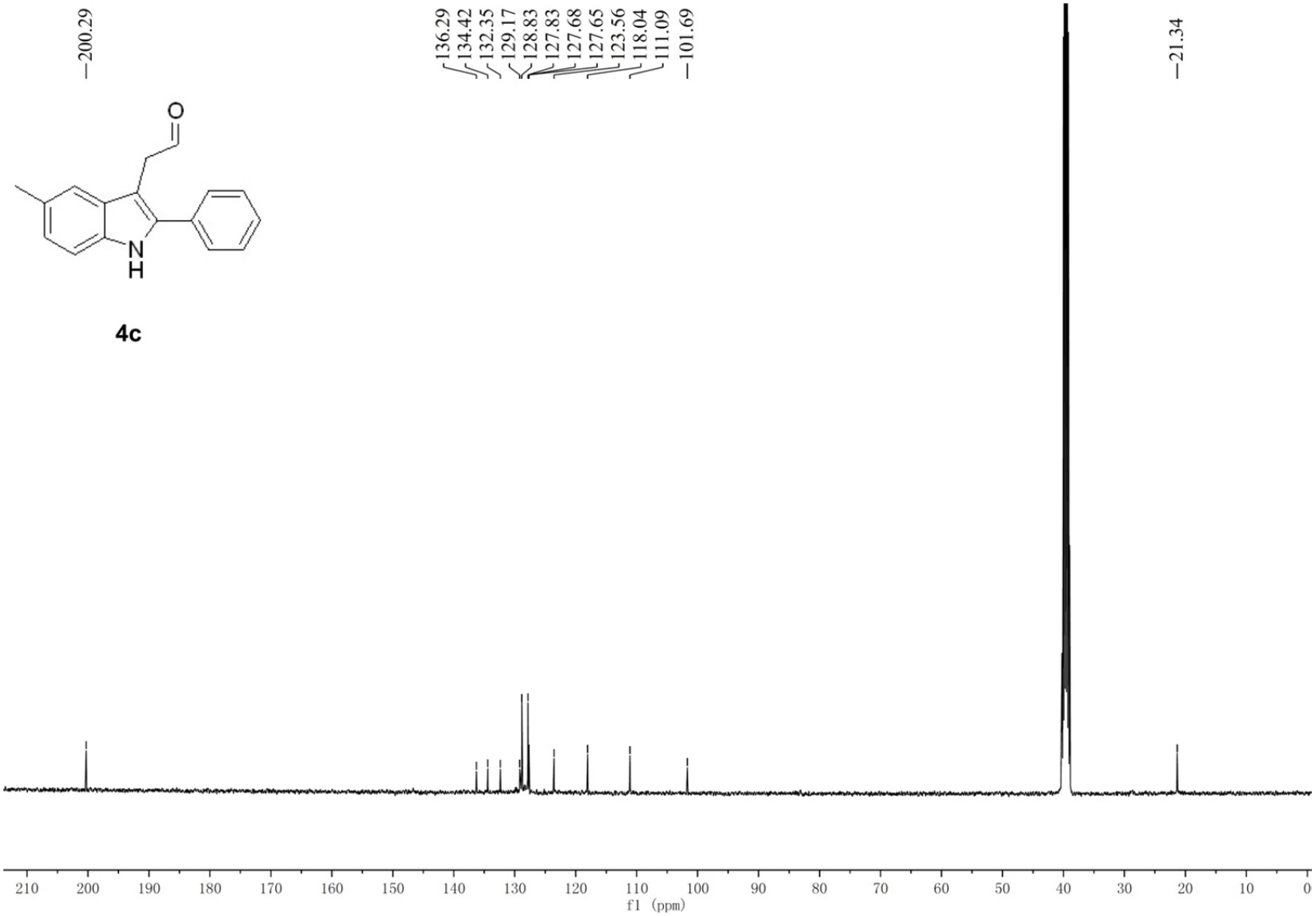
7.61
7.61
7.60
7.59
7.59
7.54
7.53
7.53
7.52
7.51
7.50
7.50
7.49
7.42
7.42
7.42
7.41
7.41
7.41
7.41
7.40
7.40
7.39
7.39
7.39
7.39
7.38
7.38
7.16
7.16
7.15
7.14
7.14
7.13
7.12
7.05
7.05
7.04
7.03
7.03
7.02
7.01
3.95
O
N
H
4a
0.94
0.99
1.99
2.98
2.01
1.03
1.03
1.99
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 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
f1 (ppm)

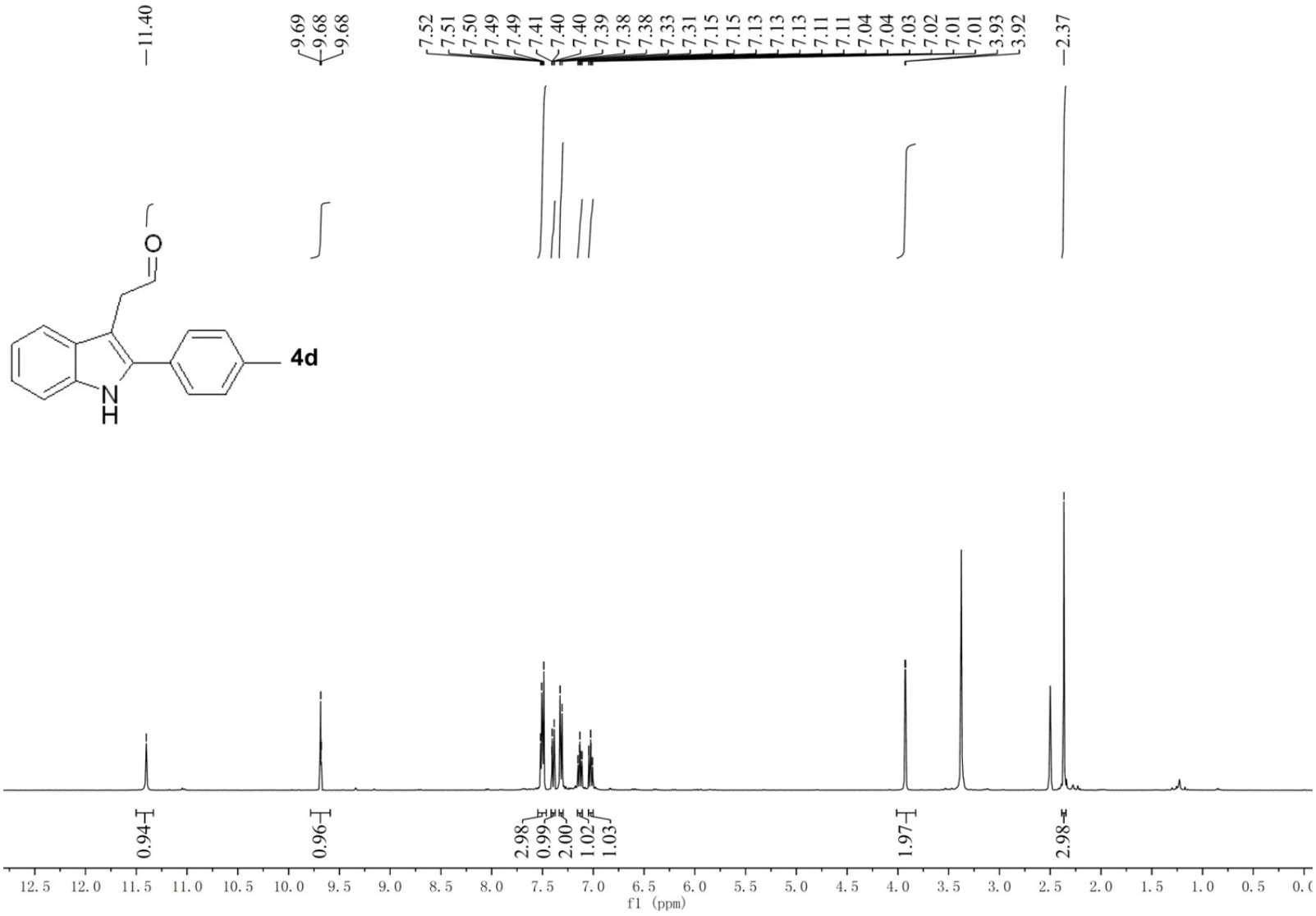

200.30
136.25
136.04
132.25
128.94
128.88
128.84
127.93
127.78
121.95
119.19
118.57
111.36
102.24
O
N
H
4a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


9.79
9.78
9.77
8.30
7.52
7.51
7.50
7.50
7.50
7.49
7.48
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.41
7.40
7.33
7.33
7.31
7.31
7.21
7.20
7.18
7.18
3.87
3.87
O
Cl
N
H
4b
0.96
0.92
6.00
0.98
0.98
1.96
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)


199.36
138.13
134.09
131.59
130.14
129.14
128.62
128.08
126.02
123.11
118.17
112.07
102.83
39.94
O
Cl
N
H
4b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.30
9.69
9.69
9.68
7.60
7.60
7.59
7.58
7.58
7.57
7.52
7.51
7.50
7.50
7.48
7.48
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.37
7.37
7.30
7.28
6.98
6.98
6.96
6.96
3.91
3.90
2.38
O
N
H
4c
0.91
0.98
1.99
1.98
1.10
1.99
0.96
1.98
2.97
f1 (ppm)


200.29
136.29
134.42
132.35
129.17
128.83
127.83
127.68
127.65
123.56
118.04
111.09
101.69
21.34
O
N
H
4c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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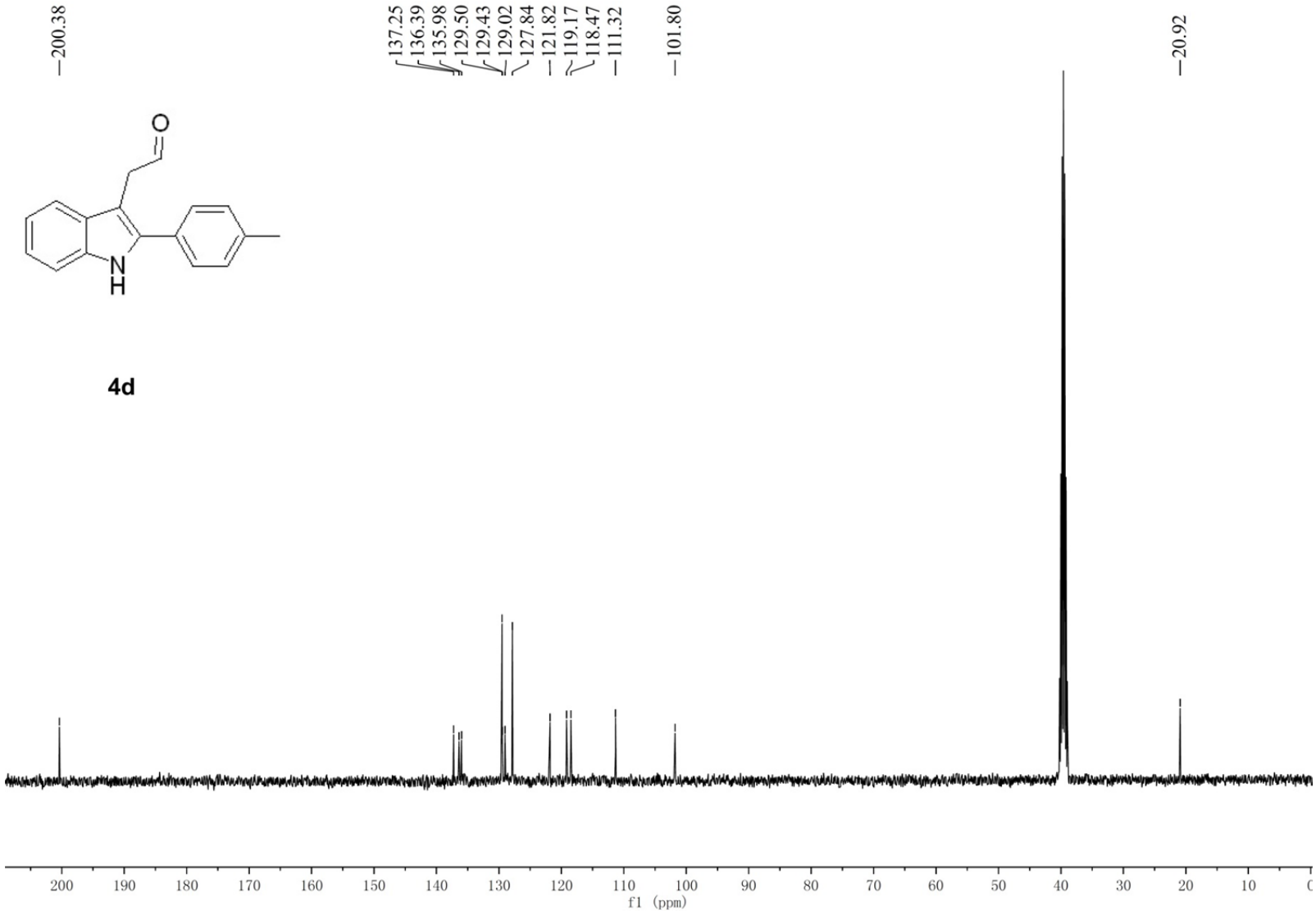
9.68
9.68
7.52
7.51
7.50
7.49
7.49
7.41
7.40
7.40
7.39
7.38
7.38
7.33
7.31
7.15
7.15
7.13
7.13
7.13
7.11
7.11
7.04
7.04
7.03
7.02
7.01
7.01
3.93
3.92
2.37
O
4d
N
H
0.94
0.96
2.98
0.99
2.00
1.02
1.03
1.97
2.98
f1 (ppm)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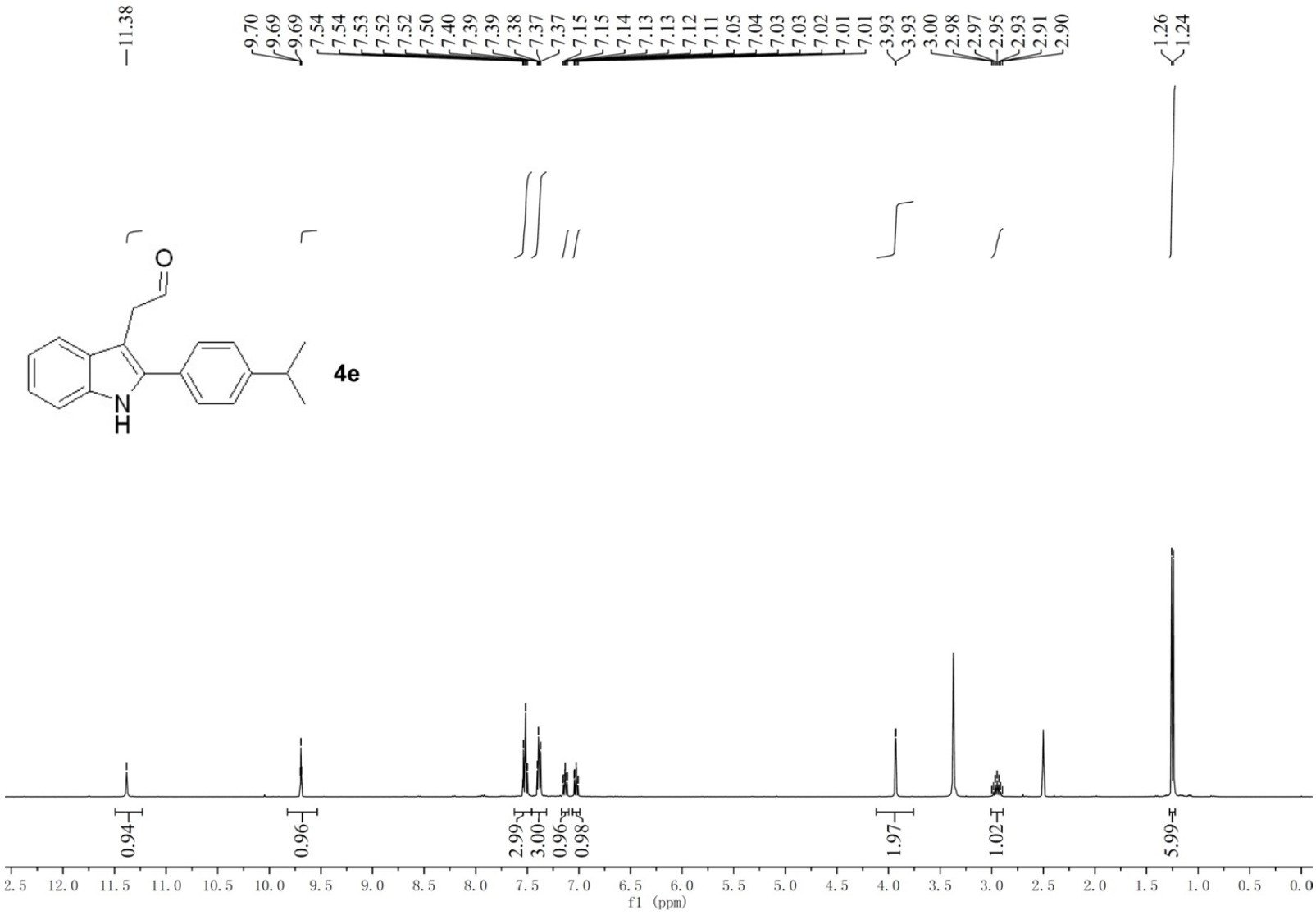
137.25
136.39
135.98
129.50
129.43
129.02
127.84
121.82
119.17
118.47
111.32
101.80
20.92
O
N
H
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

4d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9.69
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7.54
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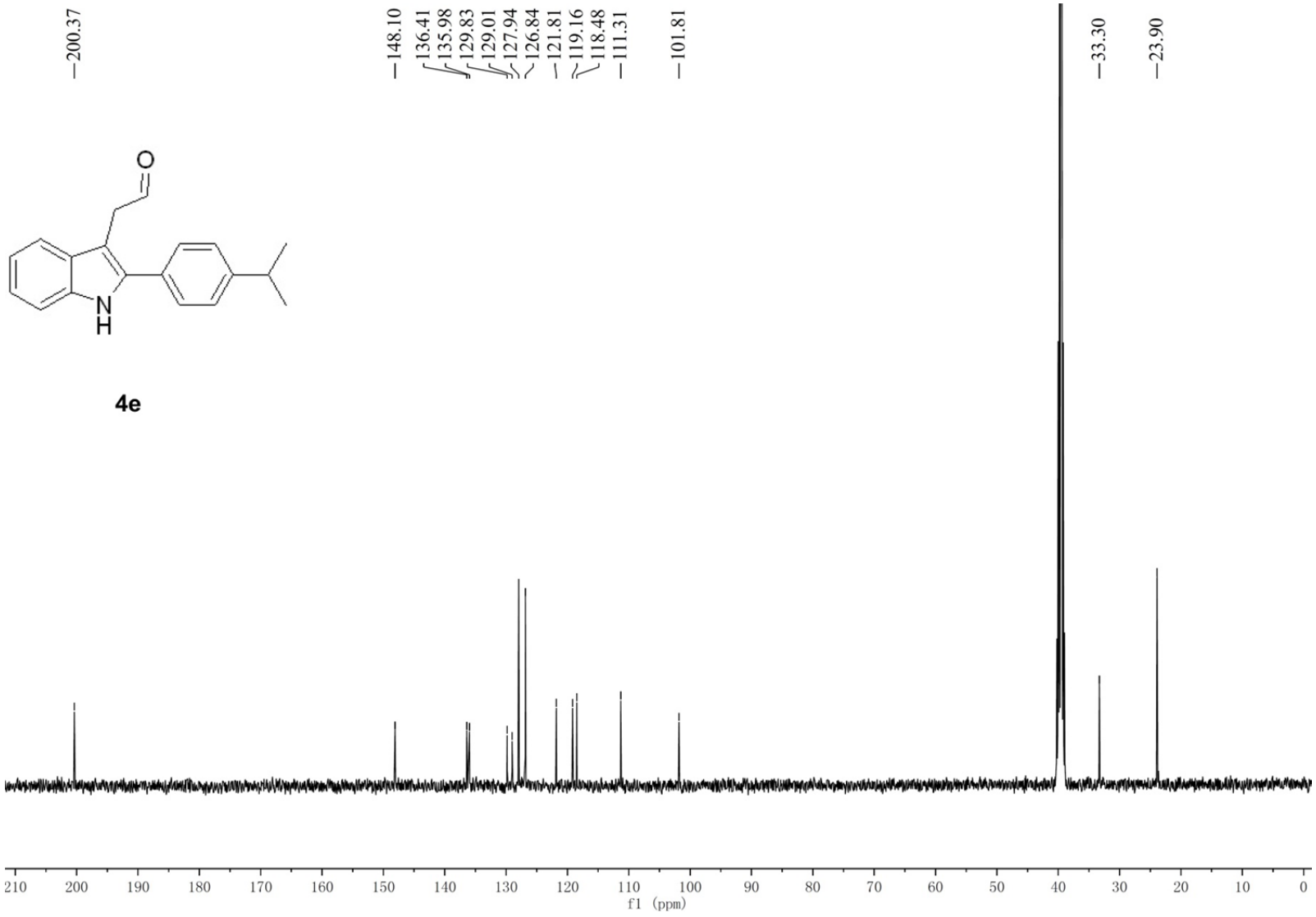
7.52
7.52
7.50
7.40
7.39
7.39
7.38
7.37
7.37
7.15
7.15
7.14
7.13
7.13
7.12
7.11
7.05
7.04
7.03
7.03
7.02
7.01
7.01
3.93
3.93
3.00
2.98
2.97
2.95
2.93
2.91
2.90
1.26
1.24
O
N
H
4e
0.94
0.96
2.99
3.00
0.96
0.98
1.97
1.02
5.99
f1 (ppm)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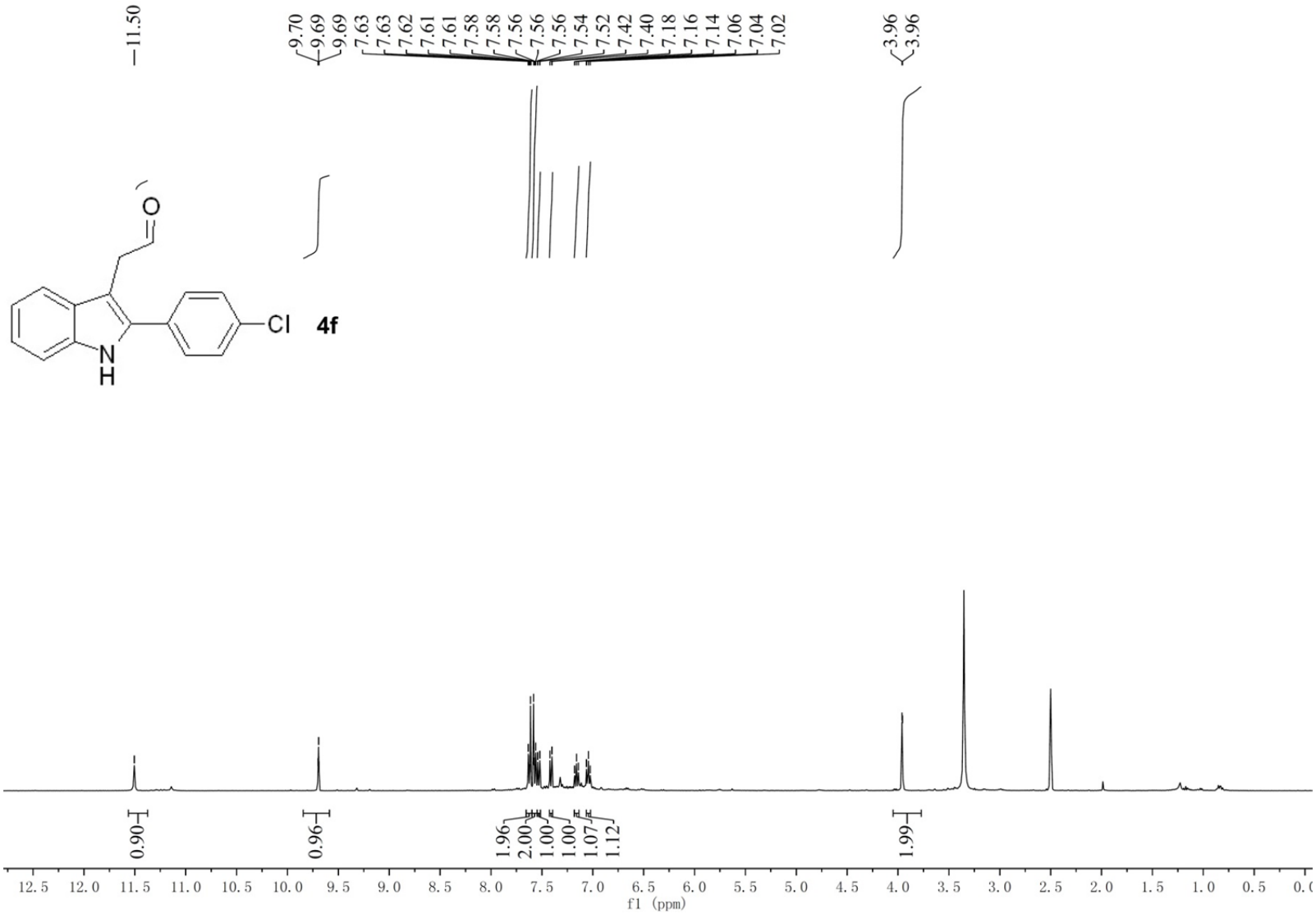
148.10
136.41
135.98
129.83
129.01
127.94
126.84
121.81
119.16
118.48
111.31
101.81
33.30
23.90
O
N
H
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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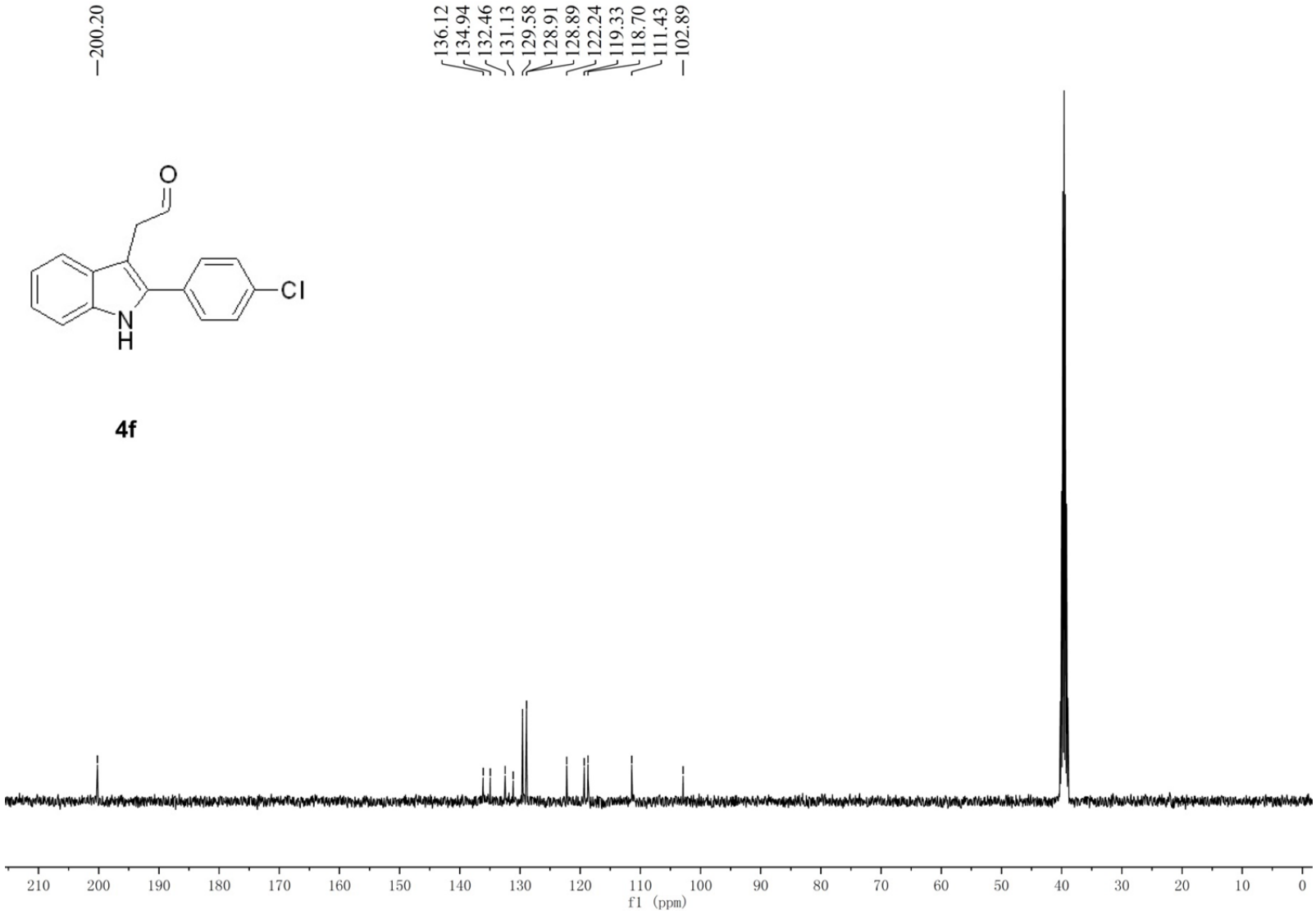
9.69
9.69
7.63
7.63
7.62
7.61
7.61
7.58
7.58
7.56
7.56
7.56
7.54
7.52
7.42
7.40
7.18
7.16
7.14
7.06
7.04
7.02
3.96
3.96
O
Cl
N
H
4f
0.90
0.96
1.96
2.00
1.00
1.00
1.07
1.12
1.99
f1 (ppm)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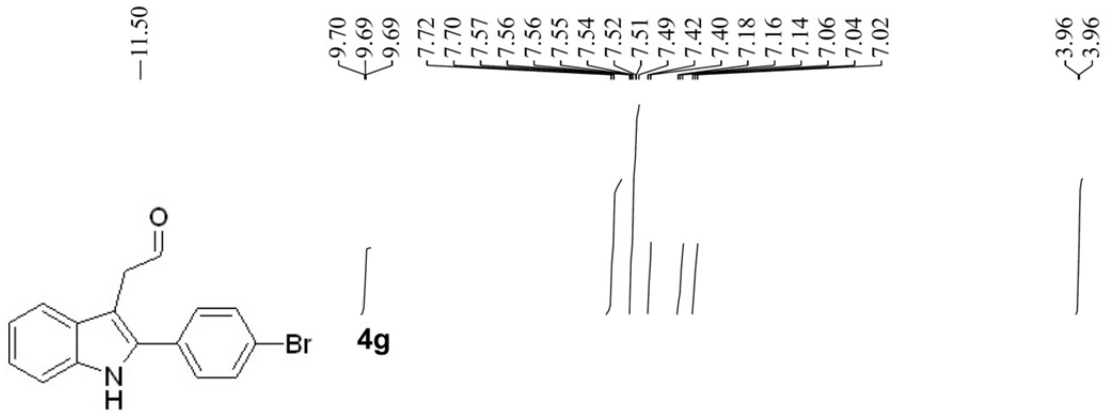
132.46
131.13
129.58
128.91
128.89
122.24
119.33
118.70
111.43
102.89
O
Cl
N
H
4f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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9.70
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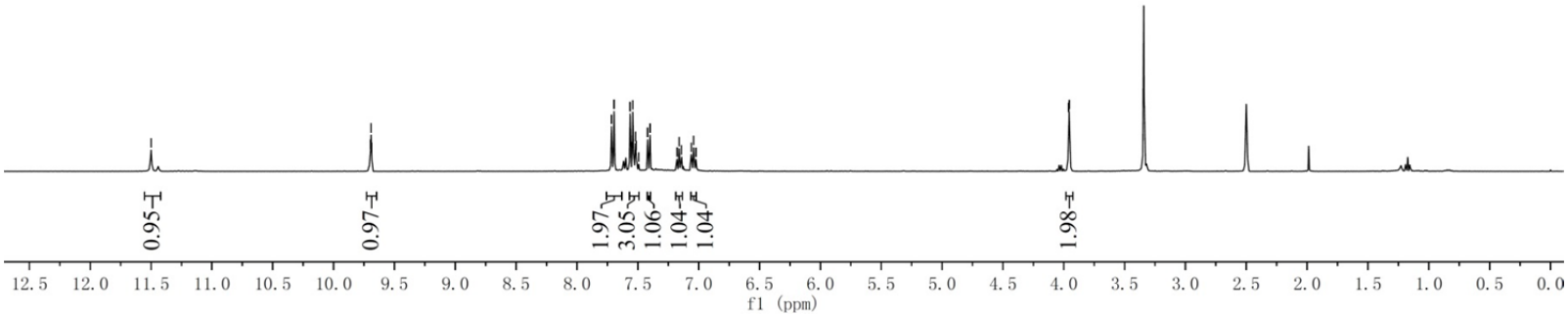
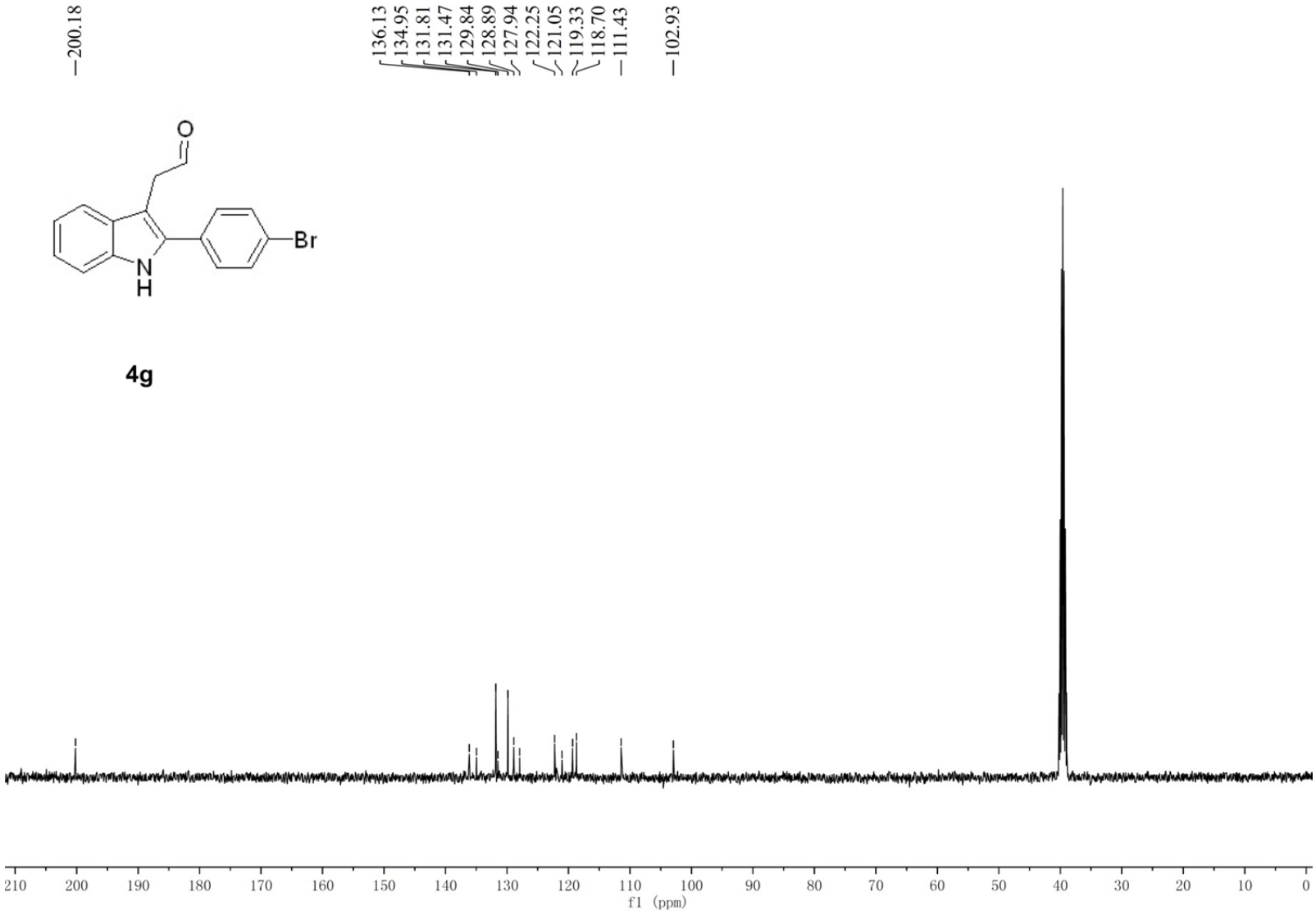
9.69
7.72
7.70
7.57
7.56
7.56
7.55
7.54
7.52
7.51
7.49
7.42
7.40
7.18
7.16
7.14
7.06
7.04
7.02
3.96
3.96
O
Br
N
H
4g


