Supporting Information for New Journal of Chemistry

Chemoselective Phosphine-Catalyzed Cyanoacylation of α-Dicarbonyl Compounds: A General Method for Synthesis of Cyanohydrin Esters with One Quaternary Stereocenter

Honghui Zhang,[‡a] *Rongfang Liu,*[‡a] *Jialin Liu,*[a] *Binbin Fan,*[a] *Ruifeng Li,*[a] *Yan Qiao,*[b] *and Rong Zhou**[a]

[a] College of Chemistry and Chemical Engineering, TaiyuanUniversity of Technology, Taiyuan, 030024,P. R. China

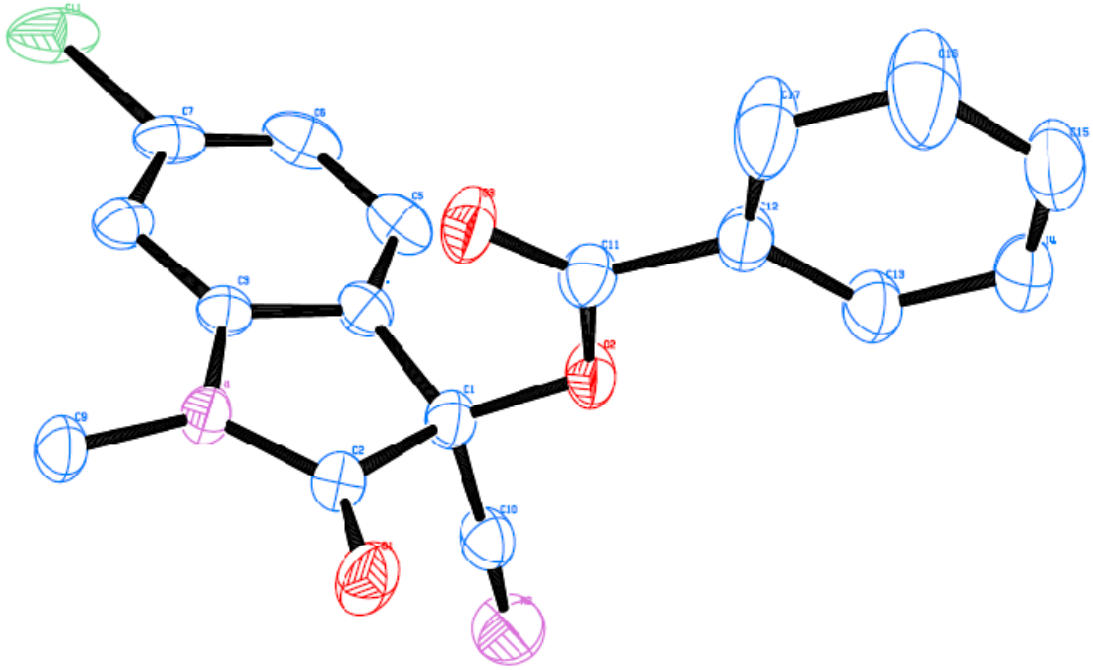
[b] The State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, 030001, P. R. China

