Supporting Information

Condensation of 1,2-Dicarbonyl Compounds with Modified Huisgen Zwitterions: Synthesis of *N*-Aryl-*N*-Acyl Hydrazones

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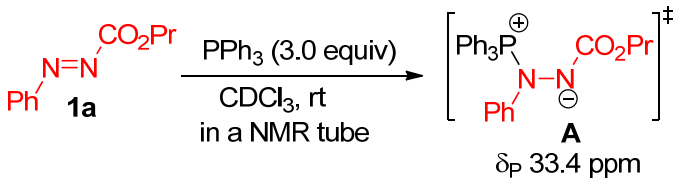
Table of Contents

I. ^{31}P NMR Tracking Experiment

Propyl 2-phenyldiazenecarboxylate **1a** (10 mg, 0.05 mmol), Ph_3P (40 mg 0.15 mmol) were added into $CDCl_3$ (1.0 mL) in an NMR tube. The resulting mixture was shaken up and immediately applied to ^{31}P NMR analysis. Then, the ^{31}P NMR data were acquired at the indicated time intervals. After that, ethyl benzoylformate **2a** (18 mg, 0.1 mmol) was added into the tube and the resulting sample was tested again to get the final ^{31}P NMR spectrum.



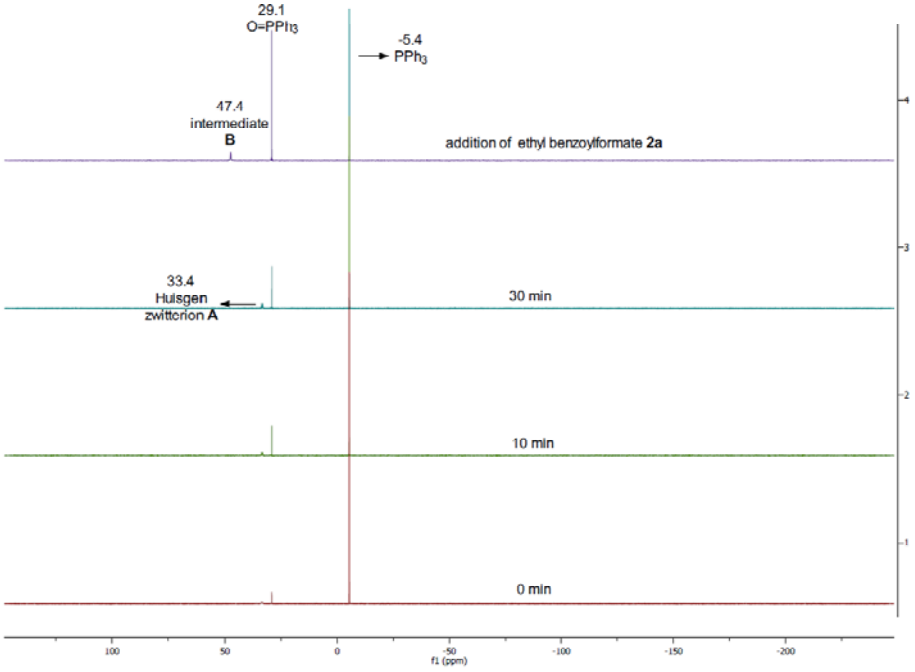
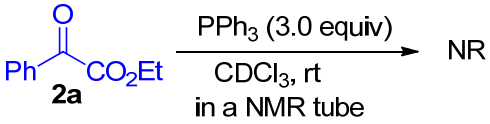


Fig S1 ^{31}P NMR tracking experiment of propyl 2-phenyldiazenecarboxylate **1a** with Ph_3P

Ethyl benzoylformate **2a** (9 mg, 0.05 mmol), Ph_3P (40 mg 0.15 mmol) were added into $CDCl_3$ (1.0 mL) in an NMR tube. The resulting mixture was shaken up and immediately applied to ^{31}P NMR analysis. After 20 min, the sample was tested again to obtain the corresponding ^{31}P NMR data.



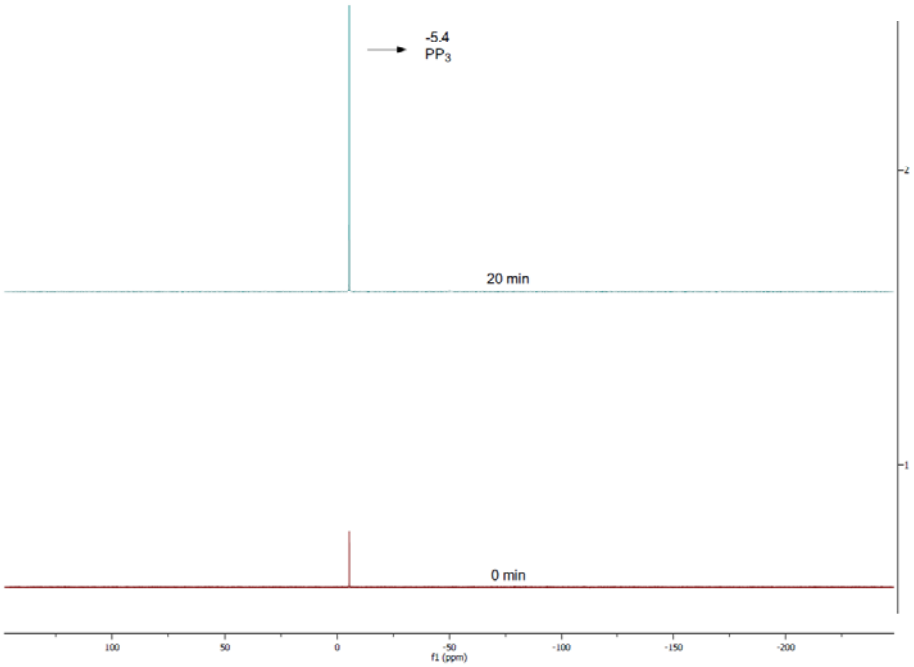
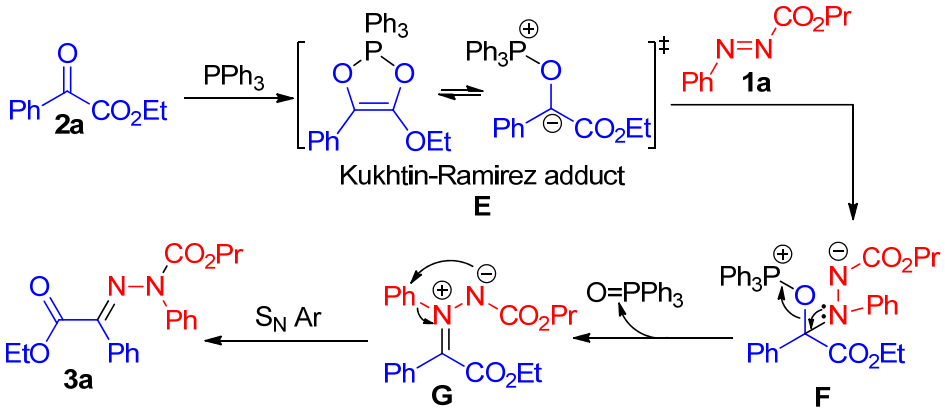


Fig S2 ^{31}P NMR tracking experiment of ethyl benzoylformate **2a** with Ph_3P

II. Proposed Kukhtin-Ramirez Adduct-Based Mechanism

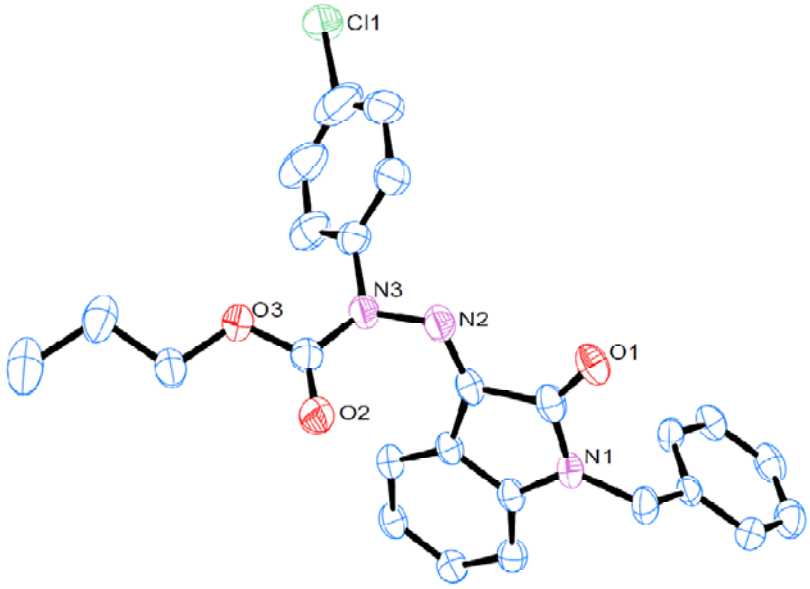
In the proposed mechanism, addition of PPh_3 to ethyl benzoylformate **2a** generates the Kukhtin-Ramirez adduct **E**, which undergoes a nucleophilic addition to propyl 2-phenyldiazenecarboxylate **1a** via its dipolar format affording intermediate **F**. Intermediate **F** eliminates triphenylphosphine oxide to give intermediate **G**. Finally, intermediate **G** undertakes an intramolecular S_NAr process to deliver the hydrazone derivative **3a**. However, this mechanism is not operative according to the above ^{31}P NMR tracking experiments.



Scheme S1 Proposed mechanism involving the Kukhtin-Ramirez adduct

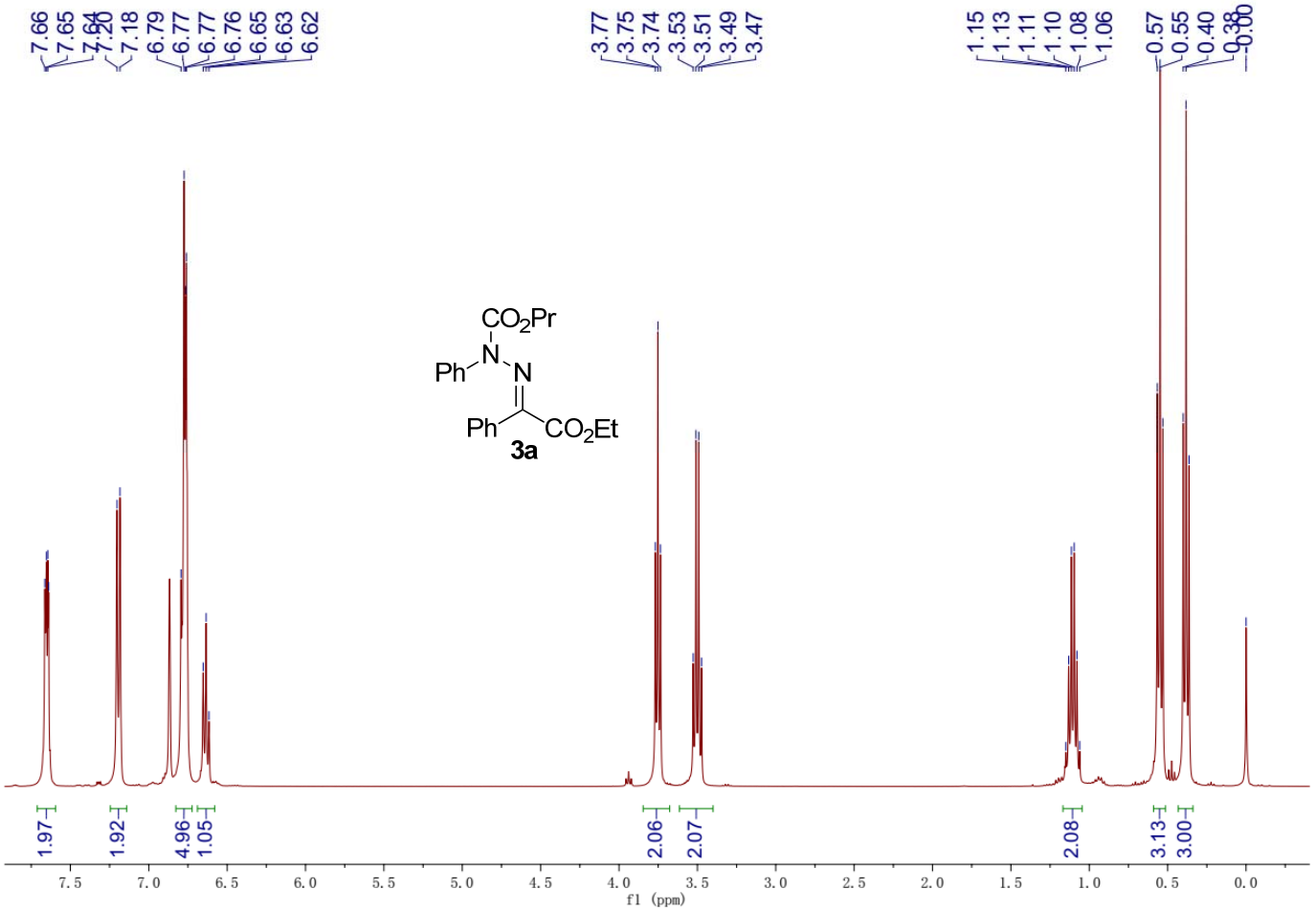
III. ORTEP Drawings for 5g.

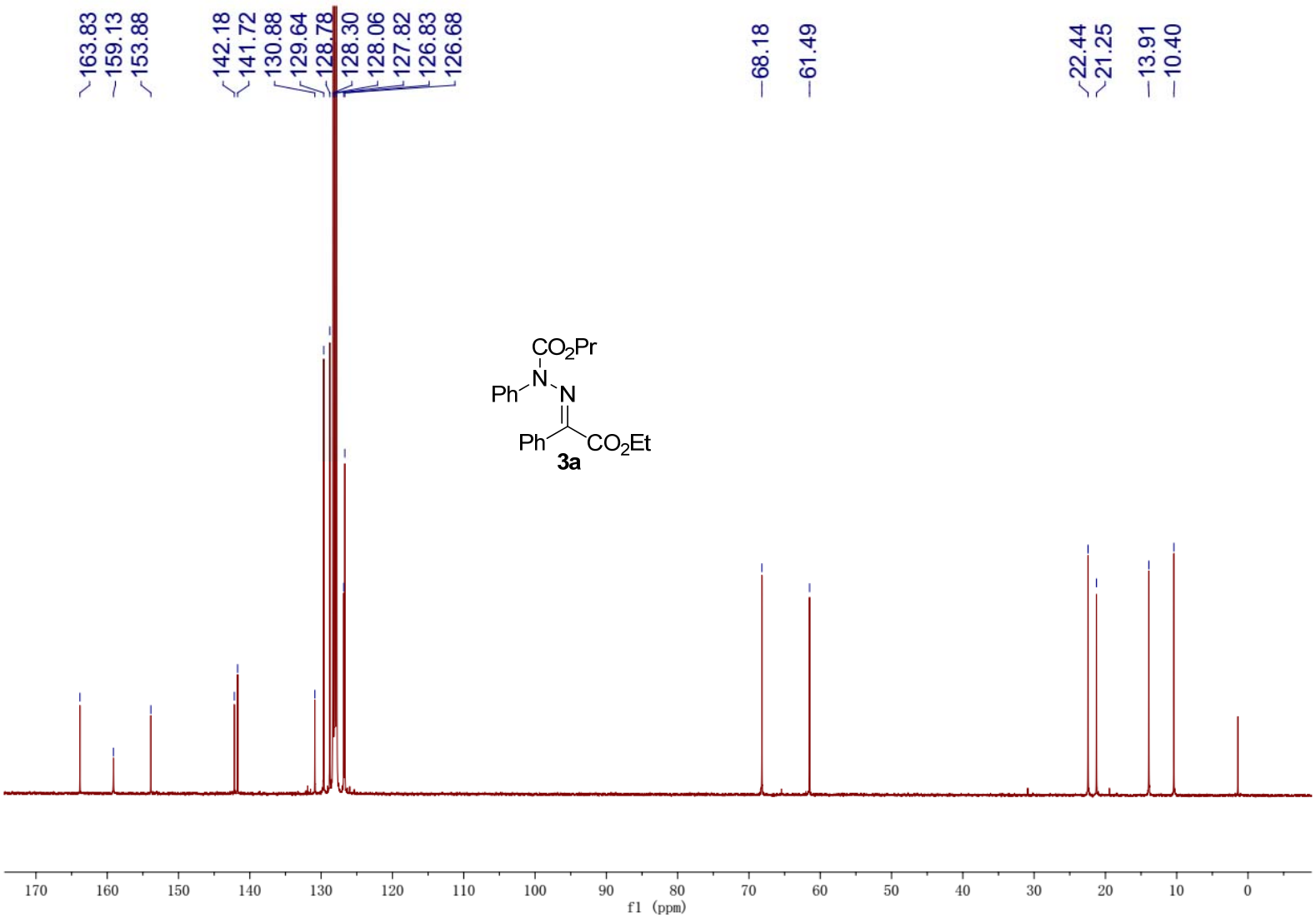
Table S1. Crystal data and structure refinement for 5g.



Identification code	**5g**
Empirical formula	$C_{25}H_{22}ClN_3O_3$
Formula weight	447.13
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 8.3937(17) Å α = 90.66(3)°
	b = 9.2600(19) Å β = 93.39(3) (9)°
	c = 13.938(3) Å γ = 95.51(3)°
Volume	1076.3(4) $Å^3$
Z, Calculated density	2, 1.329 Mg/m^3
Absorption coefficient	0.148 mm^{-1}
F(000)	452
Crystal size	0.200 x 0.180 x 0.120 mm^3
Theta range for data collection	2.210 to 25.018°
Limiting indices	-9<=h<=9, -10<=k<=11, -16<=l<=16
Reflections collected / unique	10248 / 3777 [R(int) = 0.0470]
Completeness to the θ = 25.018°	99.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3777 / 0 / 291
Goodness-of-fit on F^2	1.058
Final R indices [I>2σ(I)]	R1 = 0.0555, wR2 = 0.1340
R indices (all data)	R1 = 0.0863, wR2 = 0.1474
Largest diff. peak and hole	0.229 and -0.286 e. $Å^{-3}$