0.95
0.97
1.97
3.05
1.06
1.04
1.04
1.98
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
f1 (ppm)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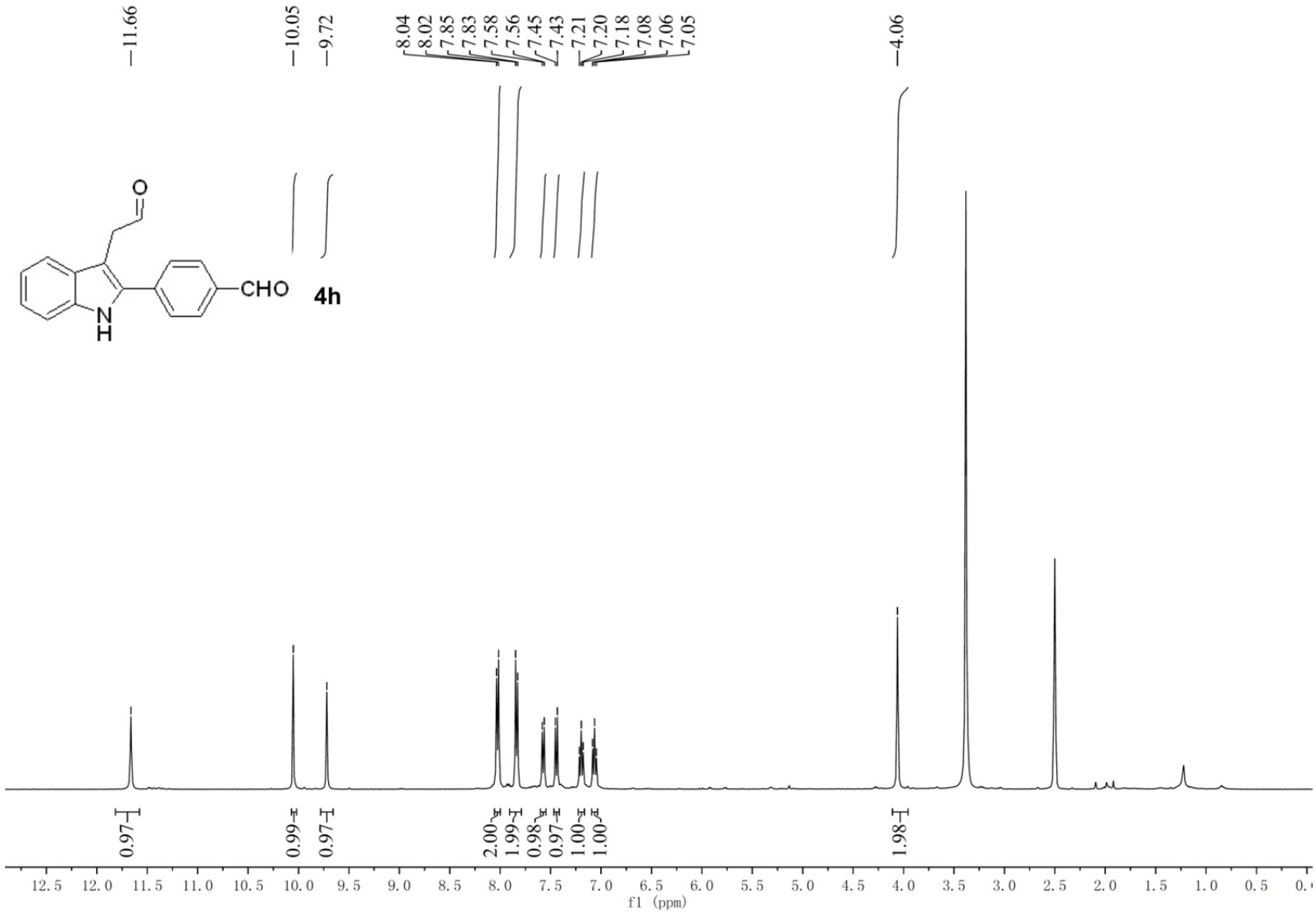
131.81
131.47
129.84
128.89
127.94
122.25
121.05
119.33
118.70
111.43
102.93
O
Br
N
H
4g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


11.66
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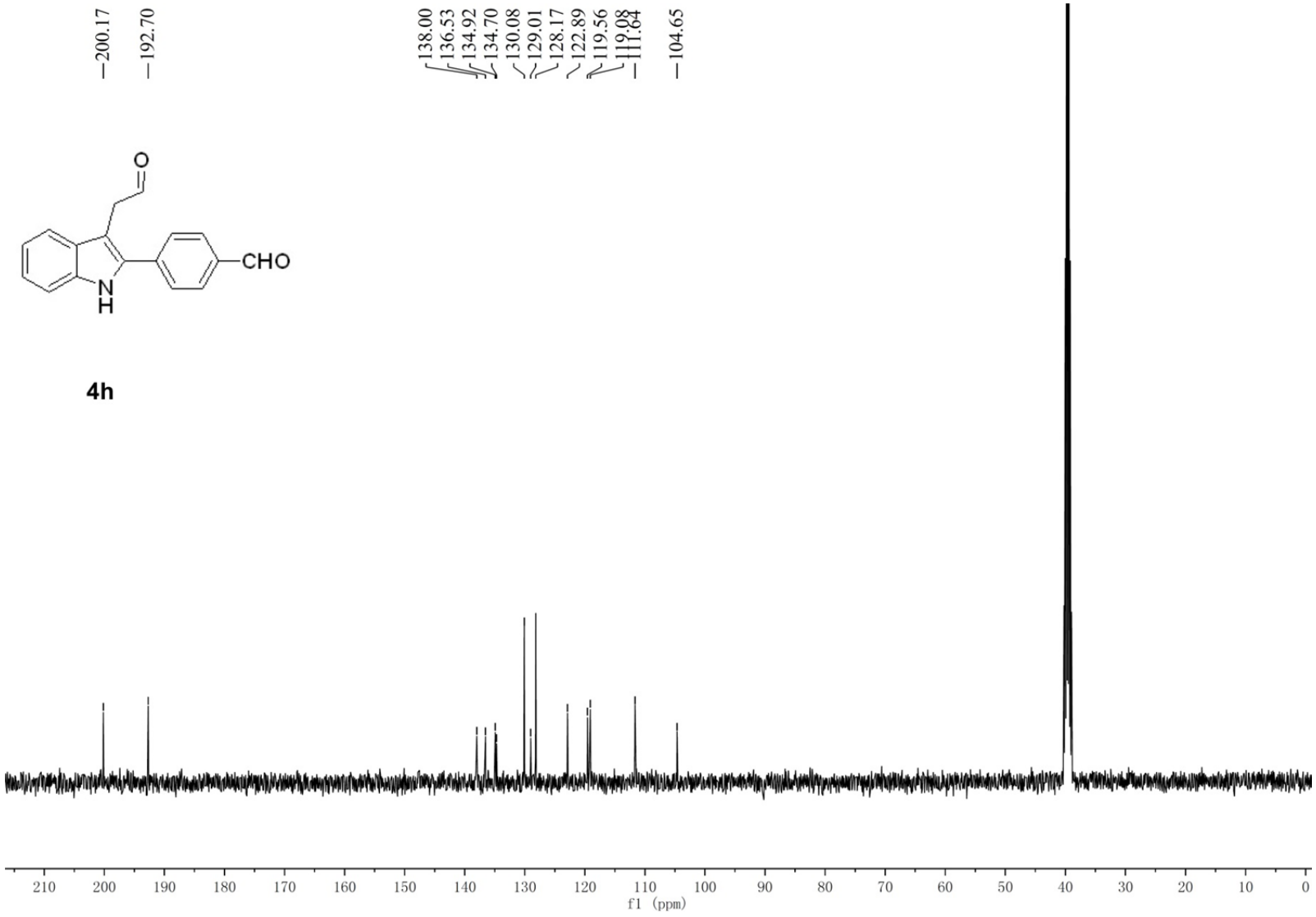
8.04
8.02
7.85
7.83
7.58
7.56
7.45
7.43
7.21
7.20
7.18
7.08
7.06
7.05
4.06
O
CHO
N
H
4h
0.97
0.99
0.97
2.00
1.99
0.98
0.97
1.00
1.00
1.98
f1 (ppm)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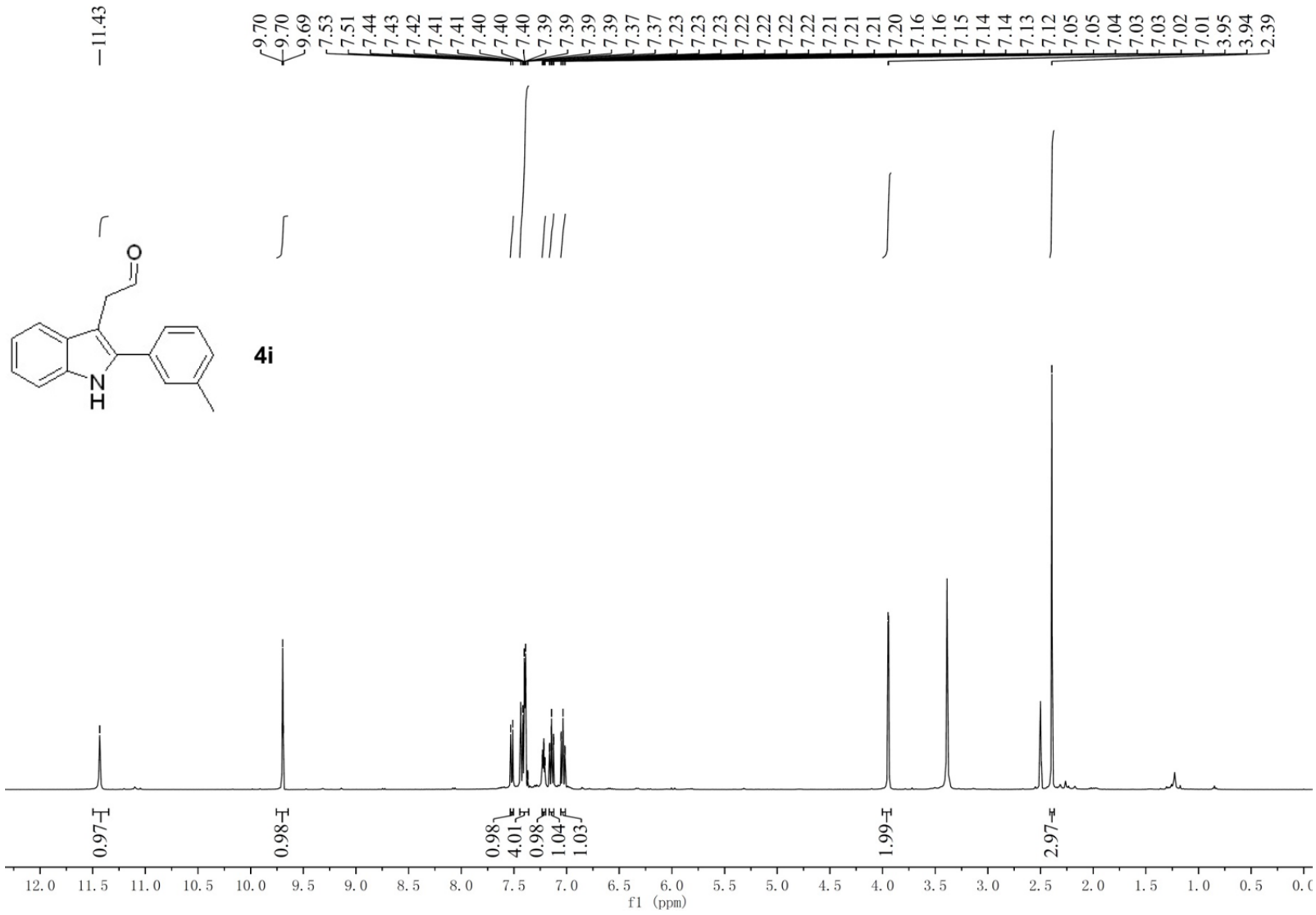
134.92
134.70
130.08
129.01
128.17
122.89
119.56
111.64
104.65
O
CHO
N
H
4h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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9.70
9.69
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7.51
7.44
7.43
7.42
7.41
7.41
7.40
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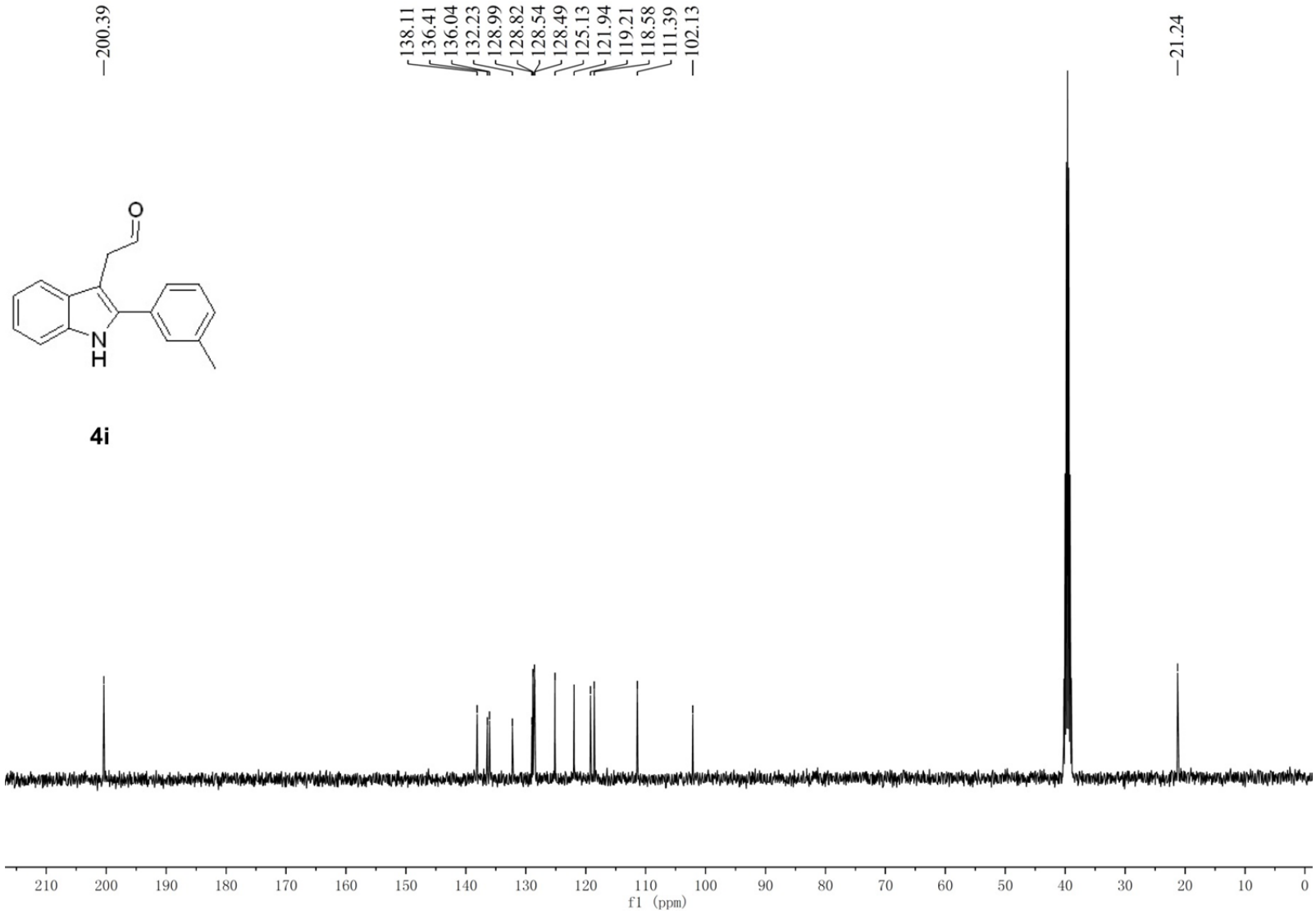
7.40
7.39
7.39
7.39
7.39
7.37
7.37
7.23
7.23
7.23
7.22
7.22
7.22
7.22
7.21
7.21
7.21
7.20
7.16
7.16
7.15
7.14
7.14
7.13
7.12
7.05
7.05
7.04
7.03
7.03
7.02
7.01
3.95
3.94
2.39
O
N
H
4i
0.97
0.98
0.98
4.01
0.98
1.04
1.03
1.99
2.97
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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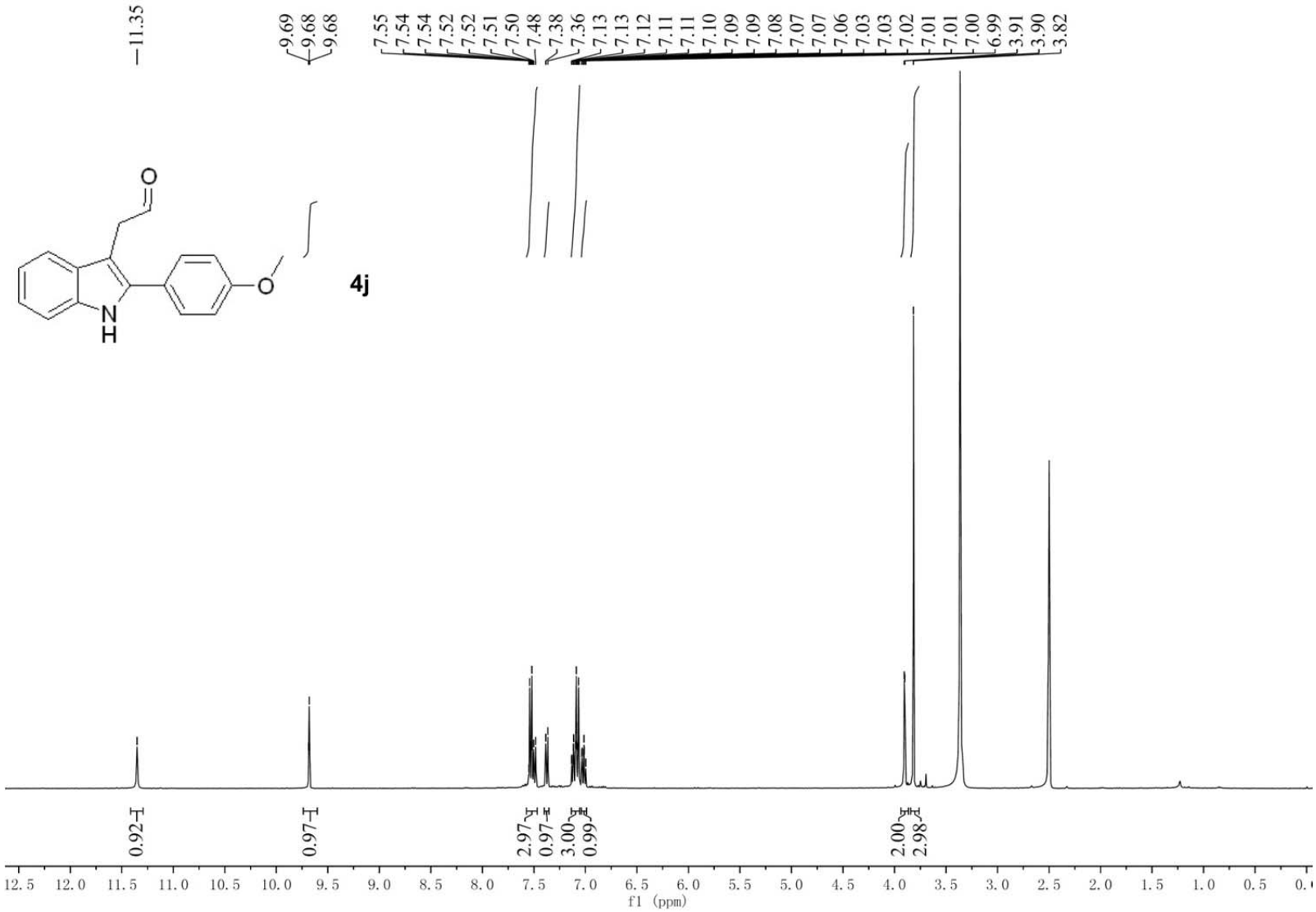
136.41
136.04
132.23
128.99
128.82
128.54
128.49
125.13
121.94
119.21
118.58
111.39
102.13
21.24
O
N
H
4i
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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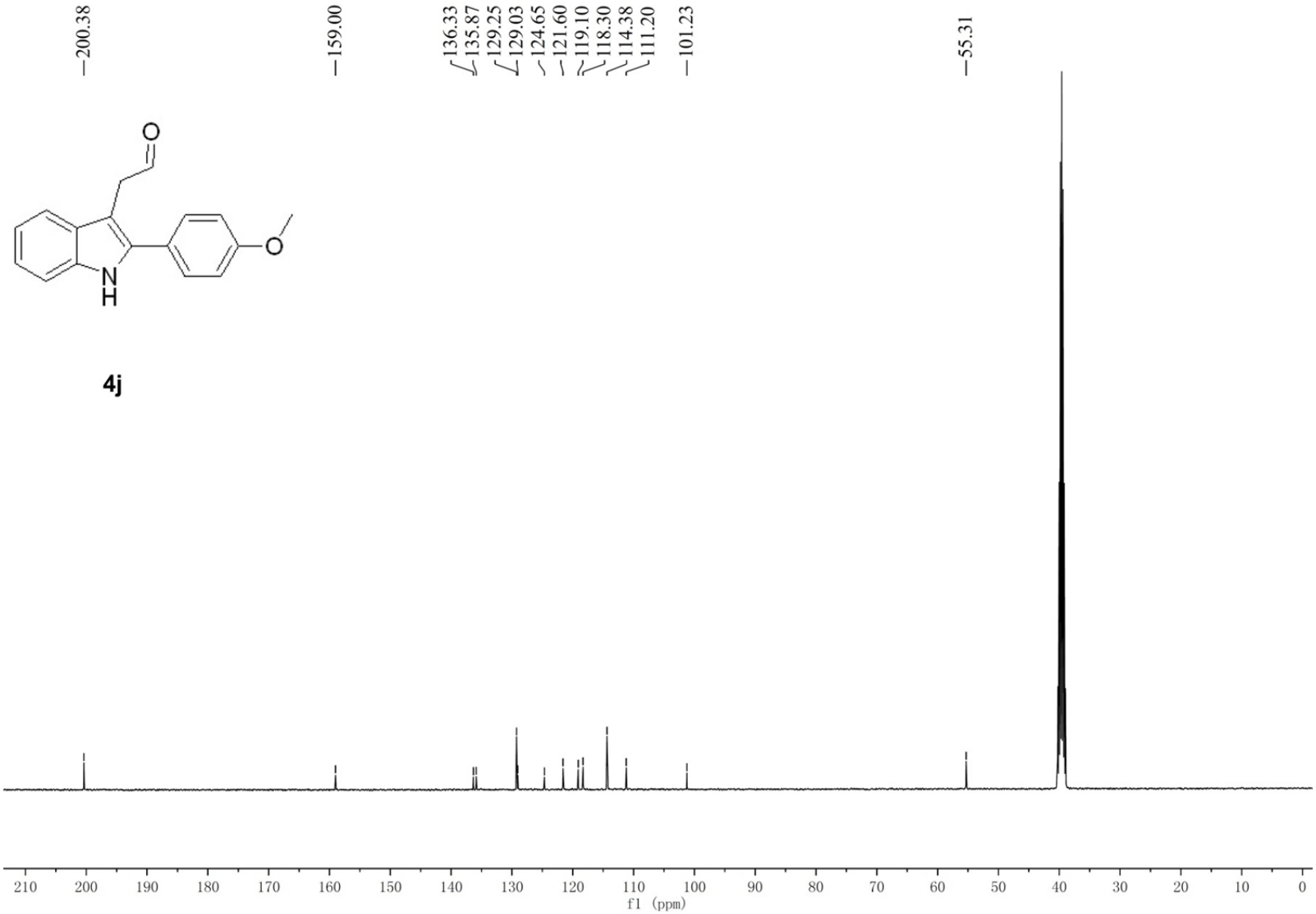
9.69
9.68
9.68
7.55
7.54
7.54
7.52
7.52
7.51
7.50
7.48
7.38
7.36
7.13
7.13
7.12
7.11
7.11
7.10
7.09
7.09
7.08
7.07
7.07
7.06
7.03
7.03
7.02
7.01
7.01
7.00
6.99
3.91
3.90
3.82
O
O
N
H
4j
0.92
0.97
2.97
0.97
3.00
0.99
2.00
2.98
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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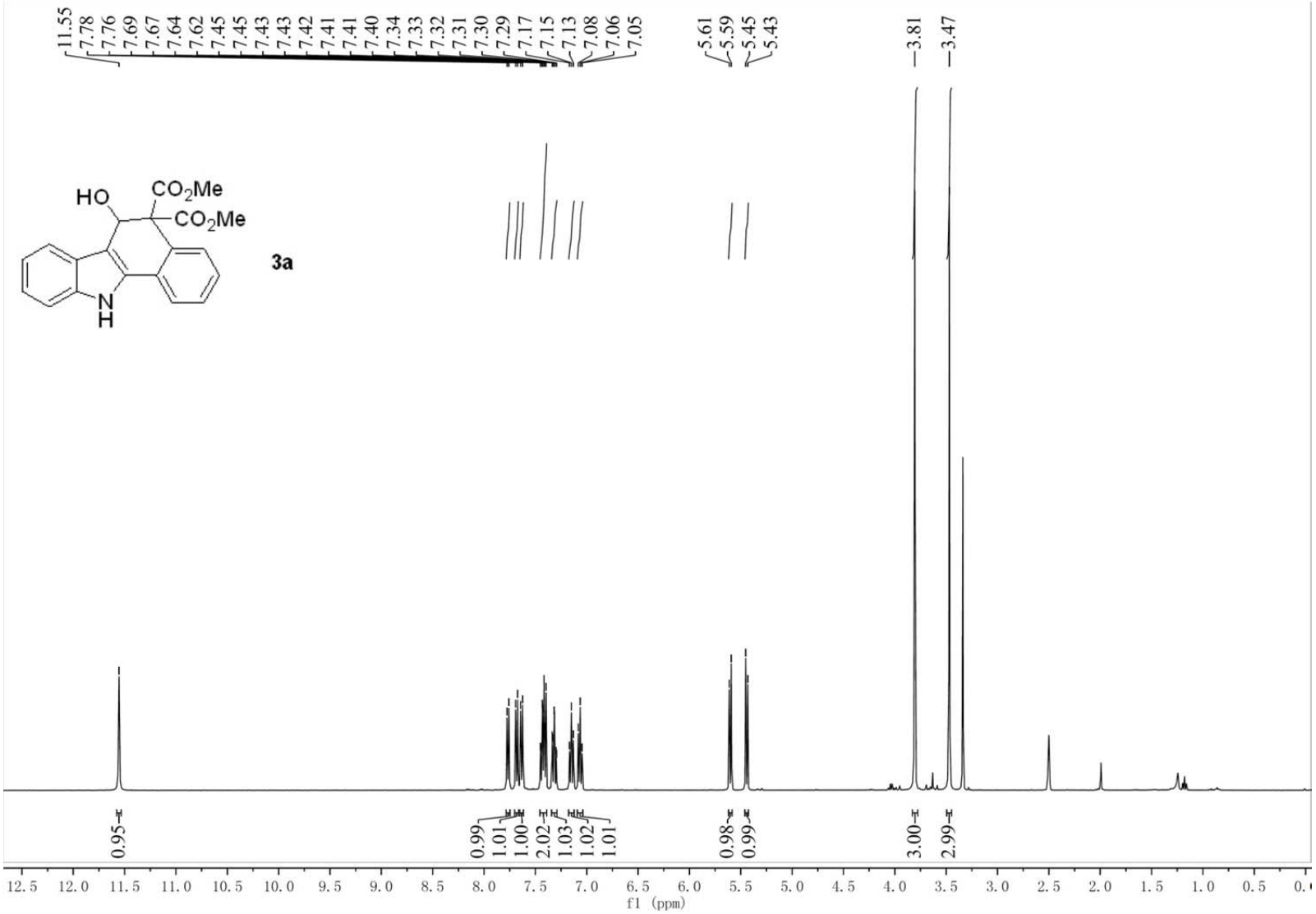
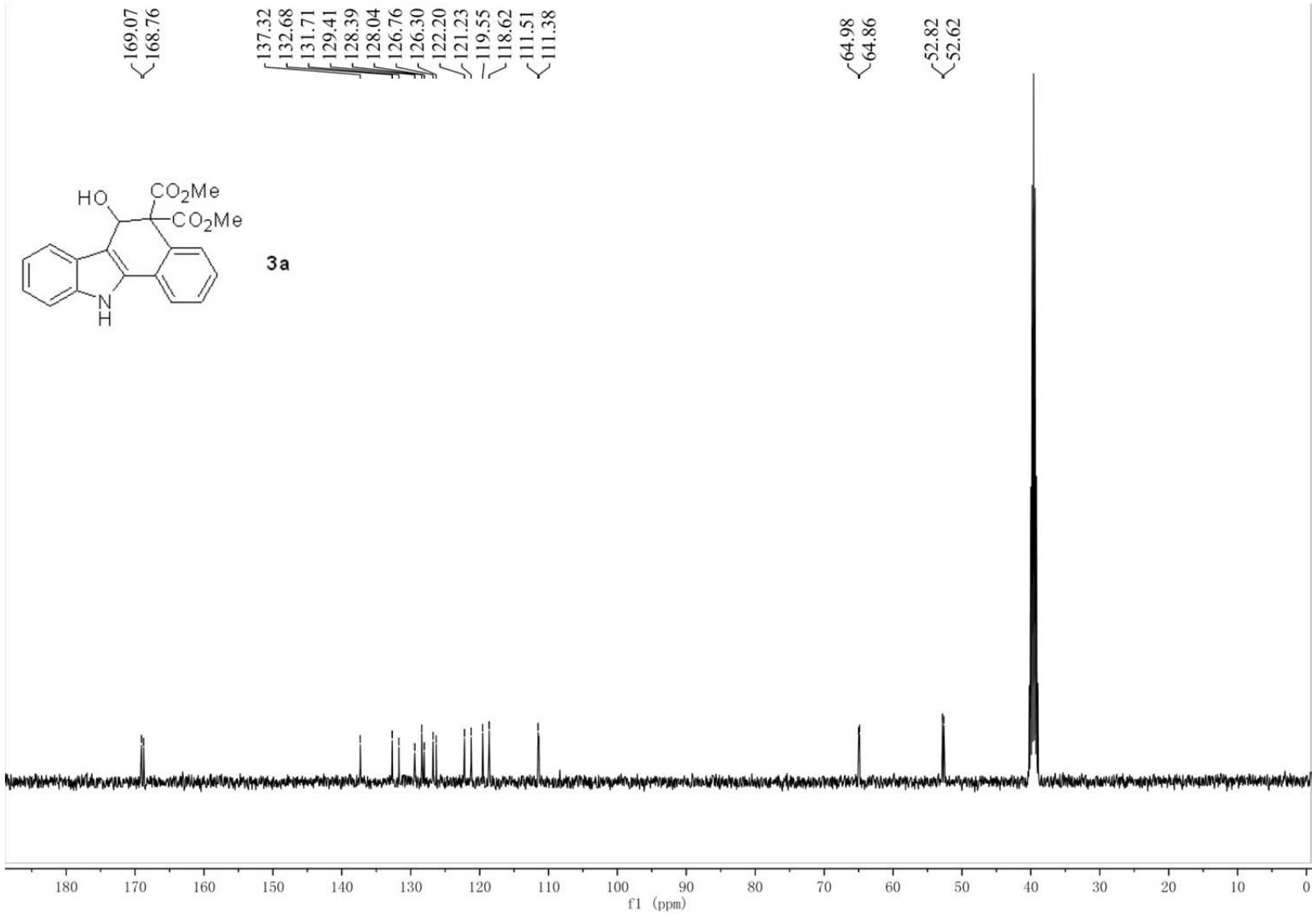
159.00
136.33
135.87
129.25
129.03
124.65
121.60
119.10
118.30
114.38
111.20
101.23
55.31
O
O
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