[‡] These authors contributed equally

E-mail: zhourong@tyut.edu.cn

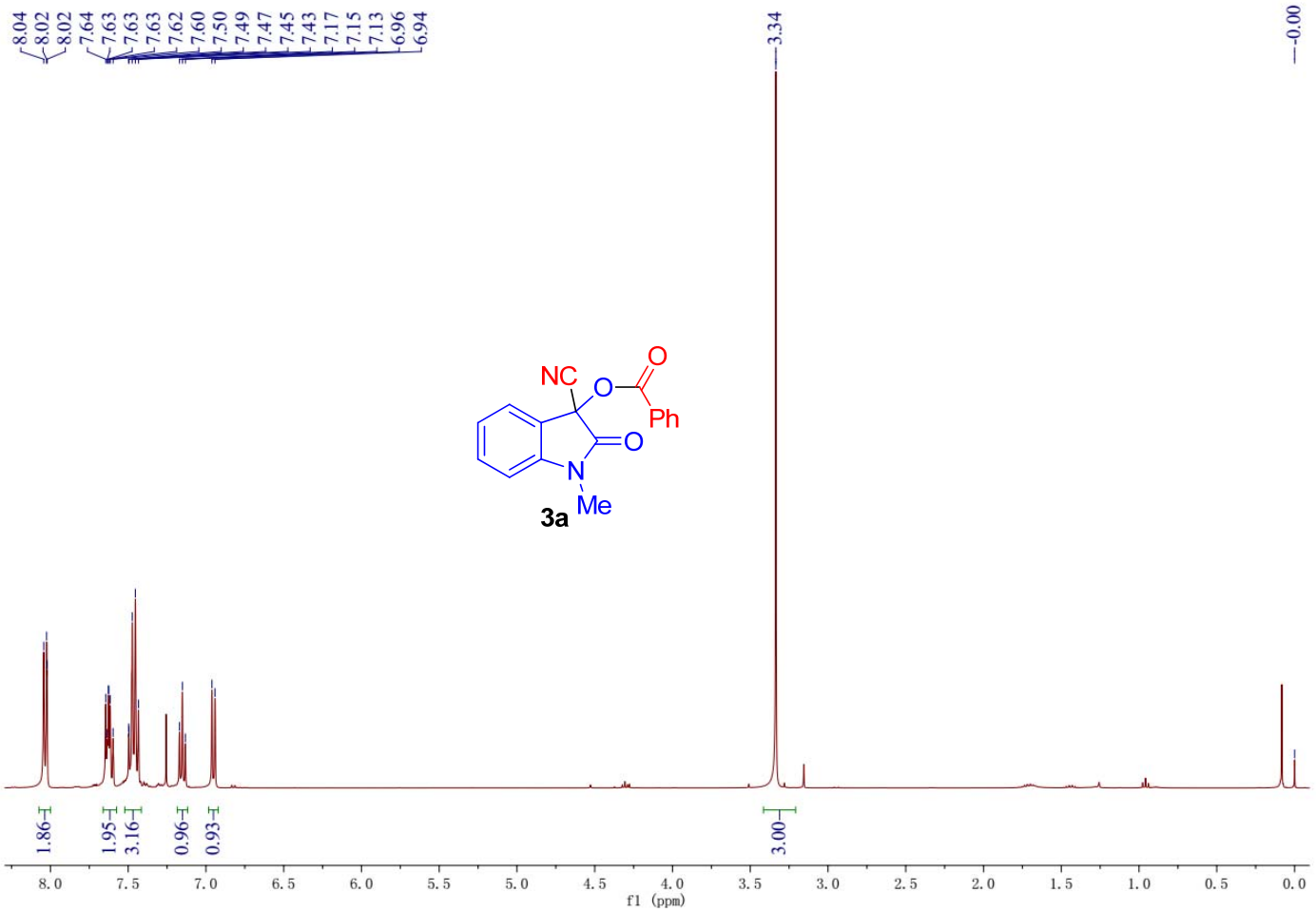
Table of Contents

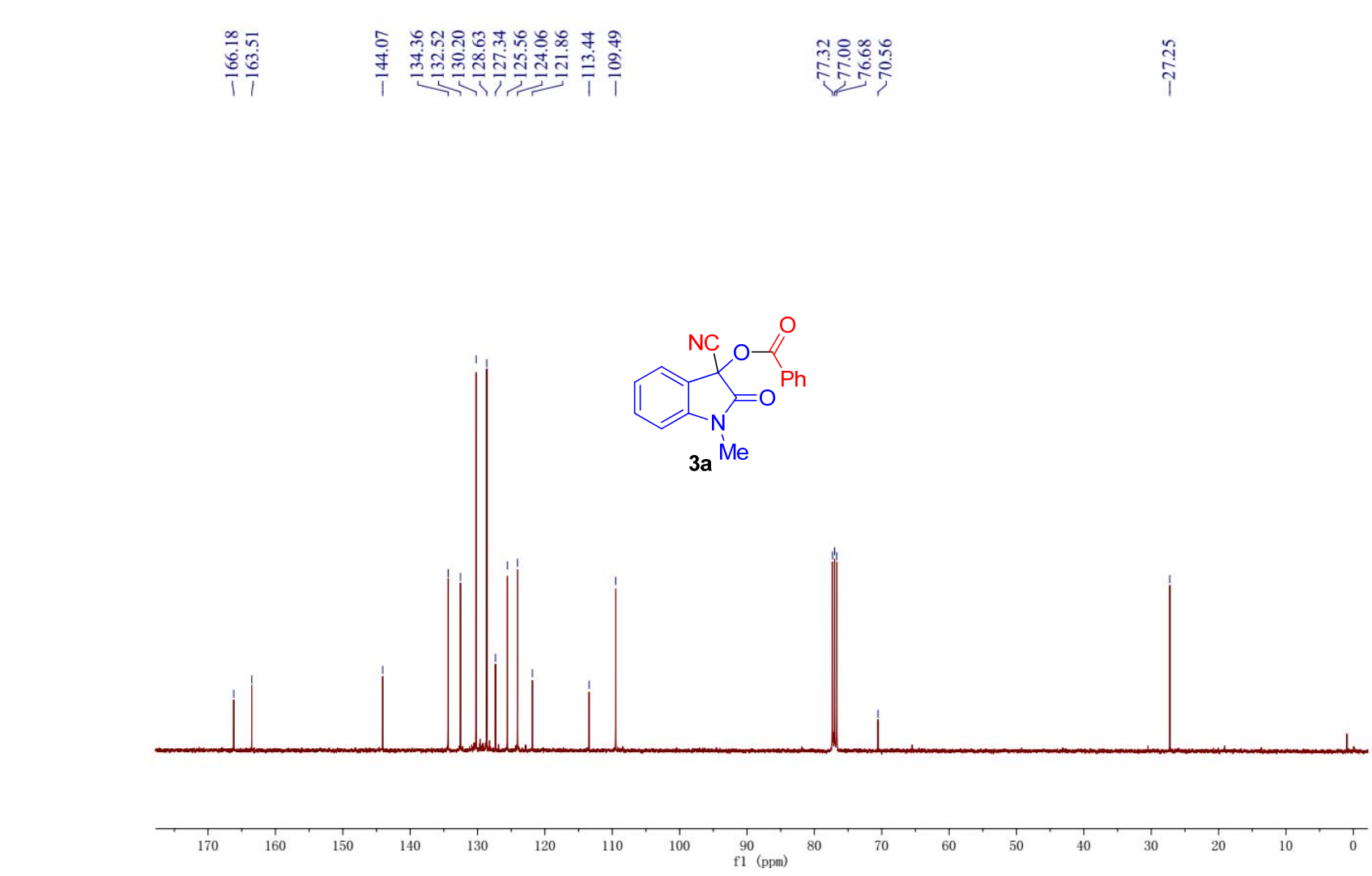
I.ORTEP Drawings for 3f.