IV. ^{1}H and ^{13}C NMR Spectra of Compounds 3, 5 and 6

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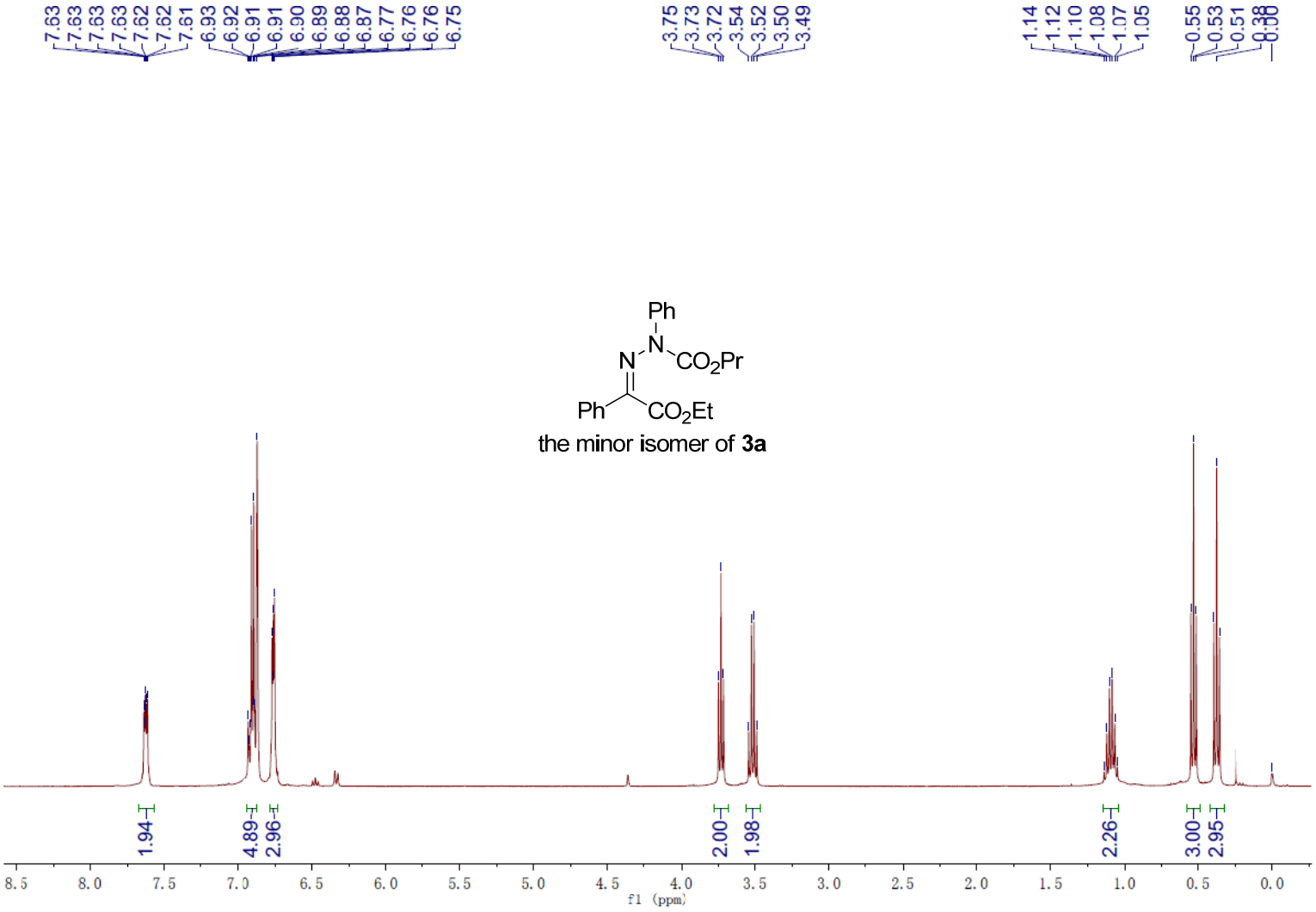
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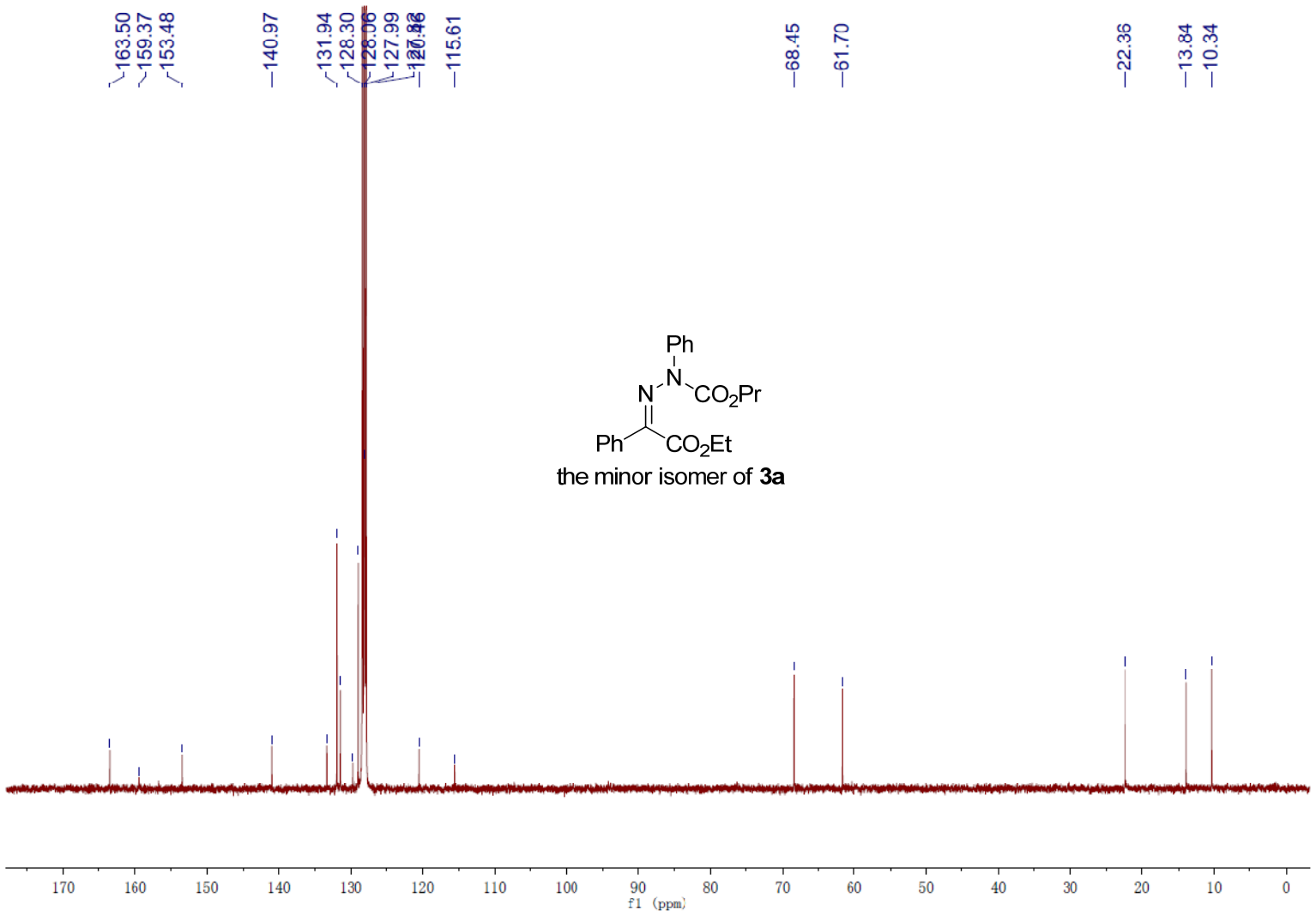
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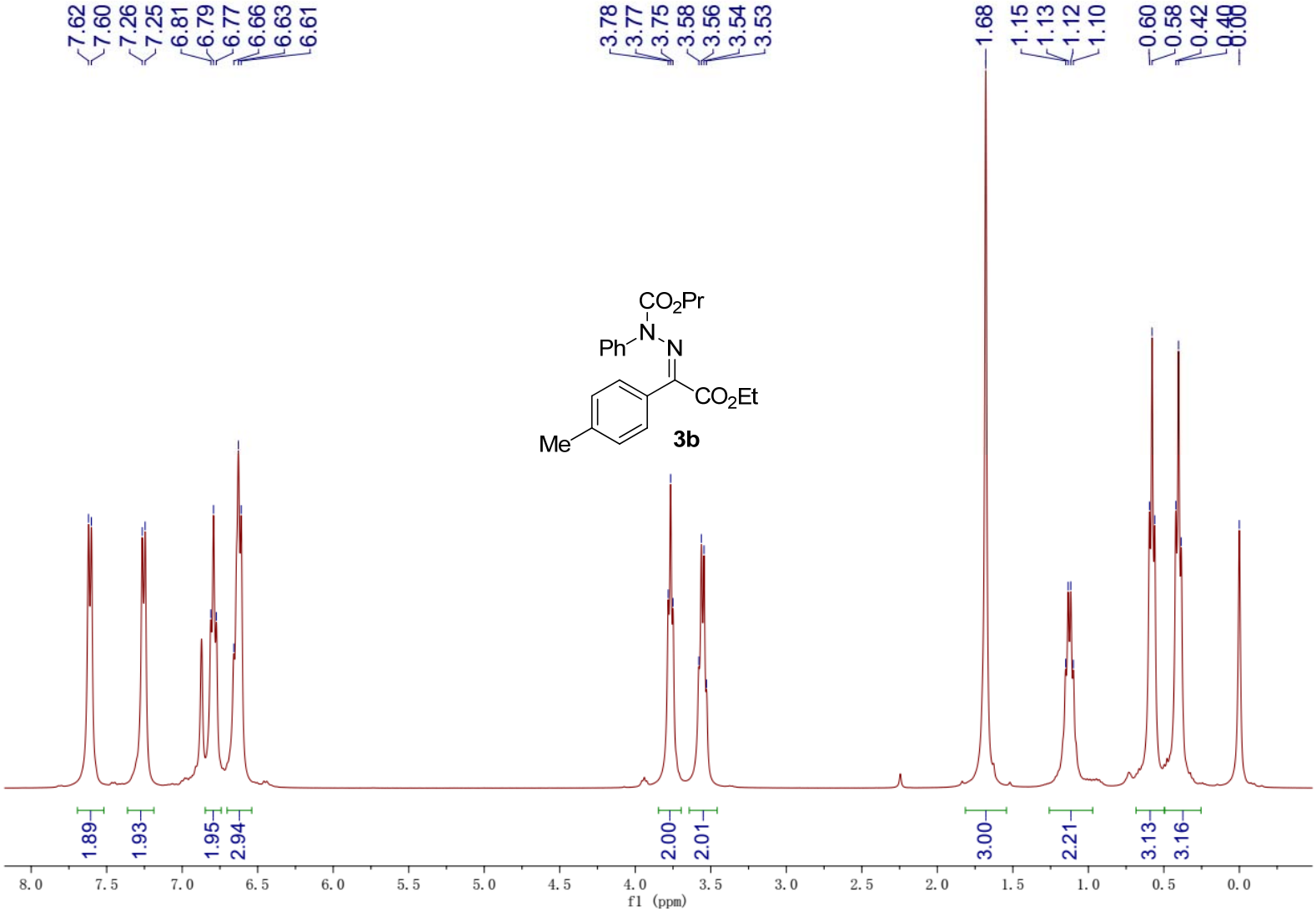
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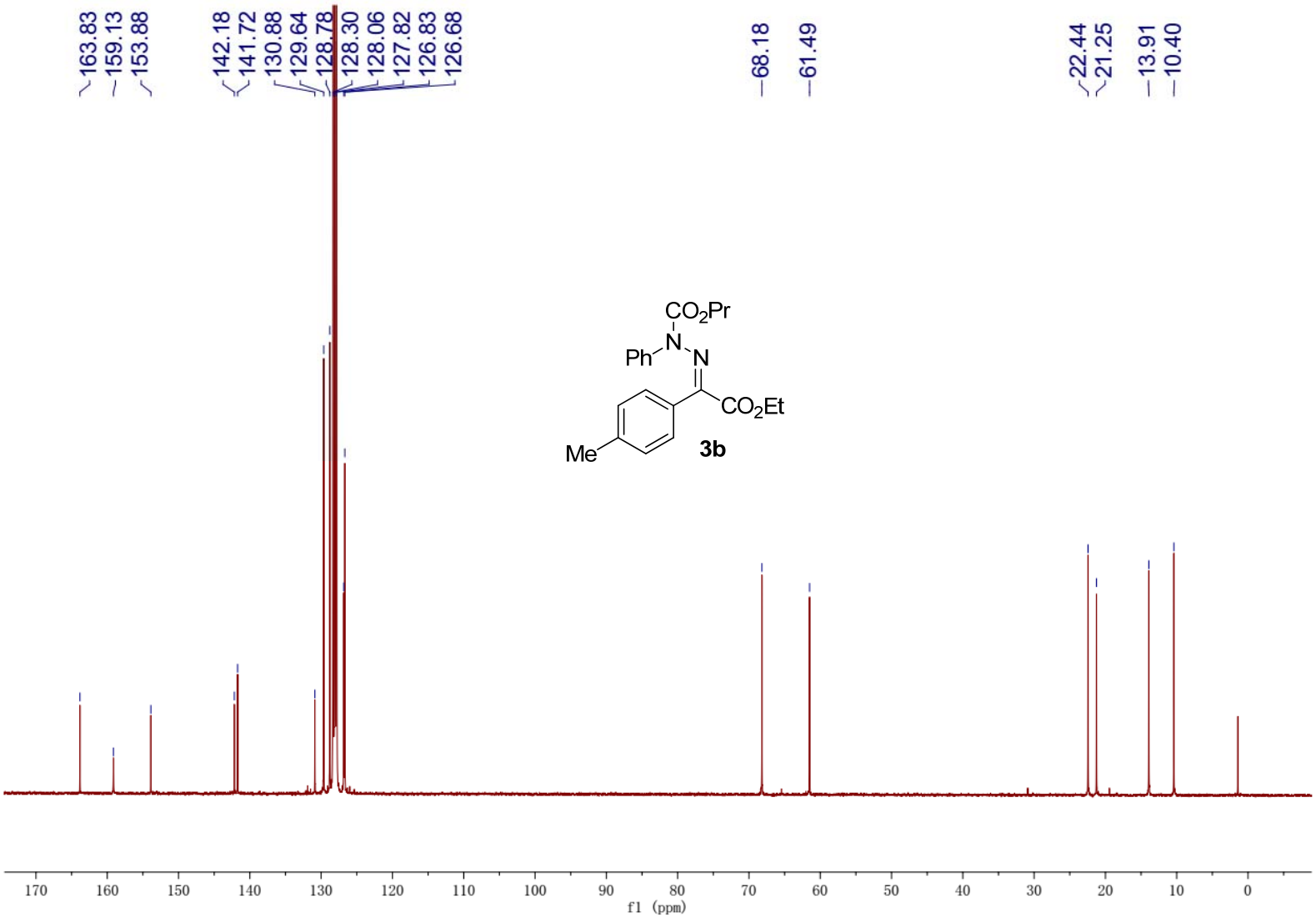
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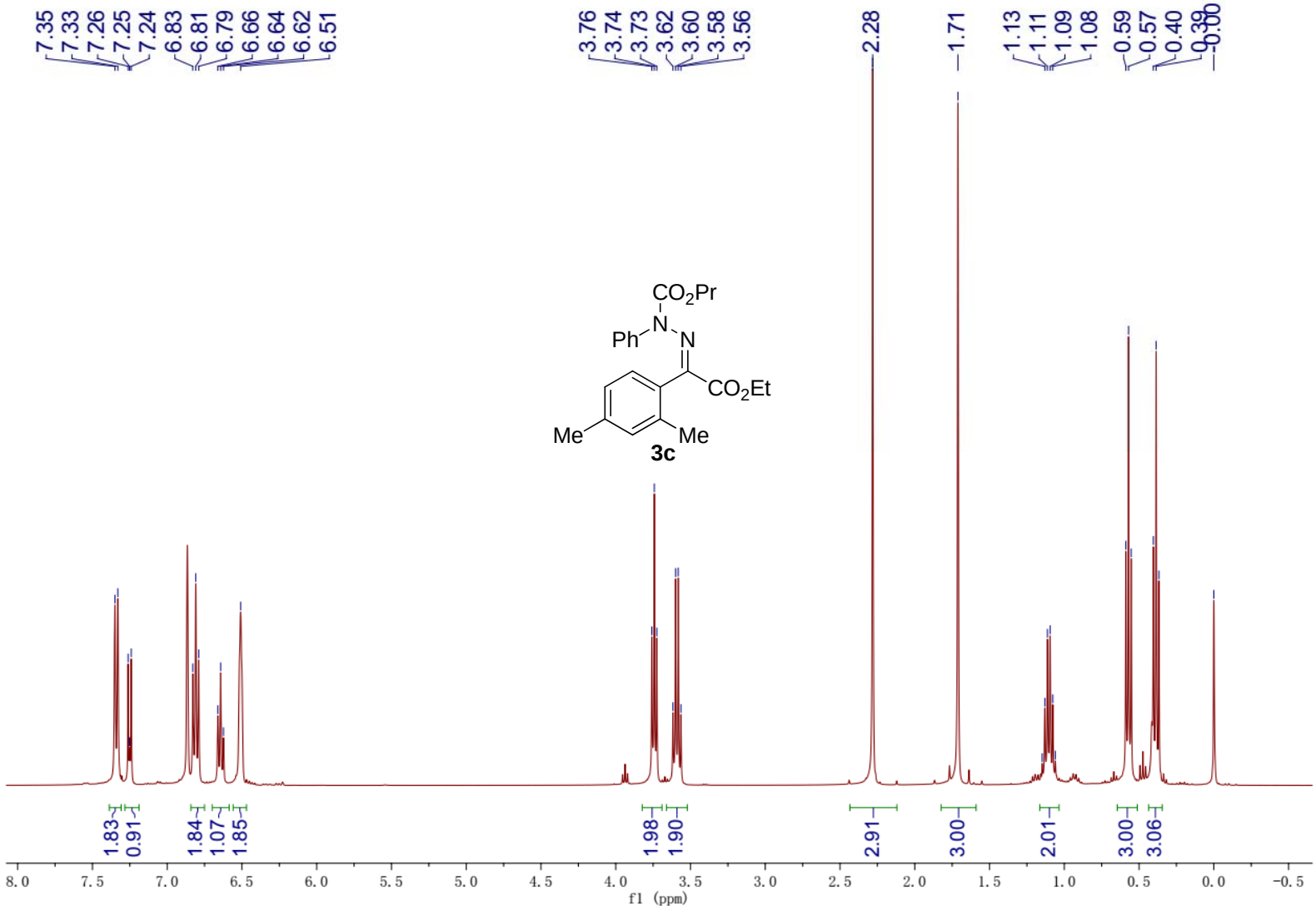
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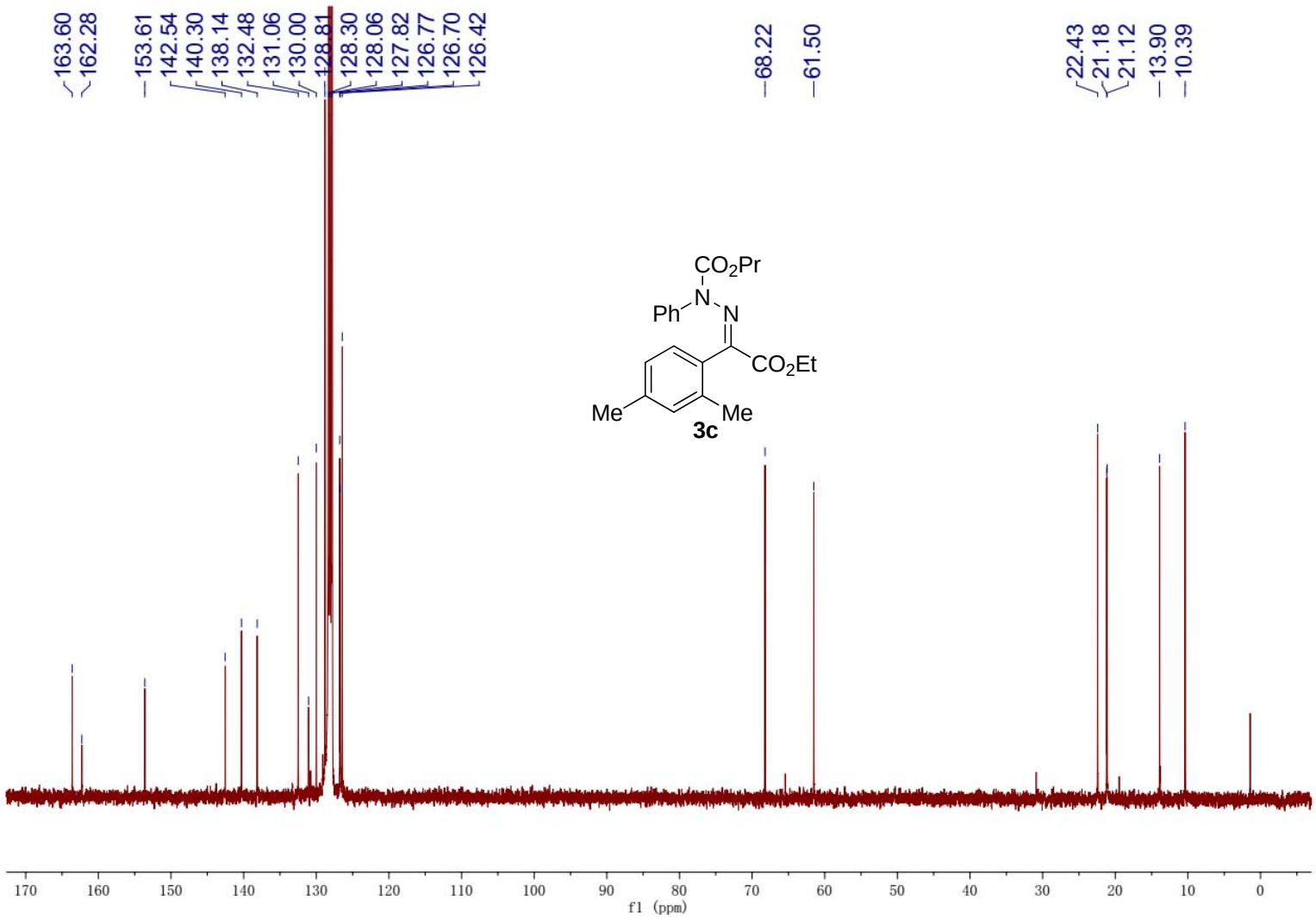
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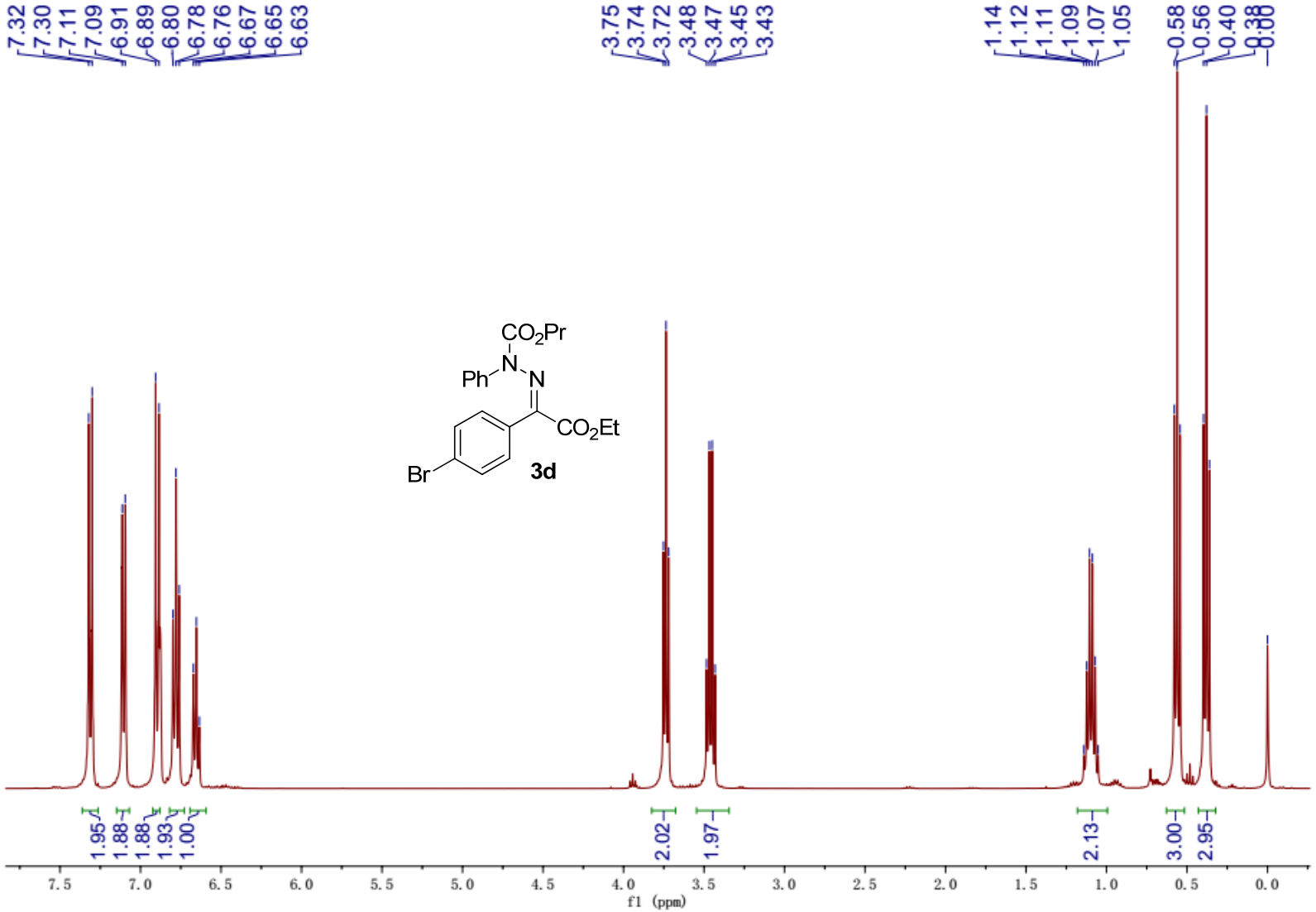
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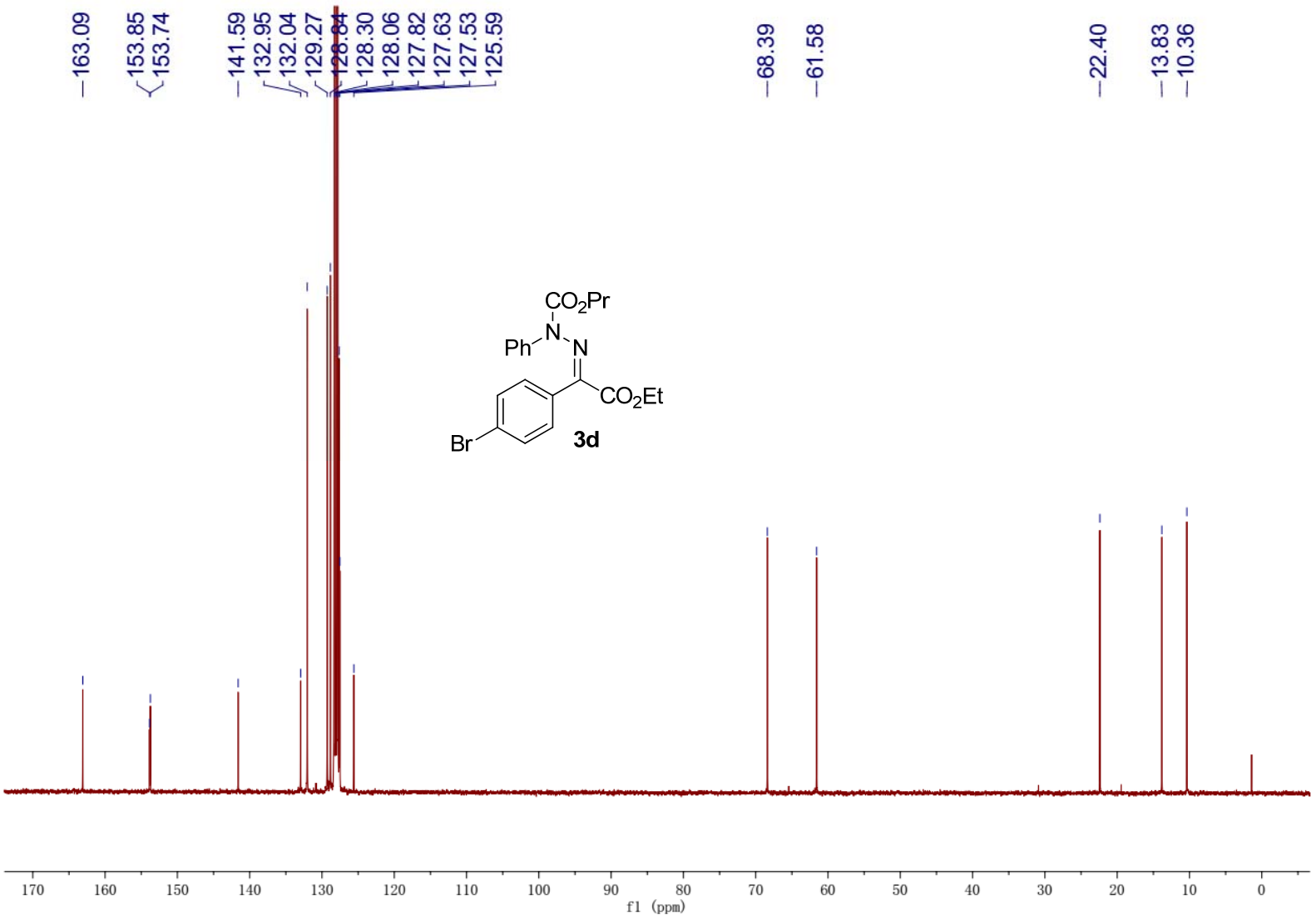
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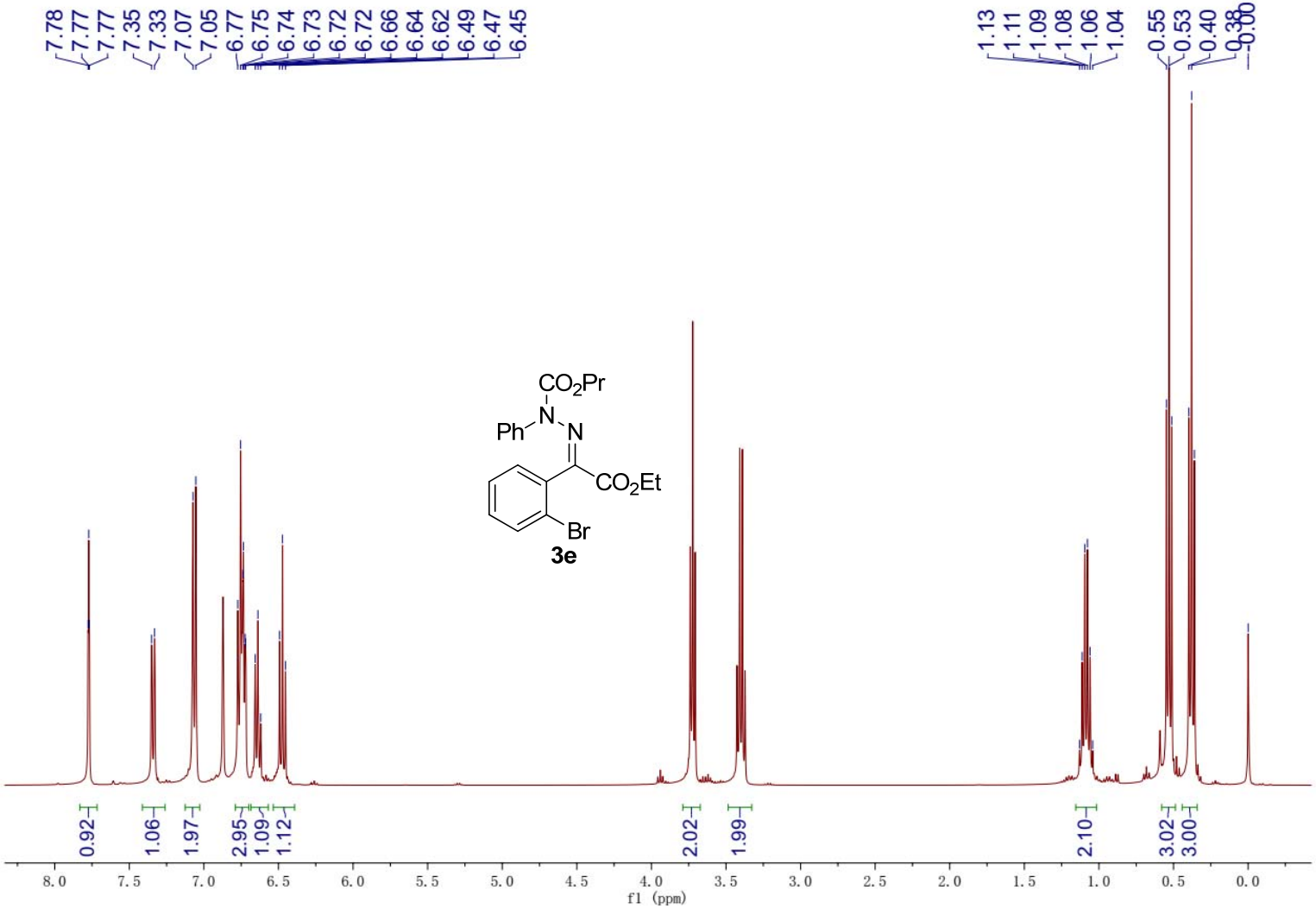
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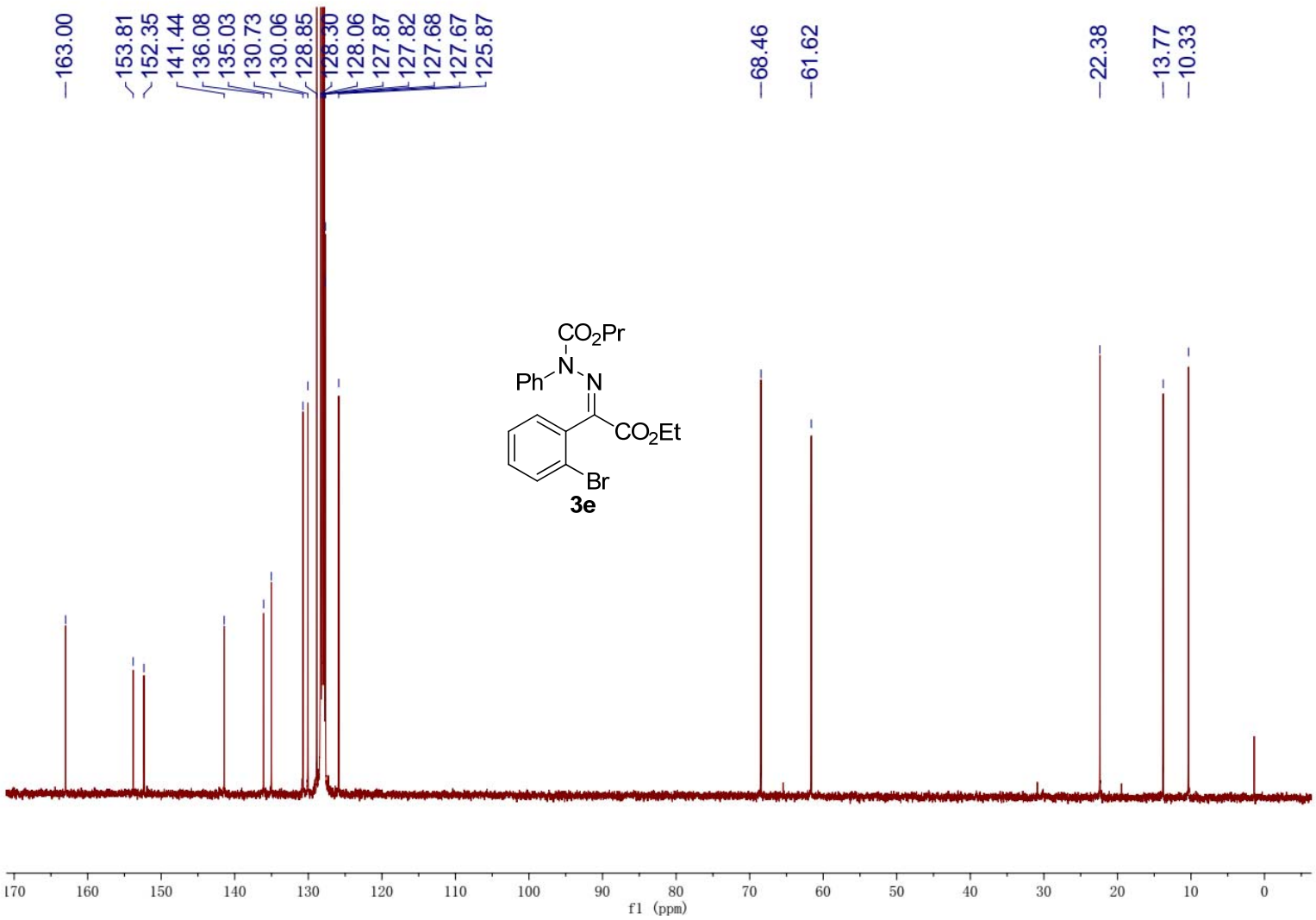
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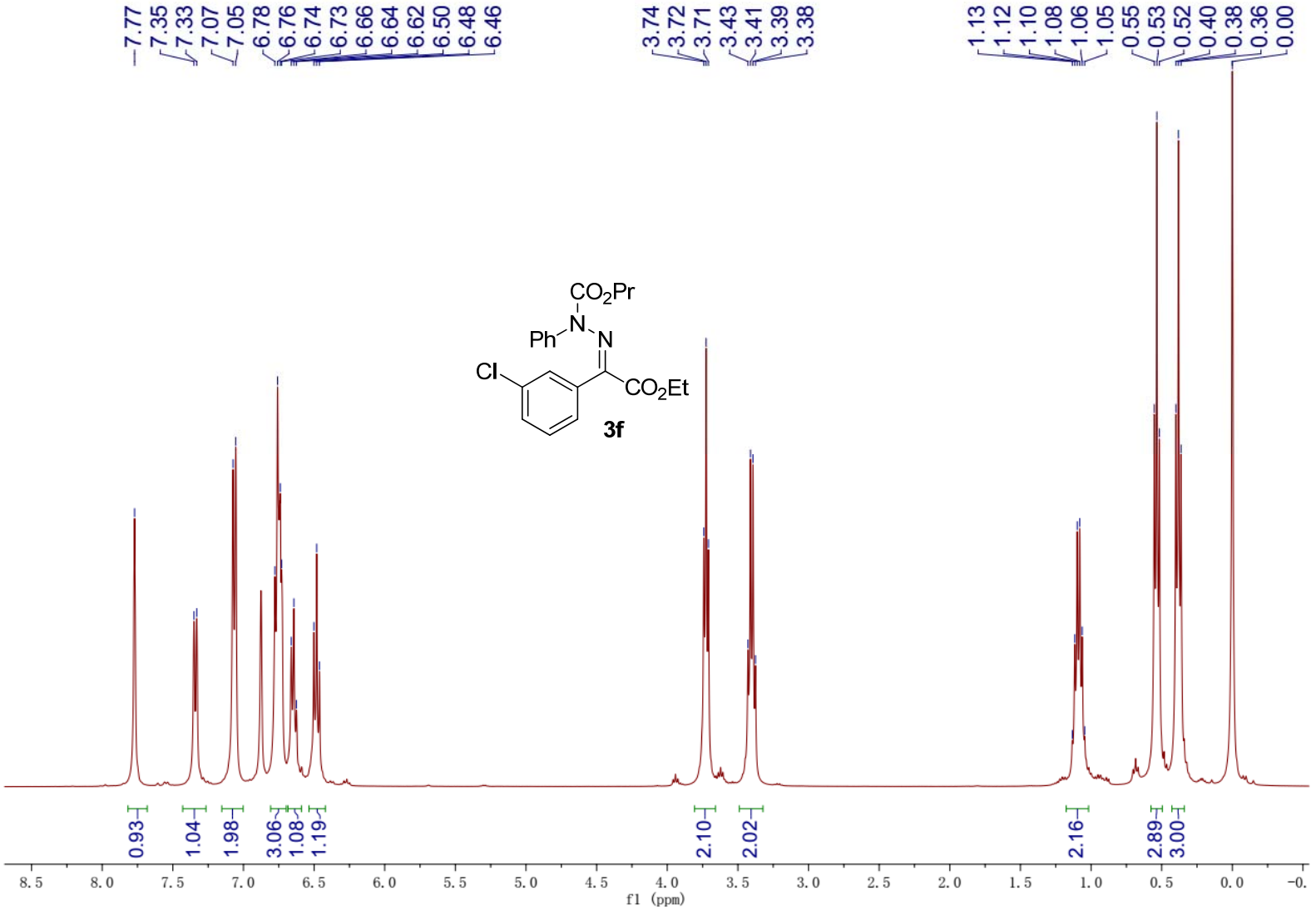
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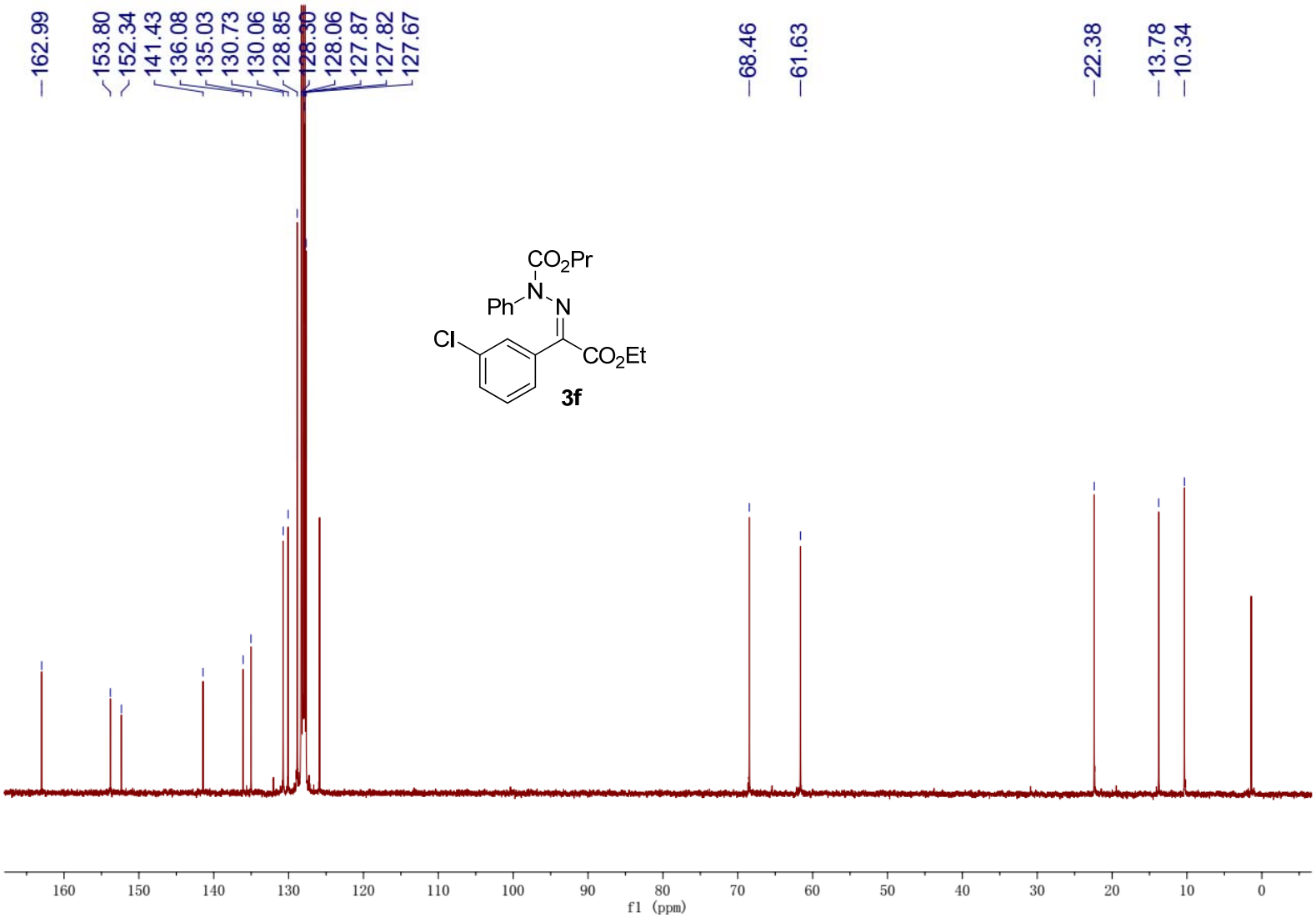
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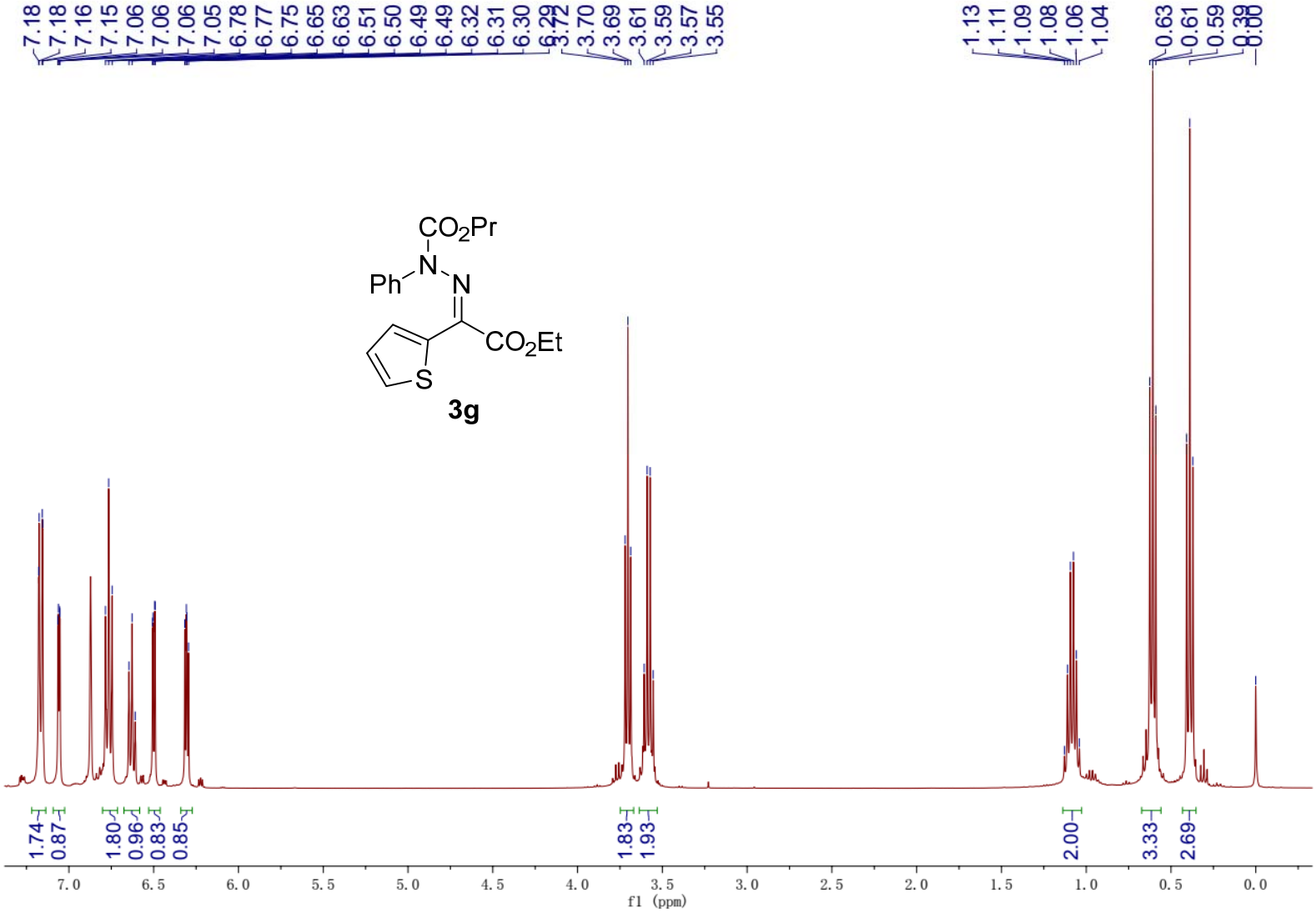
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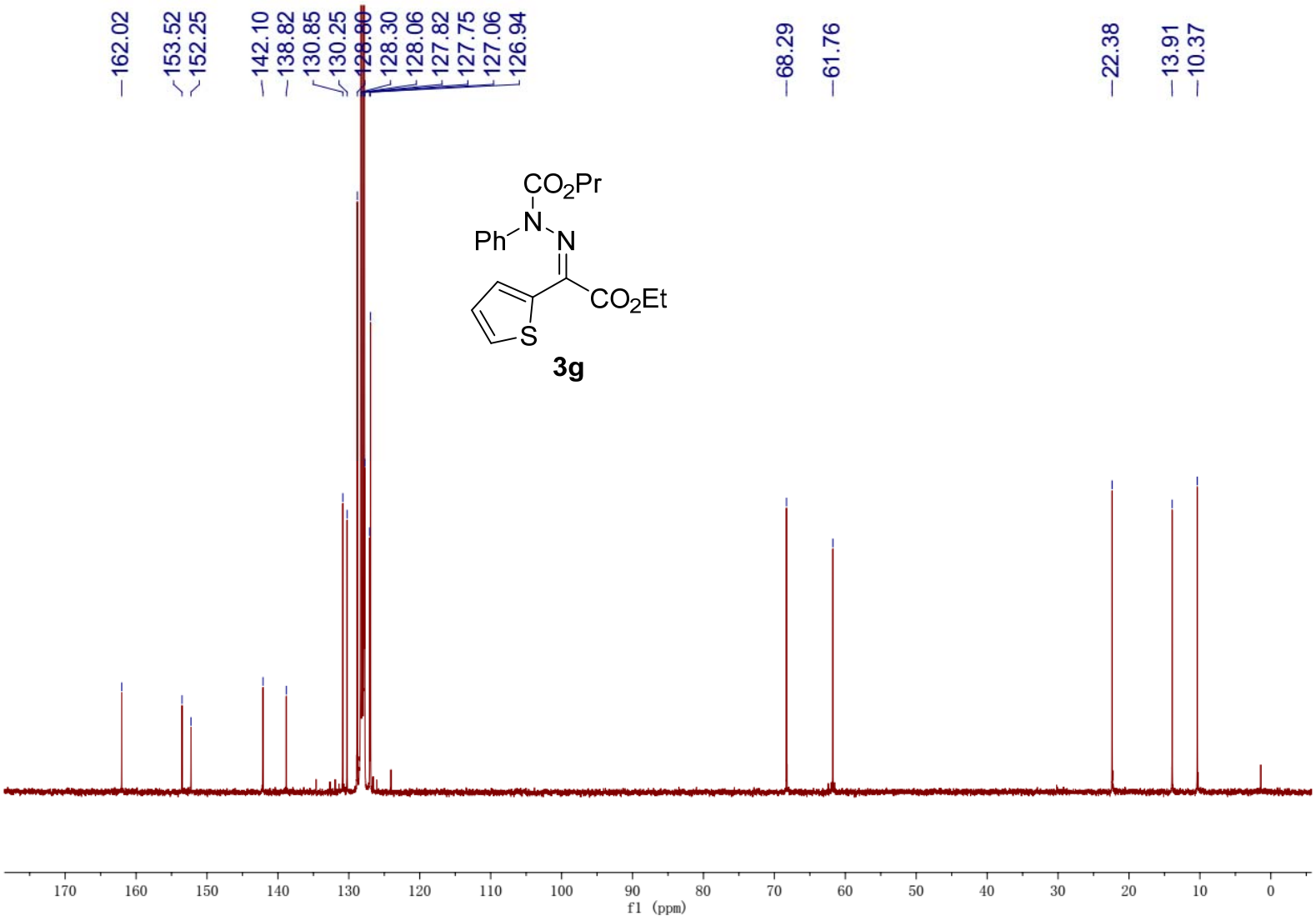
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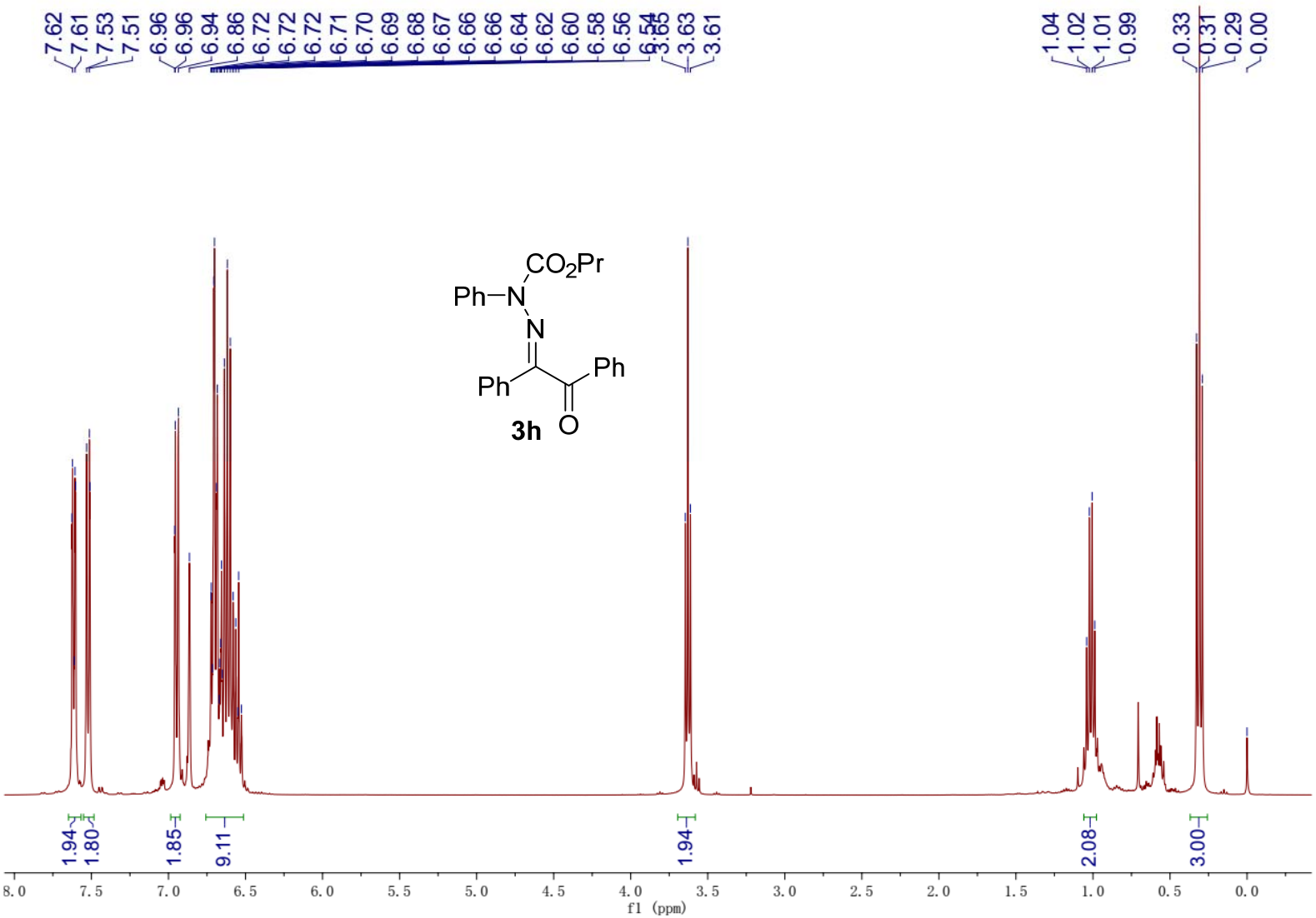
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6.72
6.71
6.70
6.69
6.68
6.67
6.66
6.66
6.64
6.62
6.60
6.58
6.56
6.54
3.65
3.63
3.61
1.04
1.02
1.01
0.99
0.33
0.31
0.29
0.00
CO2Pr
Ph—N
N
Ph
Ph
O
3h
1.94
1.80
1.85
9.11
1.94
2.08
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
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1.5
1.0
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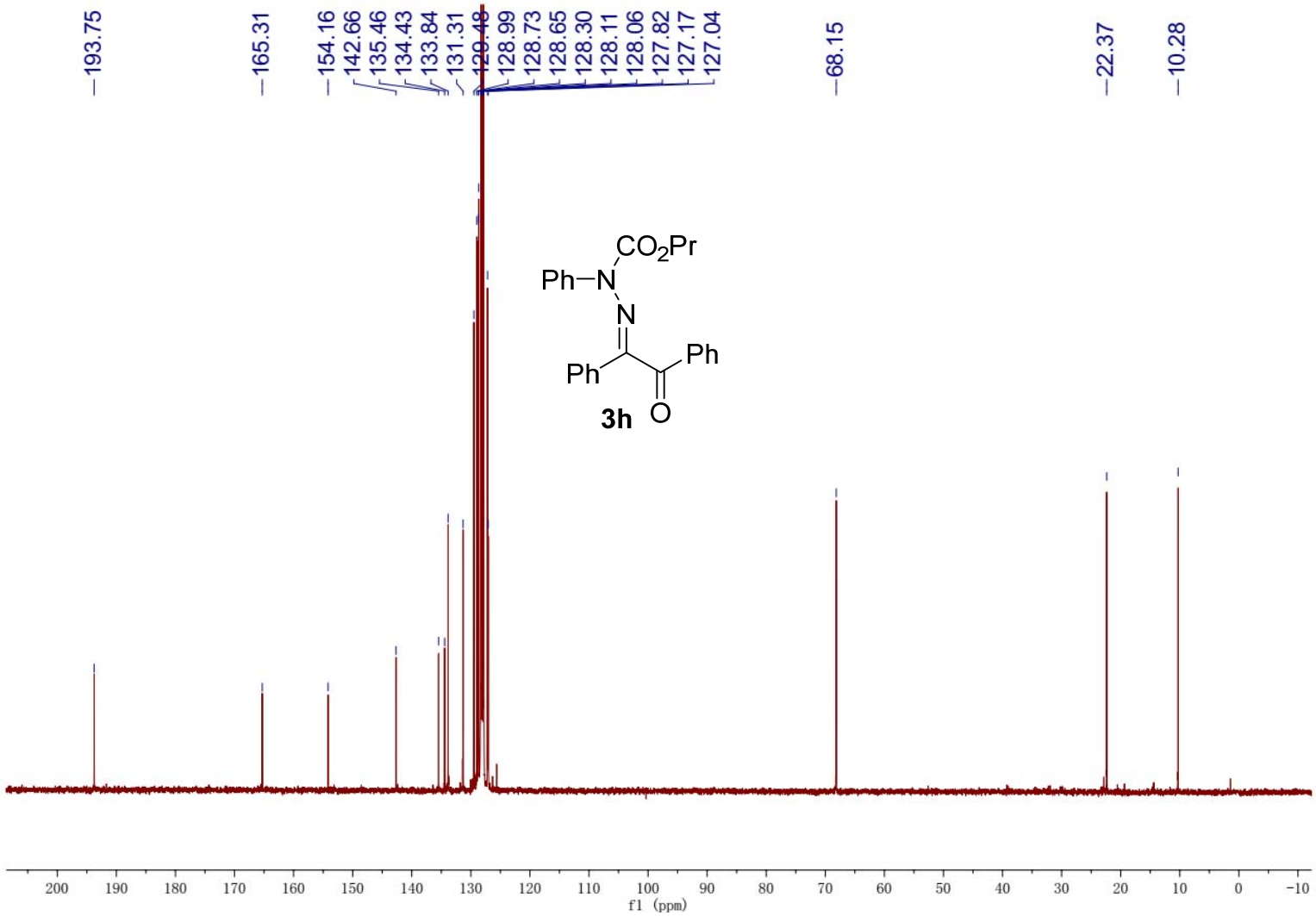
0.0
f1 (ppm)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131.31
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128.73