4j

3. Copies of ^{1}H and ^{13}C NMR charts for products

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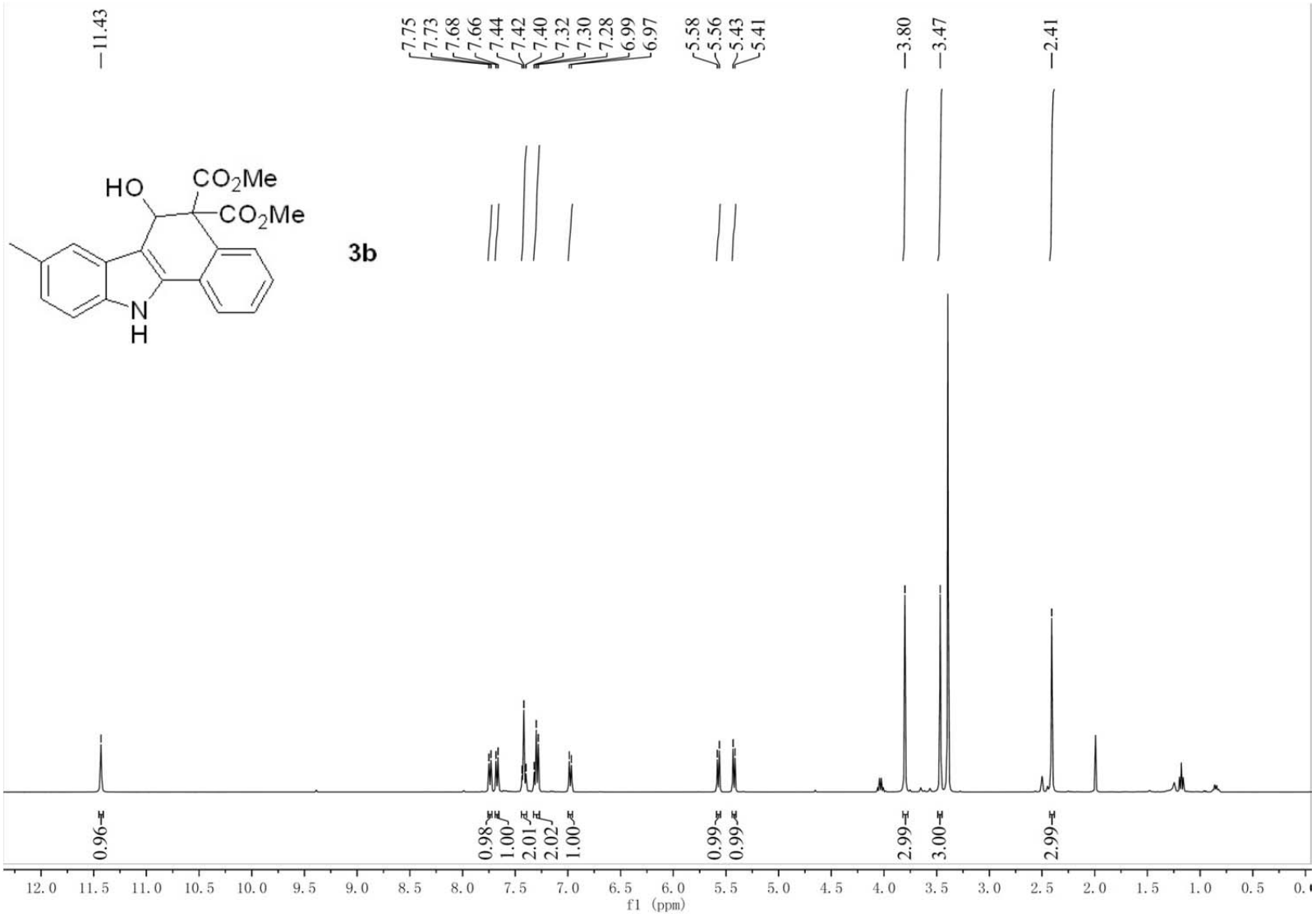
168.76
137.32
132.68
131.71
129.41
128.39
128.04
126.76
126.30
122.20
121.23
119.55
118.62
111.51
111.38
64.98
64.86
52.82
52.62
HO
CO2Me
CO2Me
N
H
3a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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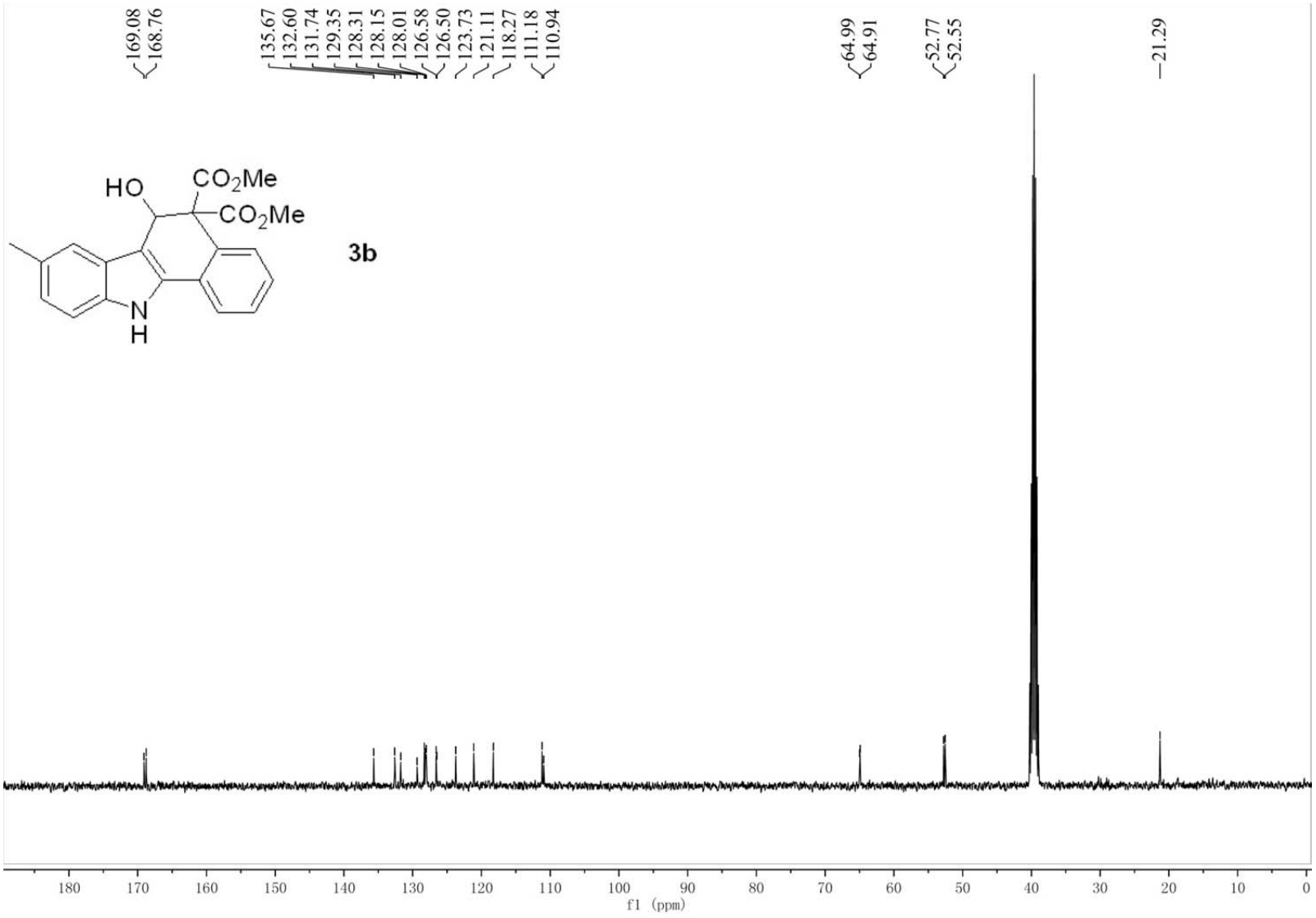
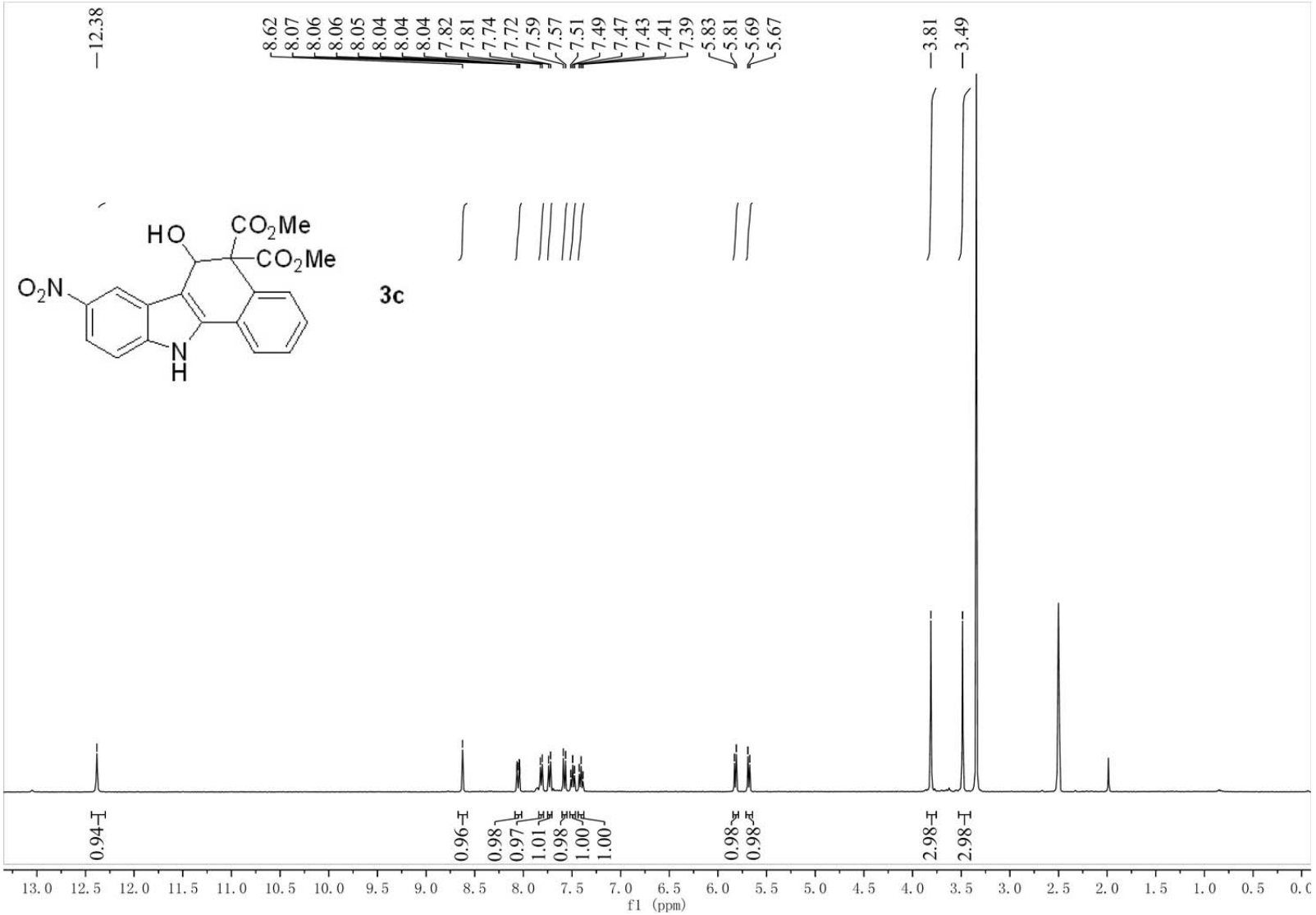
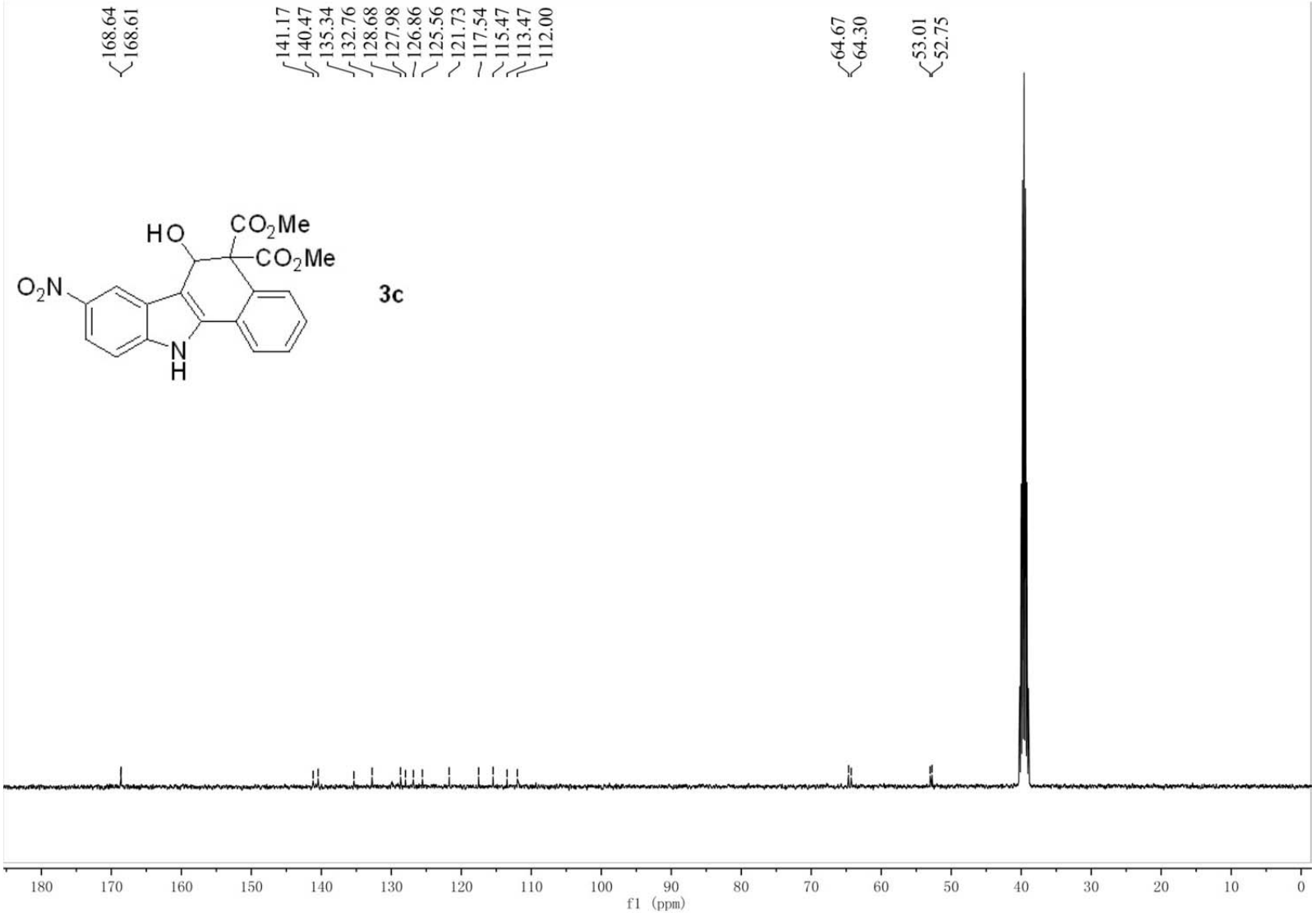
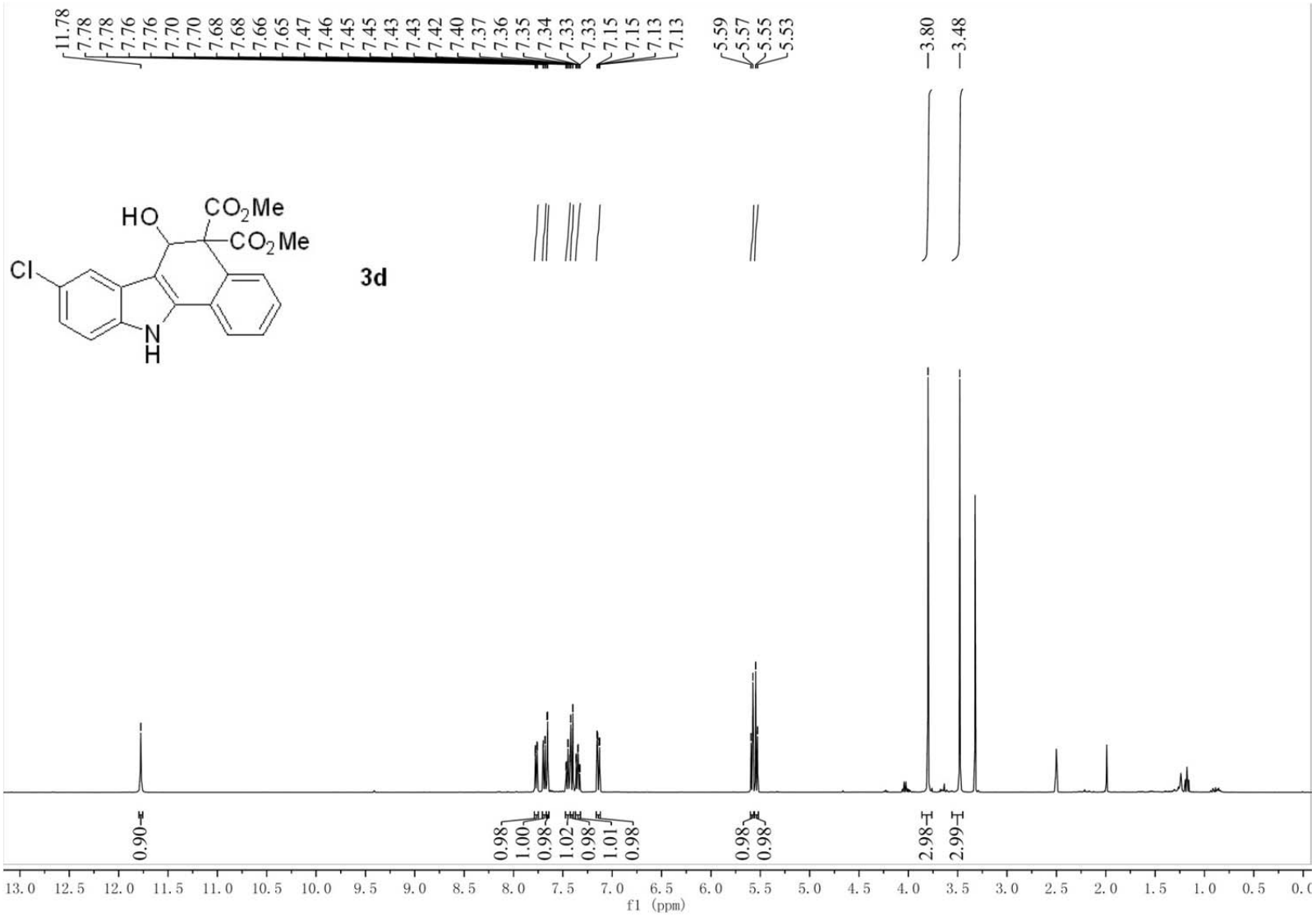
7.75
7.73
7.68
7.66
7.44
7.42
7.40
7.32
7.30
7.28
6.99
6.97
5.58
5.56
5.43
5.41
3.80
3.47
2.41
HO
CO2Me
CO2Me
N
H
3b
0.96
0.98
1.00
2.01
2.02
1.00
0.99
0.99
2.99
3.00
2.99
f1 (ppm)


169.08
168.76
135.67
132.60
131.74
129.35
128.31
128.15
128.01
126.58
126.50
123.73
121.11
118.27
111.18
110.94
64.99
64.91
52.77
52.55
21.29
HO
CO2Me
CO2Me
N
H
3b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.38
8.62
8.07
8.06
8.06
8.05
8.04
8.04
8.04
7.82
7.81
7.74
7.72
7.59
7.57
7.51
7.49
7.47
7.43
7.41
7.39
5.83
5.81
5.69
5.67
3.81
3.49
HO
CO2Me
CO2Me
O2N
N
H
3c
0.94
0.96
0.98
0.97
1.01
0.98
1.00
1.00
0.98
0.98
2.98
2.98
f1 (ppm)