128.65
128.30
128.11
128.06
127.82
127.17
127.04
68.15
22.37
10.28
CO2Pr
Ph
N
N
Ph
Ph
O
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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40
30
20
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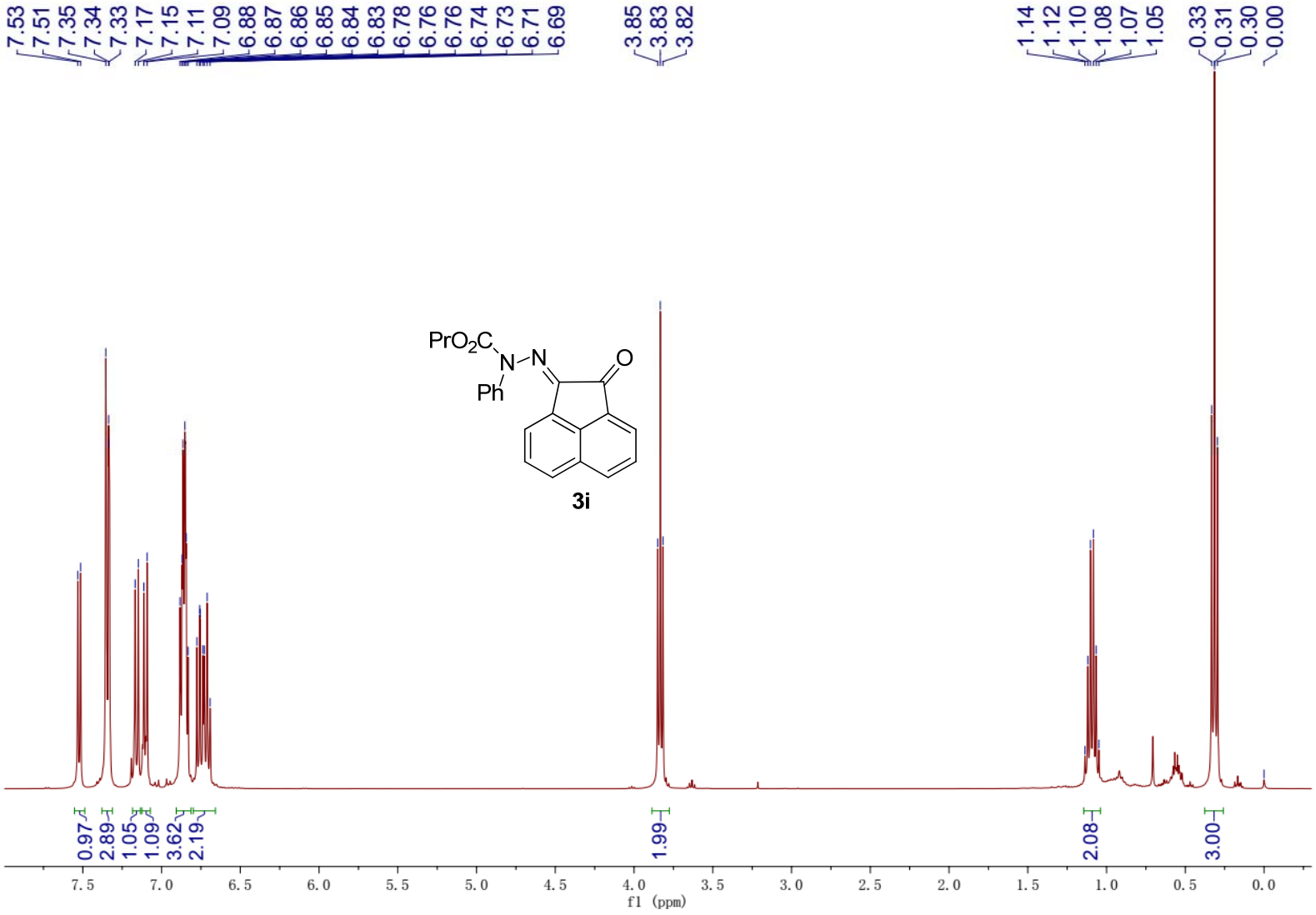
f1 (ppm)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6.86
6.85
6.84
6.83
6.78
6.76
6.76
6.74
6.73
6.71
6.69
3.85
3.83
3.82
1.14
1.12
1.10
1.08
1.07
1.05
0.33
0.31
0.30
0.00
PrO2C
N
N
Ph
O
3i
0.97
2.89
1.05
1.09
3.62
2.19
1.99
2.08
3.00
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
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2.5
2.0
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1.0
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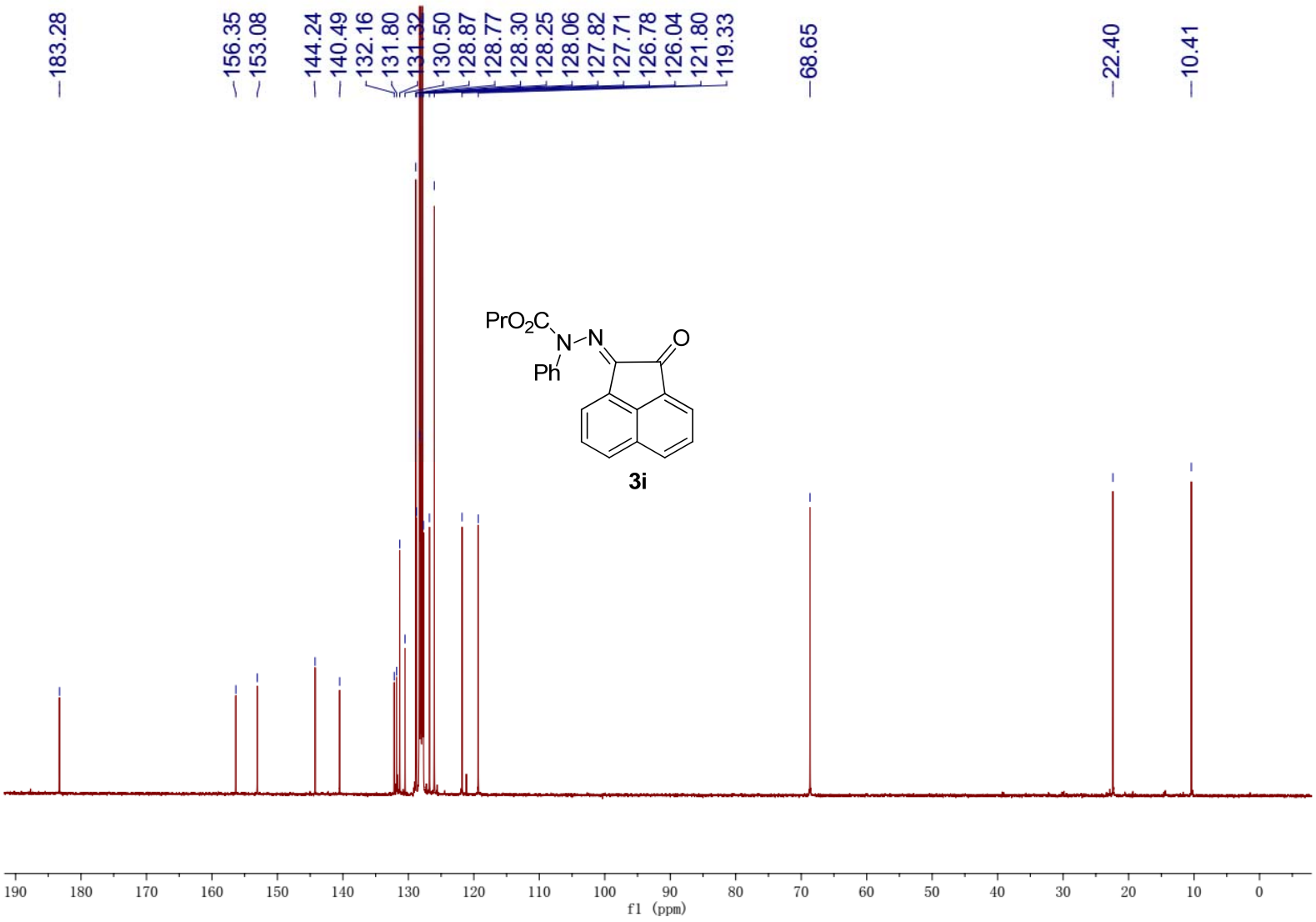
0.0
f1 (ppm)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128.25
128.06
127.82
127.71
126.78
126.04
121.80
119.33
68.65
22.40
10.41
PrO2C
N
N
O
Ph
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
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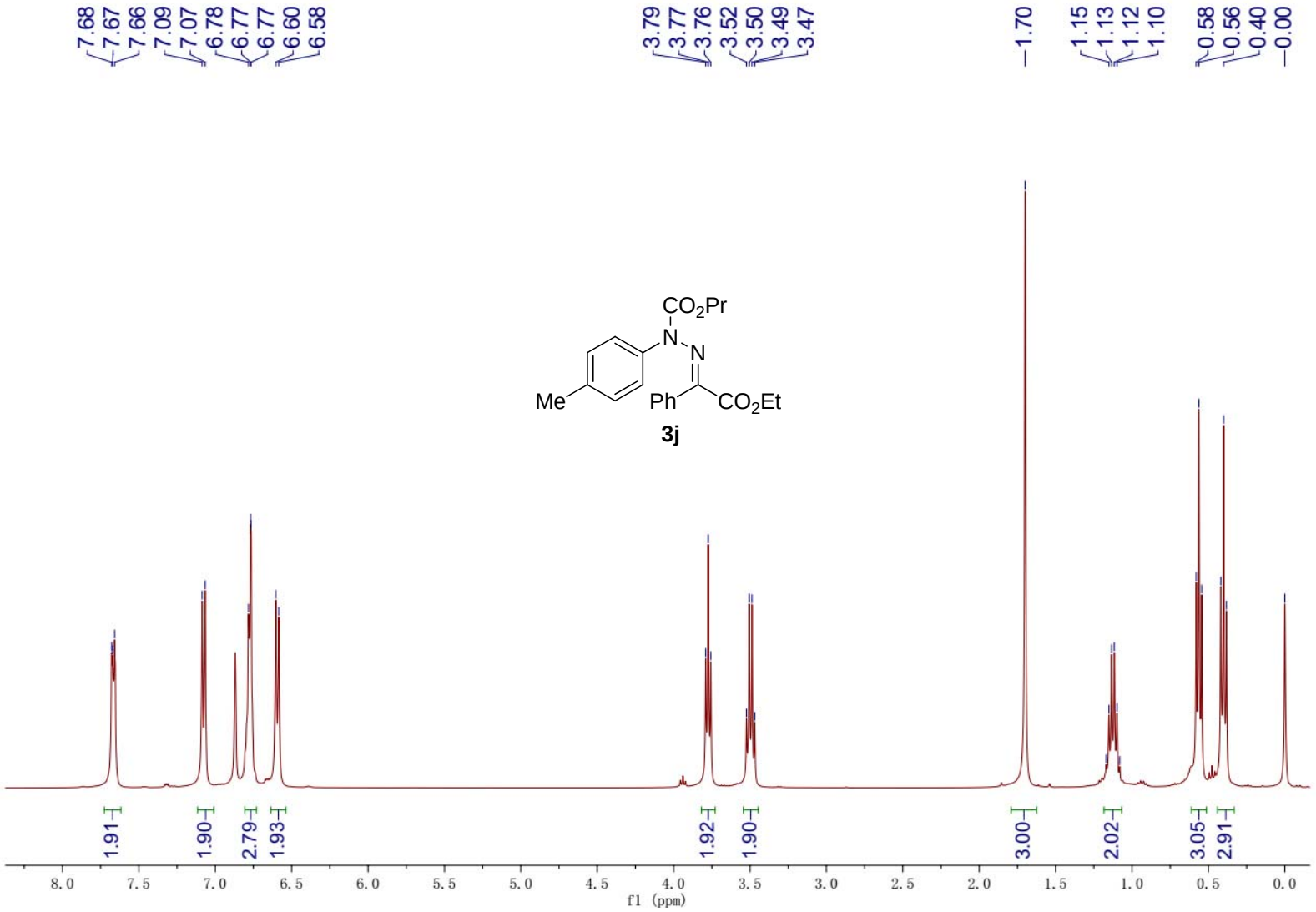
50
40
30
20
10
0
f1 (ppm)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7.67
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6.77
6.77
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6.58
3.79
3.77
3.76
3.52
3.50
3.49
3.47
1.70
1.15
1.13
1.12
1.10
0.58
0.56
0.40
0.00
CO2Pr
N
N
Me
Ph
CO2Et
3j
1.91
1.90
2.79
1.93
1.92
1.90
3.00
2.02
3.05
2.91
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
2.5
2.0
1.5
1.0
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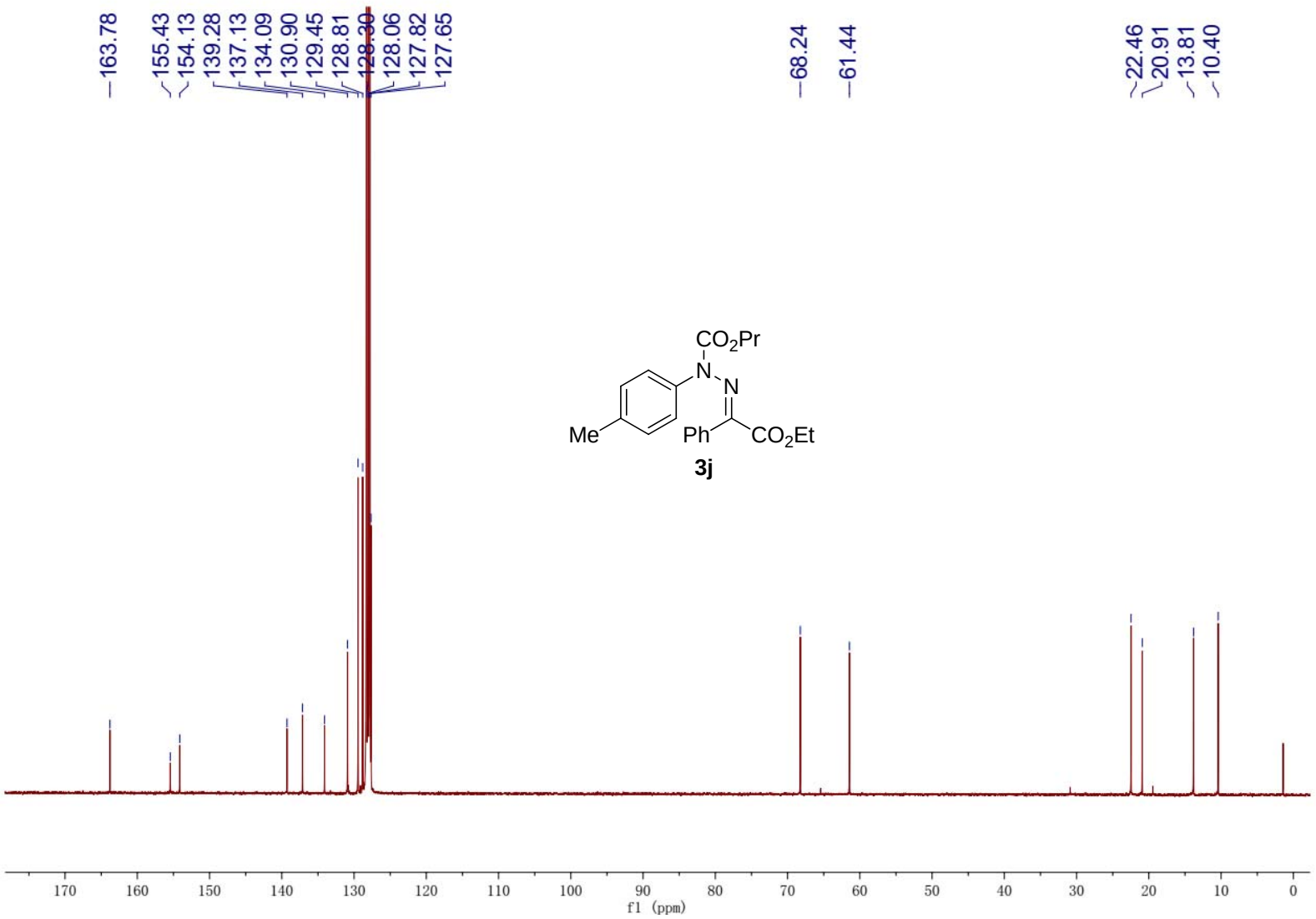
0.0
f1 (ppm)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129.45
128.81
128.30
128.06
127.82
127.65
68.24
61.44
22.46
20.91
13.81
10.40
CO2Pr
N
N
Me
Ph
CO2Et
3j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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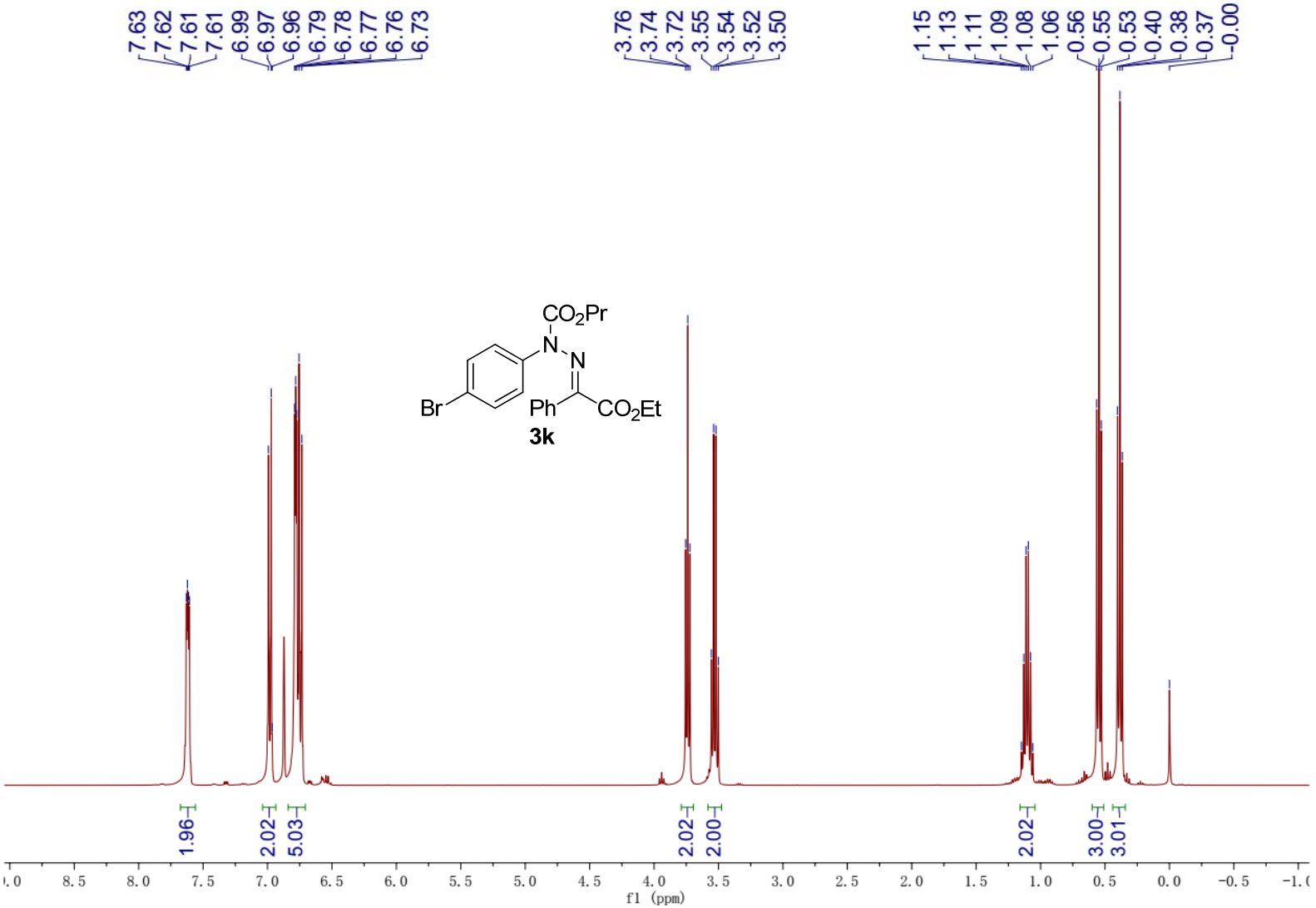
f1 (ppm)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7.62
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7.61
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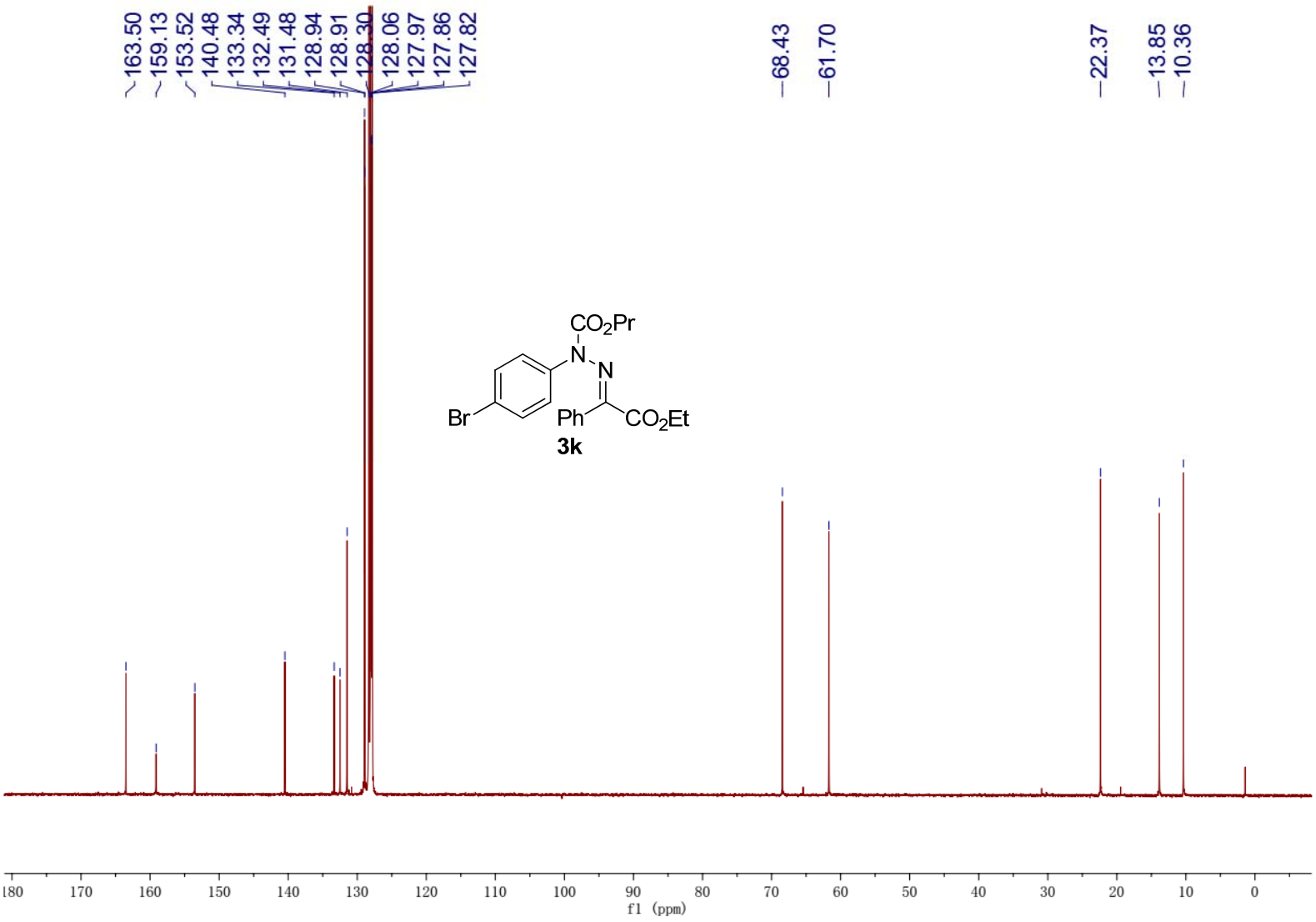
6.79
6.78
6.77
6.76
6.73
3.76
3.74
3.72
3.55
3.54
3.52
3.50
1.15
1.13
1.11
1.09
1.08
1.06
0.56
0.55
0.53
0.40
0.38
0.37
-0.00
CO2Pr
N
N
Br
Ph
CO2Et
3k
1.96
2.02
5.03
2.02
2.00
2.02
3.00
3.01
f1 (ppm)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132.49
131.48
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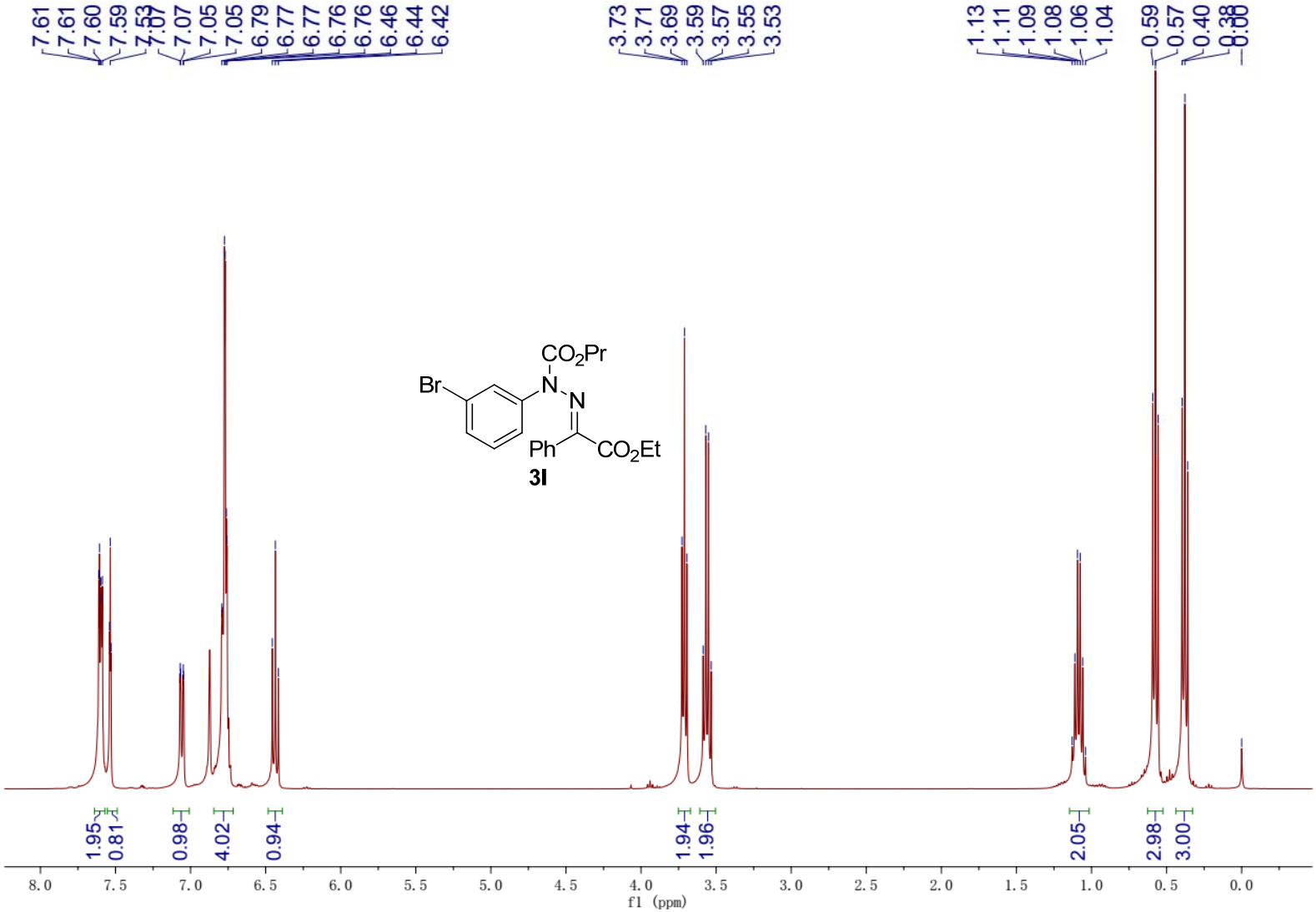
128.91
128.30
128.06
127.97
127.86
127.82
68.43
61.70
22.37
13.85
10.36
CO2Pr
N
N
Br
Ph
CO2Et
3k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.61
7.60
7.59
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7.07
7.07
7.05
7.05
6.79
6.77
6.77
6.76
6.76
6.46
6.44
6.42
3.73
3.71
3.69
3.59
3.57
3.55
3.53
1.13
1.11
1.09
1.08
1.06
1.04
0.59
0.57
0.40
0.38
0.00
CO2Pr
Br
N
N
Ph
CO2Et
3l
1.95
0.81
0.98
4.02
0.94
1.94
1.96
2.05
2.98
3.00
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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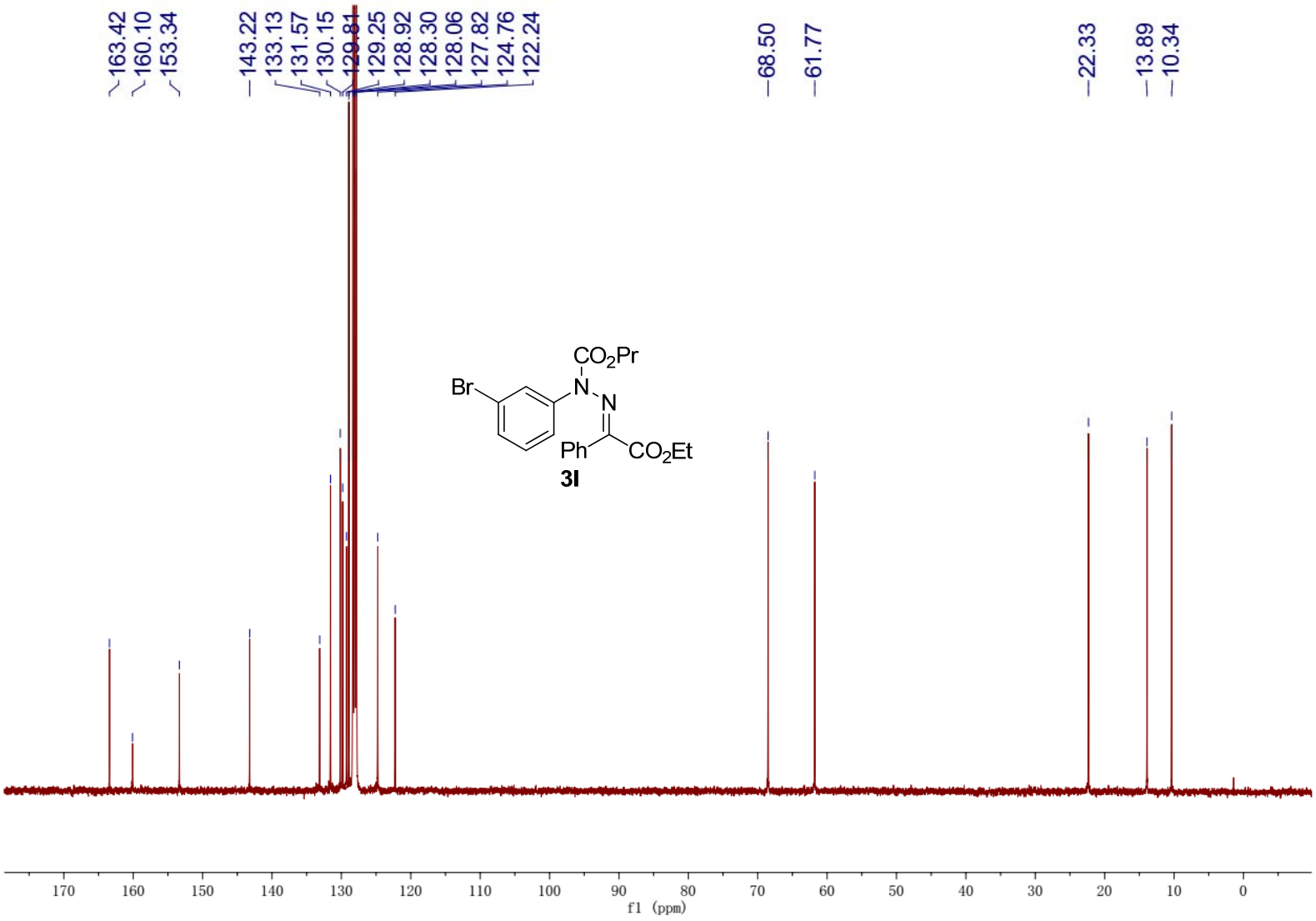
0.0
f1 (ppm)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129.81
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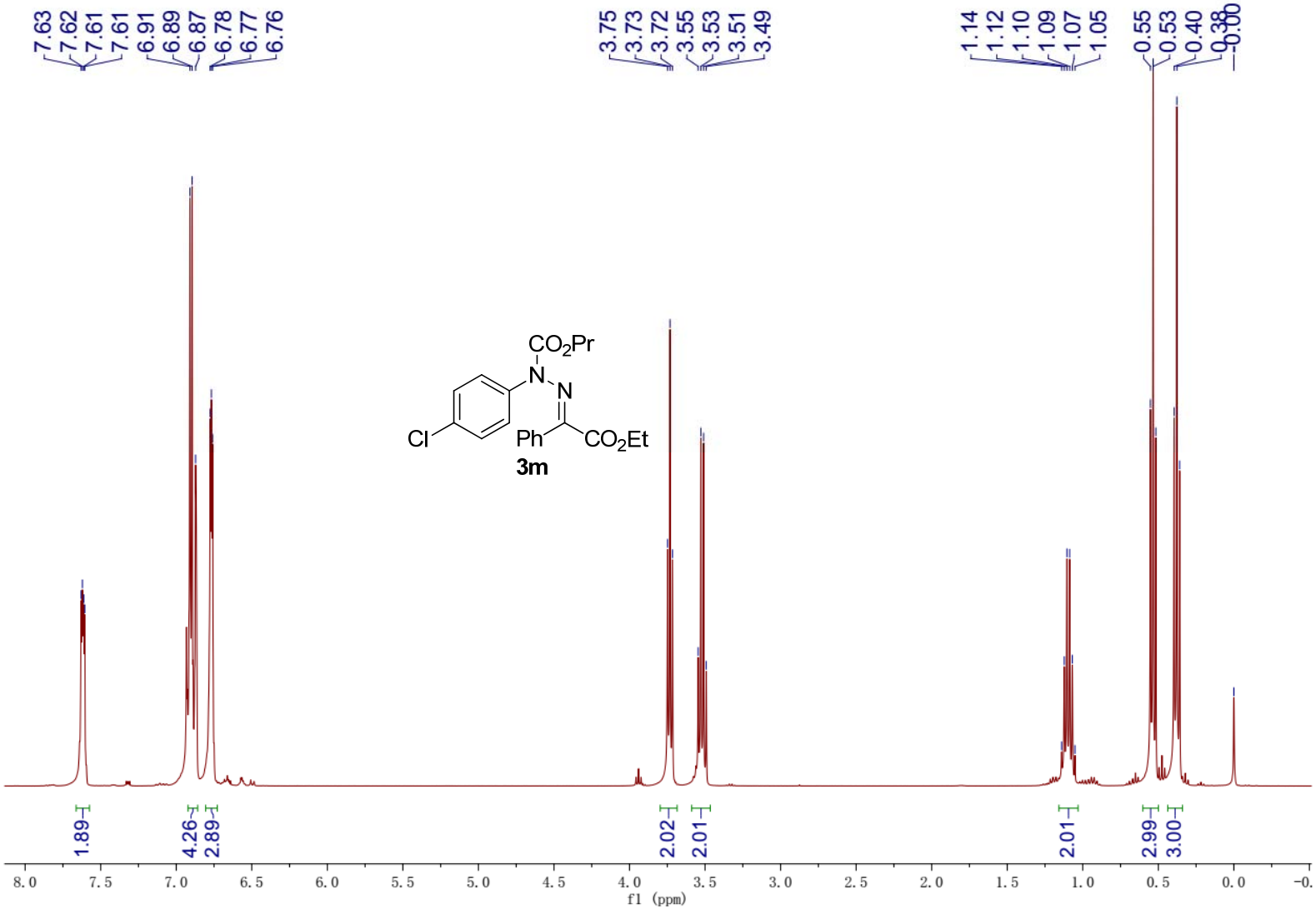
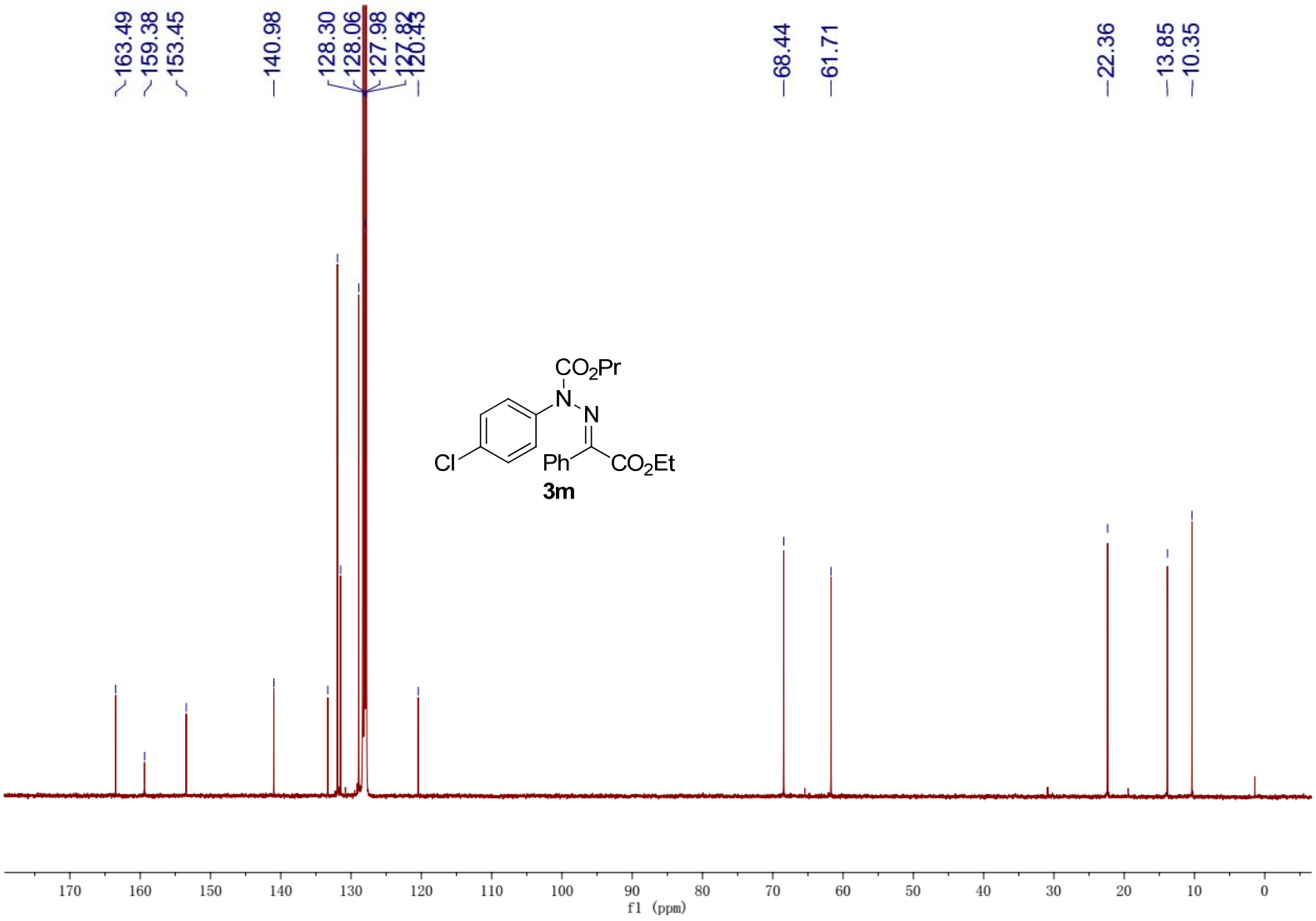
128.92
128.30
128.06
127.82
124.76
122.24
68.50
61.77
22.33
13.89
10.34
CO2Pr
Br
N
N
Ph
CO2Et
3l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.63
7.62
7.61
7.61
6.91
6.89
6.87
6.78
6.77
6.76
3.75
3.73
3.72
3.55
3.53
3.51
3.49
1.14
1.12
1.10
1.09
1.07
1.05
0.55
0.53
0.40
0.38
0.00
CO2Pr
N
N
Cl
Ph
CO2Et
3m
1.89
4.26
2.89
2.02
2.01
2.01
2.99
3.00
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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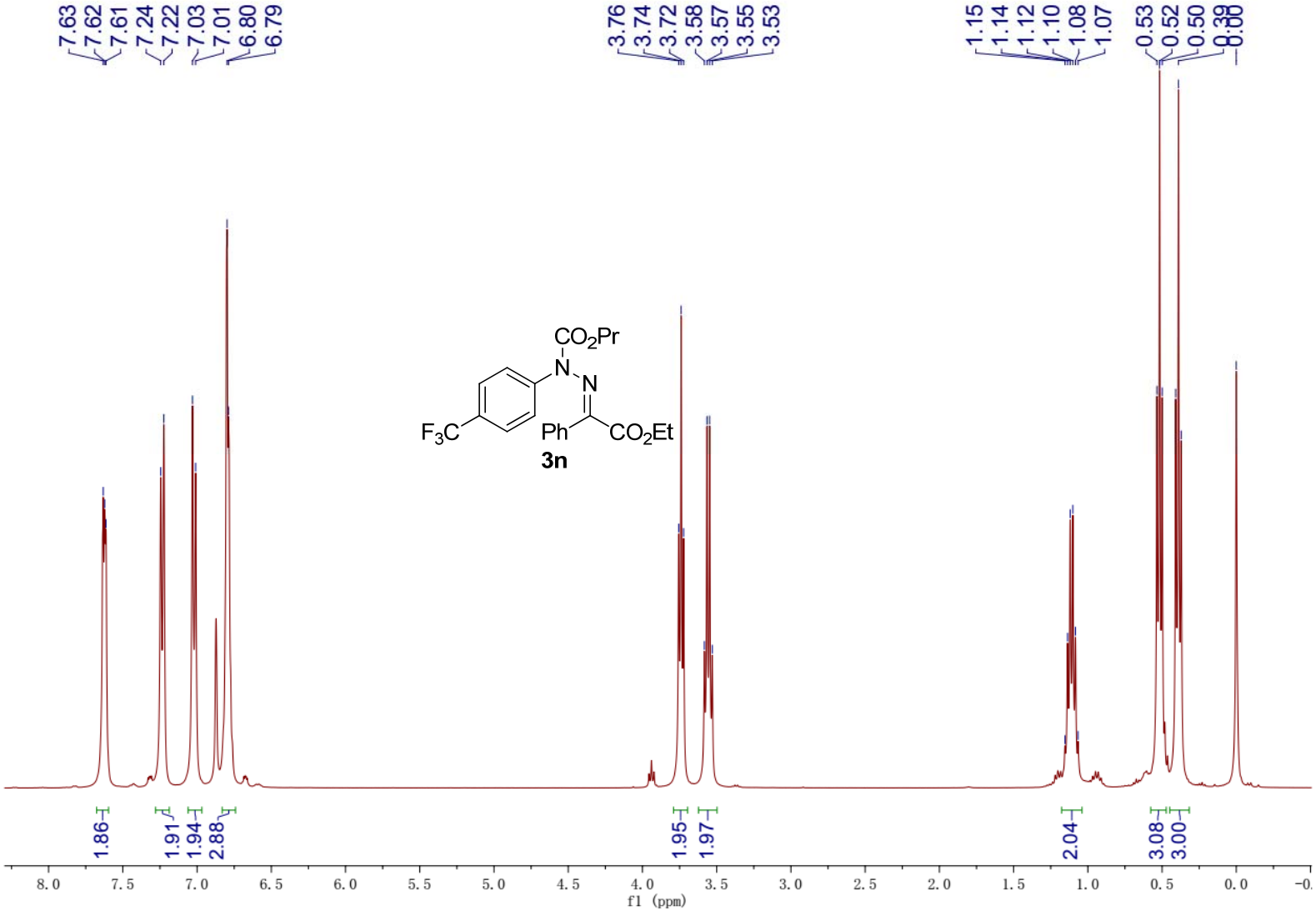
127.82
120.43
68.44
61.71
22.36
13.85
10.35
CO2Pr
N
N
Cl
Ph
CO2Et
3m
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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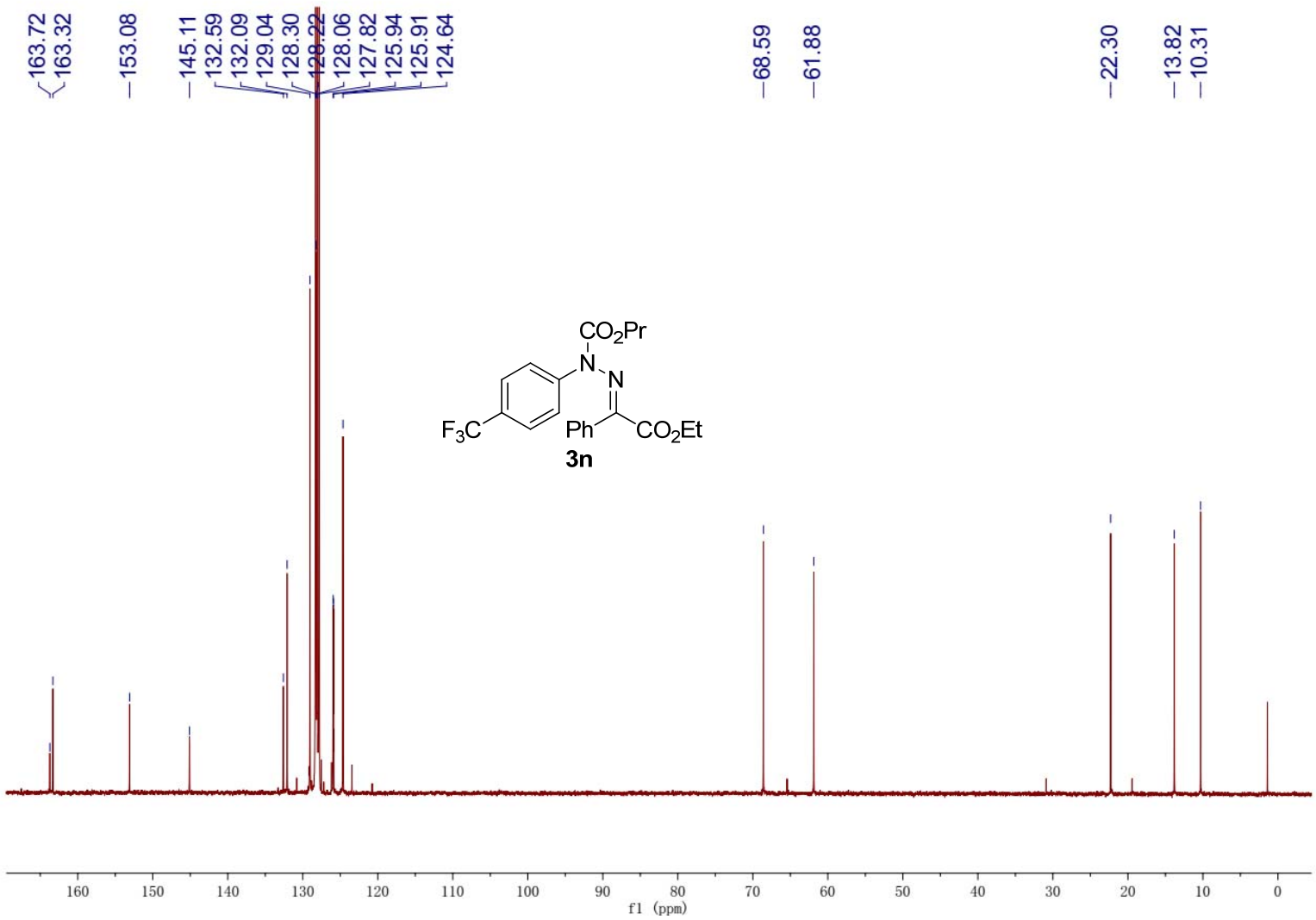
7.62
7.61
7.24
7.22
7.03