168.64
168.61
141.17
140.47
135.34
132.76
128.68
127.98
126.86
125.56
121.73
117.54
115.47
113.47
112.00
64.67
64.30
53.01
52.75
HO
CO2Me
CO2Me
O2N
N
H
3c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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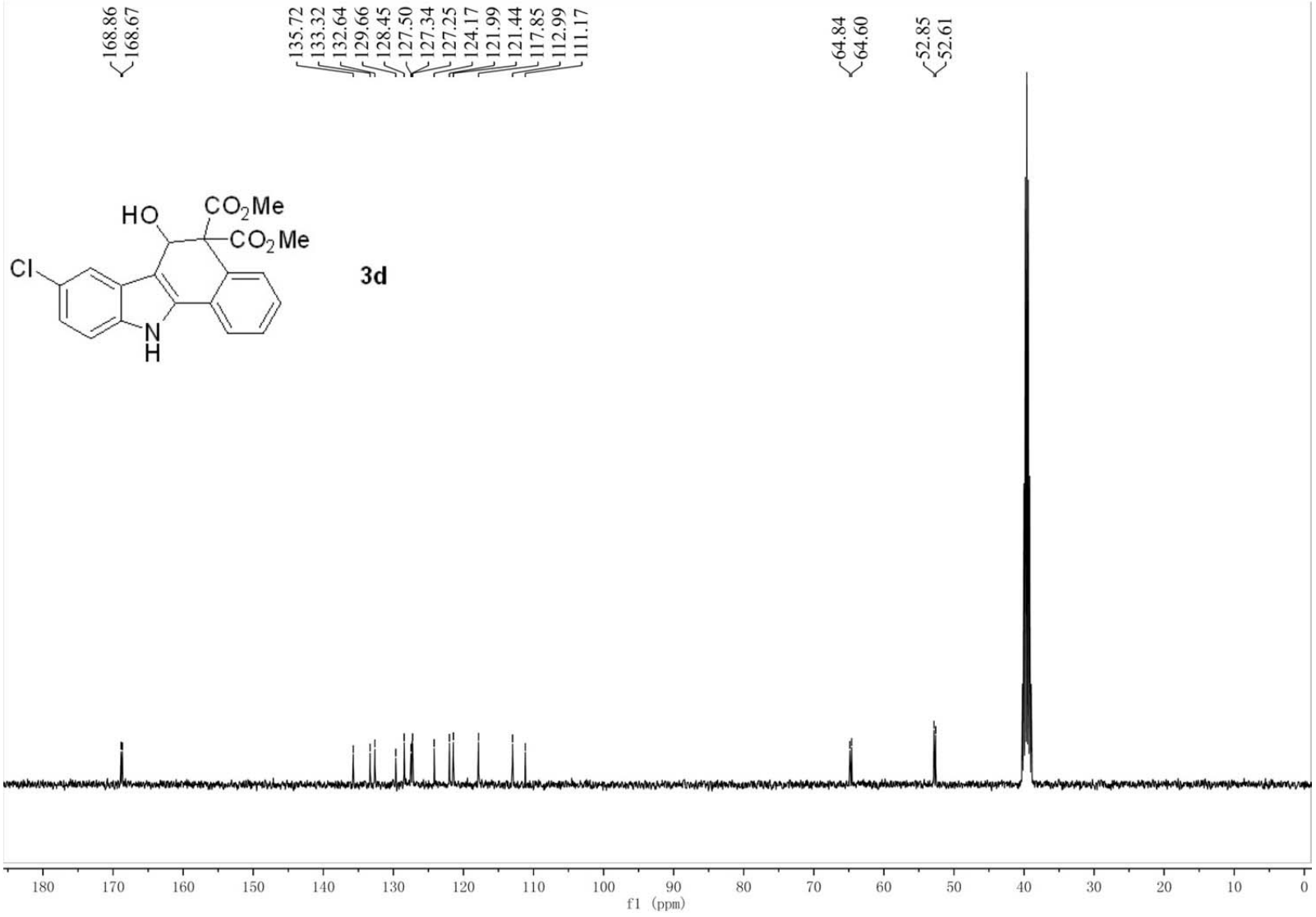
7.78
7.76
7.76
7.70
7.70
7.68
7.68
7.66
7.65
7.47
7.46
7.45
7.45
7.43
7.43
7.42
7.40
7.37
7.36
7.35
7.34
7.33
7.33
7.15
7.15
7.13
7.13
5.59
5.57
5.55
5.53
3.80
3.48
HO
CO2Me
CO2Me
Cl
N
H
3d
0.90
0.98
1.00
0.98
1.02
0.98
1.01
0.98
0.98
0.98
2.98
2.99
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 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
f1 (ppm)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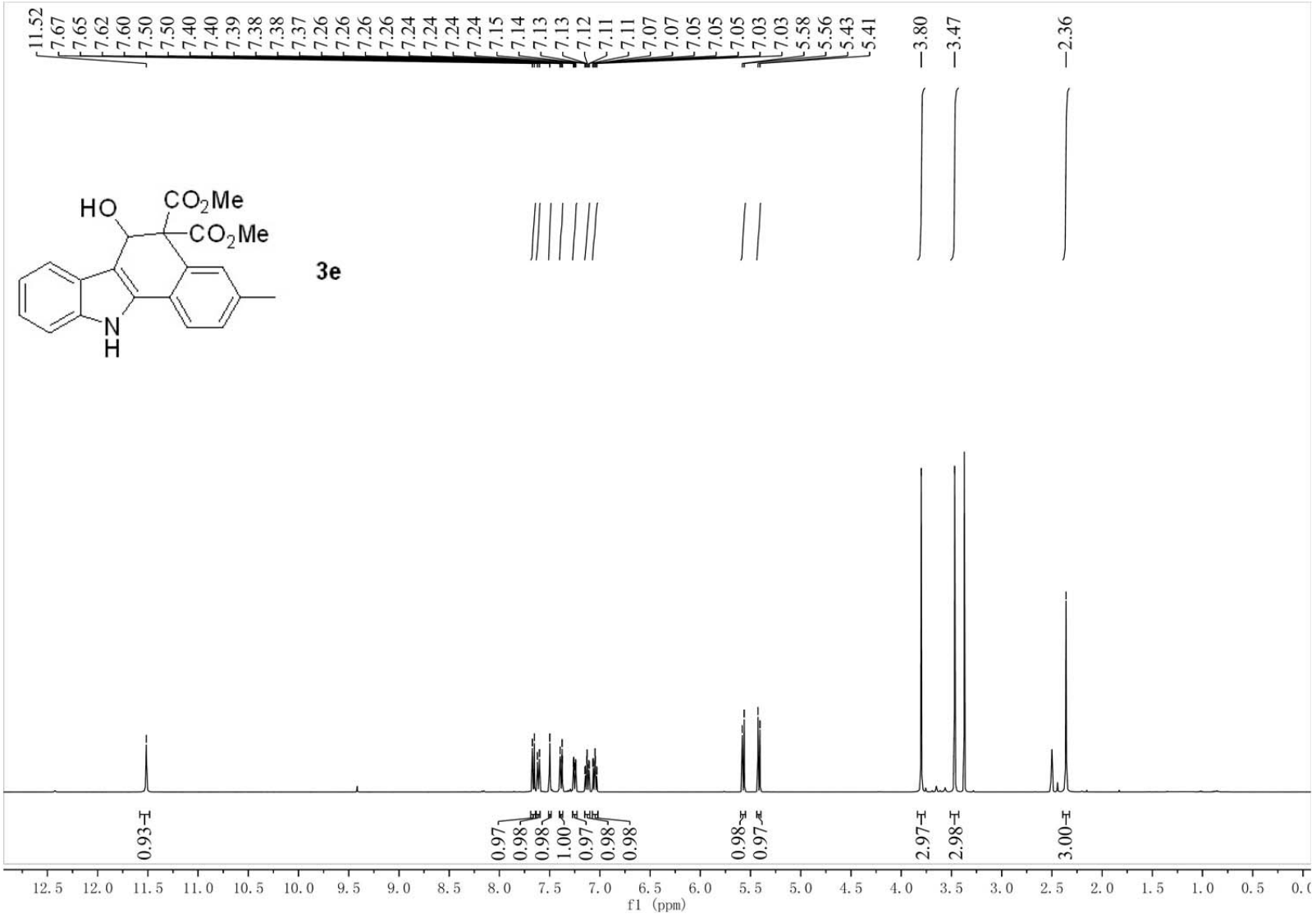
168.67
135.72
133.32
132.64
129.66
128.45
127.50
127.34
127.25
124.17
121.99
121.44
117.85
112.99
111.17
64.84
64.60
52.85
52.61
HO
CO2Me
CO2Me
Cl
N
H
3d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.67
7.65
7.62
7.60
7.50
7.50
7.40
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7.39
7.38
7.38
7.37
7.26
7.26
7.26
7.26
7.24
7.24
7.24
7.24
7.15
7.14
7.13
7.13
7.12
7.11
7.11
7.07
7.07
7.05
7.05
7.05
7.03
7.03
5.58
5.56
5.43
5.41
3.80
3.47
2.36
HO
CO2Me
CO2Me
N
H
3e
0.93
0.97
0.98
0.98
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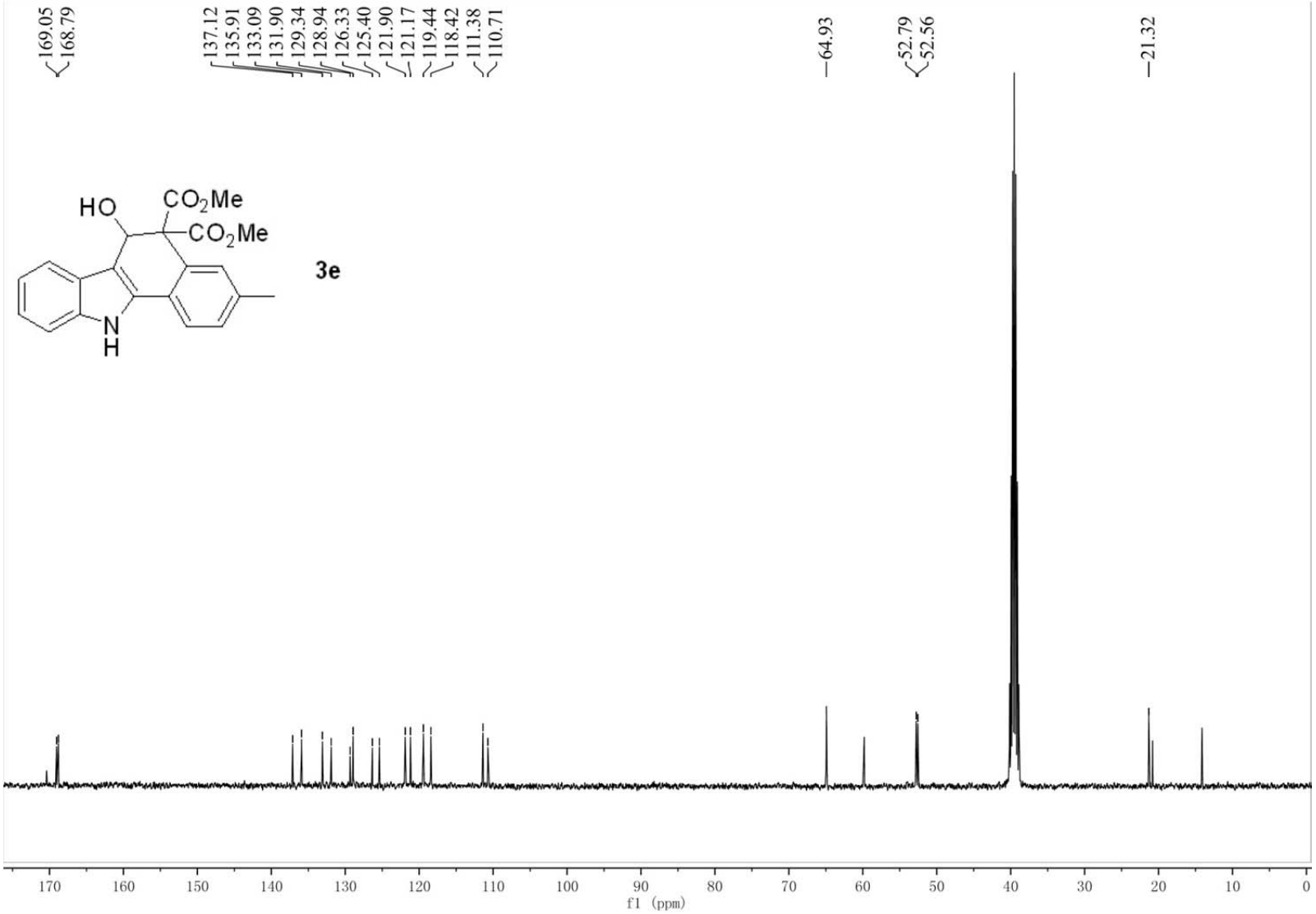
0.97
0.98
0.98
0.98
0.97
2.97
2.98
3.00
f1 (ppm)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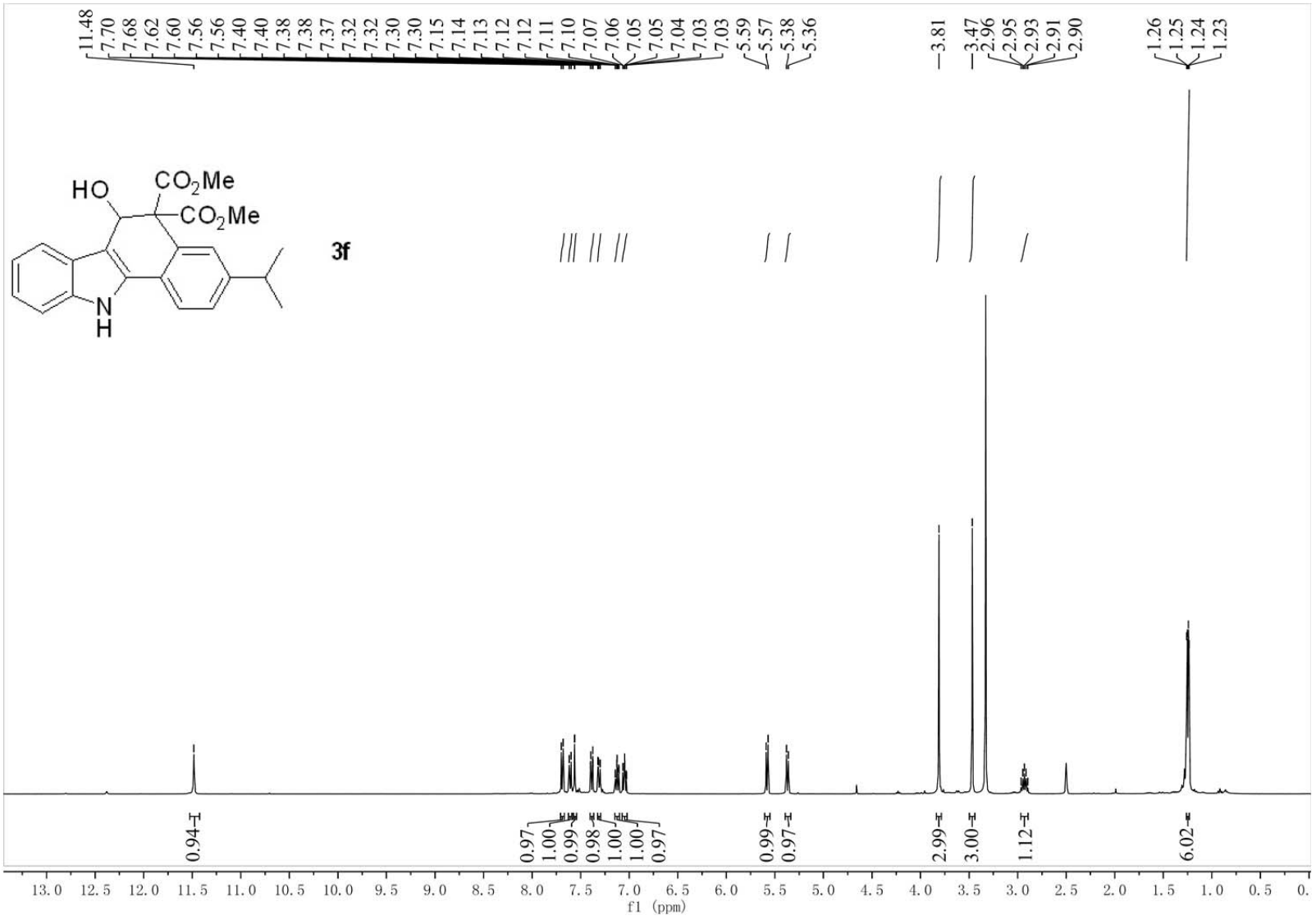
135.91
133.09
131.90
129.34
128.94
126.33
125.40
121.90
121.17
119.44
118.42
111.38
110.71
64.93
52.79
52.56
21.32
HO
CO2Me
CO2Me
N
H
3e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.68
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7.60
7.56
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7.40
7.40
7.38
7.38
7.37
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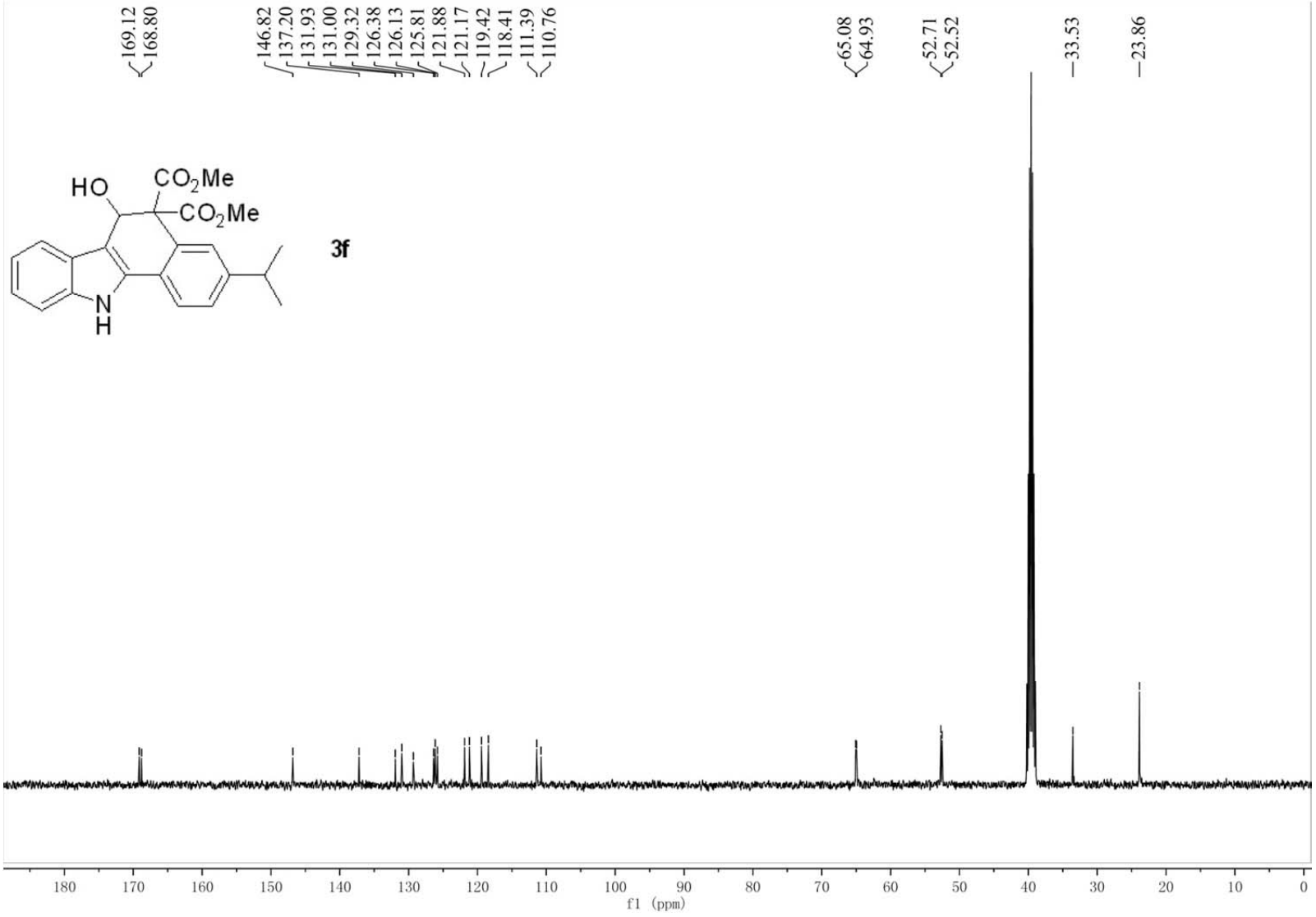
7.32
7.30
7.30
7.15
7.14
7.13
7.12
7.12
7.11
7.10
7.07
7.06
7.05
7.05
7.04
7.03
7.03
5.59
5.57
5.38
5.36
3.81
3.47
2.96
2.95
2.93
2.91
2.90
1.26
1.25
1.24
1.23
HO
CO2Me
CO2Me
N
H
3f
0.94
0.97
1.00
0.99
0.98
1.00
1.00
0.97
0.99
0.97
2.99
3.00
1.12
6.02
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 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.
f1 (ppm)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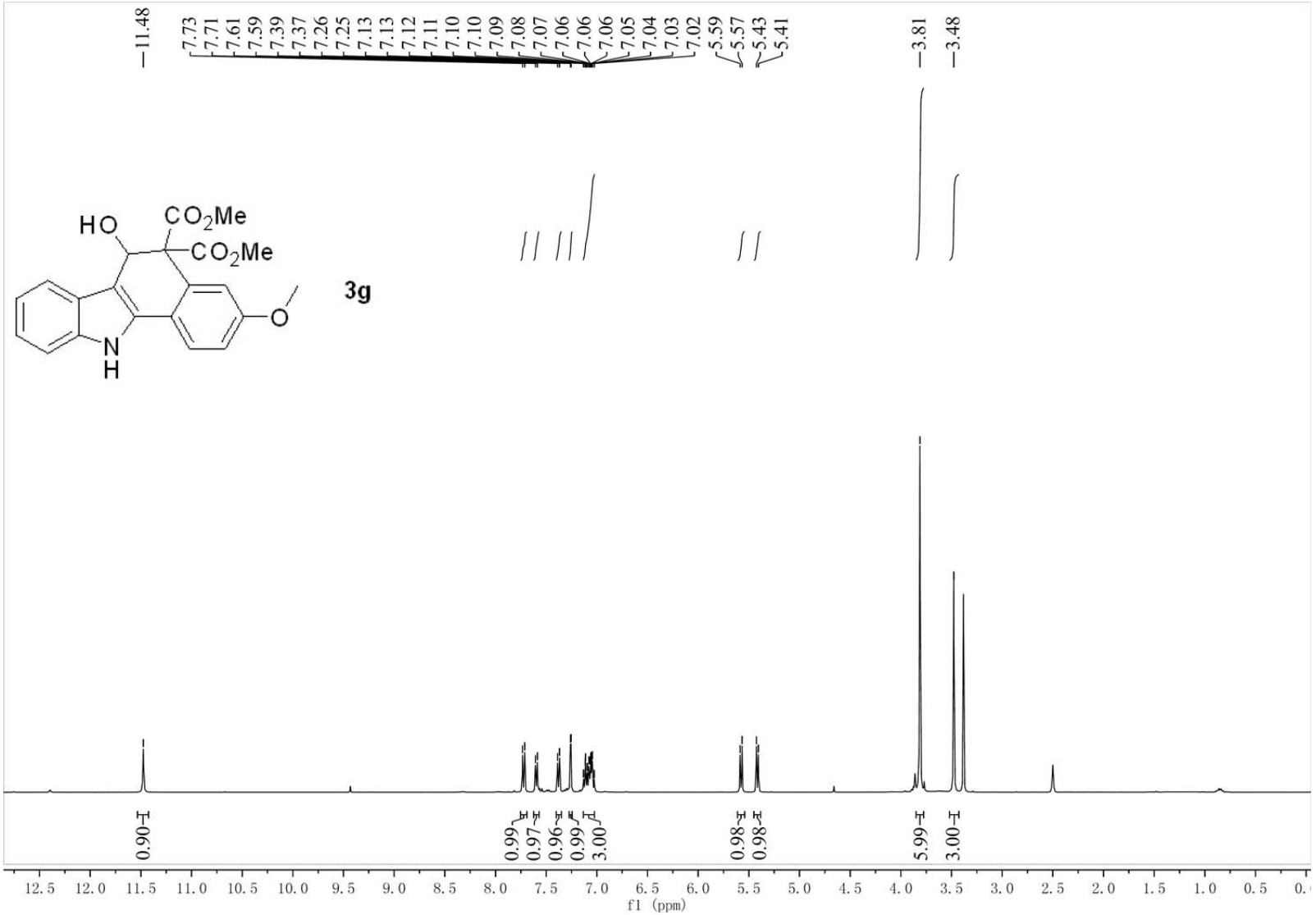
126.38
126.13
125.81
121.88
121.17
119.42
118.41
111.39
110.76
65.08
64.93
52.71
52.52
33.53
23.86
HO
CO2Me
CO2Me
N
H
3f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.71
7.61
7.59
7.39
7.37
7.26
7.25
7.13
7.13
7.12
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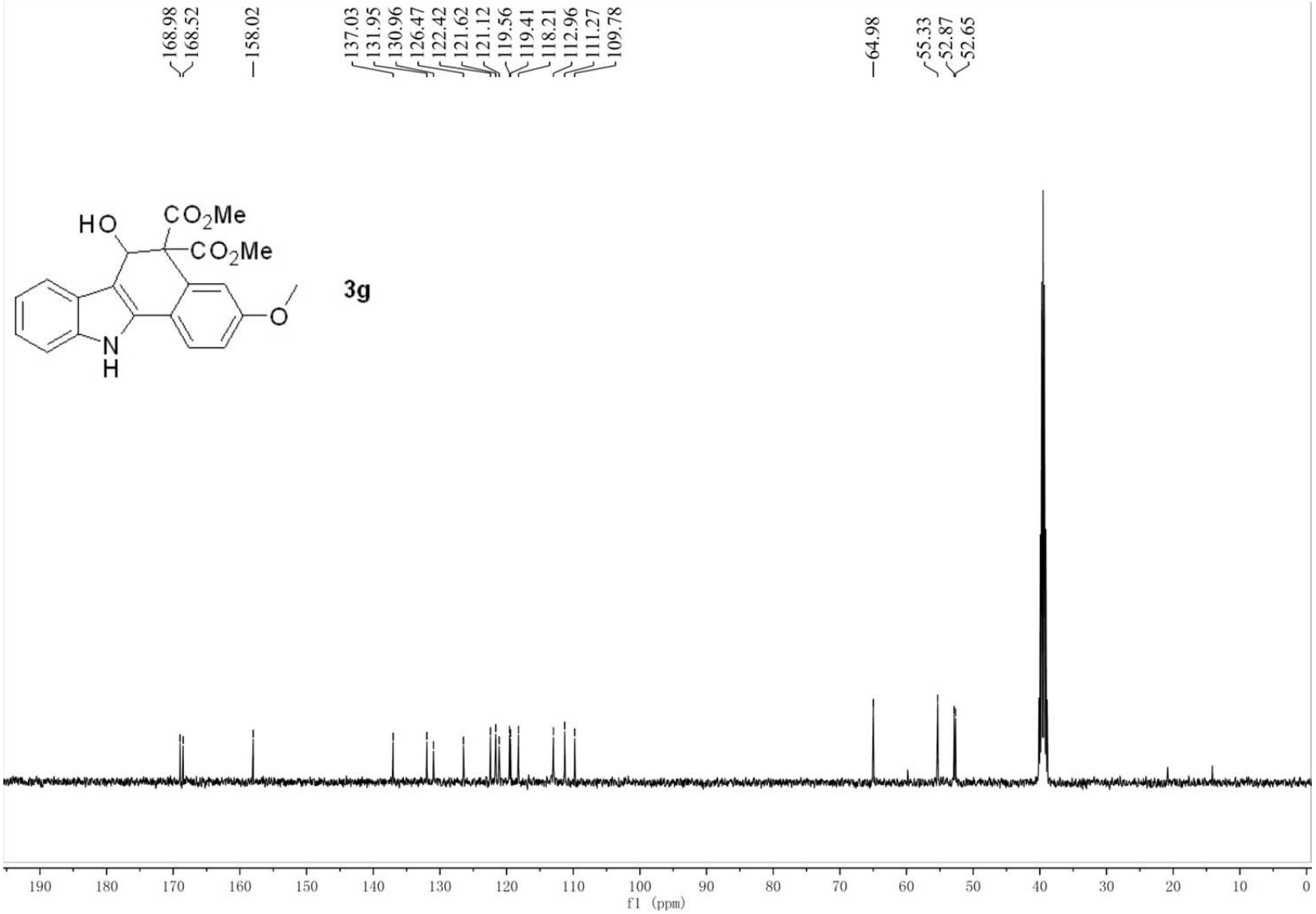
7.10
7.10
7.09
7.08
7.07
7.06
7.06
7.06
7.05
7.04
7.03
7.02
5.59
5.57
5.43
5.41
3.81
3.48
HO
CO2Me
CO2Me
O
N
H
3g
0.90
0.99
0.97
0.96
0.99
3.00
0.98
0.98
5.99
3.00
f1 (ppm)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168.52
158.02
137.03
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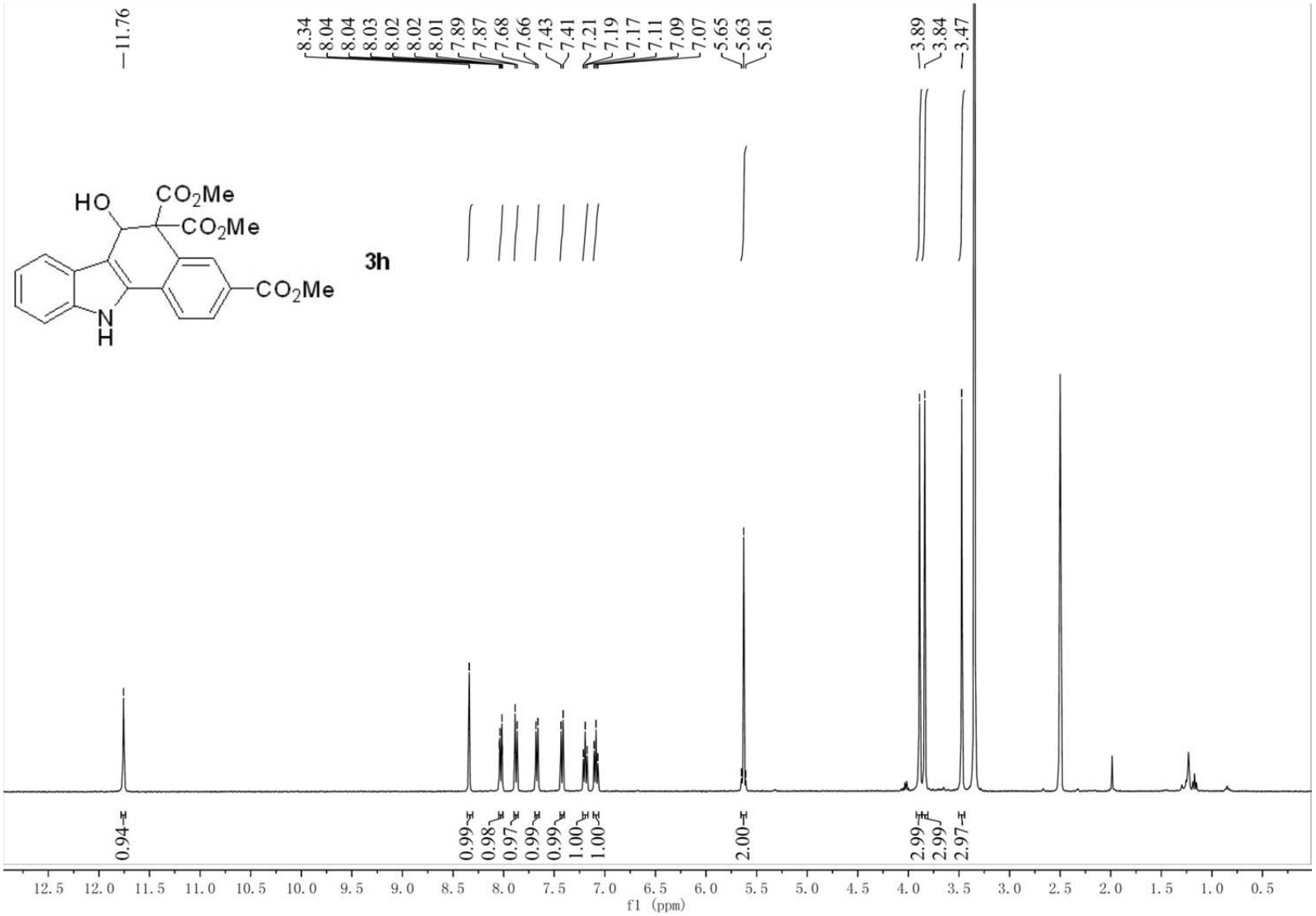
126.47
122.42
121.62
121.12
119.56
119.41
118.21
112.96
111.27
109.78
64.98
55.33
52.87
52.65
HO
CO2Me
CO2Me
O
N
H
3g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.04
8.03
8.02
8.02
8.01
7.89
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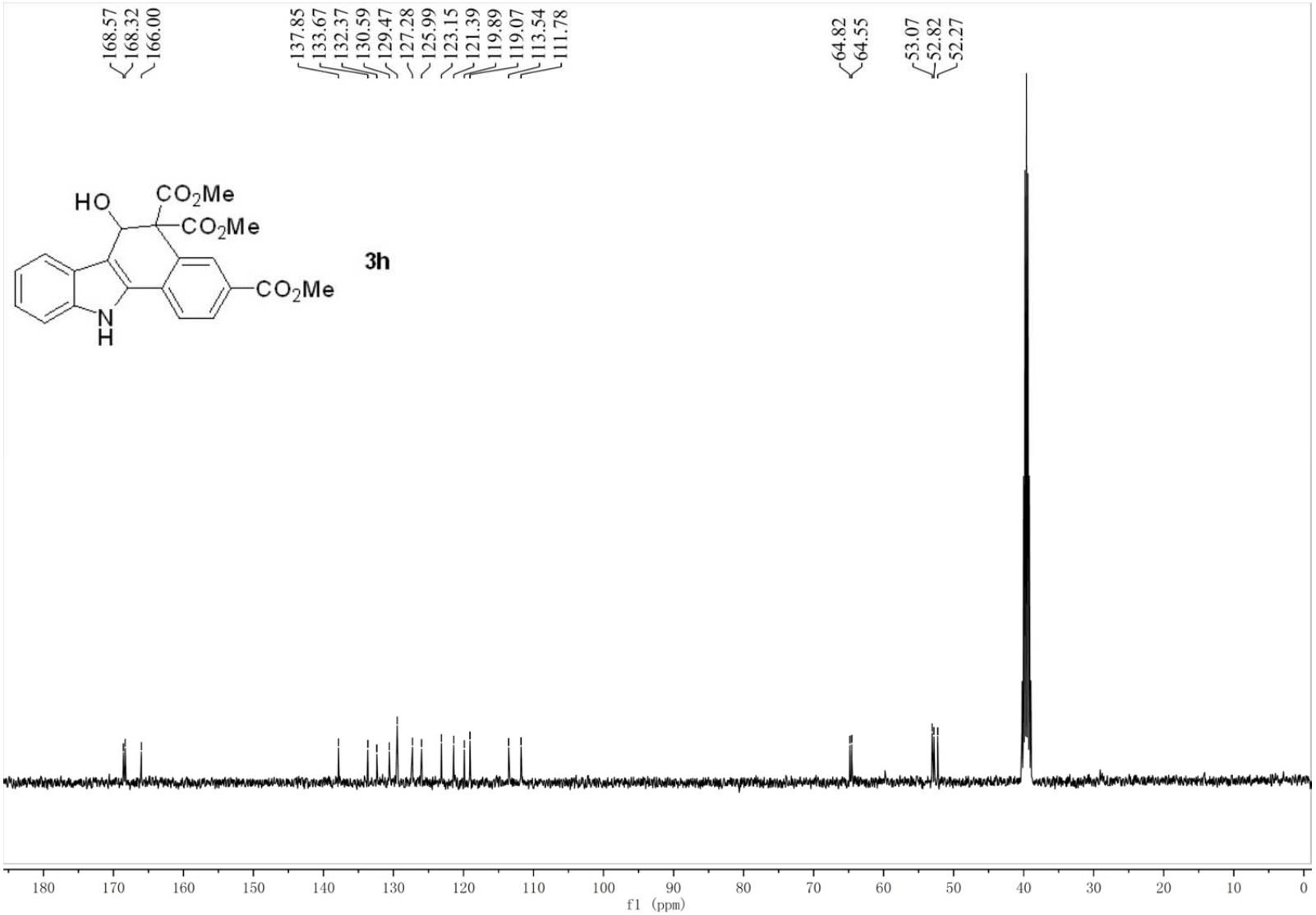
7.43
7.41
7.21
7.19
7.17
7.11
7.09
7.07
5.65
5.63
5.61
3.89
3.84
3.47
HO
CO2Me
CO2Me
CO2Me
N
H
3h
0.94
0.99
0.98
0.97
0.99
0.99
1.00
1.00
2.00
2.99
2.99
2.97
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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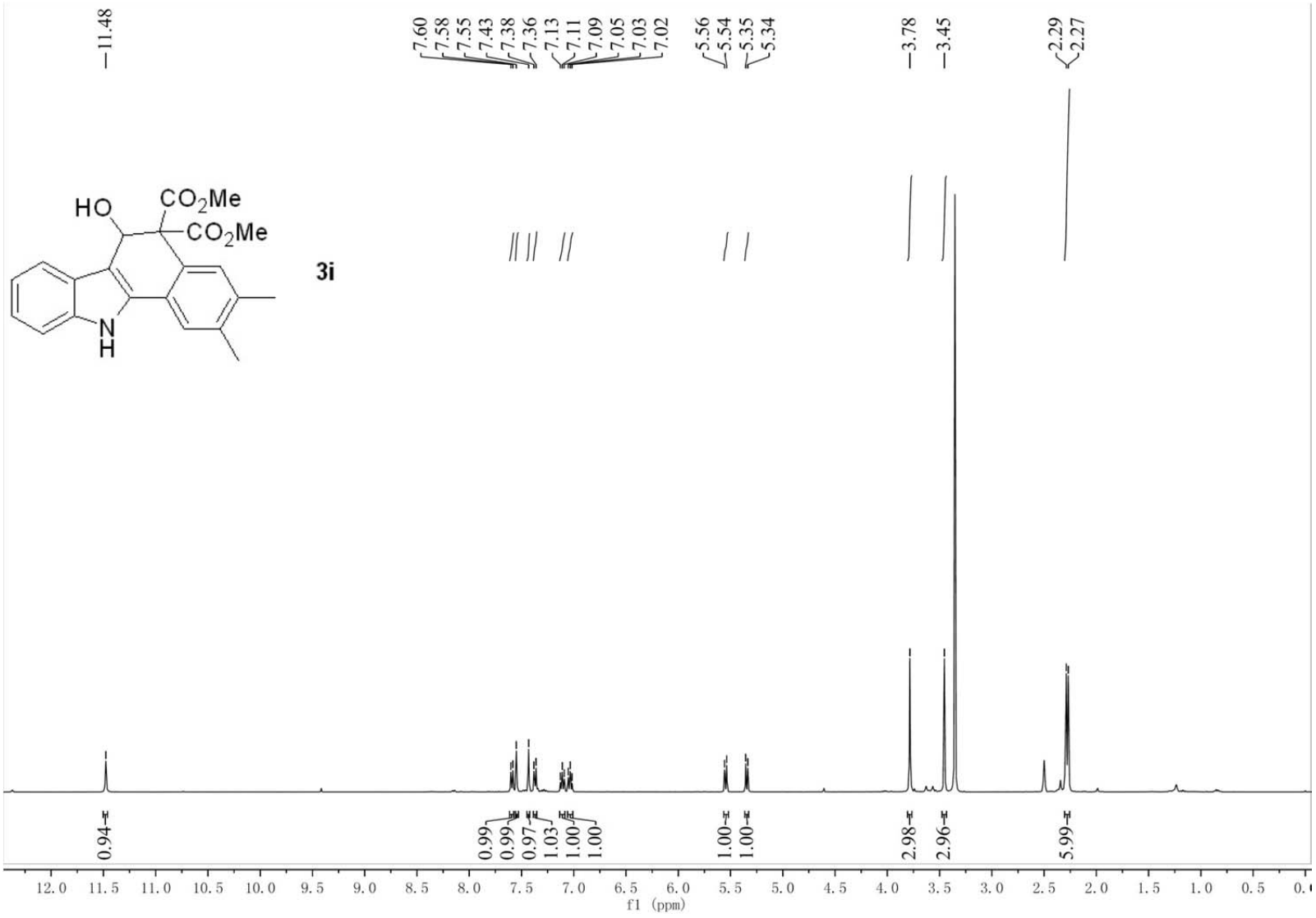
123.15
121.39
119.89
119.07
113.54
111.78
64.82
64.55
53.07
52.82
52.27
HO
CO2Me
CO2Me
CO2Me
N
H
3h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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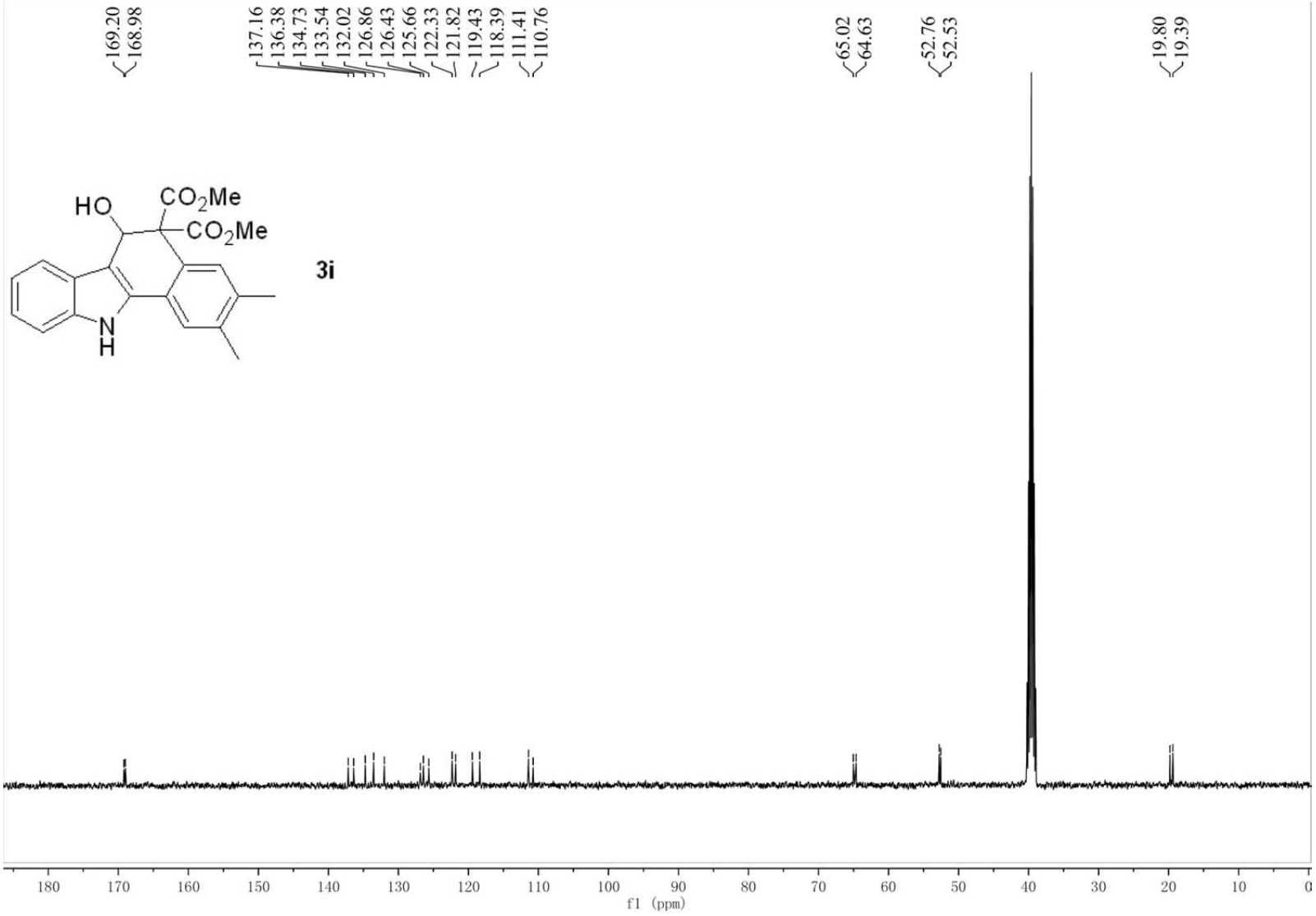
7.09
7.05
7.03
7.02
5.56
5.54
5.35
5.34
3.78
3.45
2.29
2.27
HO
CO2Me
CO2Me
N
H
3i
0.94
0.99
0.99
0.97
1.03
1.00
1.00
1.00
1.00
2.98
2.96
5.99
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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125.66
122.33
121.82
119.43
118.39
111.41
110.76
65.02
64.63
52.76
52.53
19.80
19.39
HO
CO2Me
CO2Me
N
H
3i
180
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100
90
80
70
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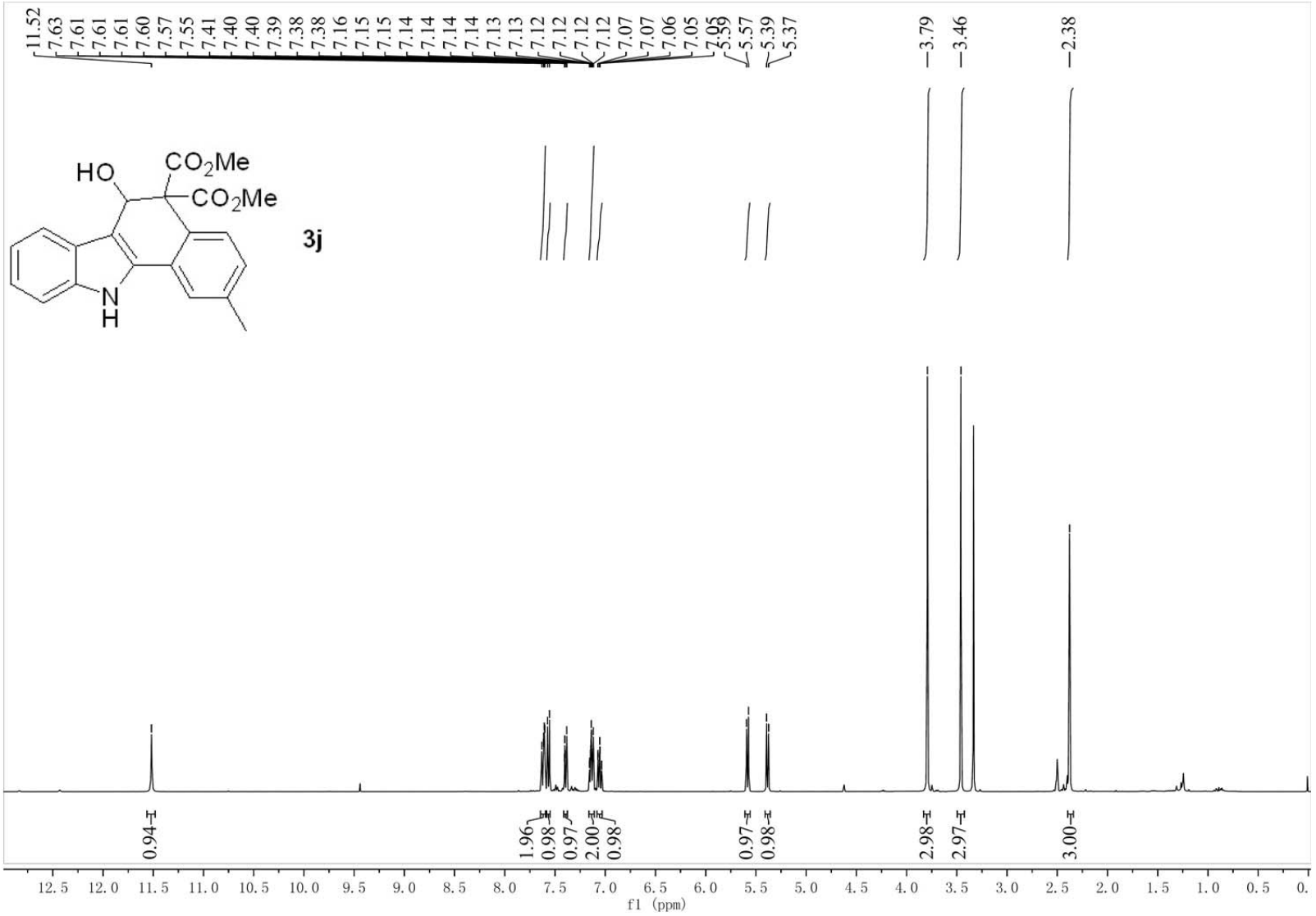
50
40
30
20
10
0
f1 (ppm)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7.61
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7.55
7.41
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7.39
7.38
7.38
7.16
7.15
7.15
7.14
7.14
7.14
7.14
7.13
7.13
7.12
7.12
7.12
7.12
7.07
7.07
7.06
7.05
5.59
5.57
5.39
5.37
3.79
3.46
2.38
HO
CO2Me
CO2Me
N
H
3j
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1.96
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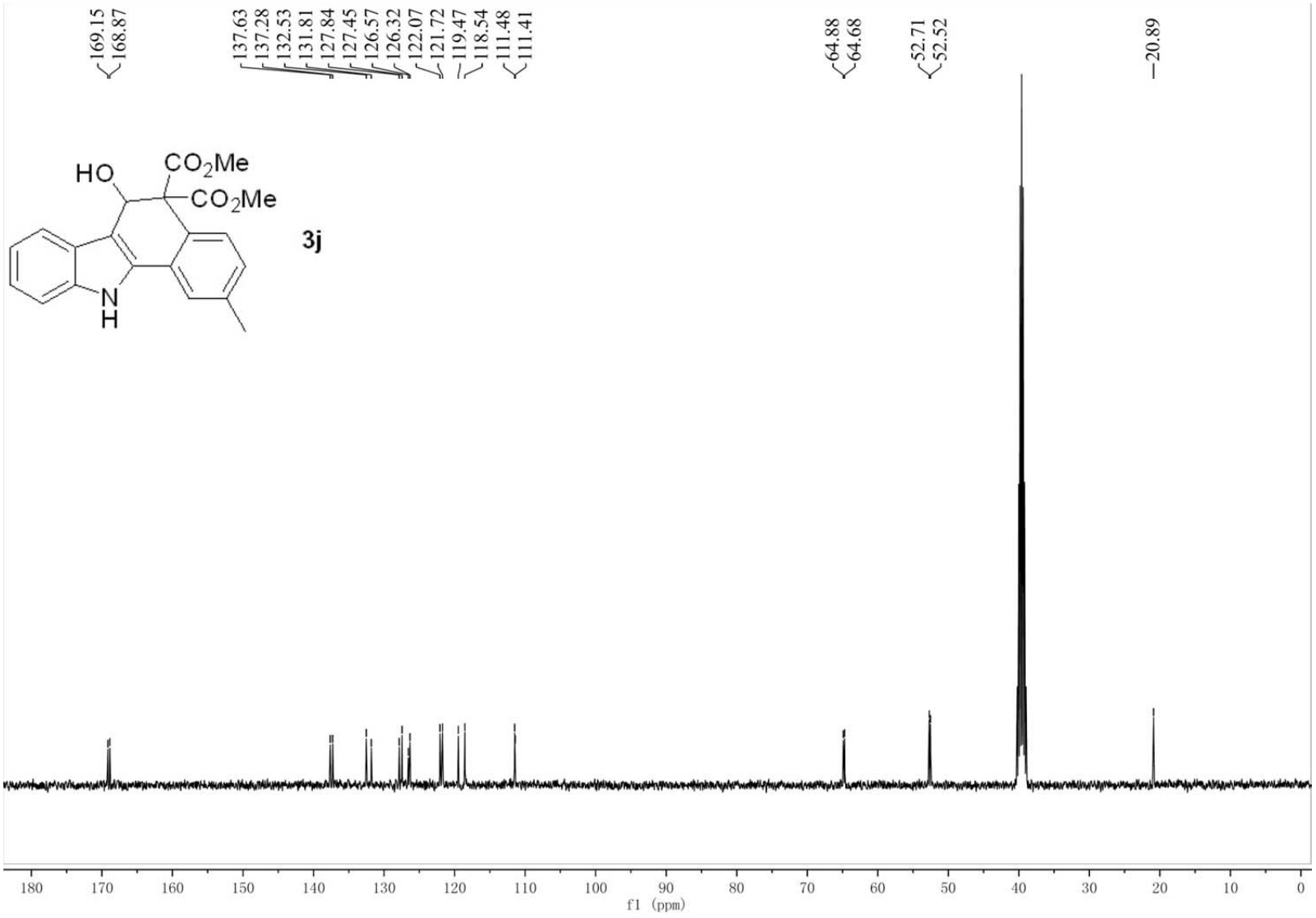
0.97
2.00
0.98
0.97
0.98
2.98
2.97
3.00
f1 (ppm)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126.32
122.07
121.72
119.47
118.54
111.48
111.41
64.88
64.68
52.71
52.52
20.89
HO
CO2Me
CO2Me
N
H
3j
180
170
160
150
140
130
120
110
100
90
80
70
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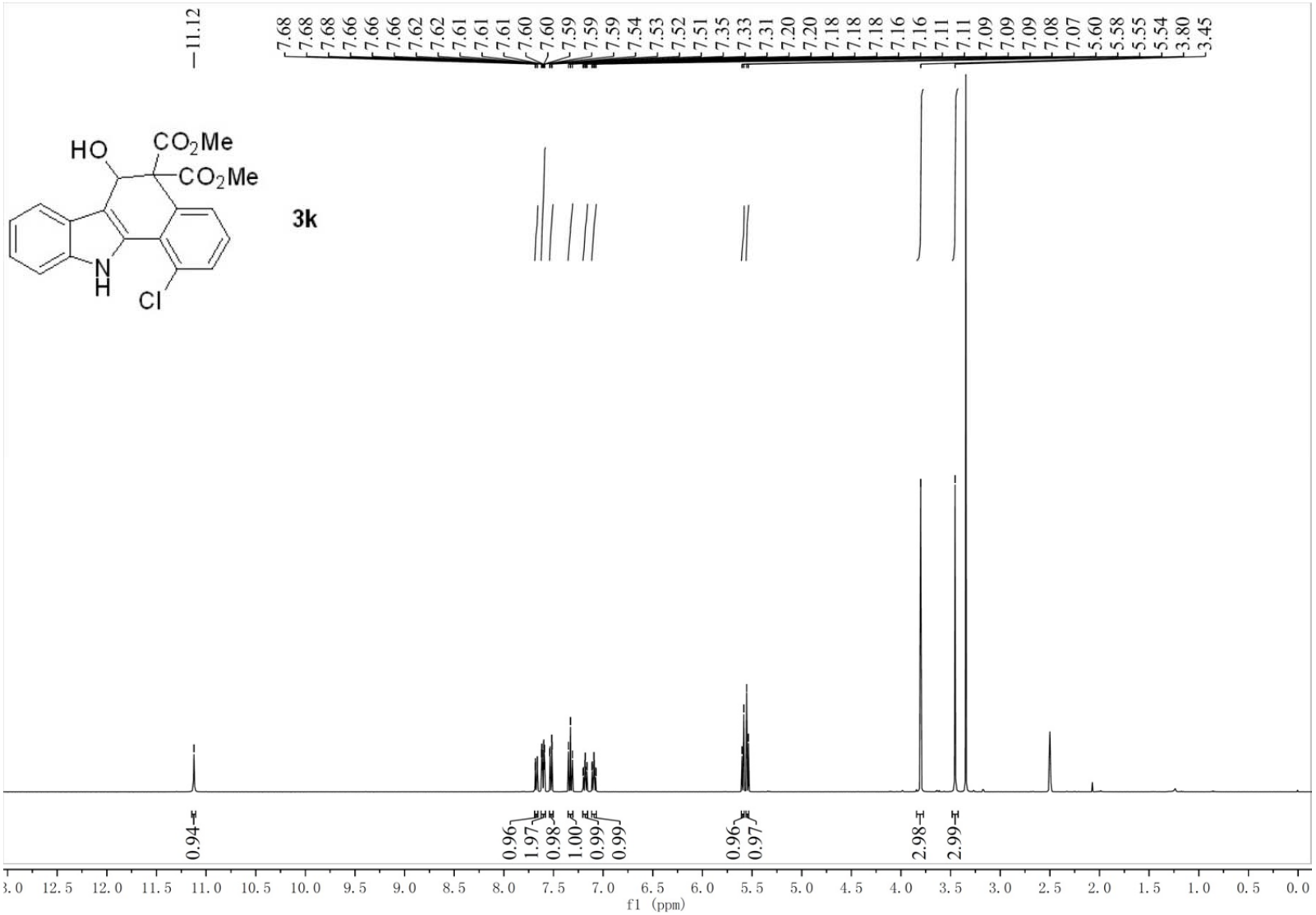
f1 (ppm)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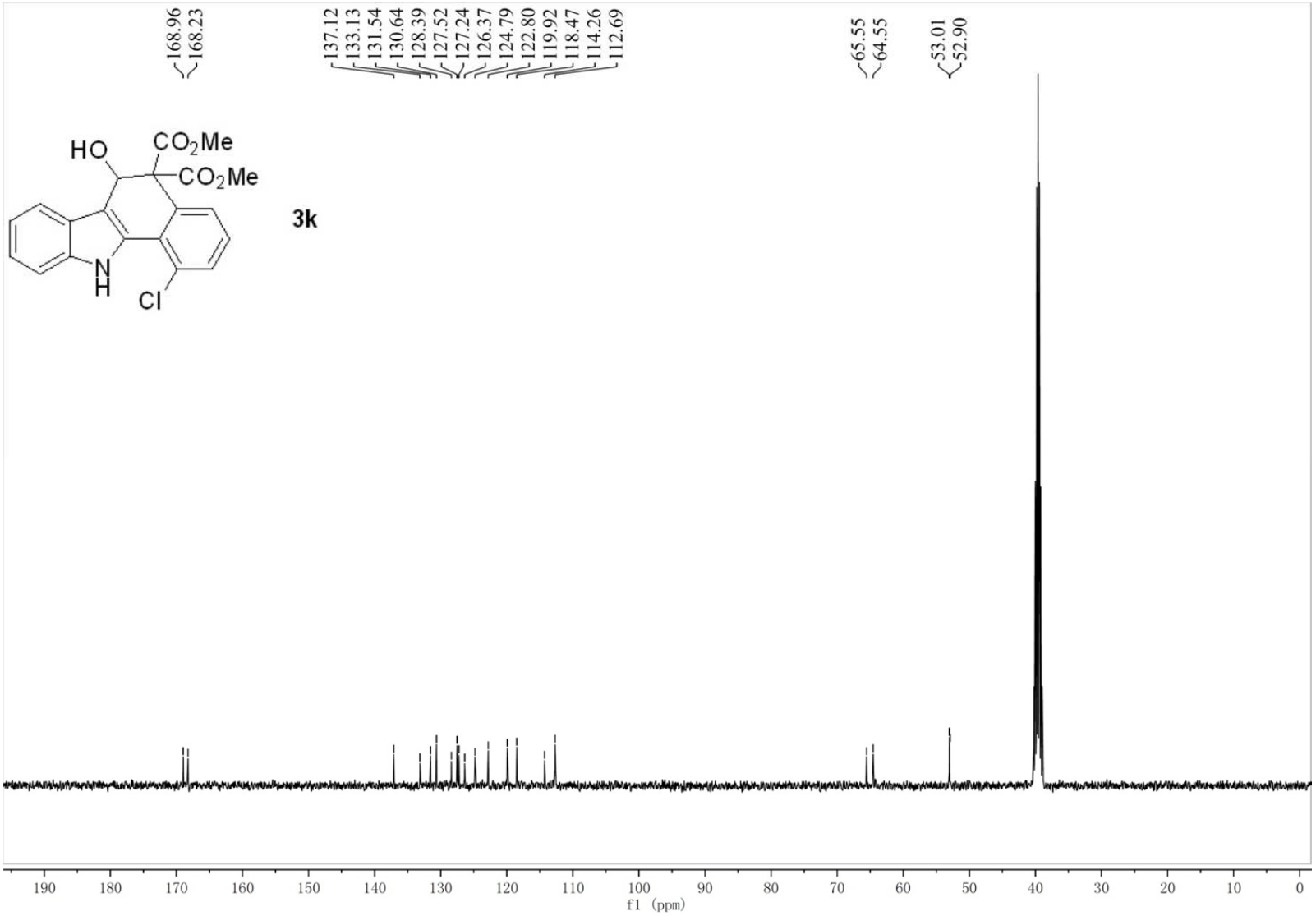
7.68
7.68
7.68
7.66
7.66
7.66
7.62
7.62
7.61
7.61
7.61
7.60
7.60
7.59
7.59
7.59
7.54
7.53
7.52
7.51
7.35
7.33
7.31
7.20
7.20
7.18
7.18
7.18
7.16
7.16
7.11
7.11
7.09
7.09
7.09
7.08
7.07
5.60
5.58
5.55
5.54
3.80
3.45
HO
CO2Me
CO2Me
N
H
Cl
3k
0.94
0.96
1.97
0.98
1.00
0.99
0.99
0.96
0.97
2.98
2.99
f1 (ppm)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130.64
128.39
127.52
127.24
126.37
124.79
122.80
119.92
118.47
114.26
112.69
65.55
64.55
53.01
52.90
HO
CO2Me
CO2Me
N
H
Cl
3k
190
180
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110
100
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50
40
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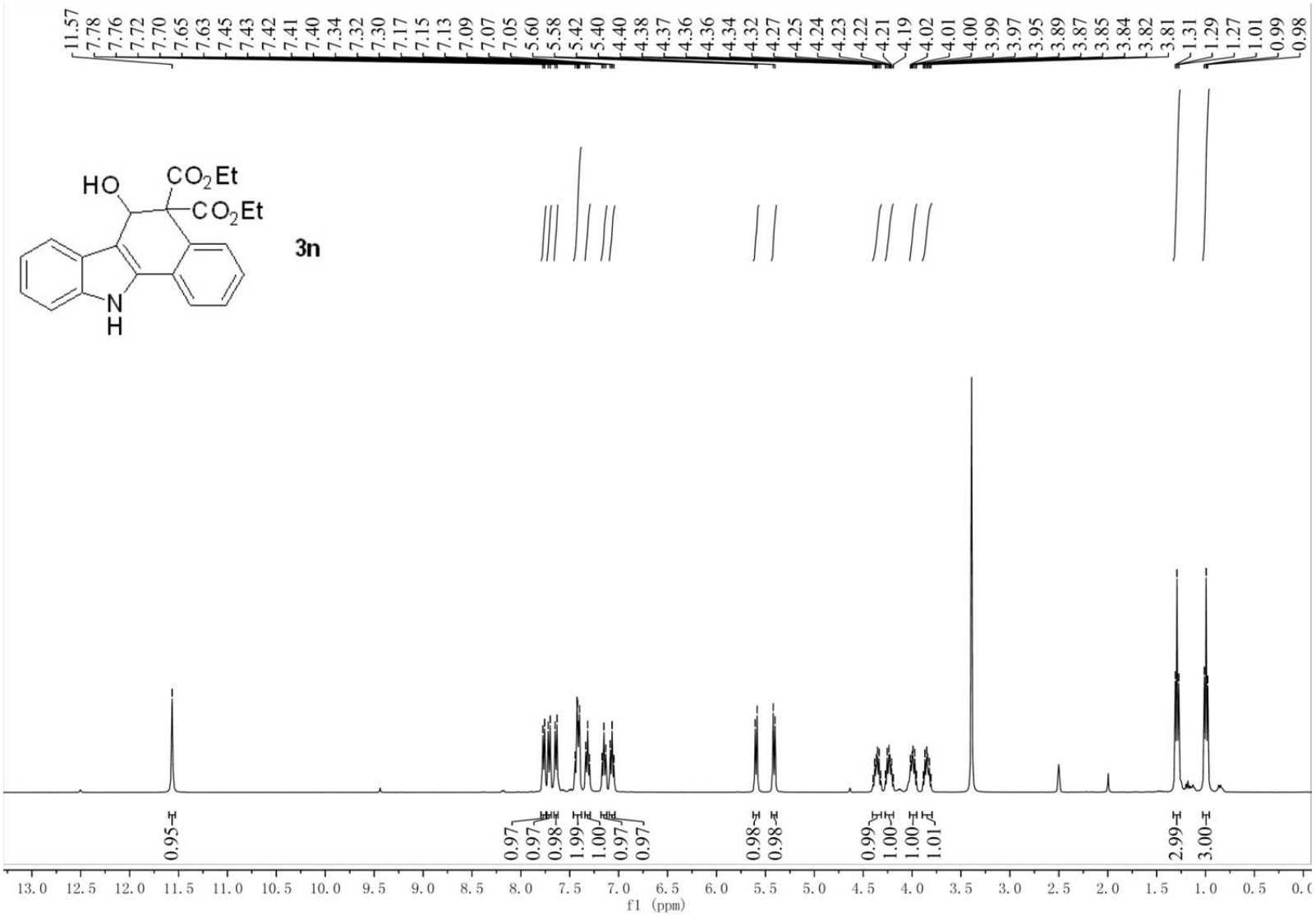
10
0
f1 (ppm)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7.45
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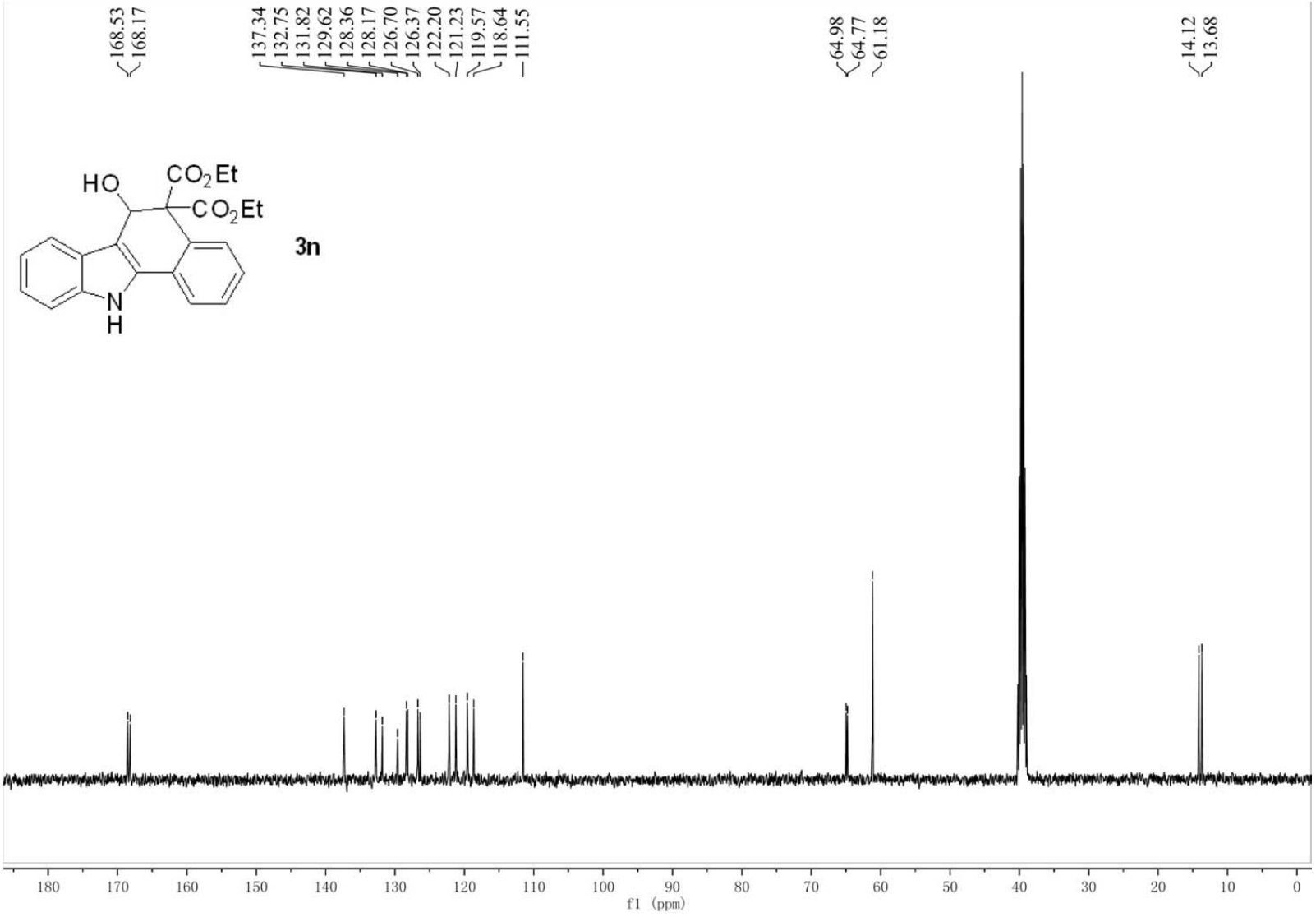
7.42
7.41
7.40
7.34
7.32
7.30
7.17
7.15
7.13
7.09
7.07
7.05
5.60
5.58
5.42
5.40
4.40
4.38
4.37
4.36
4.36
4.34
4.32
4.27
4.25
4.24
4.23
4.22
4.21
4.19
4.02
4.01
4.00
3.99
3.97
3.95
3.89
3.87
3.85
3.84
3.82
3.81
1.31
1.29
1.27
1.01
0.99
0.98
HO
CO2Et
CO2Et
N
H
3n
0.95
0.97
0.97
0.98
1.99
1.00
0.97
0.97
0.98
0.98
0.99
1.00
1.00
1.01
2.99
3.00
f1 (ppm)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131.82
129.62
128.36
128.17
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126.37
122.20
121.23
119.57
118.64
111.55
64.98
64.77
61.18
14.12
13.68
HO
CO2Et
CO2Et
N
H
3n
180
170
160
150
140
130
120
110
100
90
80
70
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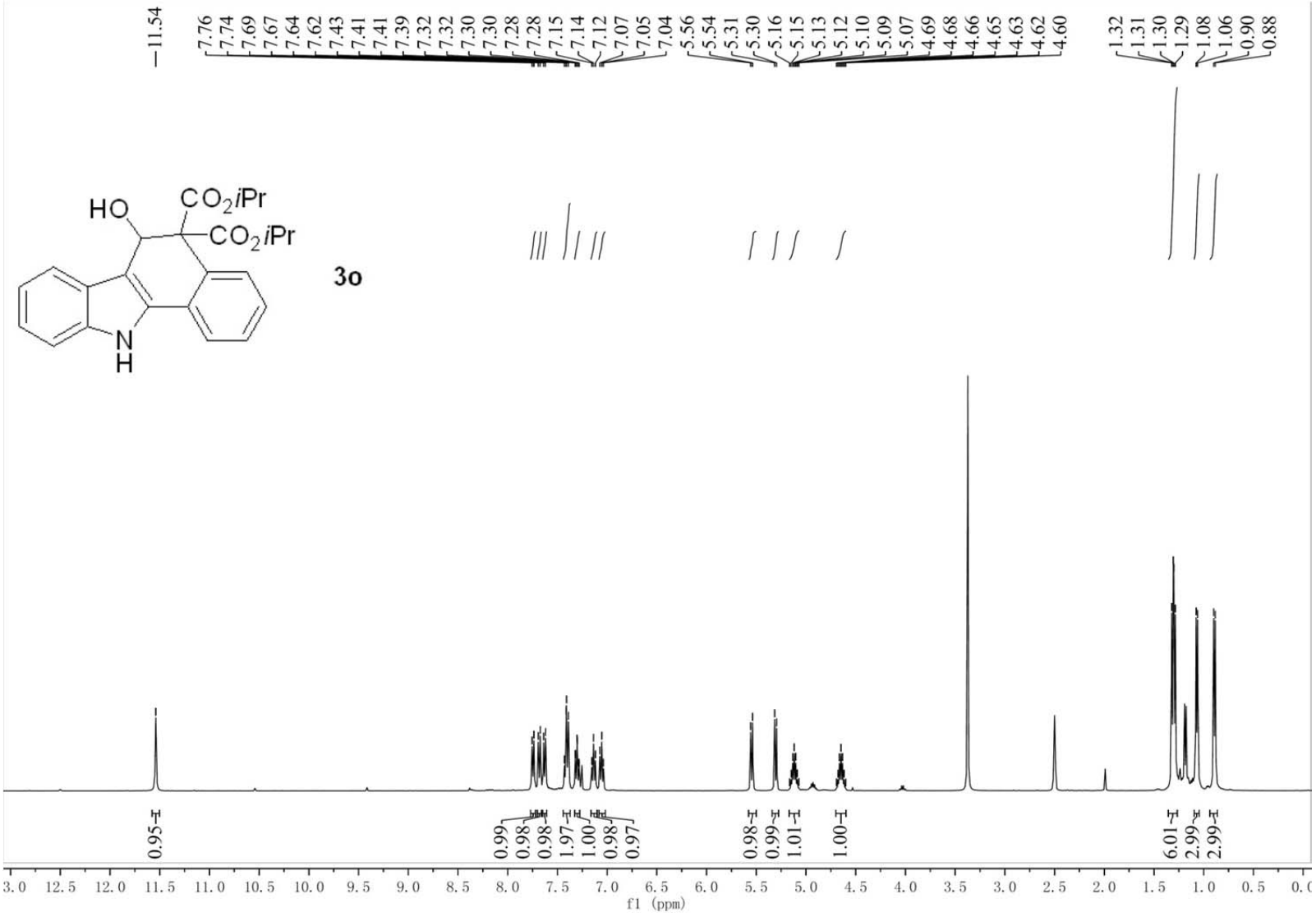
50
40
30
20
10
0
f1 (ppm)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7.74
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7.64
7.62
7.43
7.41
7.41
7.39
7.32
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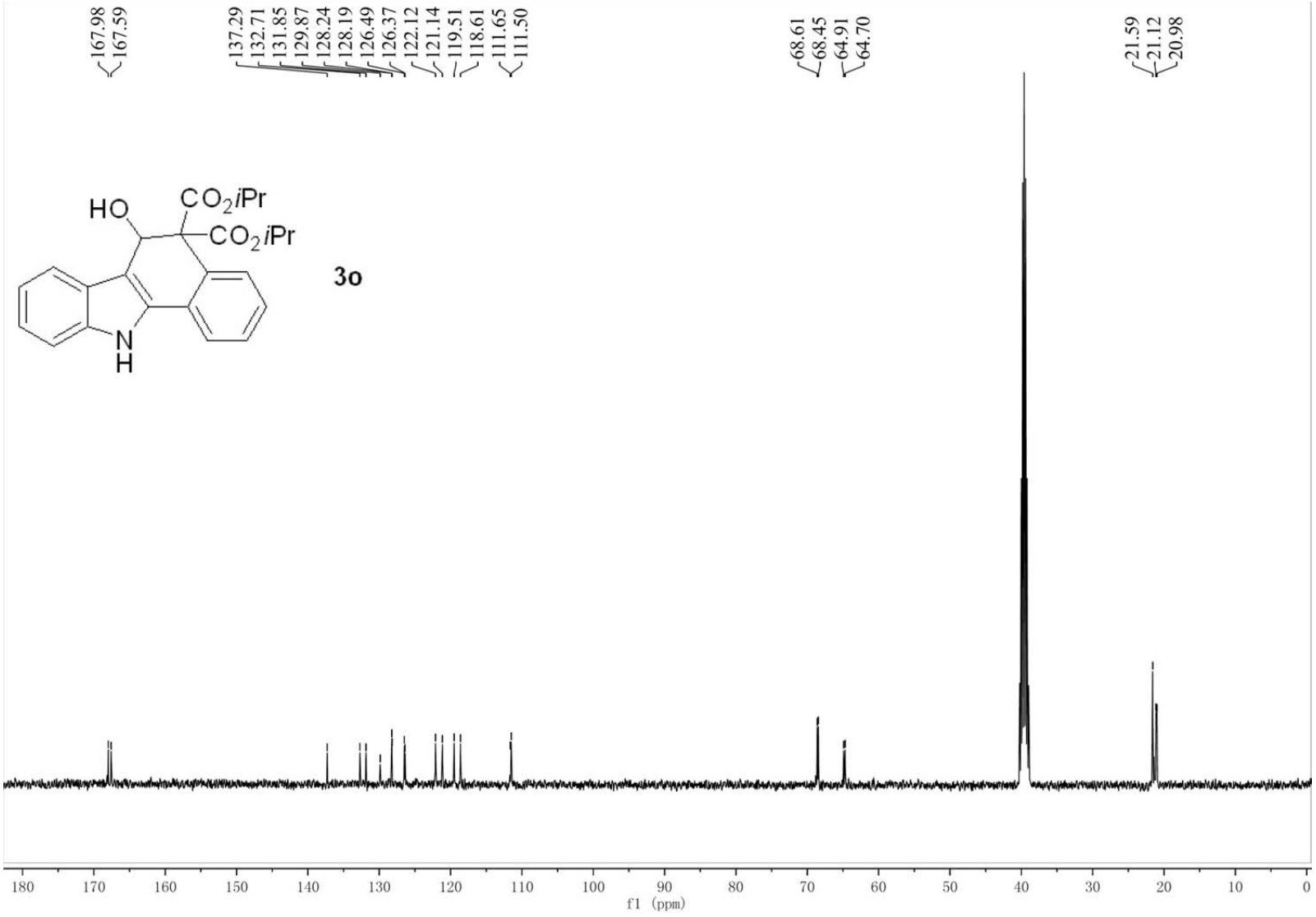
7.30
7.30
7.28
7.28
7.15
7.14
7.12
7.07
7.05
7.04
5.56
5.54
5.31
5.30
5.16
5.15
5.13
5.12
5.10
5.09
5.07
4.69
4.68
4.66
4.65
4.63
4.62
4.60
1.32
1.31
1.30
1.29
1.08
1.06
0.90
0.88
HO
CO2iPr
CO2iPr
N
H
3o
0.95
0.99
0.98
0.98
1.97
1.00
0.98
0.97
0.98
0.99
1.01
1.00
6.01
2.99
2.99
f1 (ppm)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128.19
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126.37
122.12
121.14
119.51
118.61
111.65
111.50
68.61
68.45
64.91
64.70
21.59
21.12
20.98
HO
CO2iPr
CO2iPr
N
H
3o
180
170
160
150
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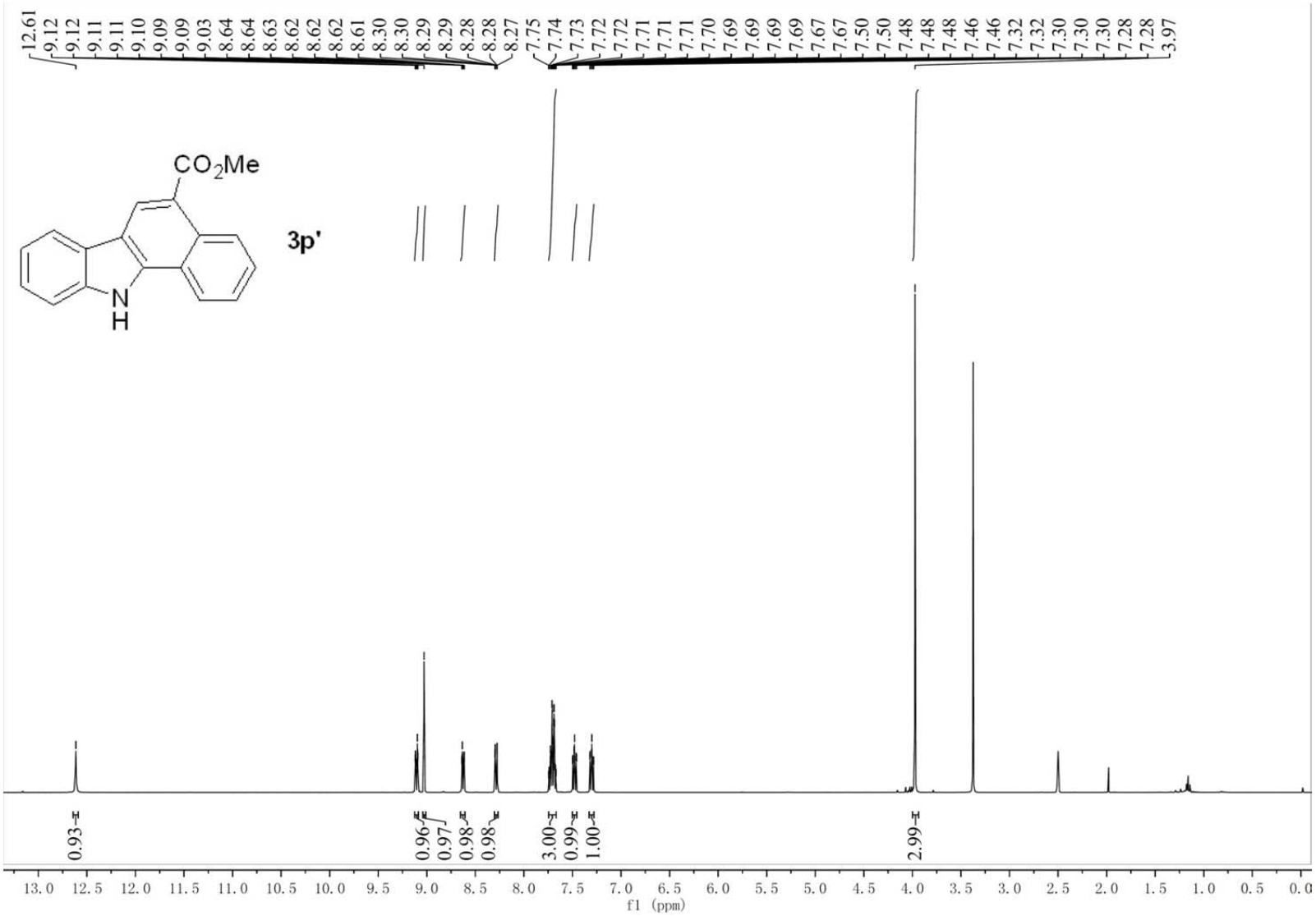
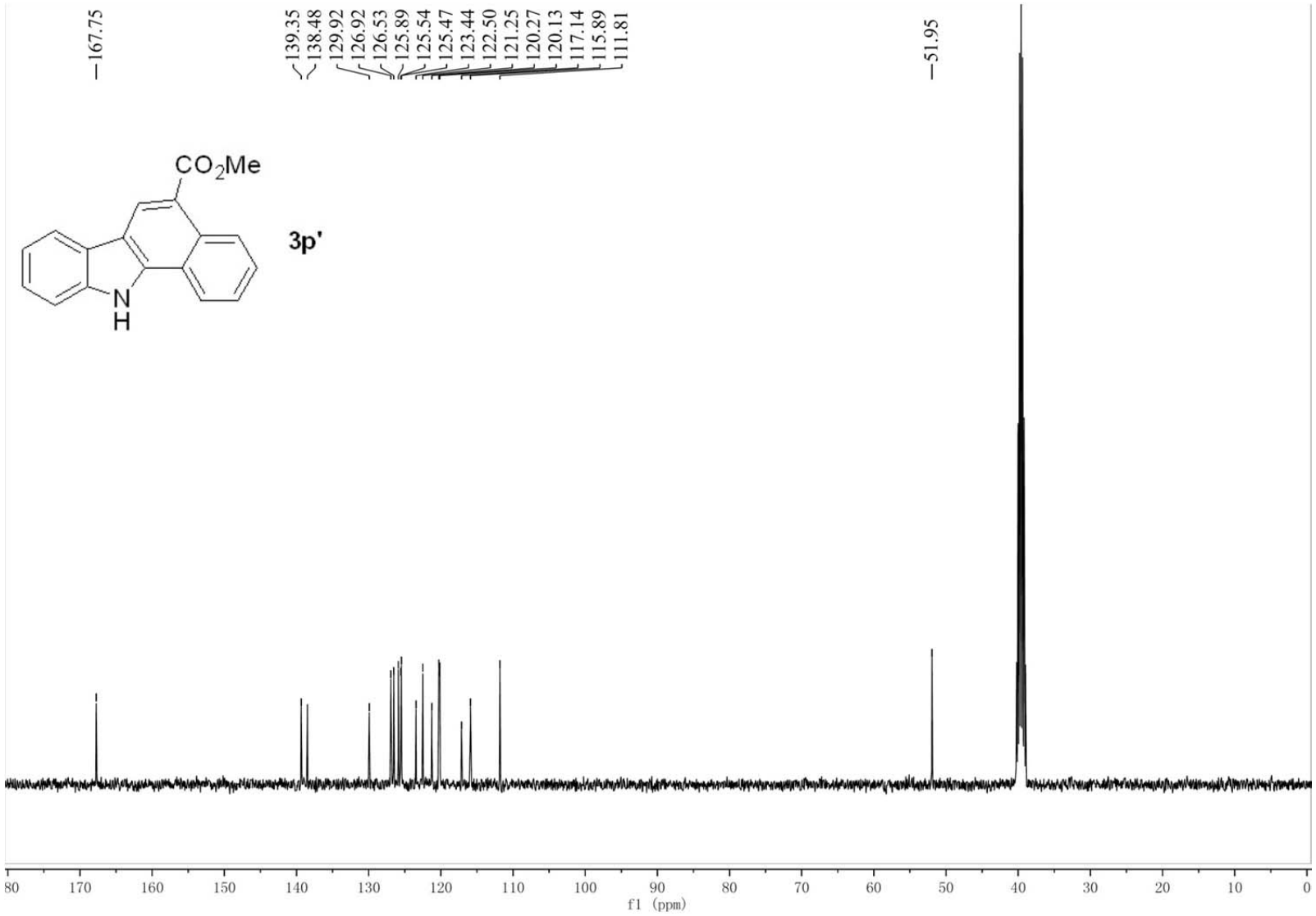
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.61
9.12
9.12
9.11
9.11
9.10
9.09
9.09
9.03
8.64
8.64
8.63
8.62
8.62
8.62
8.61
8.30
8.30
8.29
8.29
8.28
8.28
8.27
7.75
7.74
7.73
7.72
7.72
7.71
7.71
7.71
7.70
7.69
7.69
7.69
7.69
7.67
7.67
7.50
7.50
7.48
7.48
7.48
7.46
7.46
7.32
7.32
7.30
7.30
7.30
7.28
7.28
3.97
CO2Me
N
H
3p'
0.93
0.96
0.97
0.98
0.98
3.00
0.99
1.00
2.99
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
f1 (ppm)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138.48
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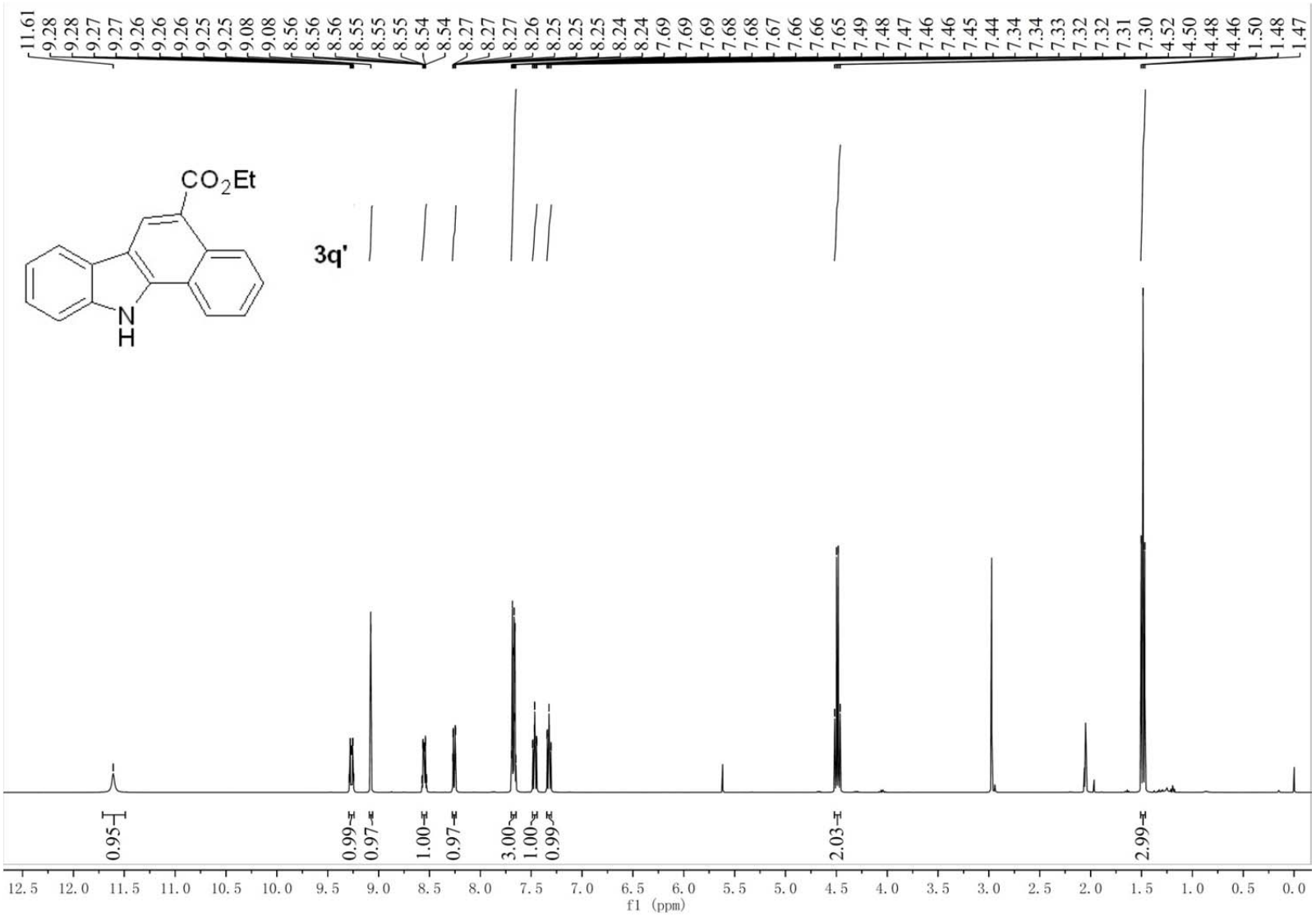
126.92
126.53
125.89
125.54
125.47
123.44
122.50
121.25
120.27
120.13
117.14
115.89
111.81
51.95
CO2Me
N
H
3p'
f1 (ppm)