7.01
6.80
6.79
3.76
3.74
3.72
3.58
3.57
3.55
3.53
1.15
1.14
1.12
1.10
1.08
1.07
0.53
0.52
0.50
0.39
0.00
CO2Pr
N
N
F3C
Ph
CO2Et
3n
1.86
1.91
1.94
2.88
1.95
1.97
2.04
3.08
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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163.32
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132.59
132.09
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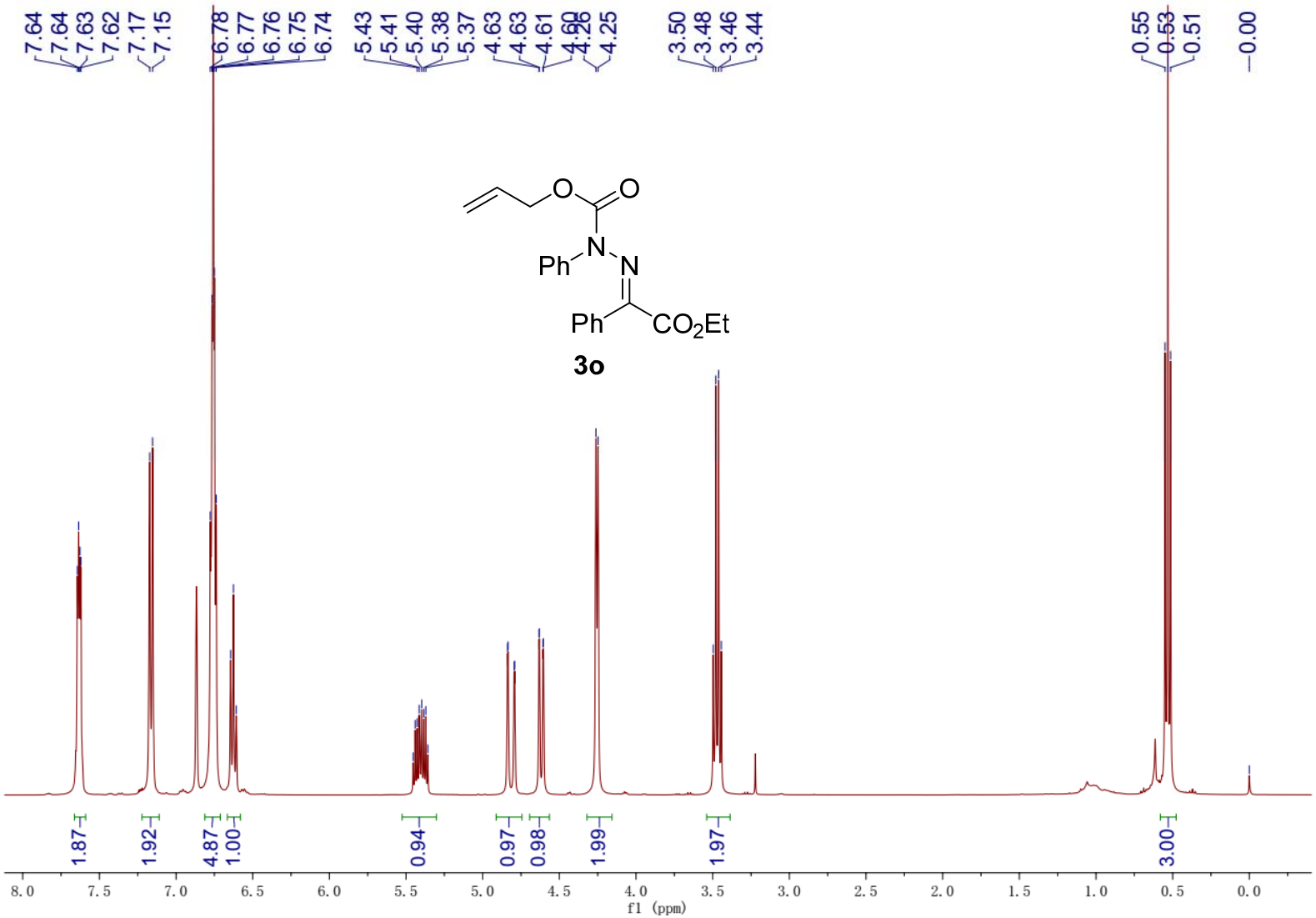
128.22
128.06
127.82
125.94
125.91
124.64
68.59
61.88
22.30
13.82
10.31
CO2Pr
N
N
F3C
Ph
CO2Et
3n
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.77
6.76
6.75
6.74
5.43
5.41
5.40
5.38
5.37
4.63
4.63
4.61
4.60
4.25
3.50
3.48
3.46
3.44
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0.53
0.51
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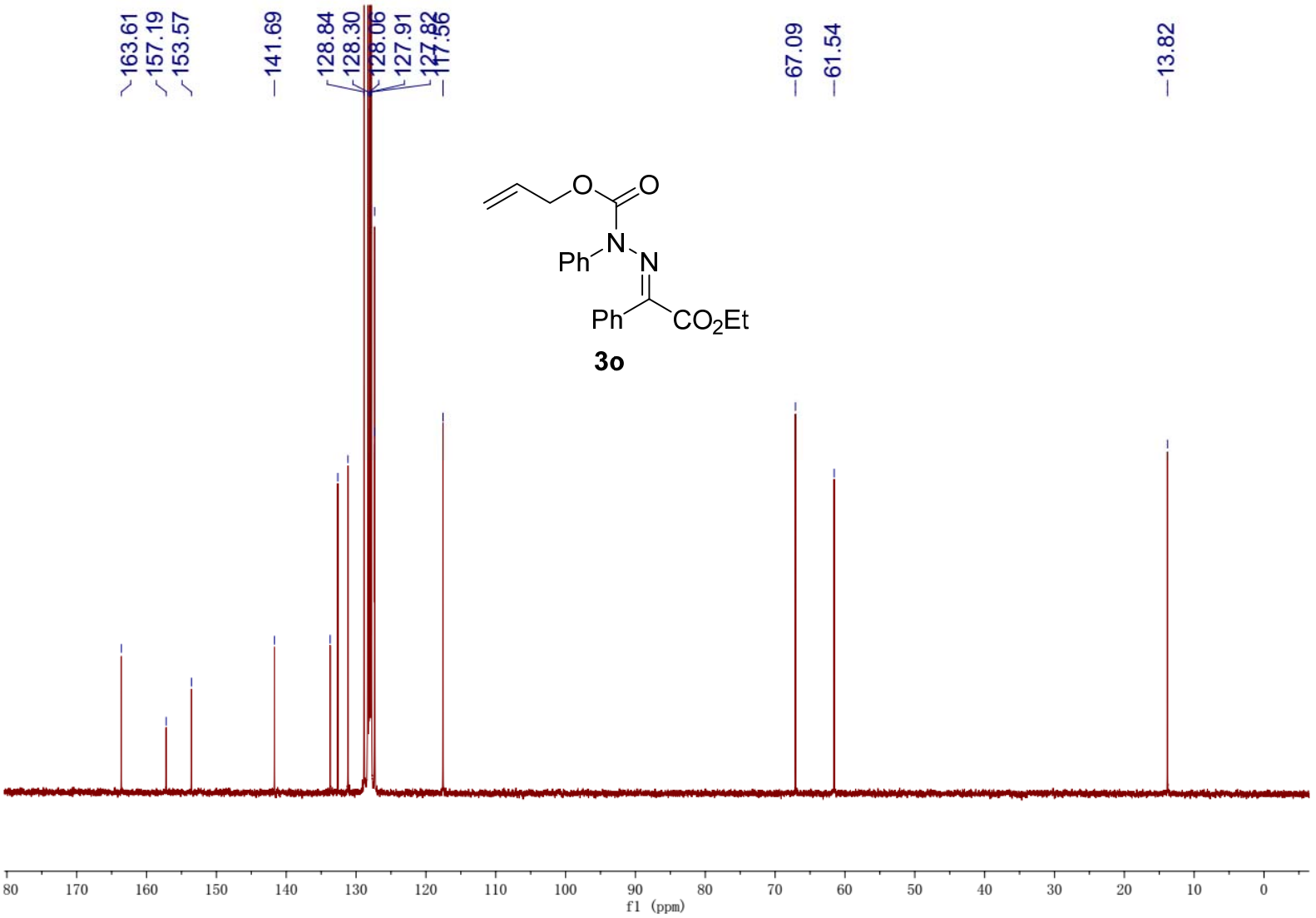
O
O
O
N
N
Ph
Ph
CO2Et
3o
1.87
1.92
4.87
1.00
0.94
0.97
0.98
1.99
1.97
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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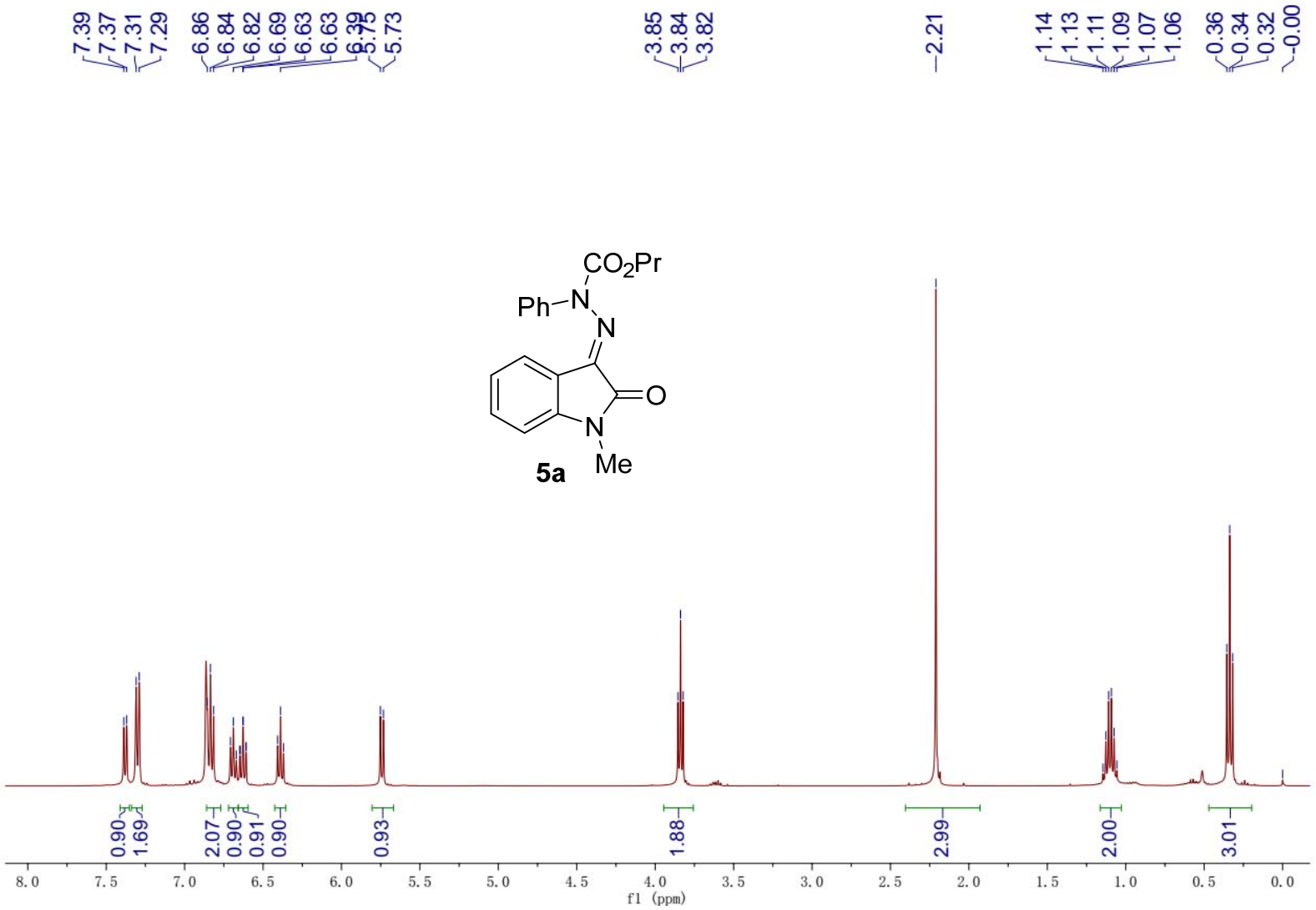
128.30
128.06
127.91
67.09
61.54
13.82
O
O
N
Ph
N
Ph
CO2Et
3o
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.37
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7.29
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6.84
6.82
6.69
6.63
6.63
5.75
5.73
3.85
3.84
3.82
2.21
1.14
1.13
1.11
1.09
1.07
1.06
0.36
0.34
0.32
-0.00
CO2Pr
Ph
N
N
O
N
Me
5a
0.90
1.69
2.07
0.90
0.91
0.90
0.93
1.88
2.99
2.00
3.01
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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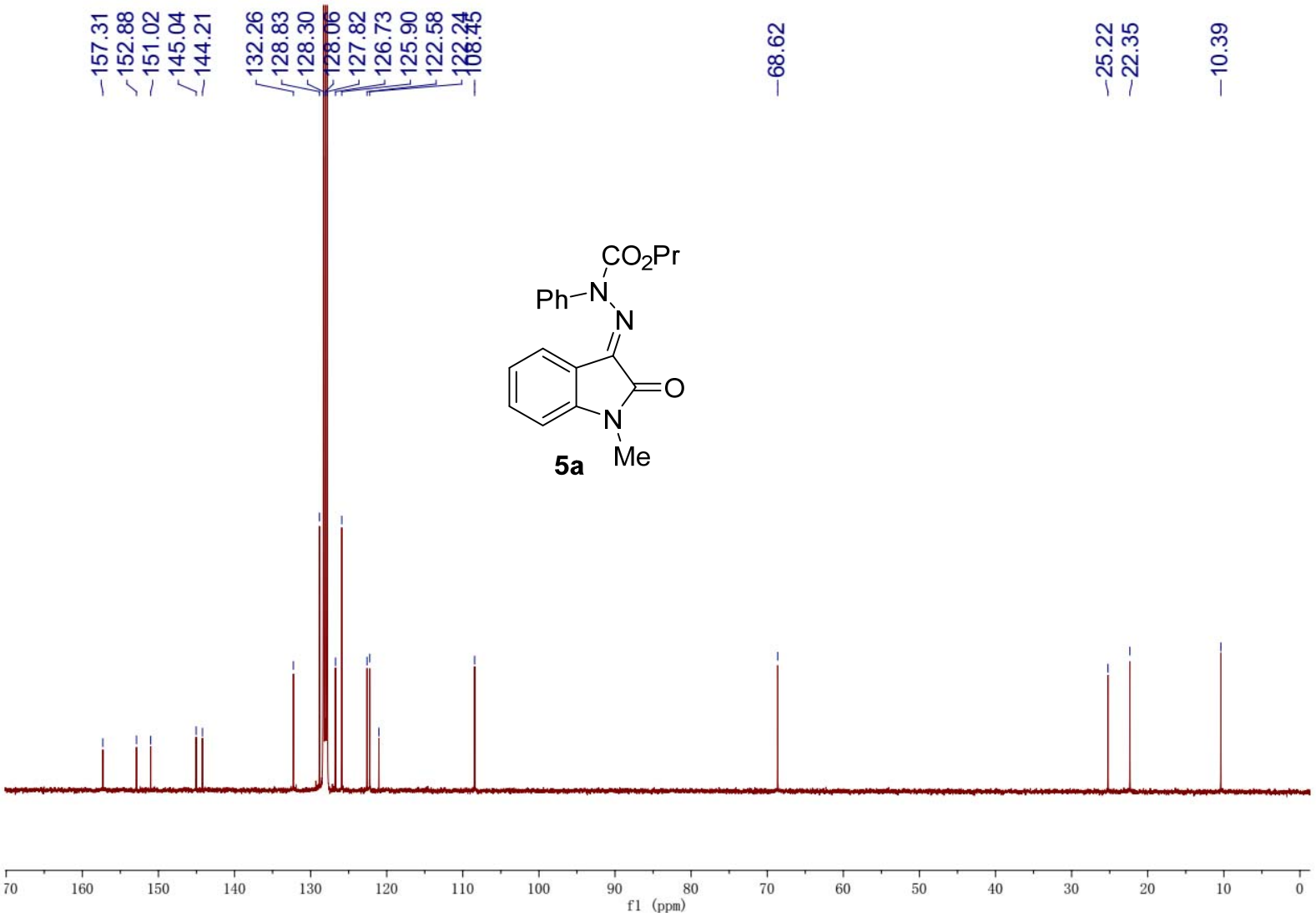
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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144.21
132.26
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128.30
128.06
127.82
126.73
125.90
122.58
68.62
25.22
22.35
10.39
CO2Pr
Ph
N
N
O
N
Me
5a
70
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130
120
110
100
90
80
70
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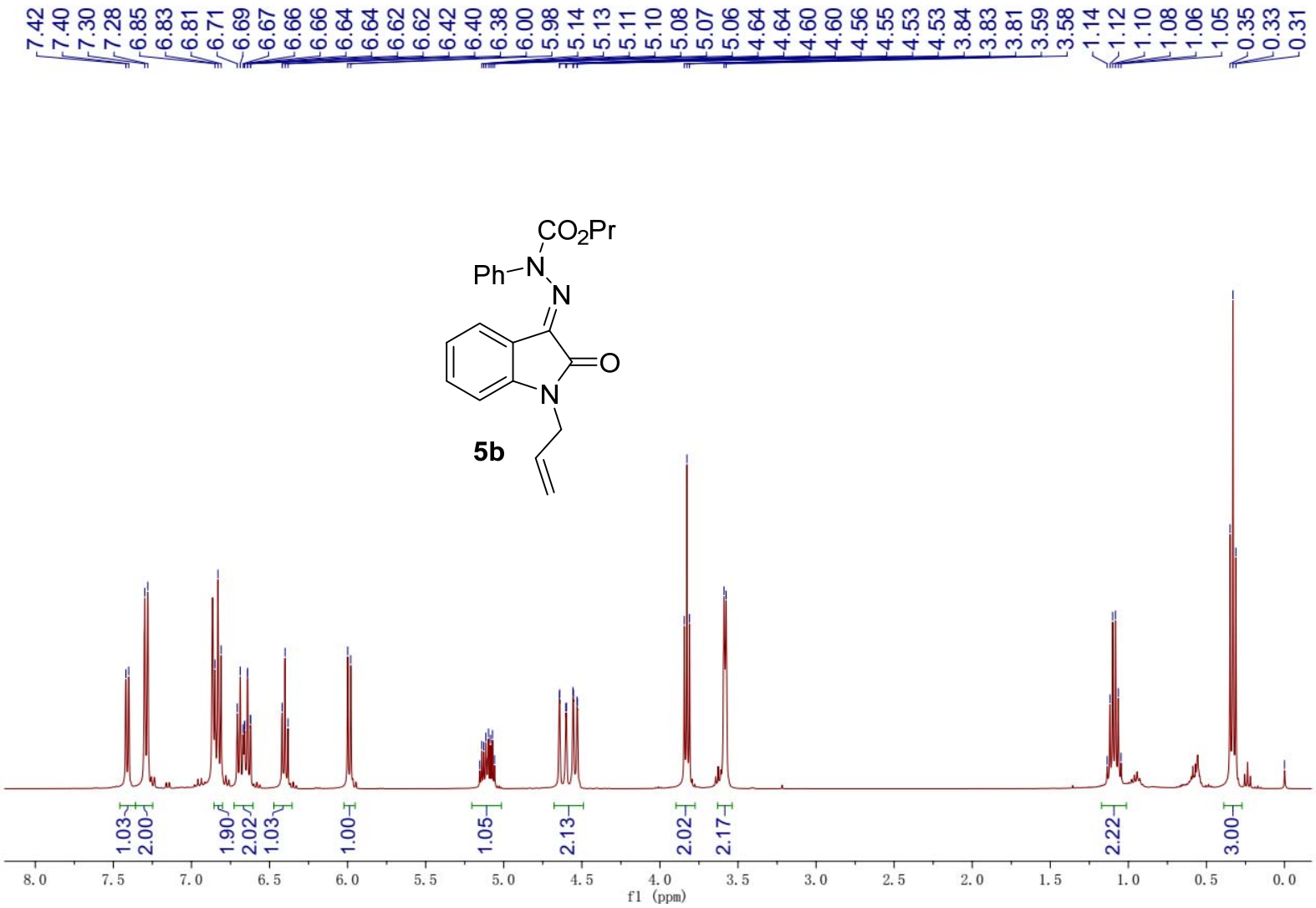