11.61
9.28
9.28
9.27
9.27
9.26
9.26
9.26
9.25
9.25
9.08
9.08
8.56
8.56
8.56
8.55
8.55
8.55
8.54
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8.27
8.27
8.27
8.26
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8.25
8.25
8.24
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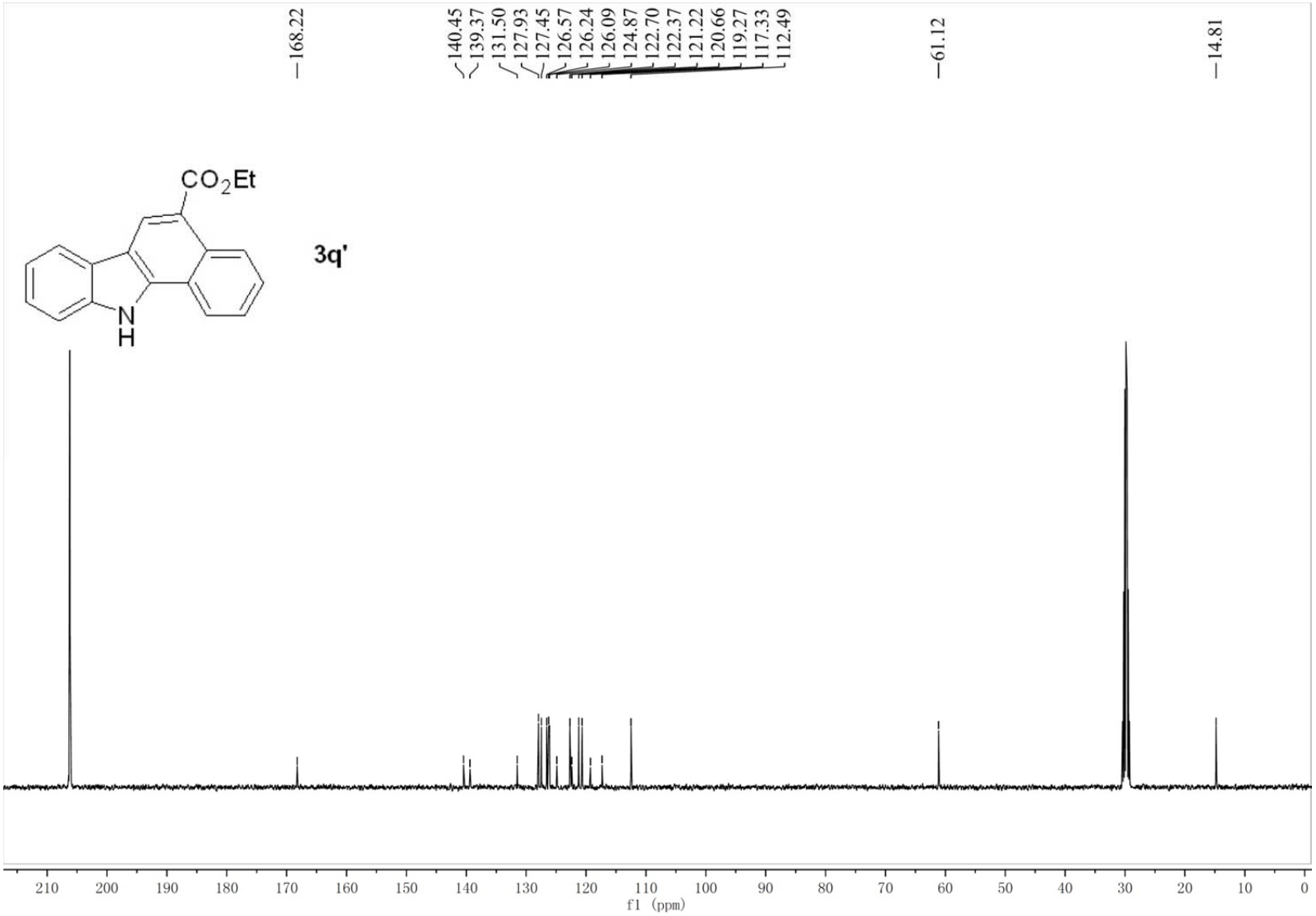
7.66
7.66
7.65
7.49
7.48
7.47
7.46
7.46
7.45
7.44
7.34
7.34
7.33
7.32
7.32
7.31
7.30
4.52
4.50
4.48
4.46
1.50
1.48
1.47
CO2Et
N
H
3q'
0.95
0.99
0.97
1.00
0.97
3.00
1.00
0.99
2.03
2.99
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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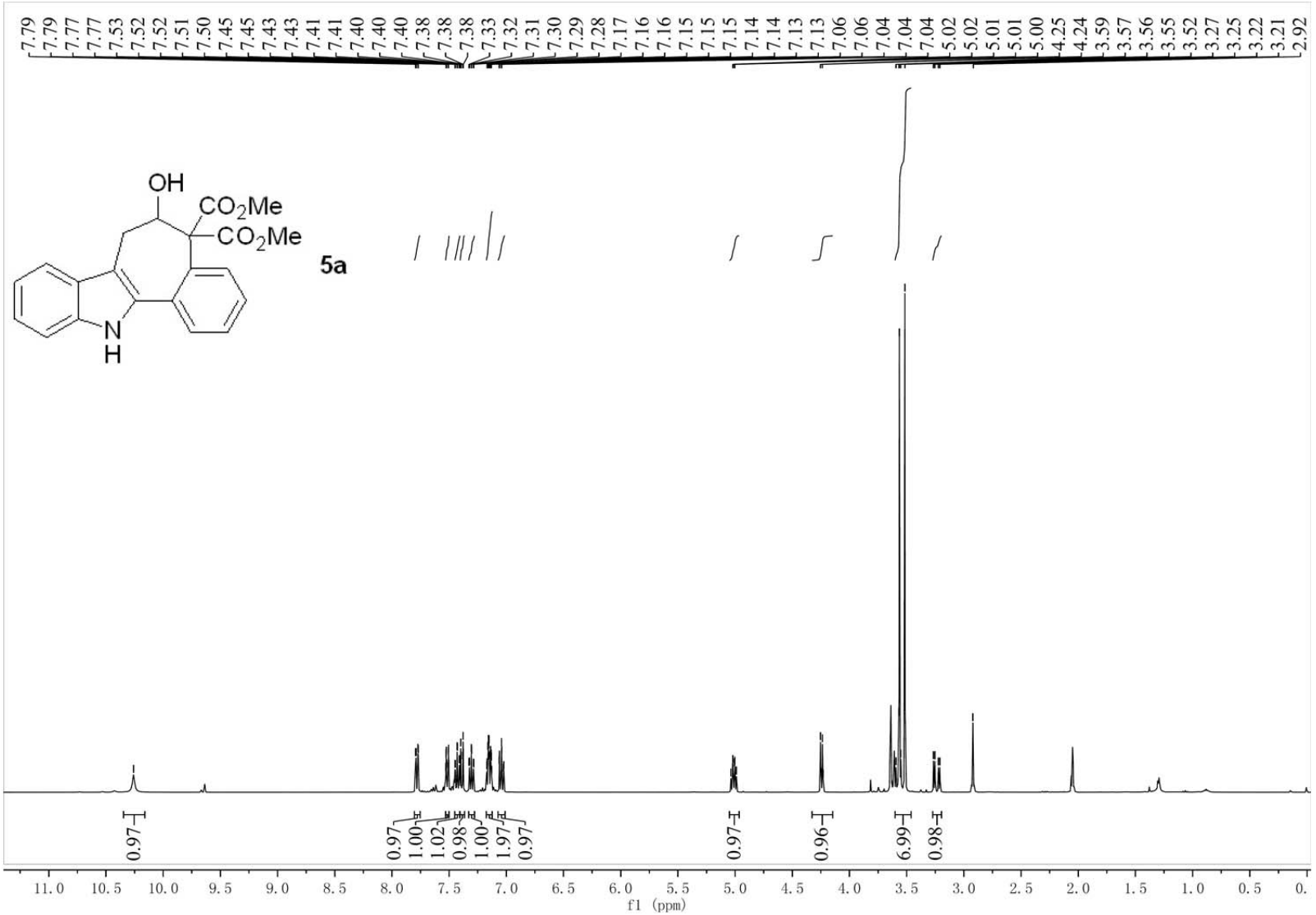
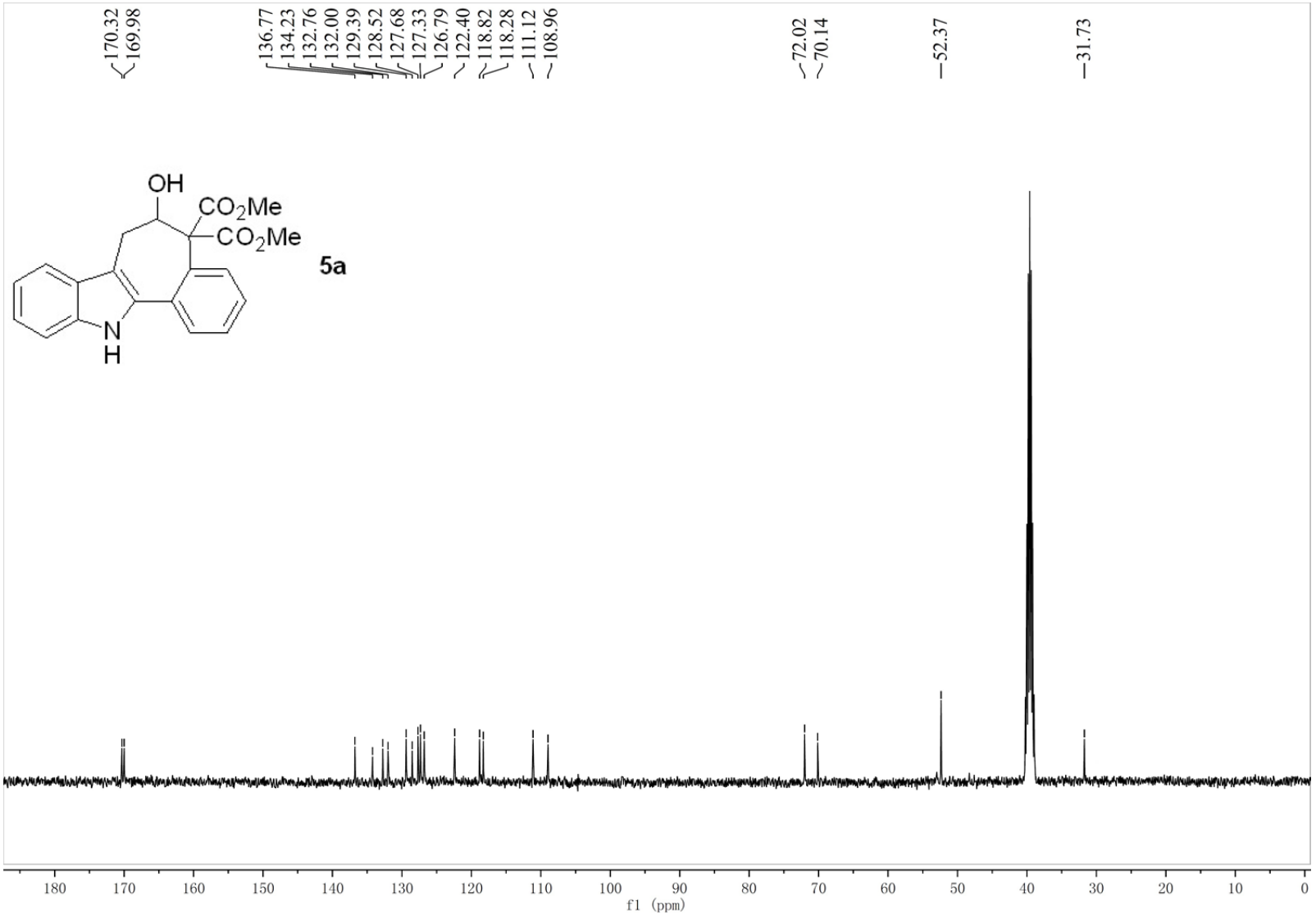
127.45
126.57
126.24
126.09
124.87
122.70
122.37
121.22
120.66
119.27
117.33
112.49
61.12
14.81
CO2Et
N
H
3q'
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OH
CO2Me
CO2Me
N
H
5a
7.79 7.79 7.77 7.77 7.53 7.52 7.52 7.51 7.50 7.45 7.45 7.43 7.43 7.41 7.41 7.40 7.40 7.40 7.38 7.38 7.38 7.33 7.32 7.31 7.30 7.29 7.28 7.17 7.16 7.16 7.15 7.15 7.15 7.14 7.14 7.13 7.13 7.06 7.06 7.04 7.04 7.04 5.02 5.02 5.01 5.01 5.00 4.25 4.24 3.59 3.57 3.56 3.55 3.52 3.27 3.25 3.22 3.21 2.92
0.97 0.97 1.00 1.02 0.98 1.00 1.97 0.97 0.97 0.96 6.99 0.98
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.
f1 (ppm)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169.98
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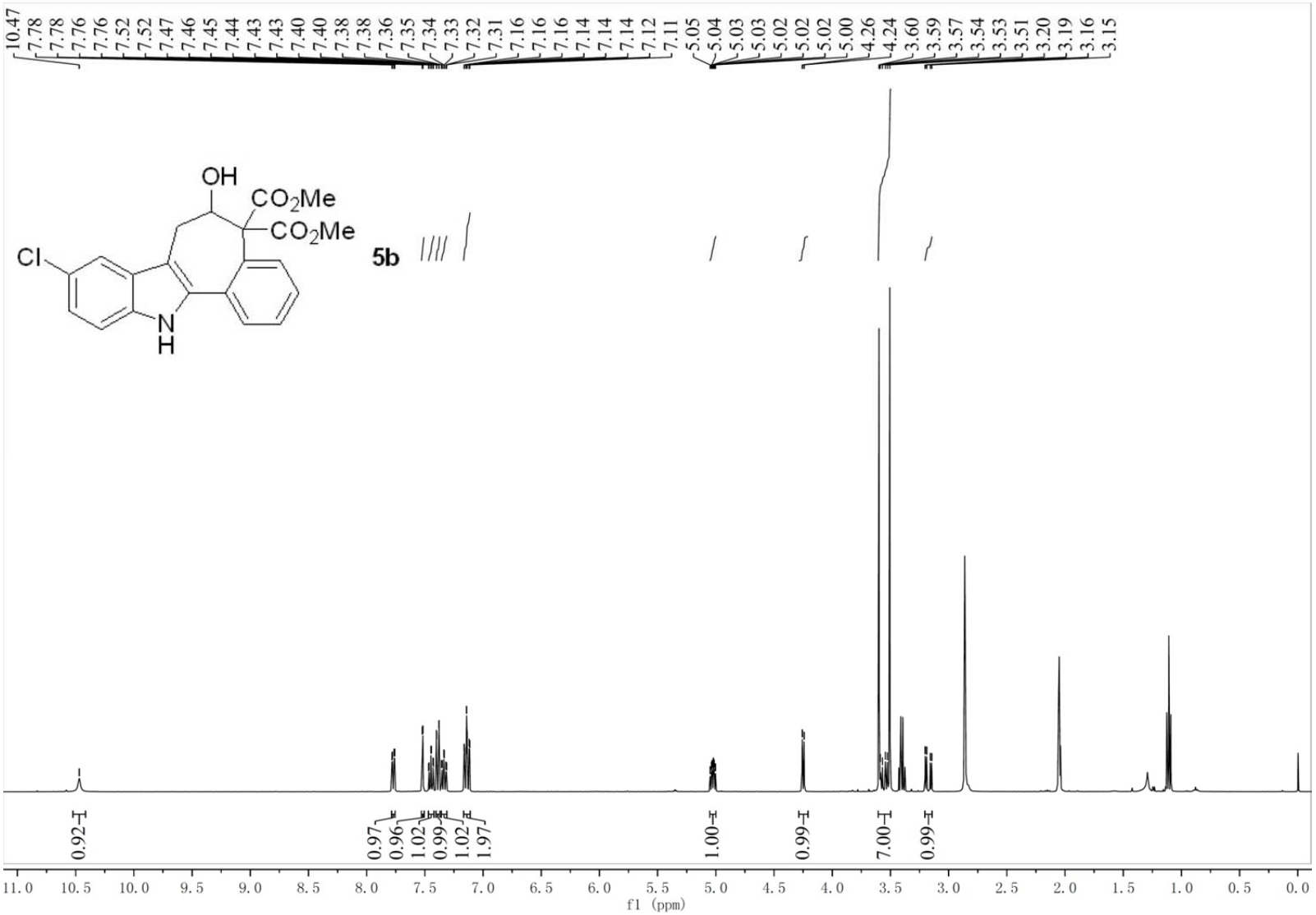
134.23
132.76
132.00
129.39
128.52
127.68
127.33
126.79
122.40
118.82
118.28
111.12
108.96
72.02
70.14
52.37
31.73
OH
CO2Me
CO2Me
N
H
5a
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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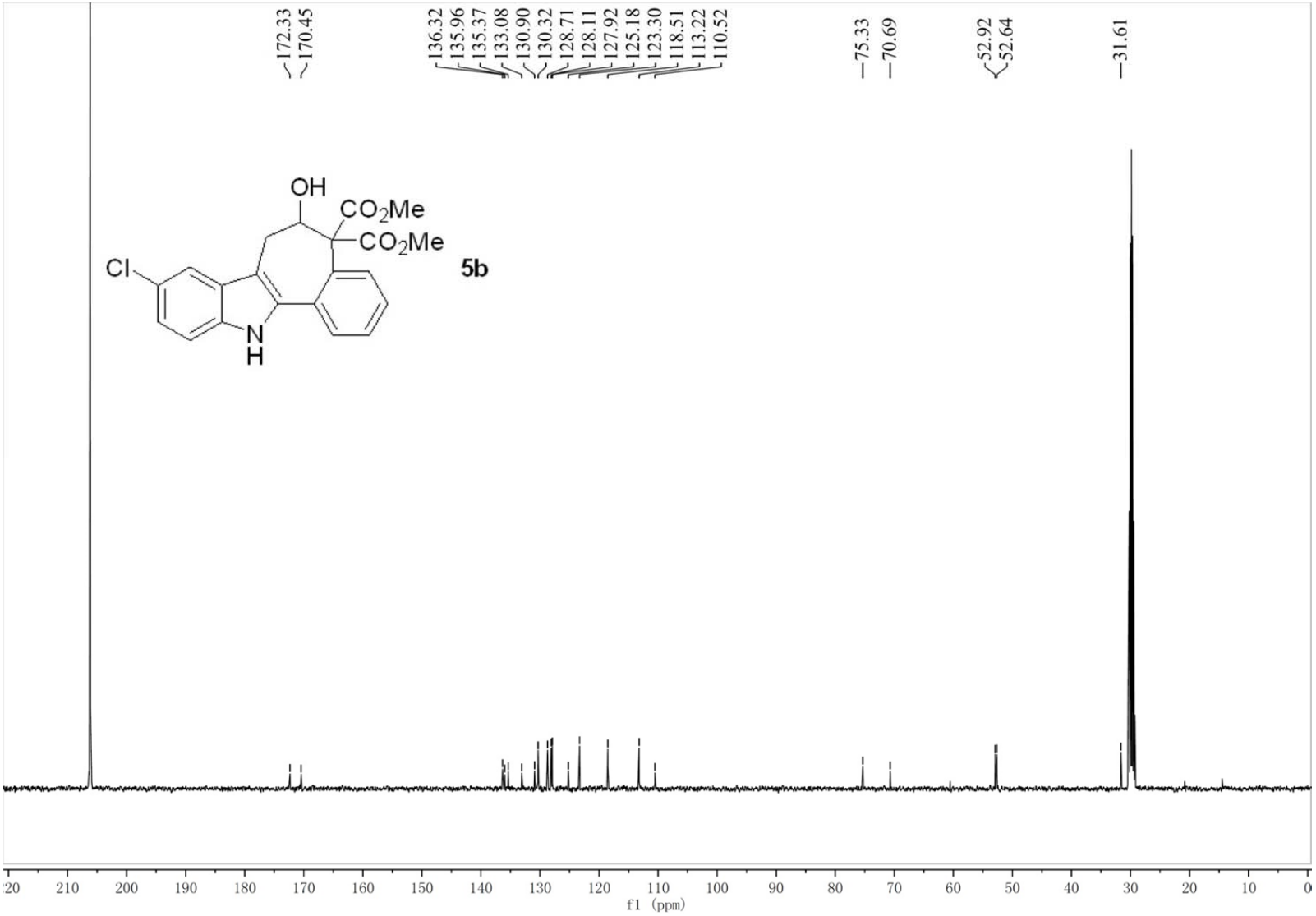
7.45
7.44
7.43
7.43
7.40
7.40
7.38
7.38
7.36
7.35
7.34
7.33
7.32
7.31
7.16
7.16
7.16
7.14
7.14
7.14
7.12
7.11
5.05
5.04
5.03
5.03
5.02
5.02
5.02
5.00
4.26
4.24
3.60
3.59
3.57
3.54
3.53
3.51
3.20
3.19
3.16
3.15
OH
CO2Me
CO2Me
Cl
N
H
5b
0.92
0.97
0.96
1.02
0.99
1.02
1.97
1.00
0.99
7.00
0.99
11.0
10.5
10.0
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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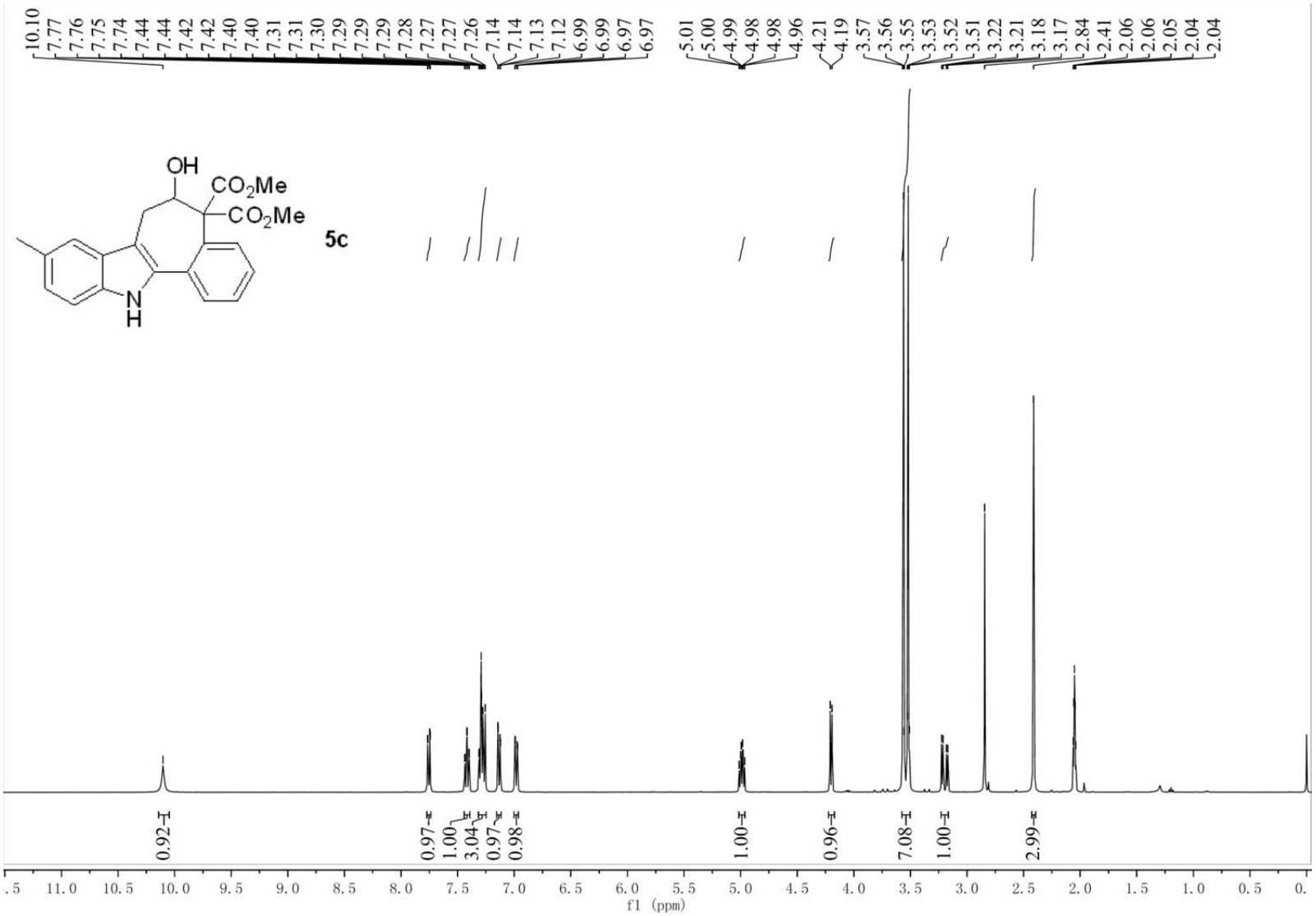
170.45
136.32
135.96
135.37
133.08
130.90
130.32
128.71
128.11
127.92
125.18
123.30
118.51
113.22
110.52
75.33
70.69
52.92
52.64
31.61
OH
CO2Me
CO2Me
Cl
N
H
5b
f1 (ppm)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7.75
7.74
7.44
7.44
7.42
7.42
7.40
7.40
7.31
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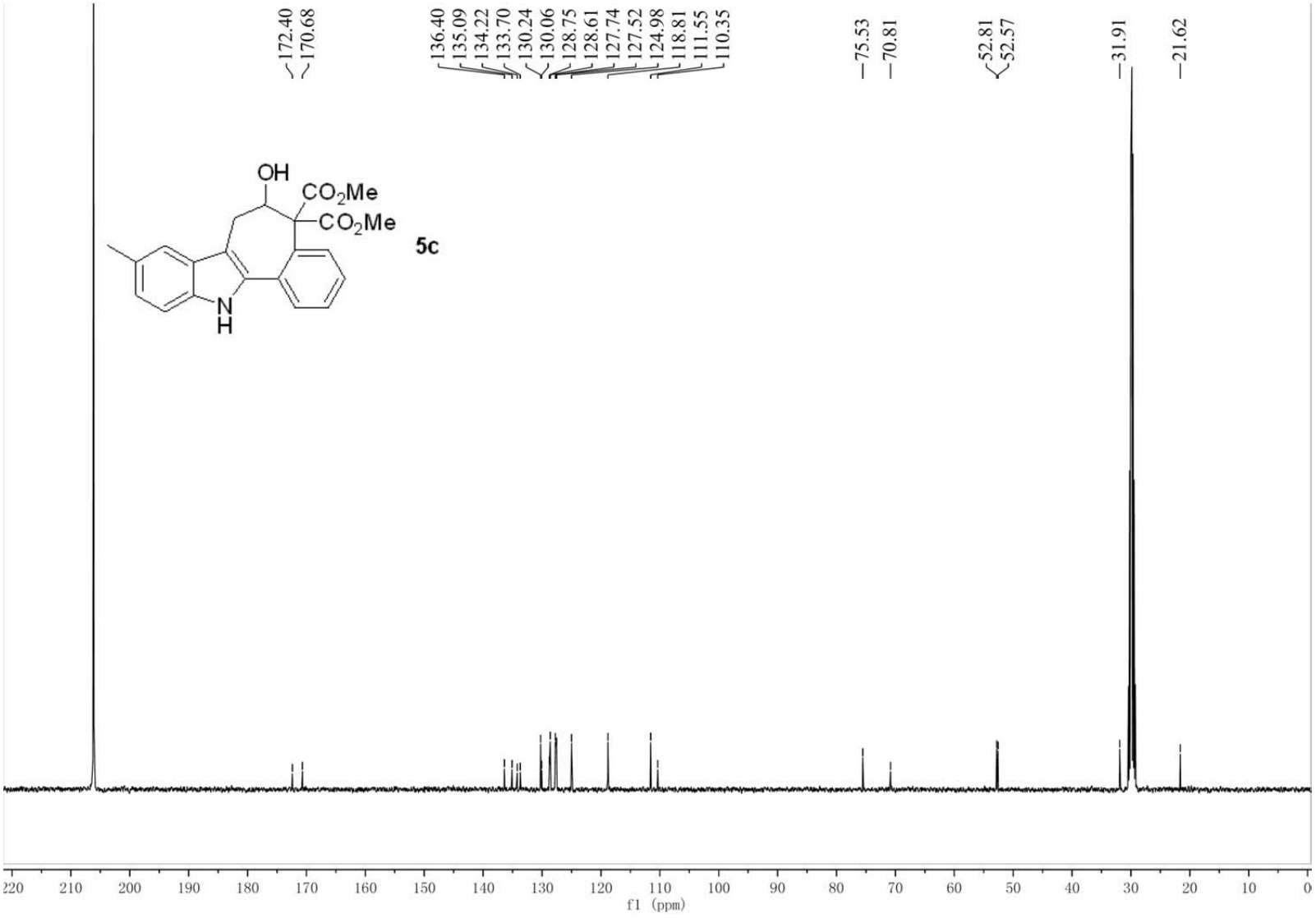
7.30
7.29
7.29
7.29
7.28
7.27
7.27
7.26
7.14
7.14
7.13
7.12
6.99
6.99
6.97
6.97
5.01
5.00
4.99
4.98
4.98
4.96
4.21
4.19
3.57
3.56
3.55
3.53
3.52
3.51
3.22
3.21
3.18
3.17
2.84
2.41
2.06
2.06
2.05
2.04
2.04
OH
CO2Me
CO2Me
5c
N
H
0.92
0.97
1.00
3.04
0.97
0.98
1.00
0.96
7.08
1.00
2.99
f1 (ppm)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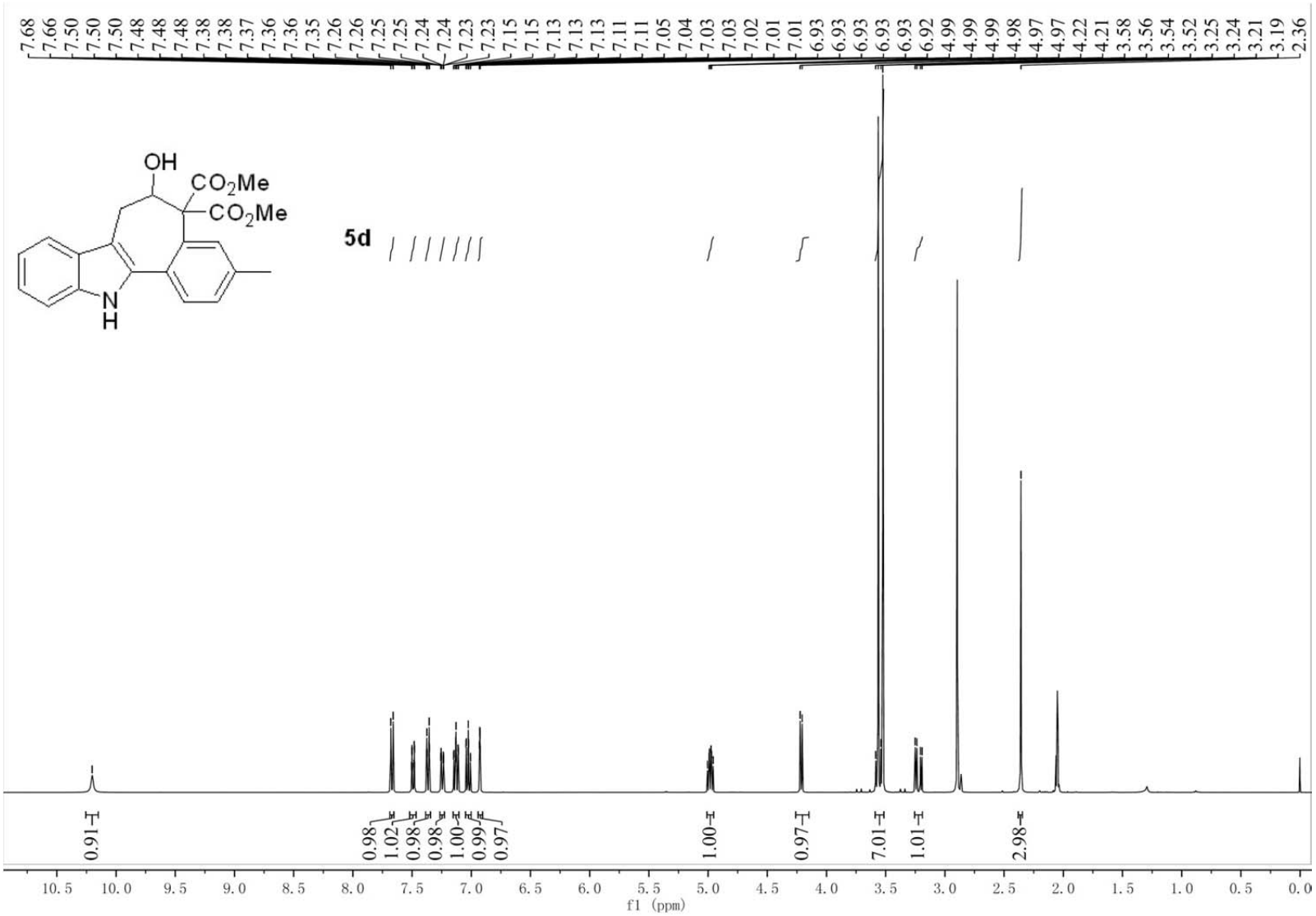
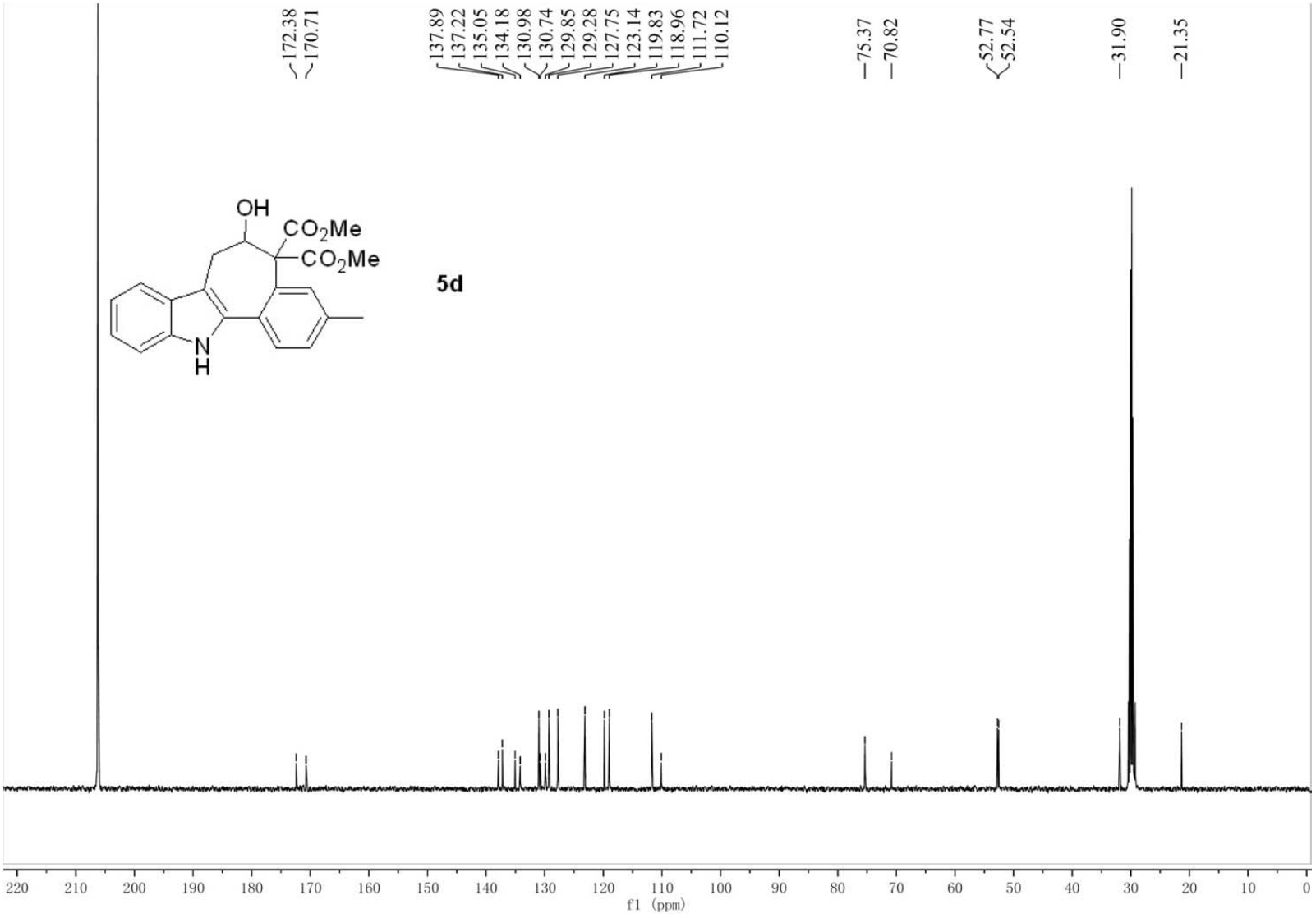
133.70
130.24
130.06
128.75
128.61
127.74
127.52
124.98
118.81
111.55
110.35
75.53
70.81
52.81
52.57
31.91
21.62
OH
CO2Me
CO2Me
N
H
5c
f1 (ppm)