50
40
30
20
10
0
f1 (ppm)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6.64
6.62
6.62
6.42
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6.38
6.00
5.98
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5.13
5.11
5.10
5.08
5.07
5.06
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4.64
4.60
4.60
4.56
4.55
4.53
4.53
3.84
3.83
3.81
3.59
3.58
1.14
1.12
1.10
1.08
1.06
1.05
0.35
0.33
0.31
CO2Pr
Ph
N
N
O
N
5b
1.03
2.00
1.90
2.02
1.03
1.00
1.05
2.13
2.02
2.17
2.22
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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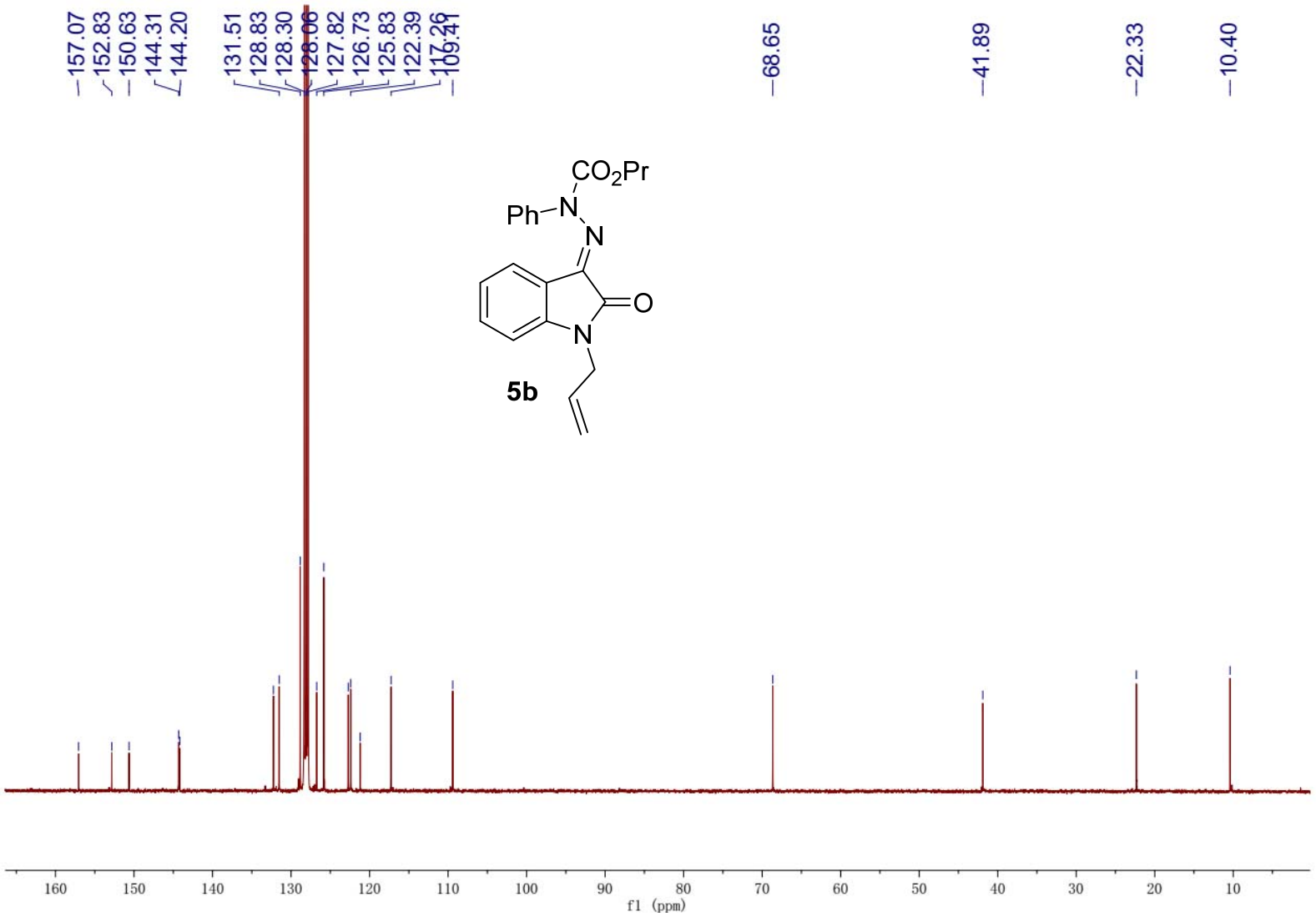
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.30
128.06
127.82
126.73
125.83
122.39
117.26
109.41
68.65
41.89
22.33
10.40
CO2Pr
Ph
N
N
O
N
5b
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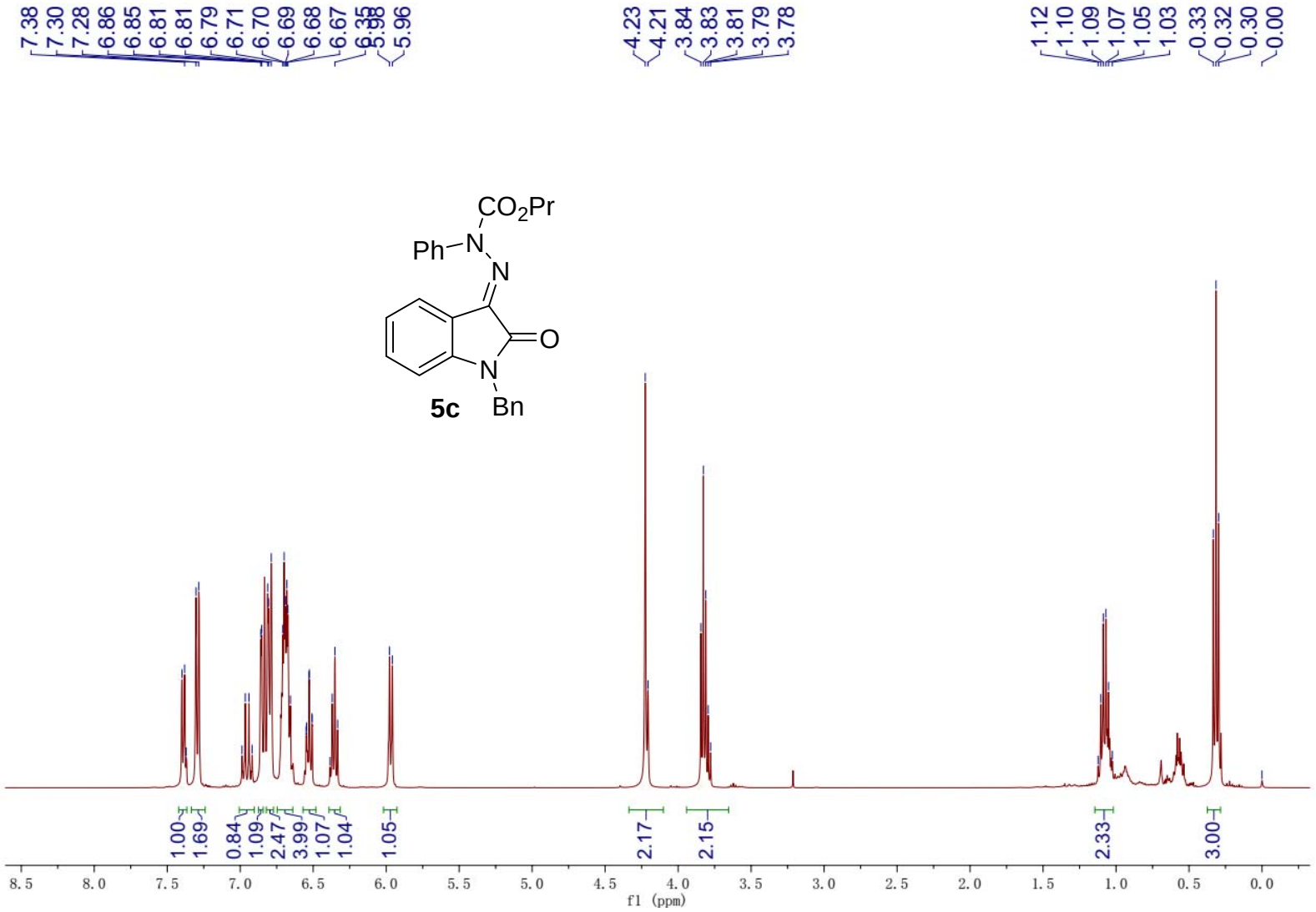
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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6.35
5.96
4.23
4.21
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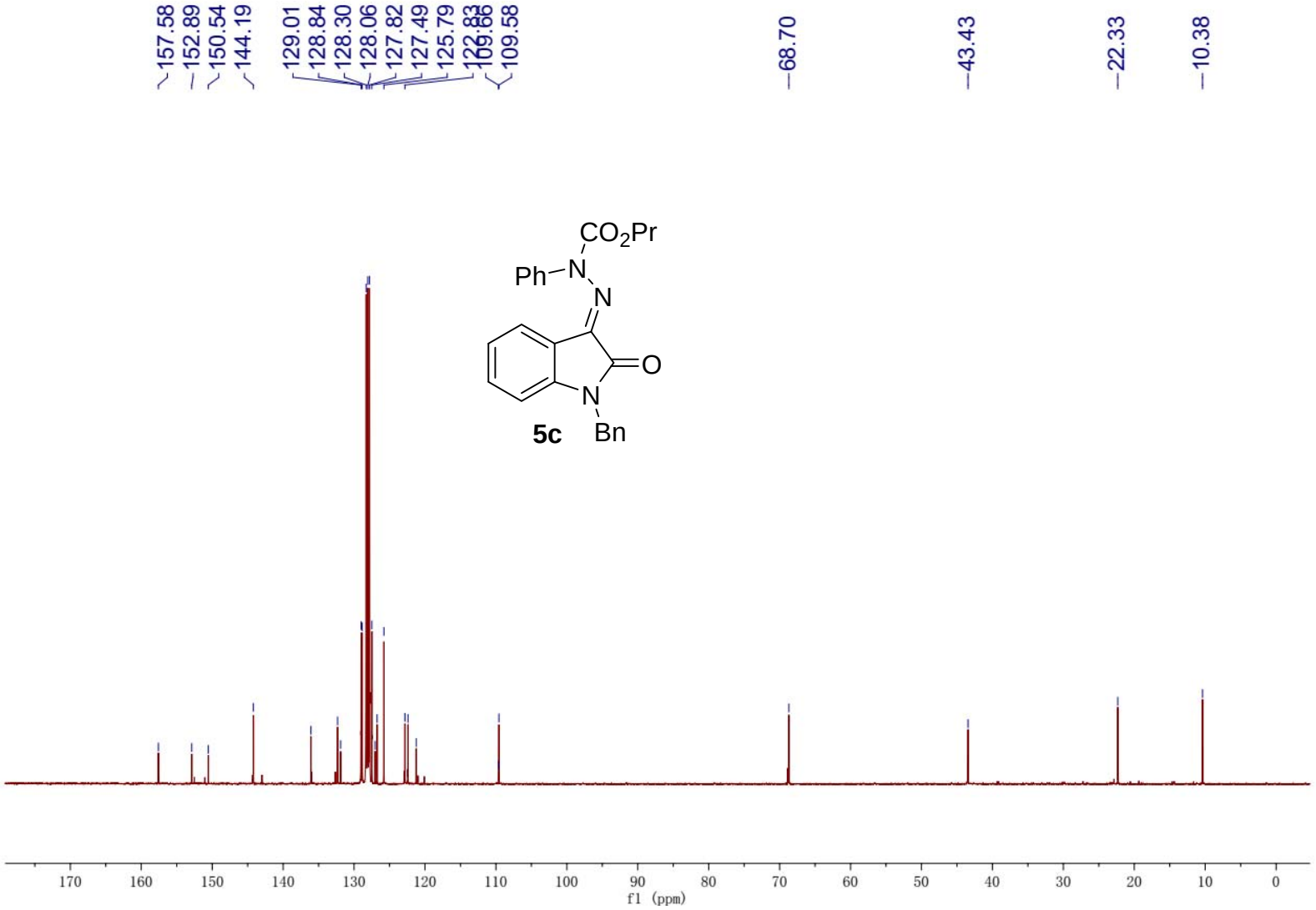
3.83
3.81
3.79
3.78
1.12
1.10
1.09
1.07
1.05
1.03
0.33
0.32
0.30
0.00
CO2Pr
Ph
N
N
O
N
Bn
5c
1.00
1.69
0.84
1.09
2.47
3.99
1.07
1.04
1.05
2.17
2.15
2.33
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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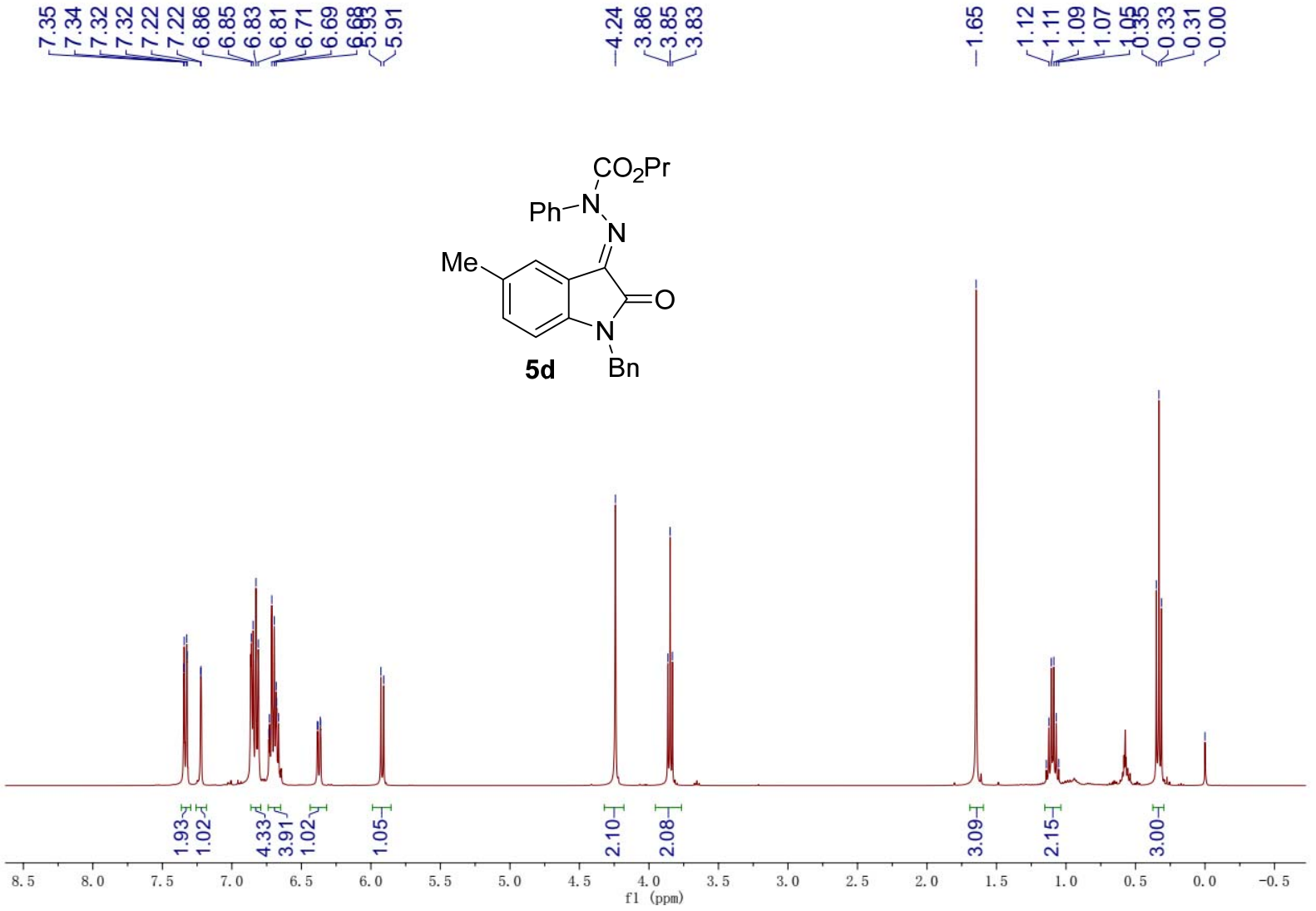
152.89
150.54
144.19
129.01
128.84
128.30
128.06
127.82
127.49
125.79
109.58
68.70
43.43
22.33
10.38
CO2Pr
Ph
N
N
O
N
Bn
5c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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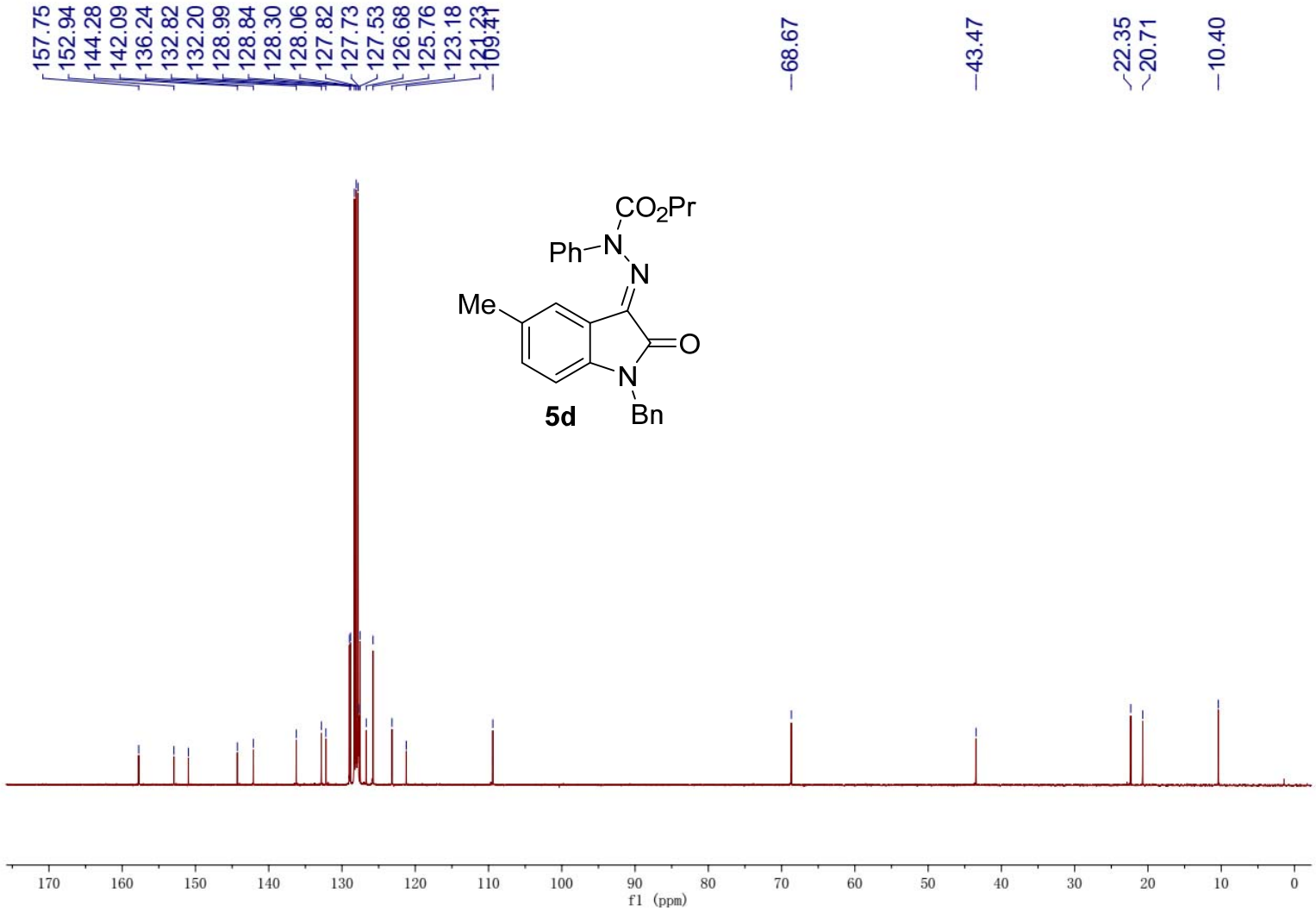
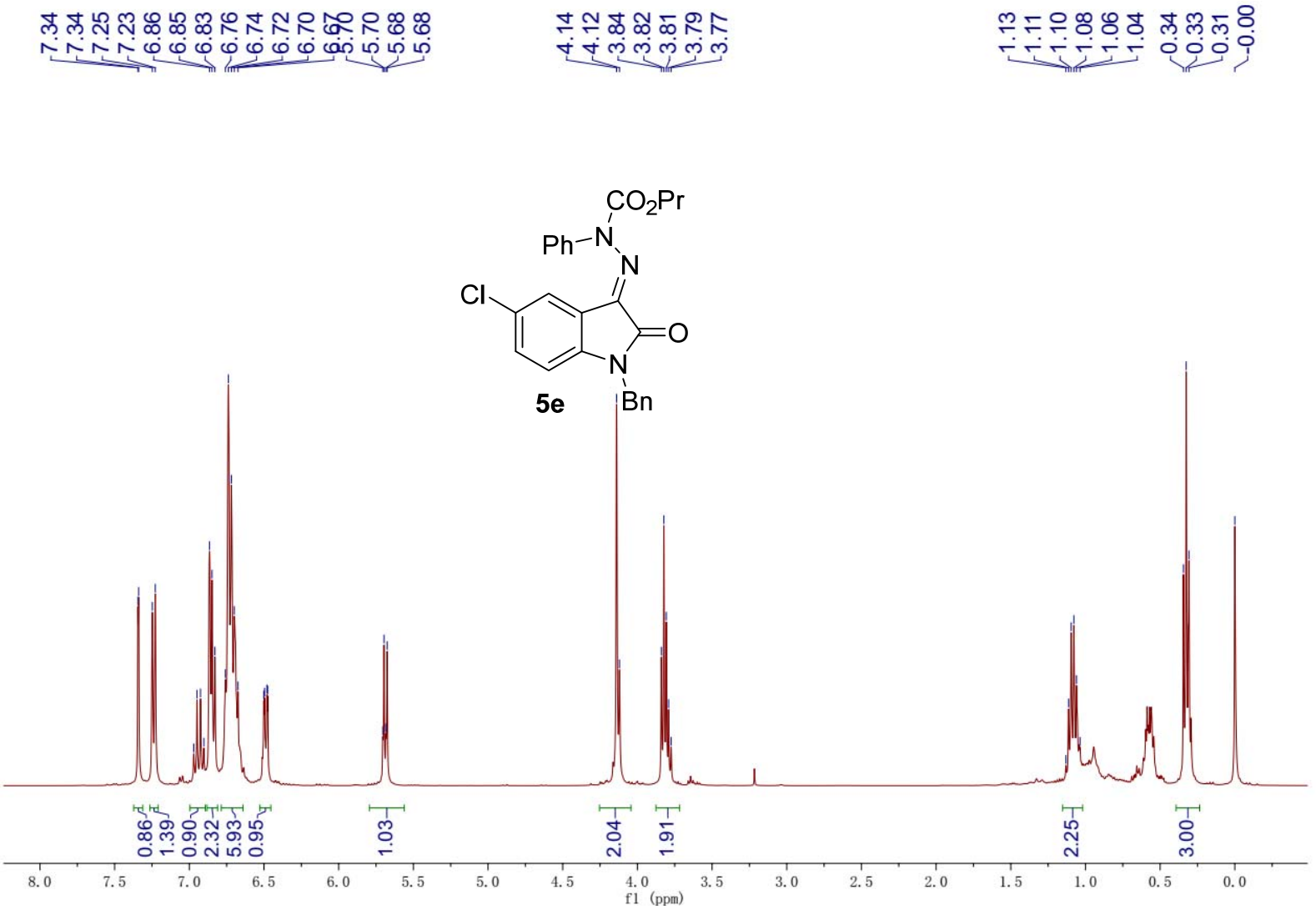
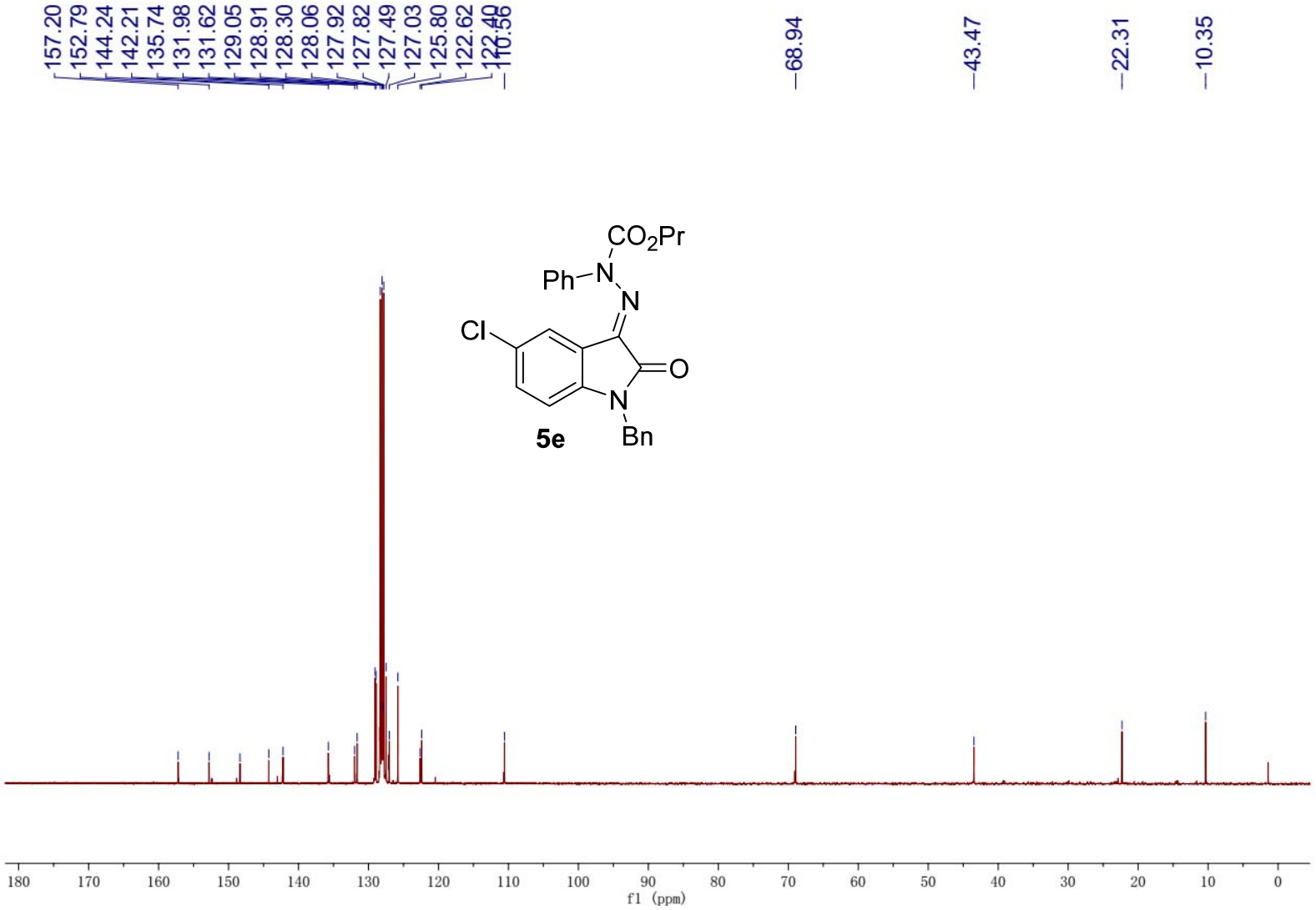
7.34
7.32
7.32
7.22
7.22
6.86
6.85
6.83
6.81
6.71
6.69
5.93
5.91
4.24
3.86
3.85
3.83
1.65
1.12
1.11
1.09
1.07
0.35
0.33
0.31
0.00
CO2Pr
Ph
N
N
Me
O
N
Bn
5d
1.93
1.02
4.33
3.91
1.02
1.05
2.10
2.08
3.09
2.15
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