7.68 7.66 7.50 7.50 7.50 7.48 7.48 7.48 7.38 7.38 7.37 7.36 7.36 7.35 7.26 7.26 7.25 7.25 7.24 7.24 7.23 7.23 7.15 7.15 7.13 7.13 7.13 7.11 7.11 7.05 7.04 7.03 7.03 7.02 7.01 7.01 6.93 6.93 6.93 6.93 6.92 4.99 4.99 4.99 4.98 4.97 4.97 4.22 4.21 3.58 3.56 3.54 3.52 3.25 3.24 3.21 3.19 2.36
OH
CO2Me
CO2Me
N
H
5d
0.91
0.98
1.02
0.98
0.98
1.00
0.99
0.97
1.00
0.97
7.01
1.01
2.98
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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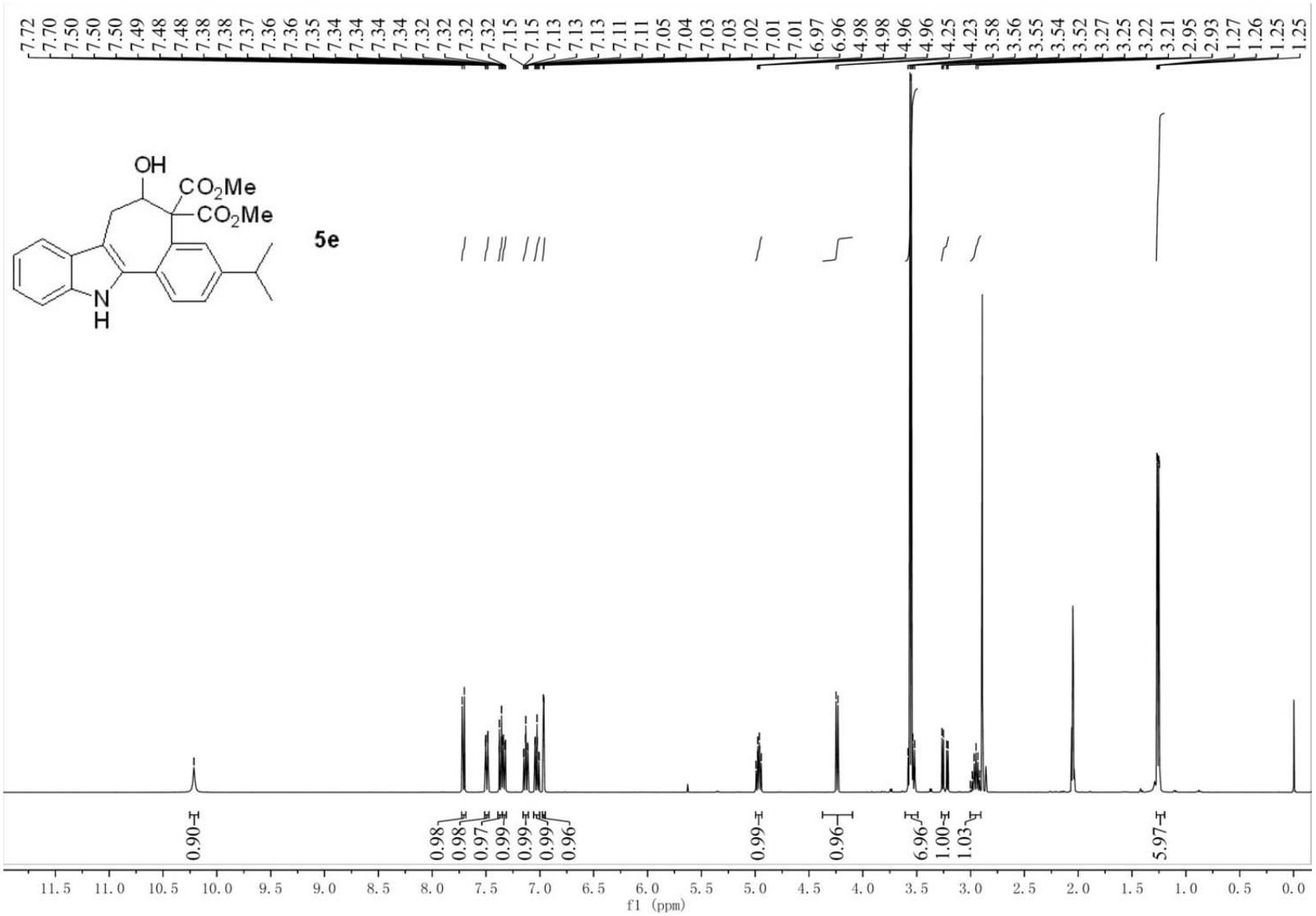
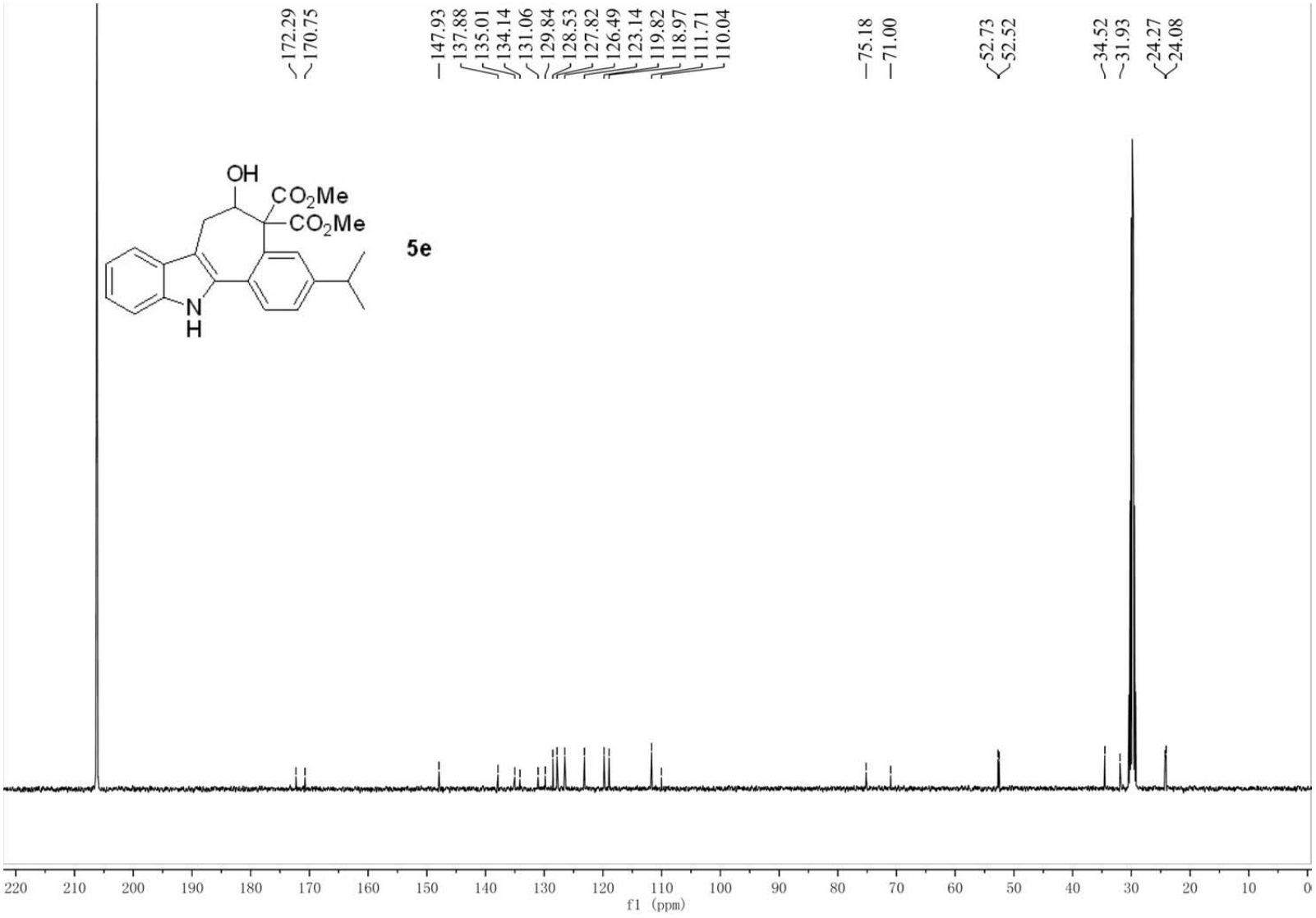
130.74
129.85
129.28
127.75
123.14
119.83
118.96
111.72
110.12
75.37
70.82
52.77
52.54
31.90
21.35
OH
CO2Me
CO2Me
N
H
5d
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.72 7.70 7.50 7.50 7.50 7.49 7.48 7.48 7.38 7.38 7.37 7.36 7.36 7.35 7.34 7.34 7.34 7.34 7.32 7.32 7.32 7.32 7.15 7.15 7.13 7.13 7.13 7.11 7.11 7.05 7.04 7.03 7.03 7.02 7.01 7.01 6.97 6.96 4.98 4.98 4.96 4.96 4.25 4.23 3.58 3.56 3.55 3.54 3.52 3.27 3.25 3.22 3.21 2.95 2.93 1.27 1.26 1.25 1.25
OH
CO2Me
CO2Me
N
H
5e
0.90
0.98
0.98
0.97
0.99
0.99
0.99
0.96
0.99
0.96
6.96
1.00
1.03
5.97
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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123.14
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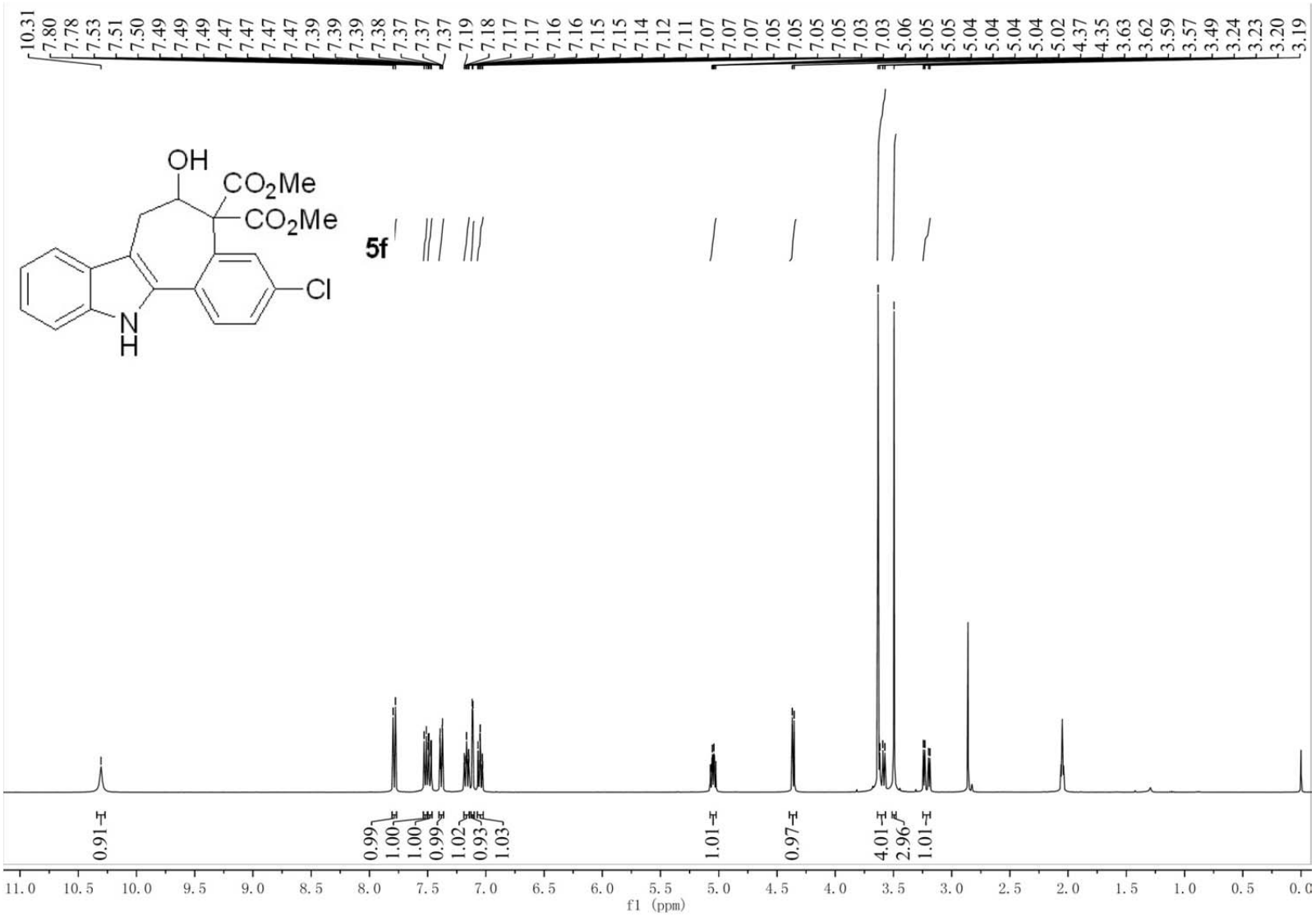
118.97
111.71
110.04
75.18
71.00
52.73
52.52
34.52
31.93
24.27
24.08
OH
CO2Me
CO2Me
N
H
5e
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.78
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7.49
7.49
7.47
7.47
7.47
7.47
7.39
7.39
7.39
7.38
7.37
7.37
7.37
7.19
7.18
7.17
7.17
7.16
7.16
7.15
7.15
7.14
7.12
7.11
7.07
7.07
7.07
7.05
7.05
7.05
7.05
7.03
7.03
5.06
5.05
5.05
5.04
5.04
5.04
5.04
5.02
4.37
4.35
3.63
3.62
3.59
3.57
3.49
3.24
3.23
3.20
3.19
OH
CO2Me
CO2Me
Cl
N
H
5f
0.91
0.99
1.00
1.00
0.99
1.02
0.93
1.03
1.01
0.97
4.01
2.96
1.01
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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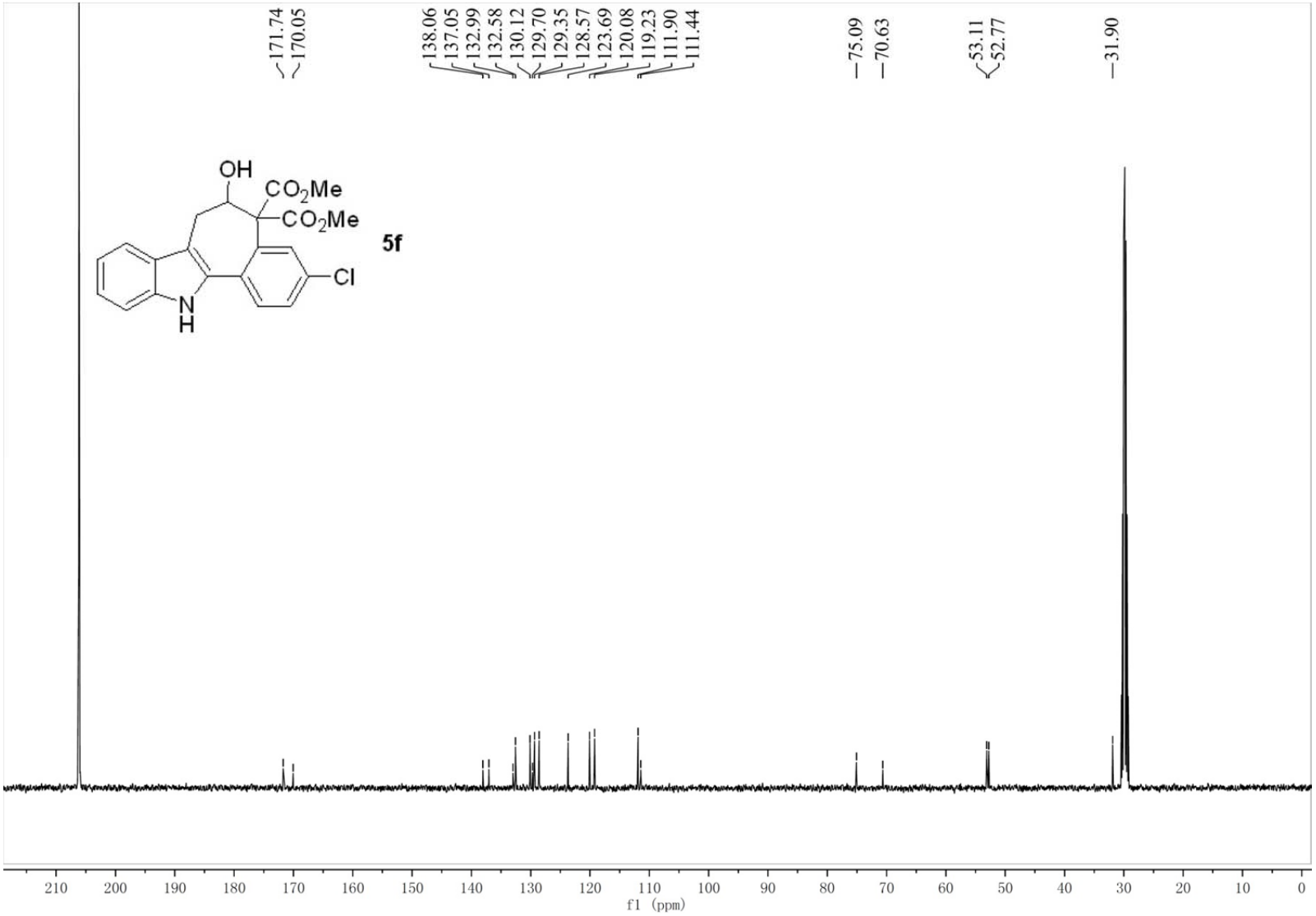
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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170.05
138.06
137.05
132.99
132.58
130.12
129.70
129.35
128.57
123.69
120.08
119.23
111.90
111.44
75.09
70.63
53.11
52.77
31.90
OH
CO2Me
CO2Me
Cl
N
H
5f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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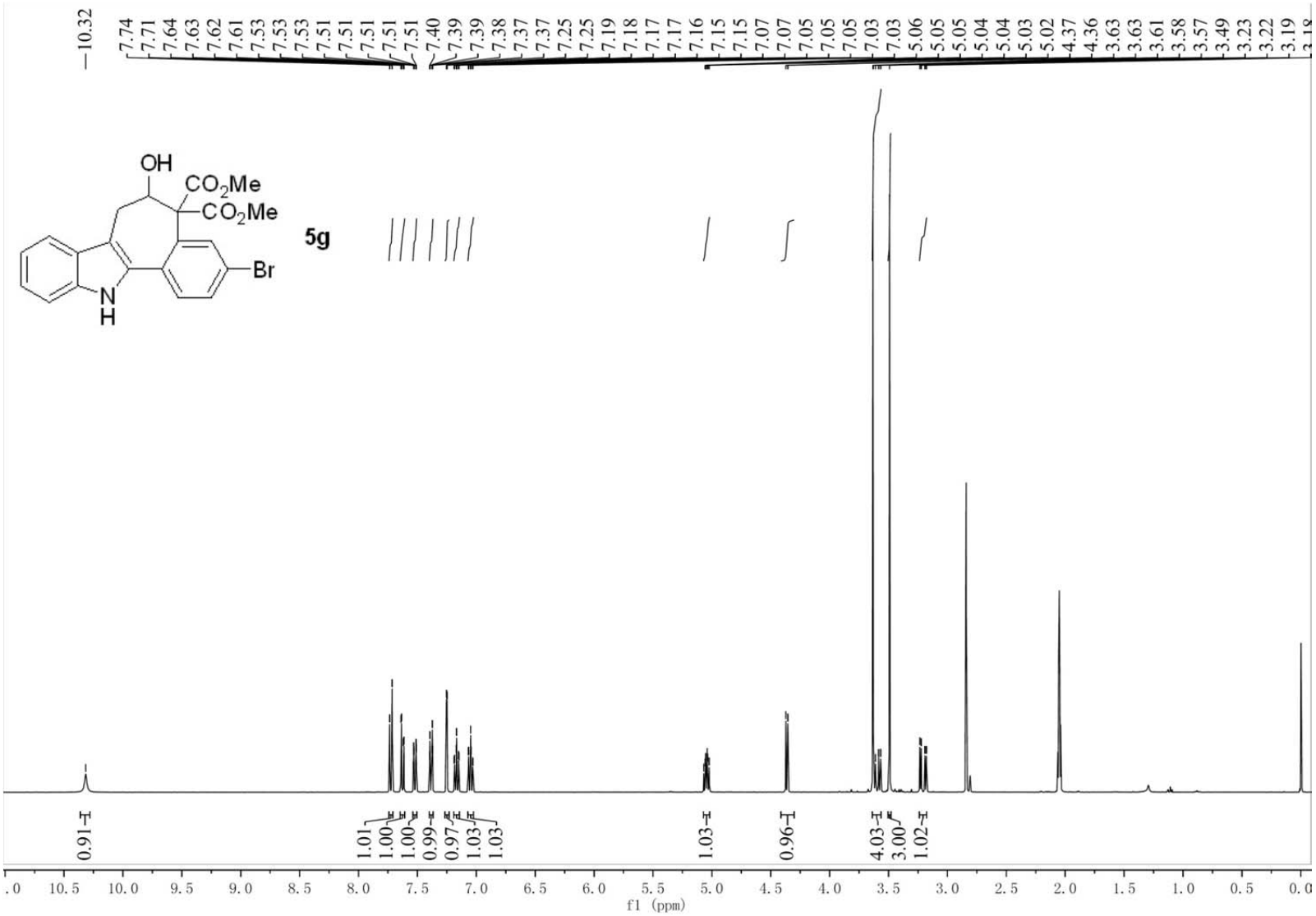
50
40
30
20
10
0
f1 (ppm)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7.63
7.62
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7.53
7.53
7.53
7.51
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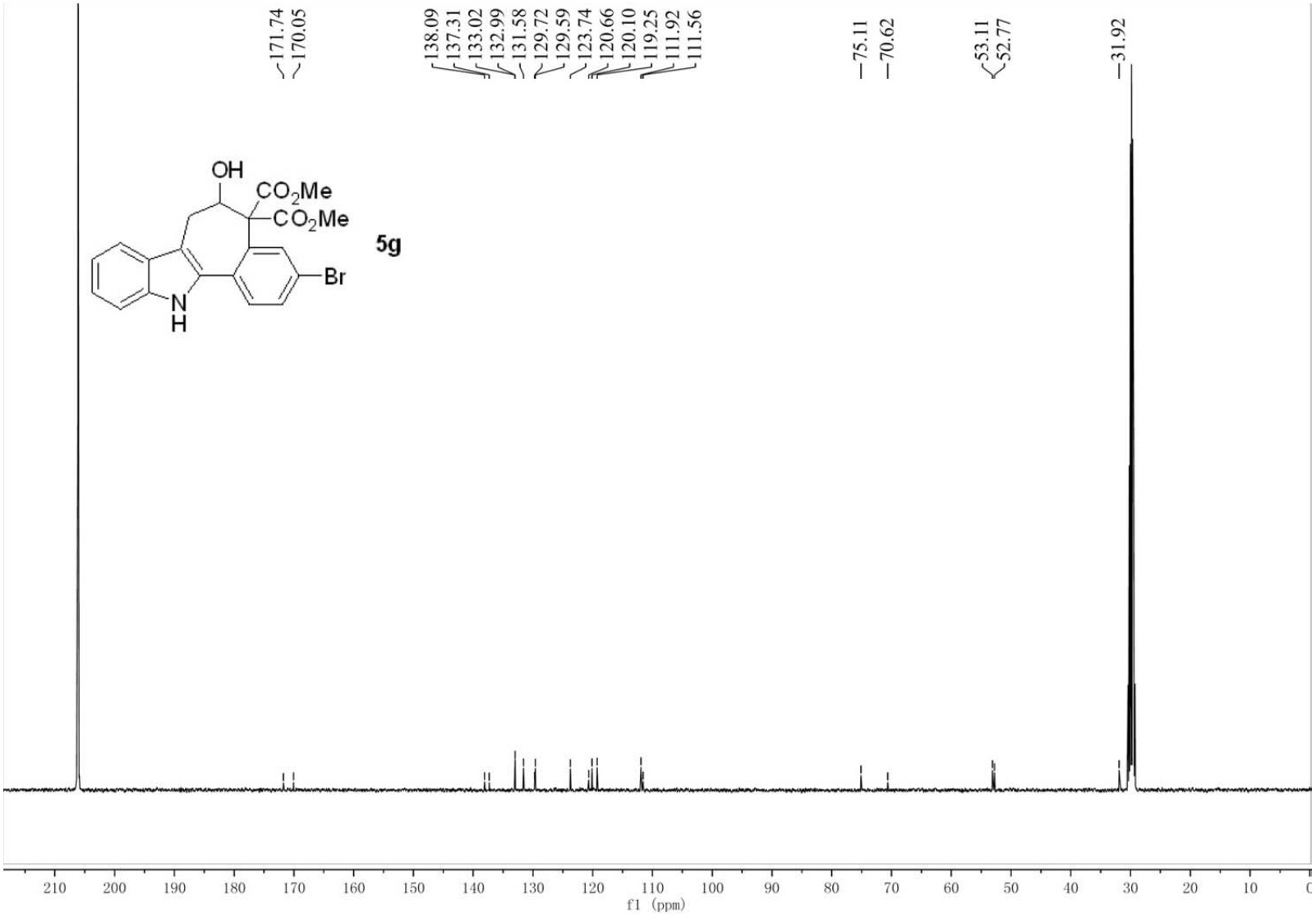
7.51
7.40
7.39
7.39
7.38
7.37
7.37
7.25
7.25
7.19
7.18
7.17
7.17
7.16
7.15
7.15
7.07
7.07
7.05
7.05
7.05
7.03
7.03
5.06
5.05
5.05
5.04
5.04
5.03
5.02
4.37
4.36
3.63
3.63
3.61
3.58
3.57
3.49
3.23
3.22
3.19
OH
CO2Me
CO2Me
Br
N
H
5g
0.91
1.01
1.00
1.00
0.99
0.97
1.03
1.03
1.03
0.96
4.03
3.00
1.02
f1 (ppm)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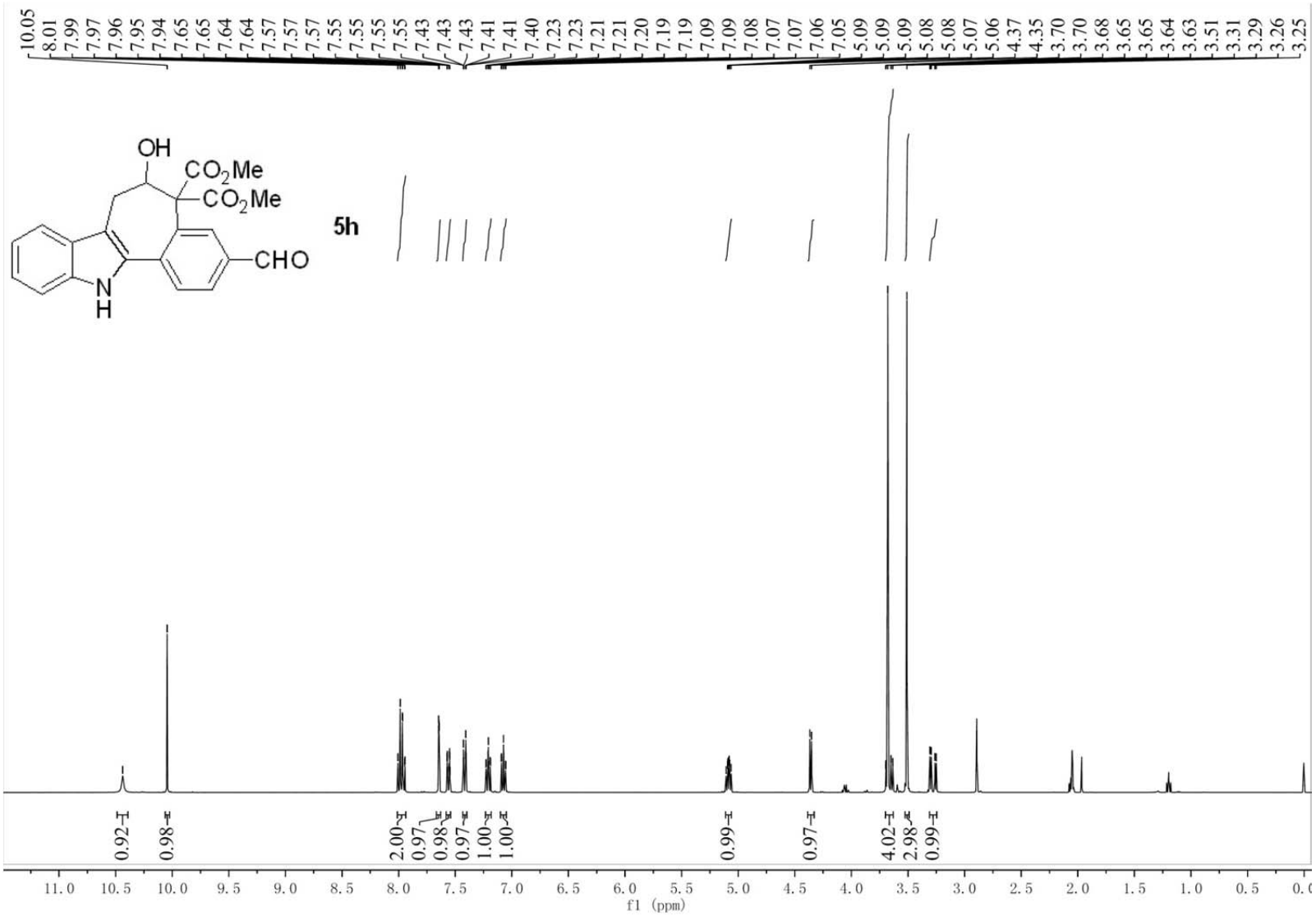
138.09
137.31
133.02
132.99
131.58
129.72
129.59
123.74
120.66
120.10
119.25
111.92
111.56
75.11
70.62
53.11
52.77
31.92
OH
CO2Me
CO2Me
Br
N
H
5g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.95
7.94
7.65
7.65
7.64
7.64
7.57
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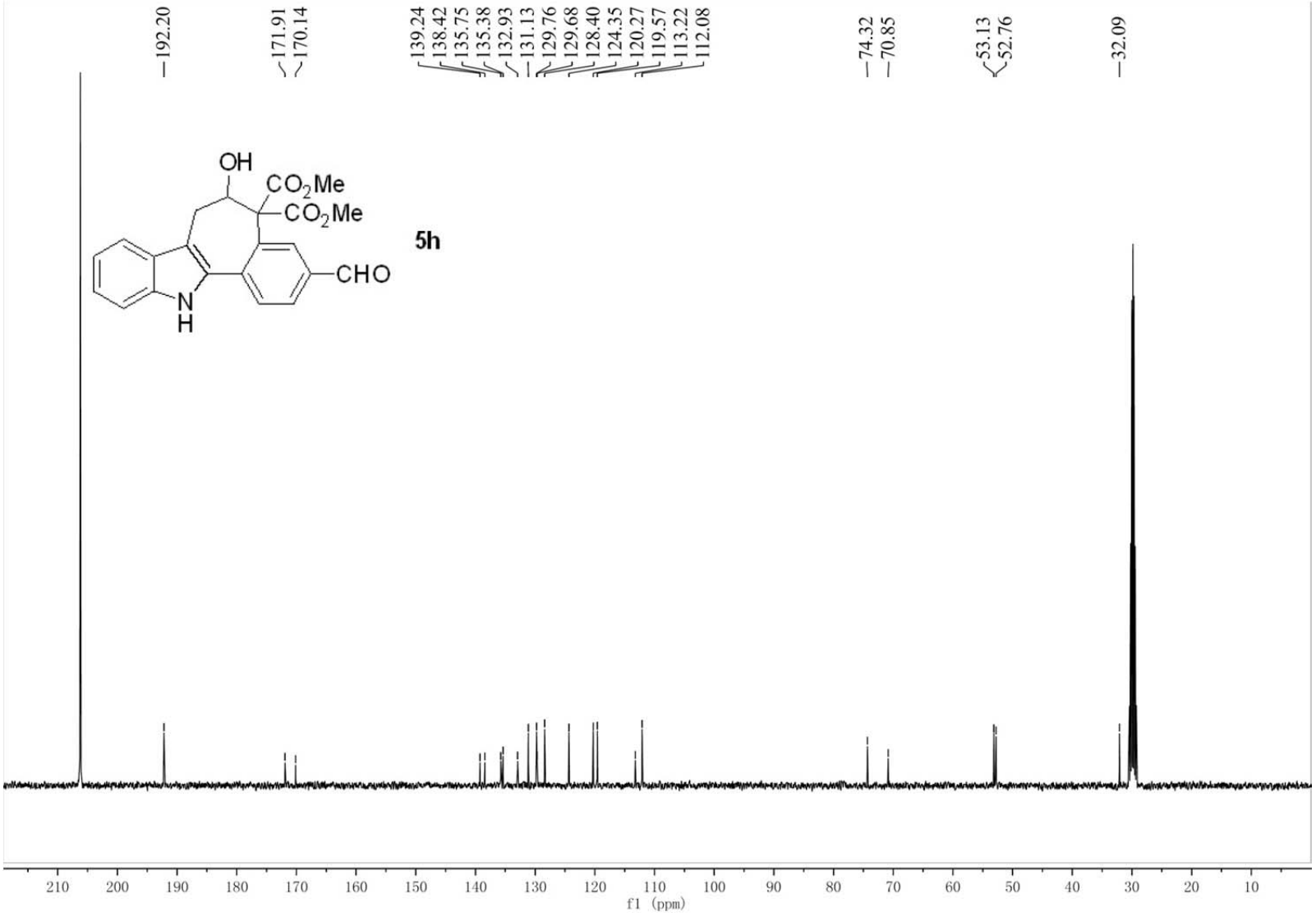
7.57
7.55
7.55
7.55
7.55
7.43
7.43
7.43
7.41
7.41
7.40
7.23
7.23
7.21
7.21
7.20
7.19
7.19
7.09
7.09
7.08
7.07
7.07
7.06
7.05
5.09
5.09
5.09
5.08
5.08
5.07
5.06
4.37
4.35
3.70
3.70
3.68
3.65
3.65
3.64
3.63
3.51
3.31
3.29
3.26
3.25
OH
CO2Me
CO2Me
CHO
N
H
5h
0.92
0.98
2.00
0.97
0.98
0.97
1.00
1.00
0.99
0.97
4.02
2.98
0.99
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
f1 (ppm)


192.20
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170.14
139.24
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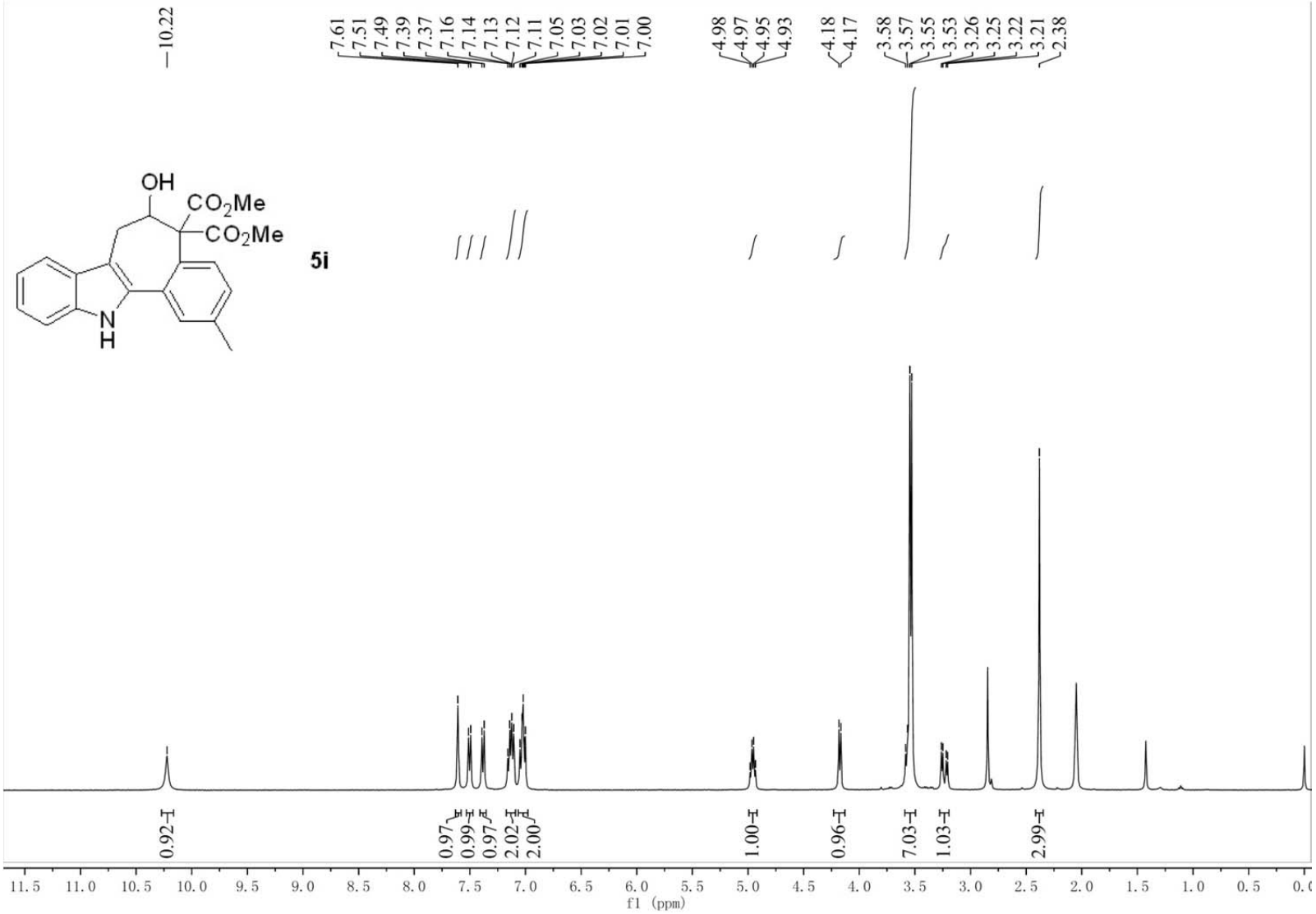
135.75
135.38
132.93
131.13
129.76
129.68
128.40
124.35
120.27
119.57
113.22
112.08
74.32
70.85
53.13
52.76
32.09
OH
CO2Me
CO2Me
CHO
N
H
5h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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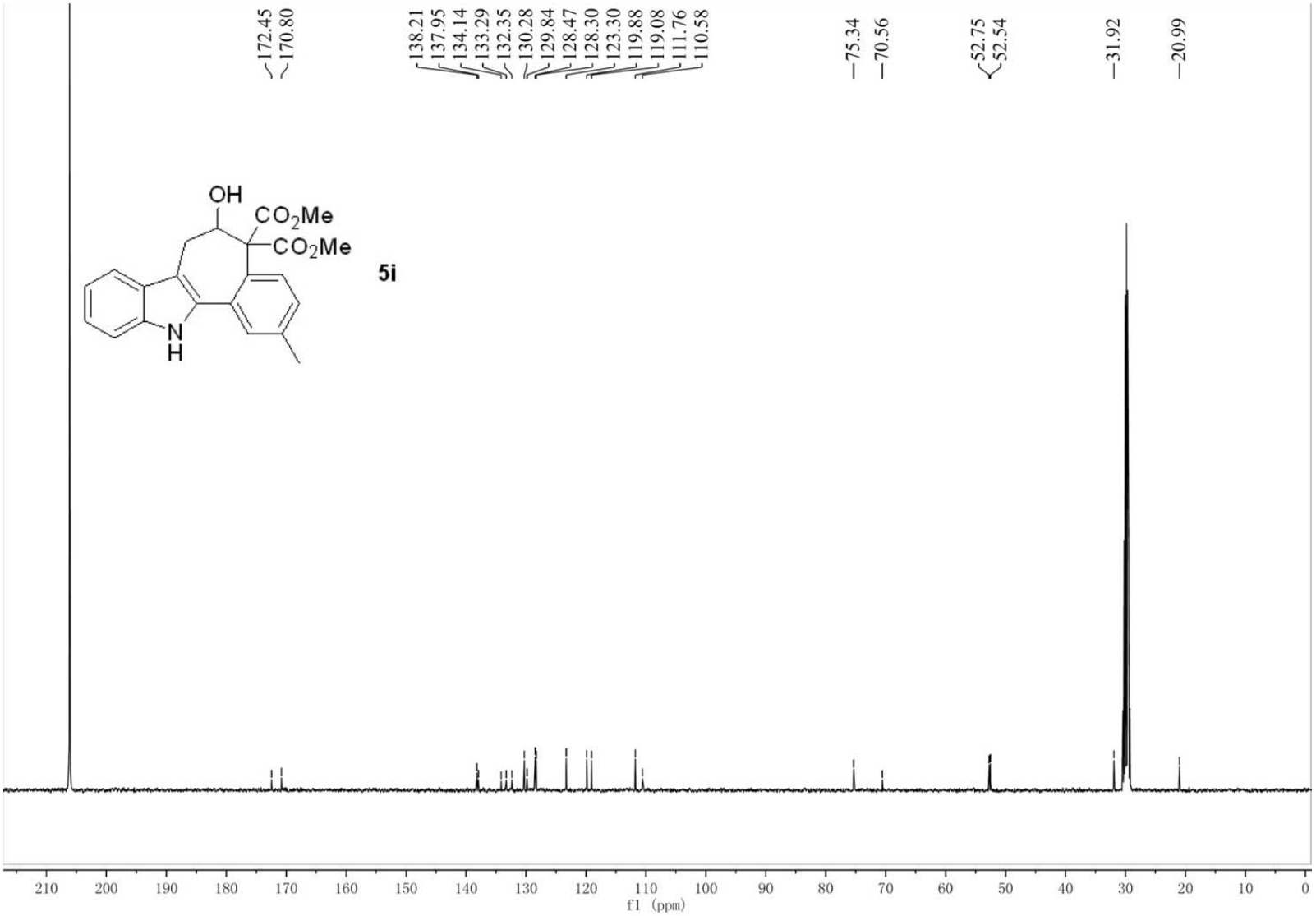
7.37
7.16
7.14
7.13
7.12
7.11
7.05
7.03
7.02
7.01
7.00
4.98
4.97
4.95
4.93
4.18
4.17
3.58
3.57
3.55
3.53
3.26
3.25
3.22
3.21
2.38
OH
CO2Me
CO2Me
N
H
5i
0.92
0.97
0.99
0.97
2.02
2.00
1.00
0.96
7.03
1.03
2.99
f1 (ppm)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132.35
130.28
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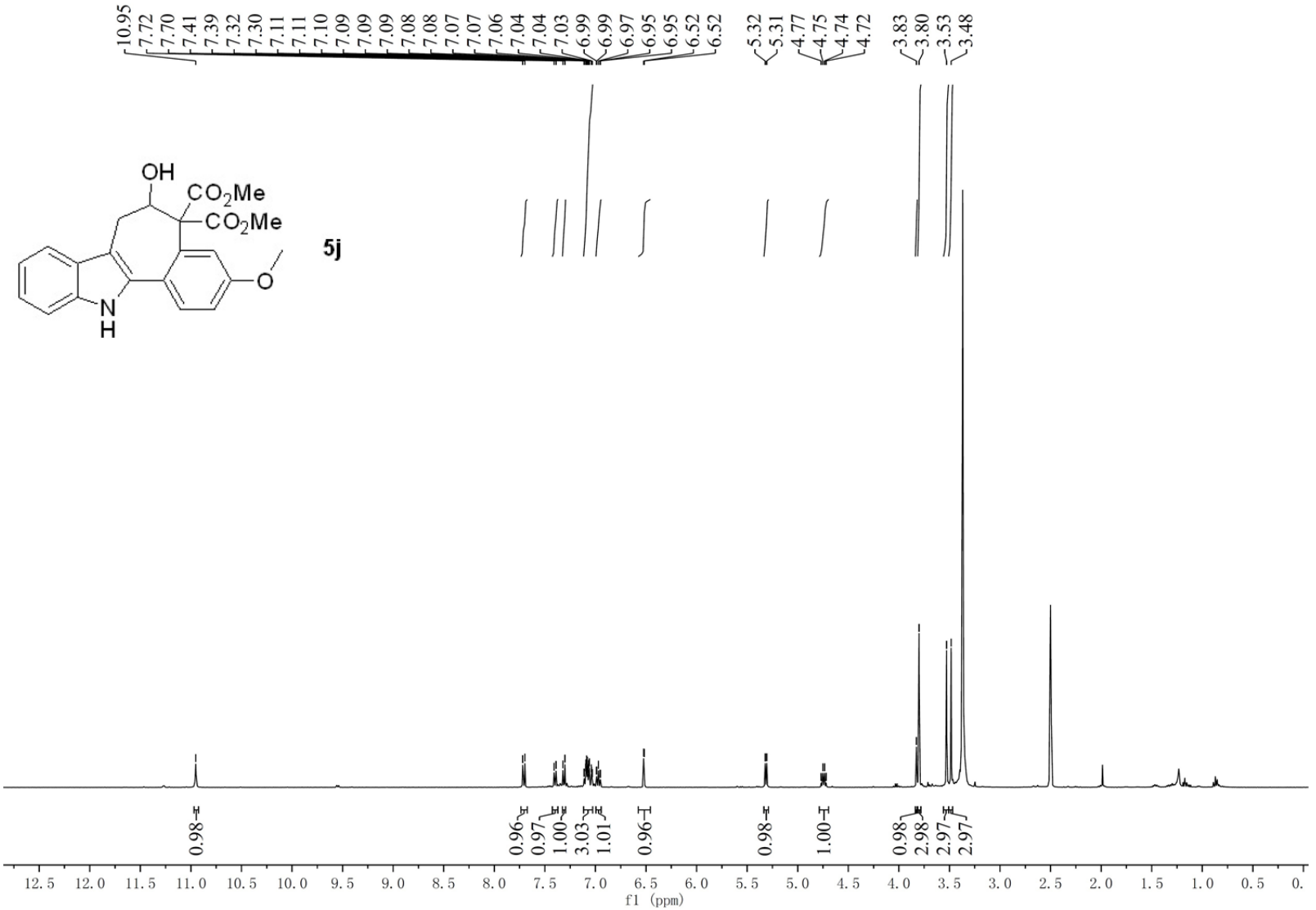
128.47
128.30
123.30
119.88
119.08
111.76
110.58
75.34
70.56
52.75
52.54
31.92
20.99
OH
CO2Me
CO2Me
N
H
5i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.11
7.11
7.10
7.09
7.09
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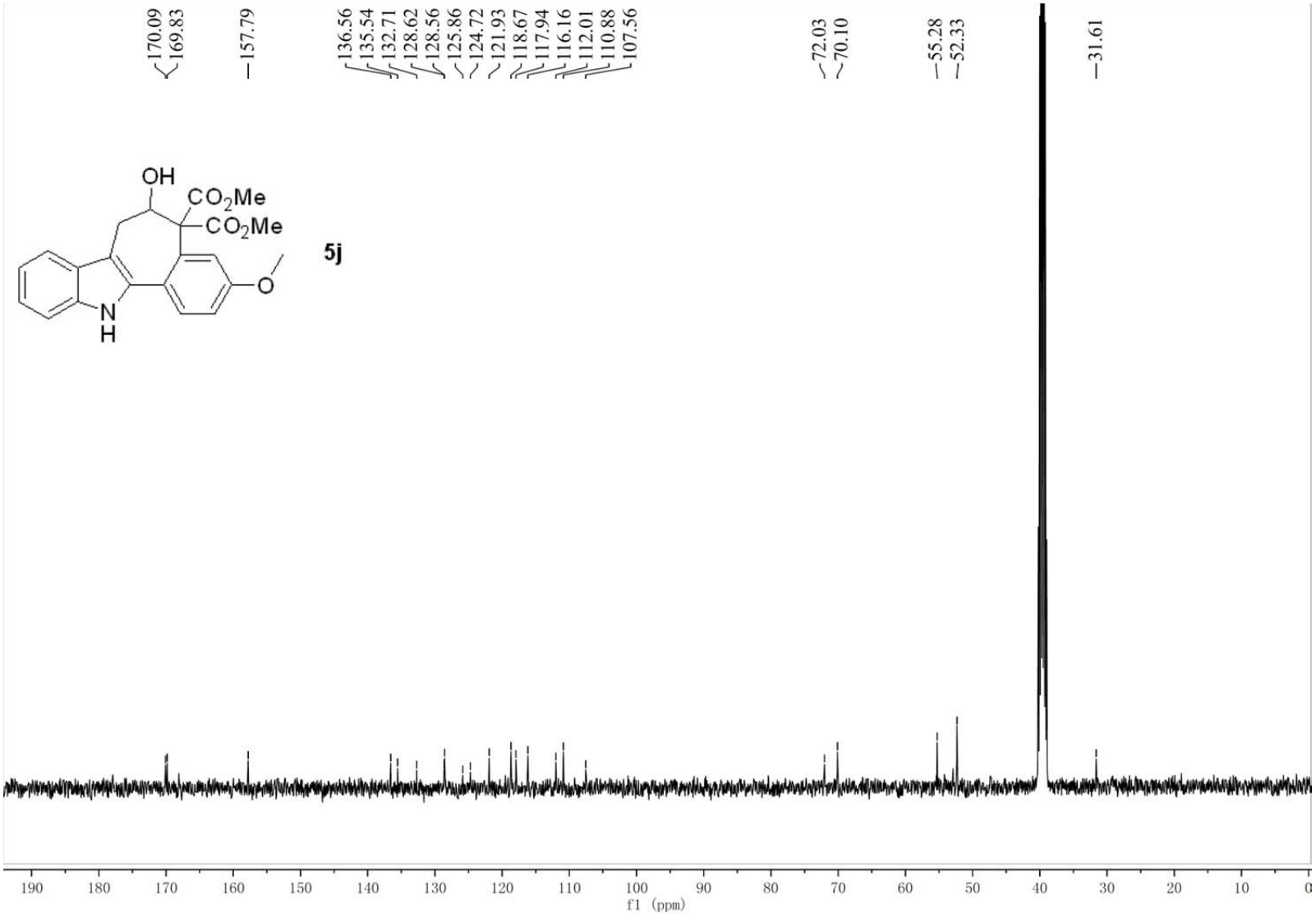
7.08
7.08
7.07
7.07
7.06
7.04
7.04
7.03
6.99
6.99
6.97
6.95
6.95
6.52
6.52
5.32
5.31
4.77
4.75
4.74
4.72
3.83
3.80
3.53
3.48
OH
CO2Me
CO2Me
O
N
H
5j
0.98
0.96
0.97
1.00
3.03
1.01
0.96
0.98
1.00
0.98
2.98
2.97
2.97
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)