157.75
152.94
144.28
142.09
136.24
132.82
132.20
128.99
128.84
128.30
128.06
127.82
127.73
127.53
126.68
125.76
123.18
121.23
109.41
68.67
43.47
22.35
20.71
10.40
CO2Pr
Ph
N
N
Me
O
N
Bn
5d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.34
7.34
7.25
7.23
6.86
6.85
6.83
6.76
6.74
6.72
6.70
6.67
5.70
5.68
5.68
4.14
4.12
3.84
3.82
3.81
3.79
3.77
1.13
1.11
1.10
1.08
1.06
1.04
0.34
0.33
0.31
-0.00
CO2Pr
Ph
N
N
Cl
O
N
Bn
5e
0.86
1.39
0.90
2.32
5.93
0.95
1.03
2.04
1.91
2.25
3.00
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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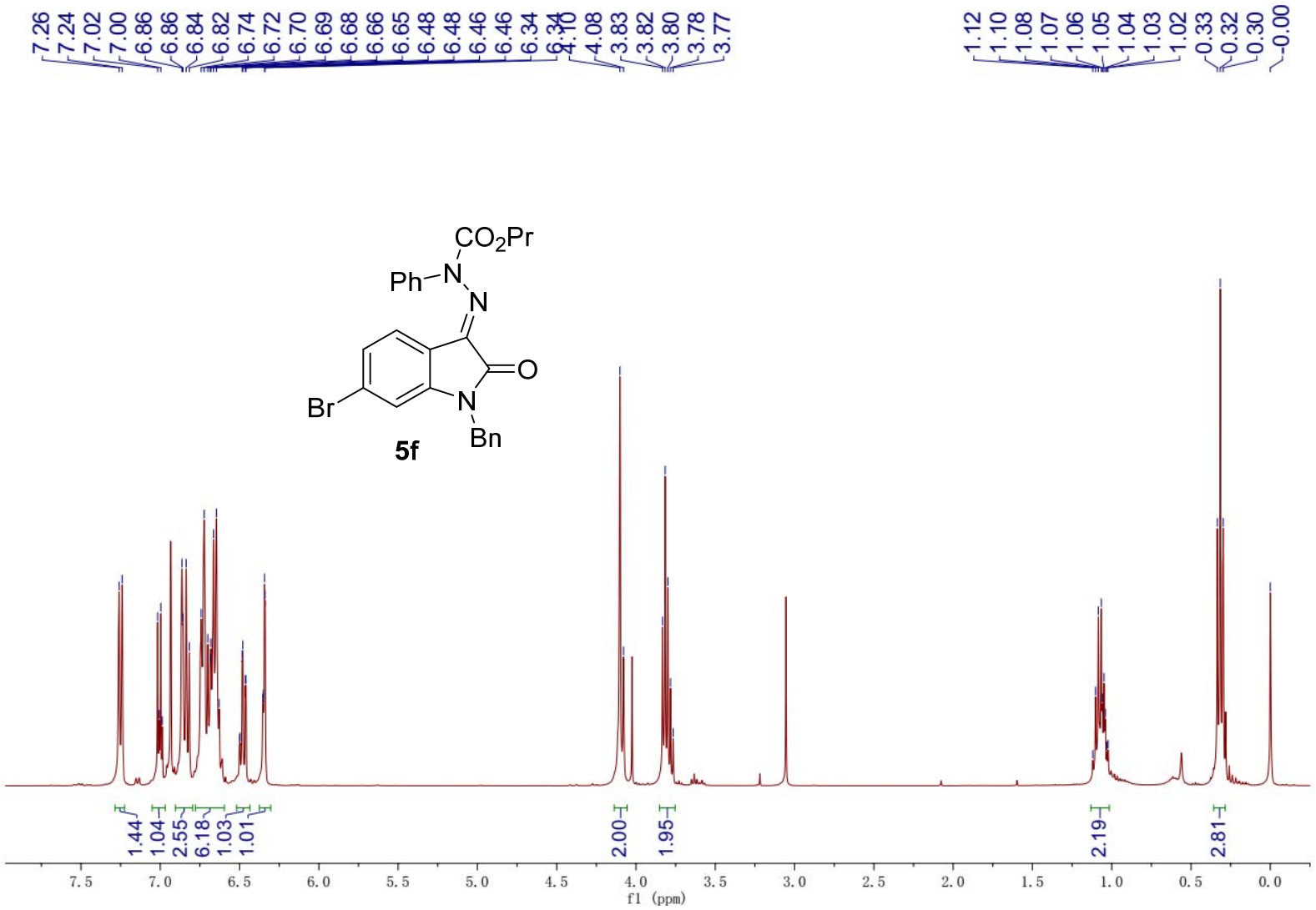
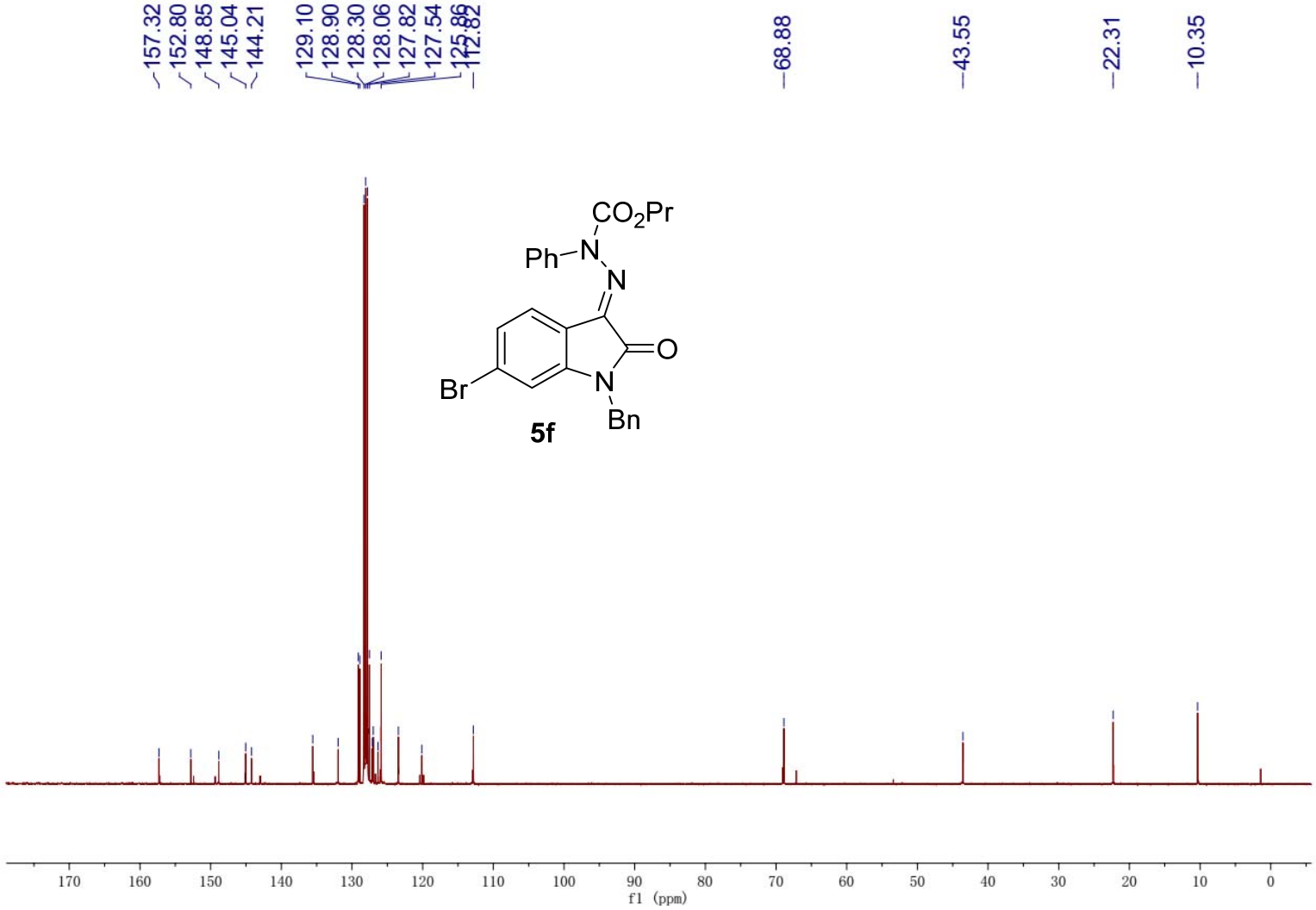
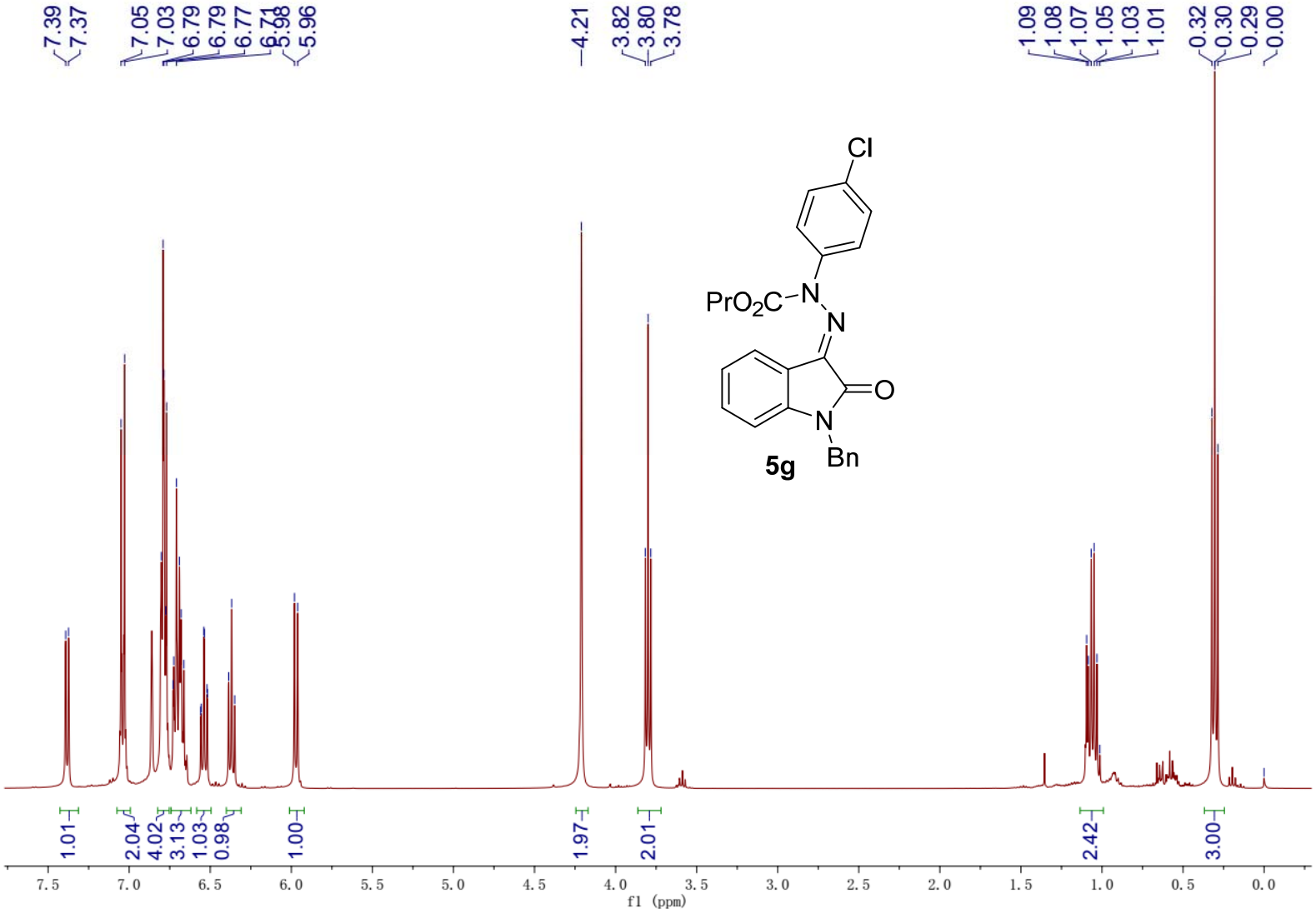
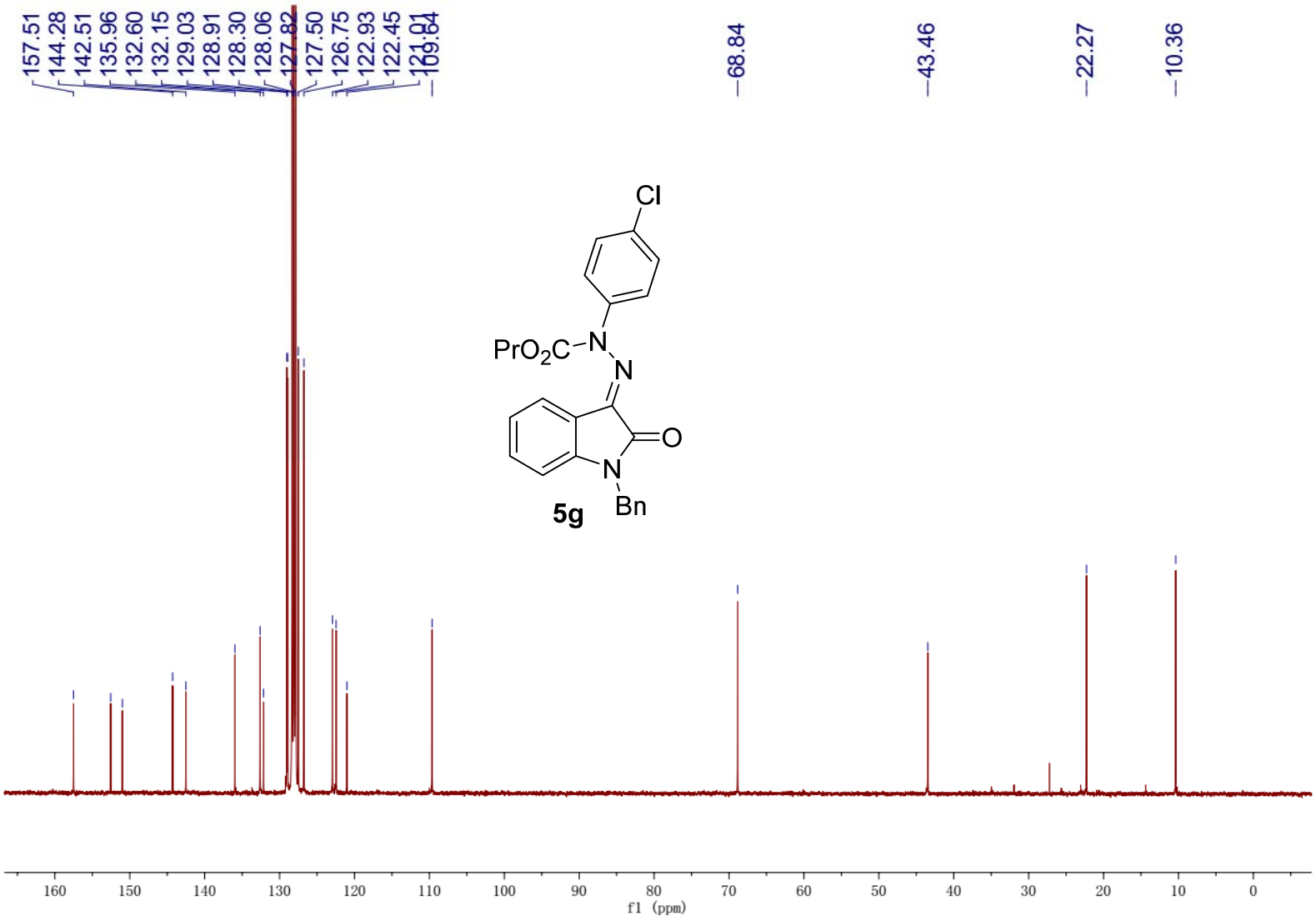
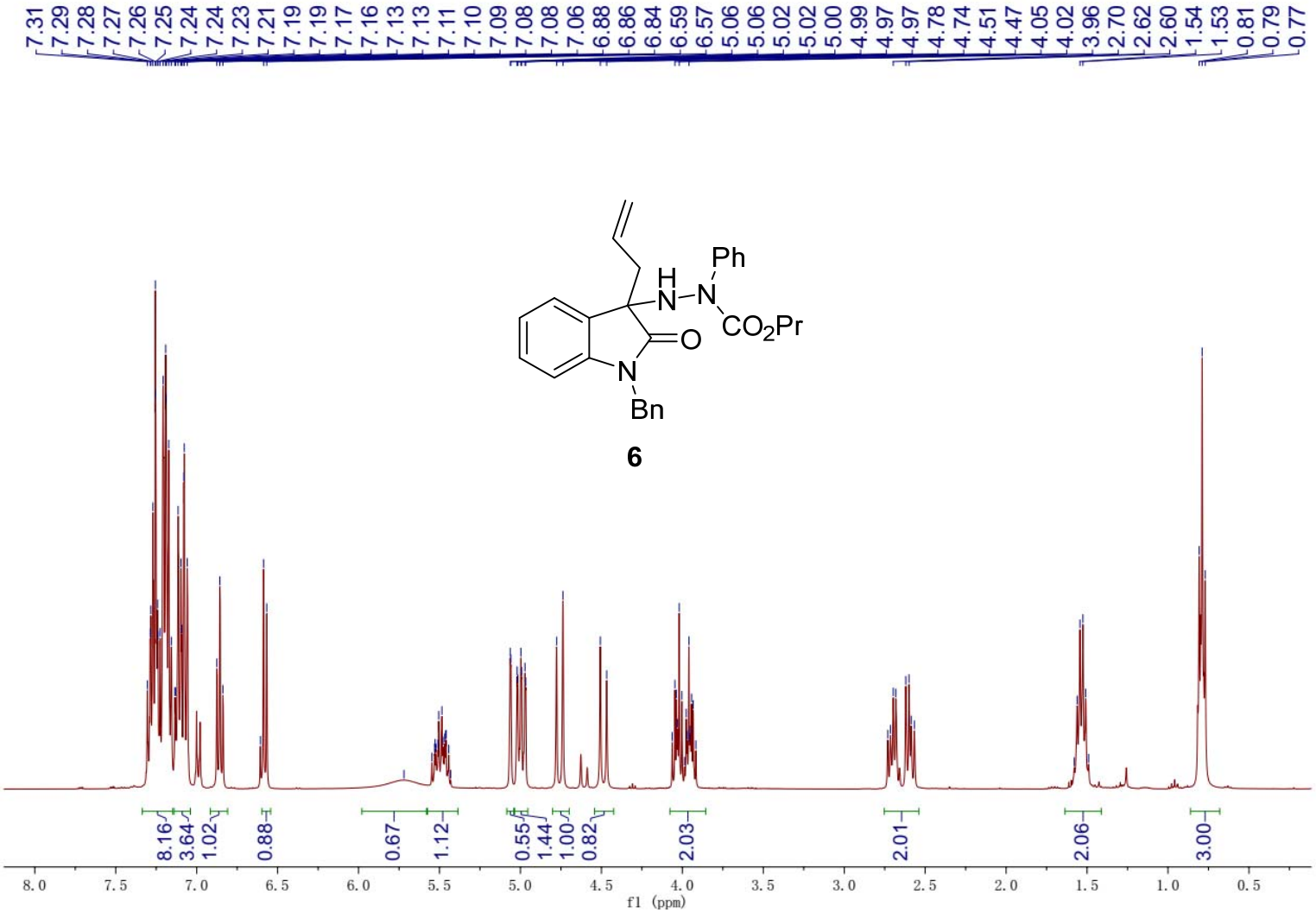
152.79
144.24
142.21
135.74
131.98
131.62
129.05
128.91
128.30
128.06
127.92
127.82
127.49
127.03
125.80
122.62
68.94
43.47
22.31
10.35
CO2Pr
Ph
N
N
Cl
O
N
Bn
5e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.26
7.24
7.02
7.00
6.86
6.86
6.84
6.82
6.74
6.72
6.70
6.69
6.68
6.66
6.65
6.48
6.48
6.46
6.46
6.34
6.34
4.10
4.08
3.83
3.82
3.80
3.78
3.77
1.12
1.10
1.08
1.07
1.06
1.05
1.04
1.03
1.02
0.33
0.32
0.30
-0.00
CO2Pr
Ph
N
N
O
Br
N
Bn
5f
1.44
1.04
2.55
6.18
1.03
1.01
2.00
1.95
2.19
2.81
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)