170.09
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157.79
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135.54
132.71
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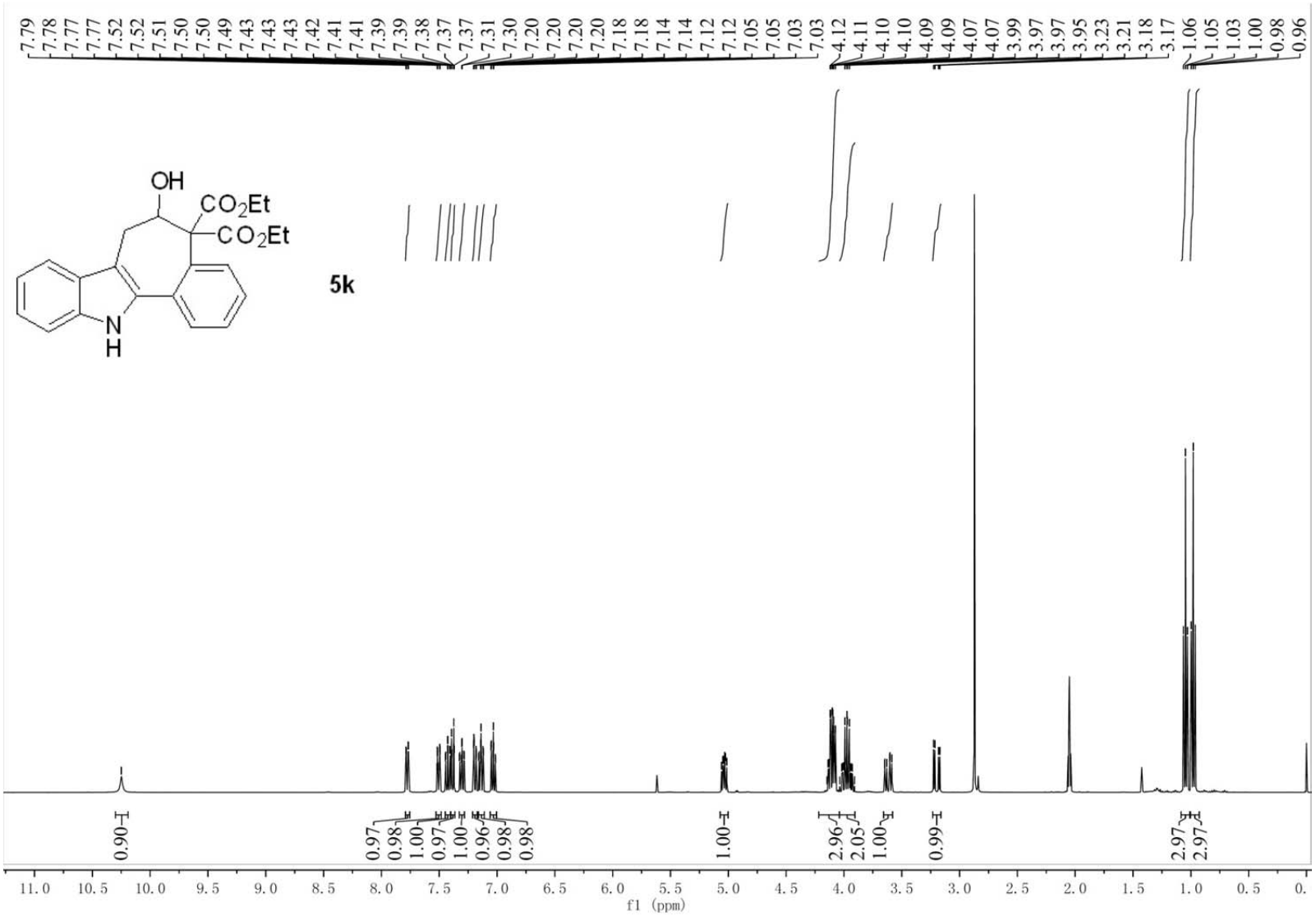
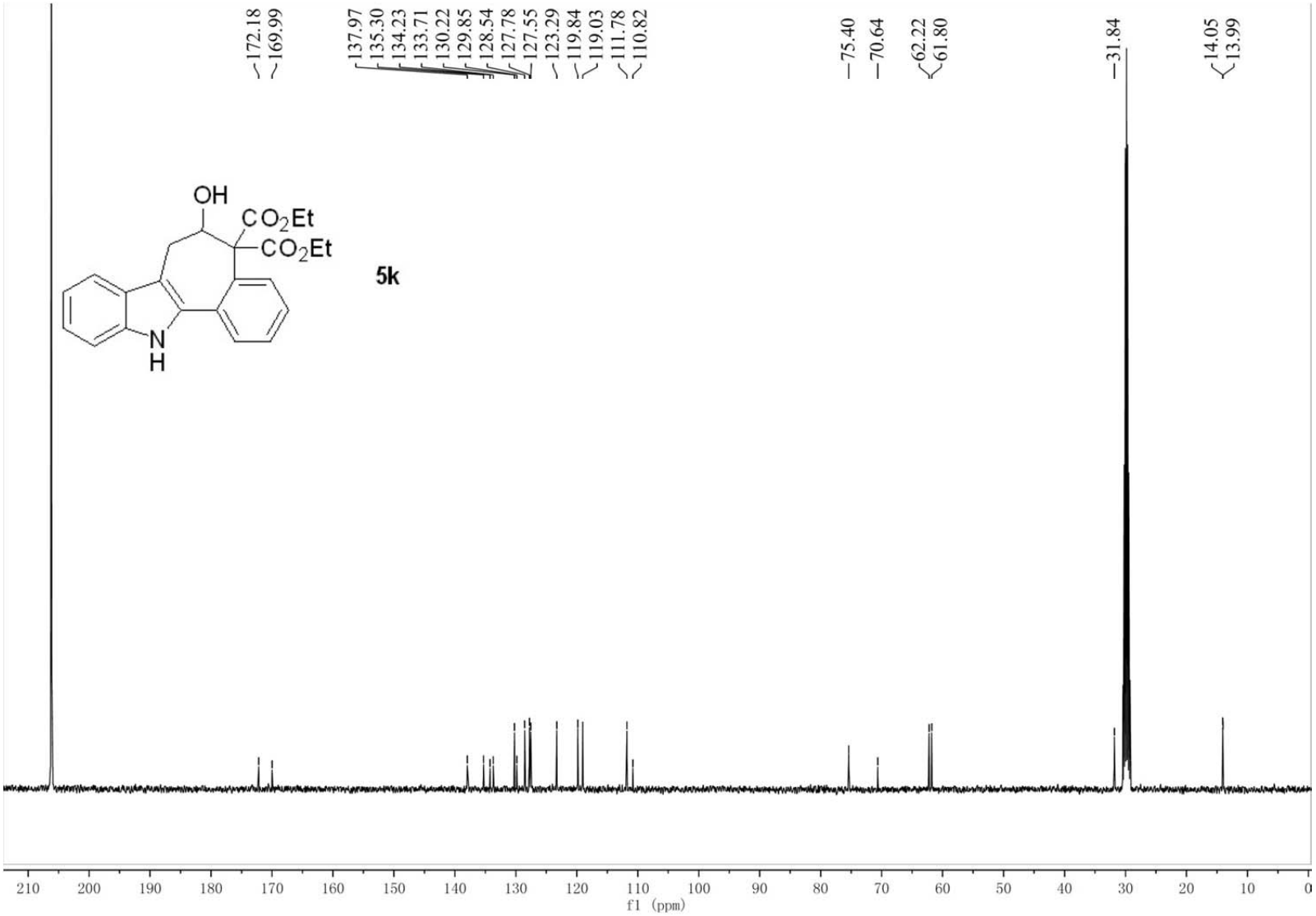
128.56
125.86
124.72
121.93
118.67
117.94
116.16
112.01
110.88
107.56
72.03
70.10
55.28
52.33
31.61
OH
CO2Me
CO2Me
O
N
H
5j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OH
CO2Et
CO2Et
N
H
5k
f1 (ppm)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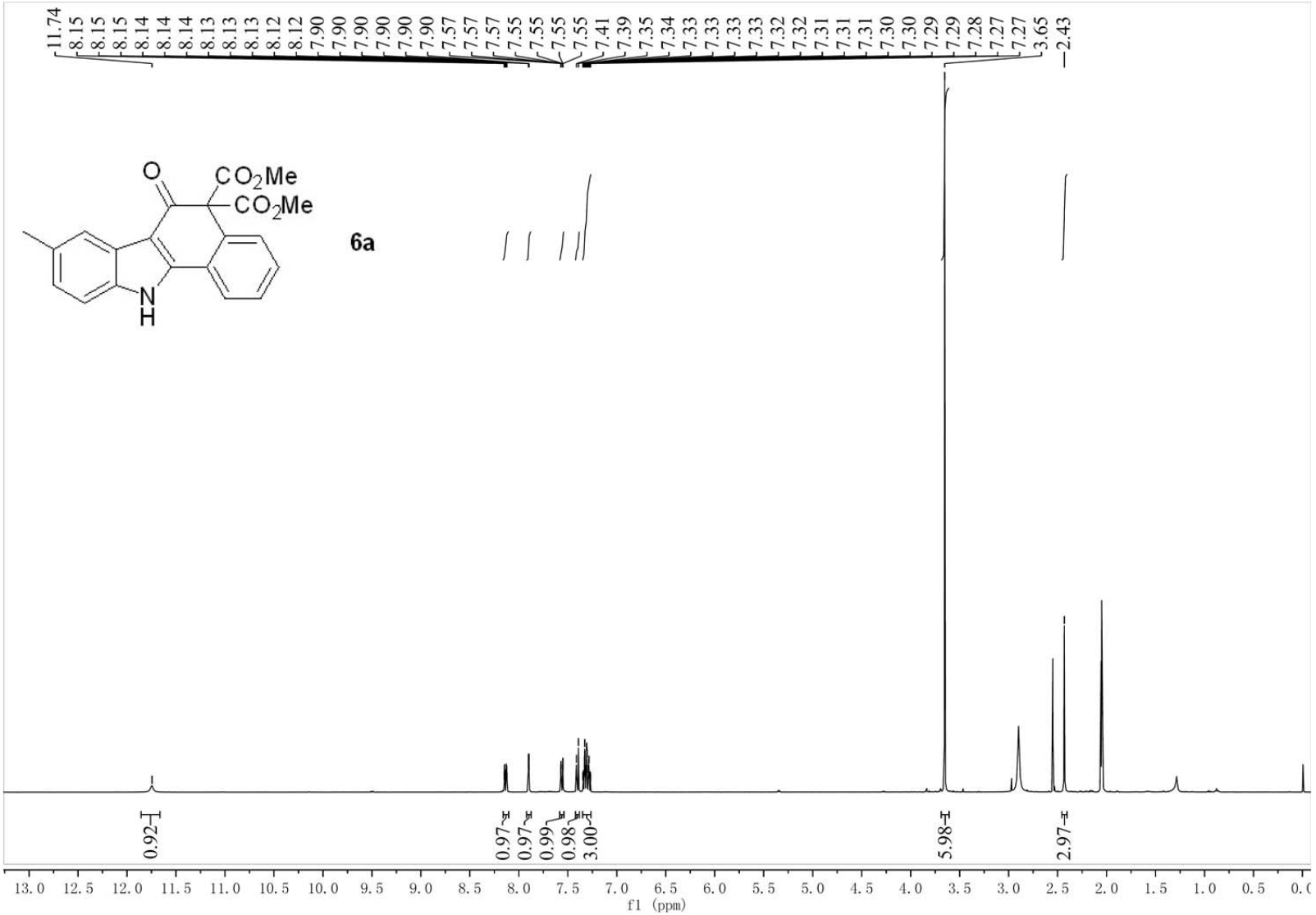
135.30
134.23
133.71
130.22
129.85
128.54
127.78
127.55
123.29
119.84
119.03
111.78
110.82
75.40
70.64
62.22
61.80
31.84
14.05
13.99
OH
CO2Et
CO2Et
N
H
5k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


11.74
8.15
8.15
8.15
8.14
8.14
8.14
8.13
8.13
8.13
8.12
8.12
7.90
7.90
7.90
7.90
7.90
7.90
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7.57
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7.55
7.55
7.55
7.41
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7.32
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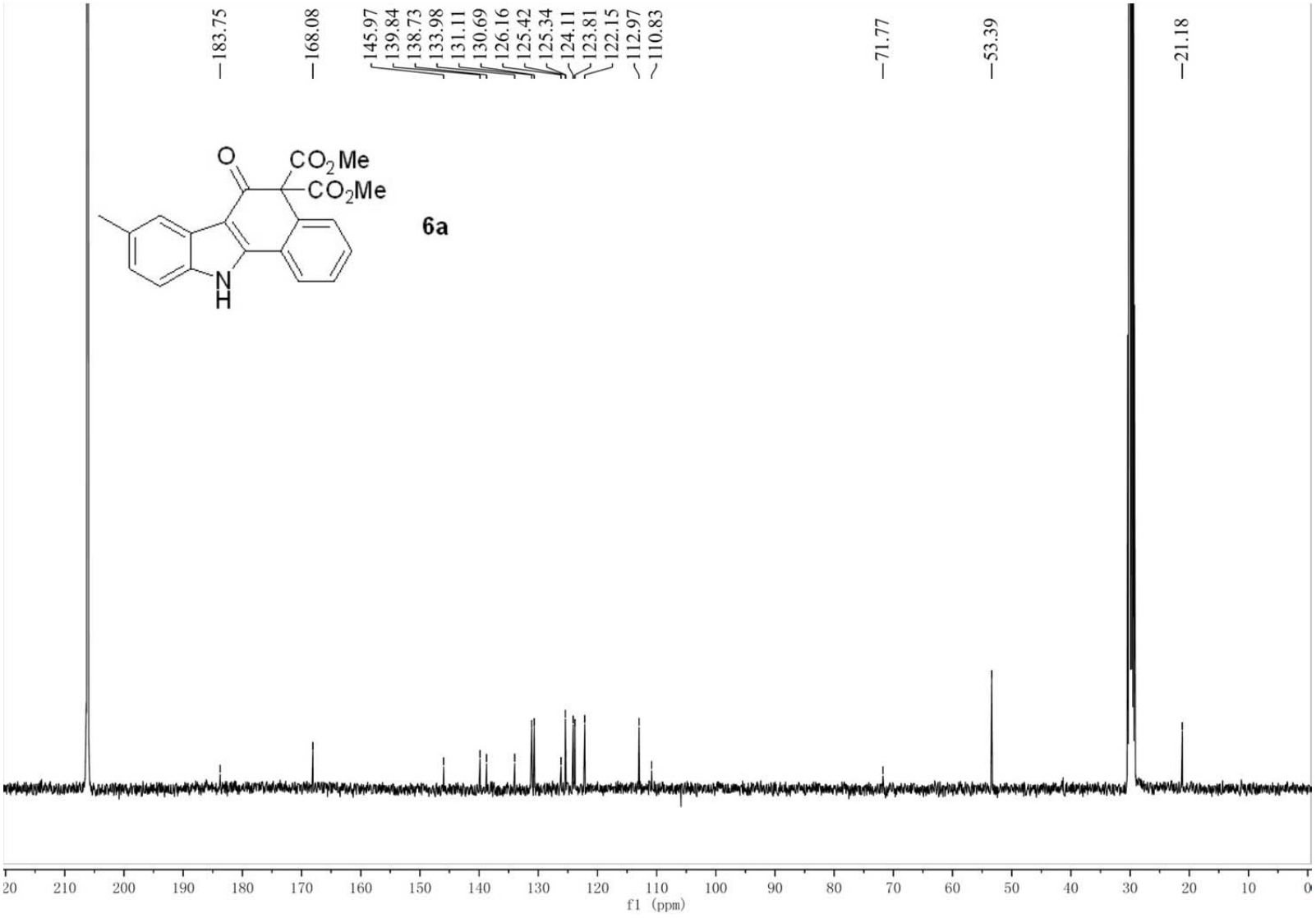
7.31
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.27
3.65
2.43
O
CO2Me
CO2Me
N
H
6a
0.92
0.97
0.97
0.99
0.98
3.00
5.98
2.97
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


183.75
168.08
145.97
139.84
138.73
133.98
131.11
130.69
126.16
125.42
125.34
124.11
123.81
122.15
112.97
110.83
71.77
53.39
21.18
O
CO2Me
CO2Me
N
H
6a
f1 (ppm)