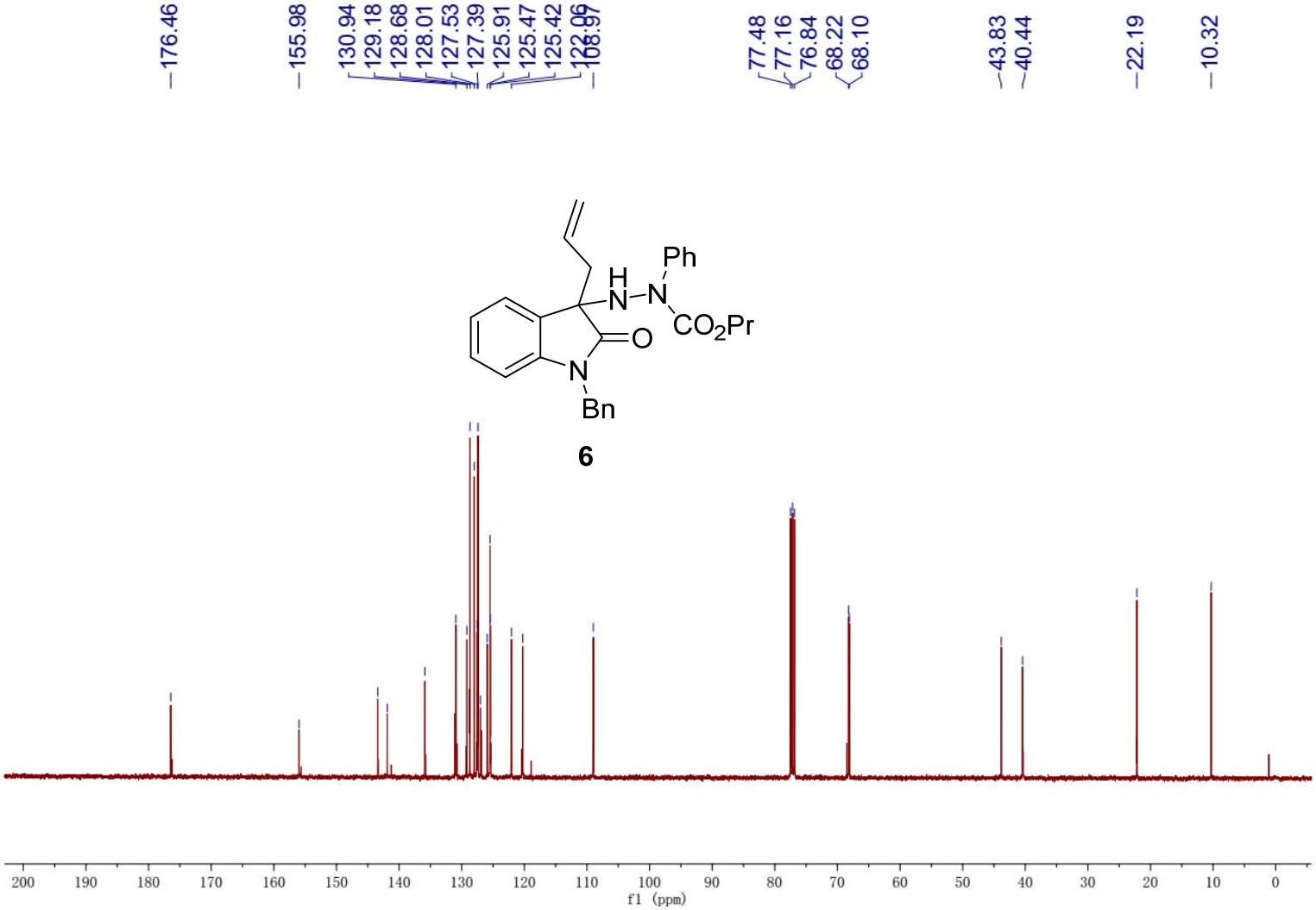

157.32
152.80
148.85
145.04
144.21
129.10
128.90
128.30
128.06
127.82
127.54
68.88
43.55
22.31
10.35
CO2Pr
Ph
N
N
O
Br
N
Bn
5f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.39
7.37
7.05
7.03
6.79
6.79
6.77
6.71
5.98
5.96
4.21
3.82
3.80
3.78
1.09
1.08
1.07
1.05
1.03
1.01
0.32
0.30
0.29
0.00
Cl
PrO2C
N
N
O
N
Bn
5g
1.01
2.04
4.02
3.13
1.03
0.98
1.00
1.97
2.01
2.42
3.00
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)


157.51
144.28
142.51
135.96
132.60
132.15
129.03
128.91
128.30
128.06
127.82
127.50
126.75
122.93
122.45
121.01
109.84
68.84
43.46
22.27
10.36
Cl
PrO2C–N
N
O
N
Bn
5g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.31
7.29
7.28
7.27
7.26
7.25
7.24
7.24
7.23
7.21
7.19
7.19
7.17
7.16
7.13
7.13
7.11
7.10
7.09
7.08
7.08
7.06
6.88
6.86
6.84
6.59
6.57
5.06
5.06
5.02
5.02
5.00
4.99
4.97
4.97
4.78
4.74
4.51
4.47
4.05
4.02
3.96
2.70
2.62
2.60
1.54
1.53
0.81
0.79
0.77
Ph
H
N
N
CO2Pr
O
N
Bn
8.16
3.64
1.02
0.88
0.67
1.12
0.55
1.44
1.00
0.82
2.03
2.01
2.06
3.00
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)

6


176.46
155.98
130.94
129.18
128.68
128.01
127.53
127.39
125.91
125.47
125.42
122.06
108.97
77.48
77.16
76.84
68.22
68.10
43.83
40.44
22.19
10.32
Ph
H
N
N
CO2Pr
O
N
Bn
6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)