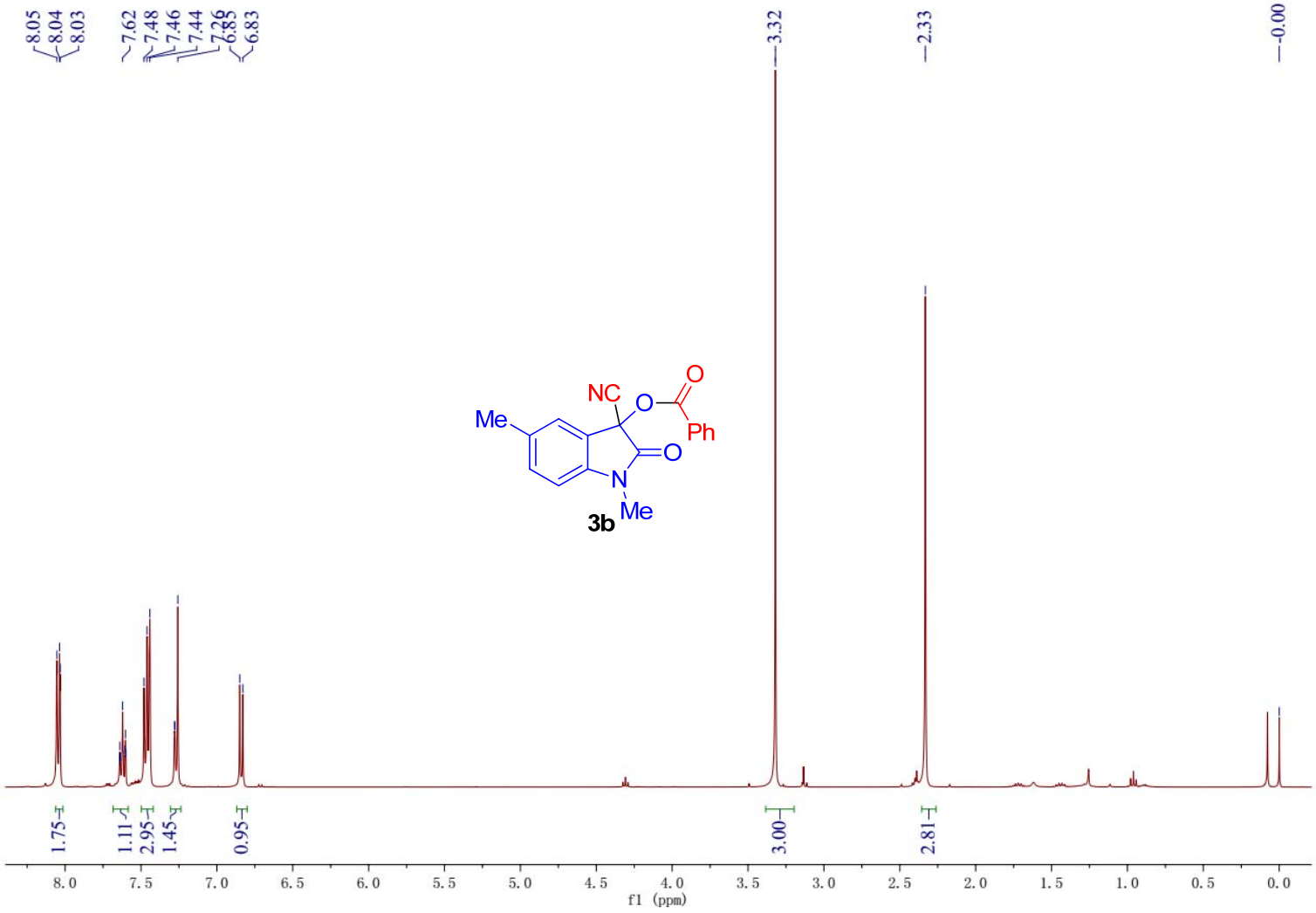


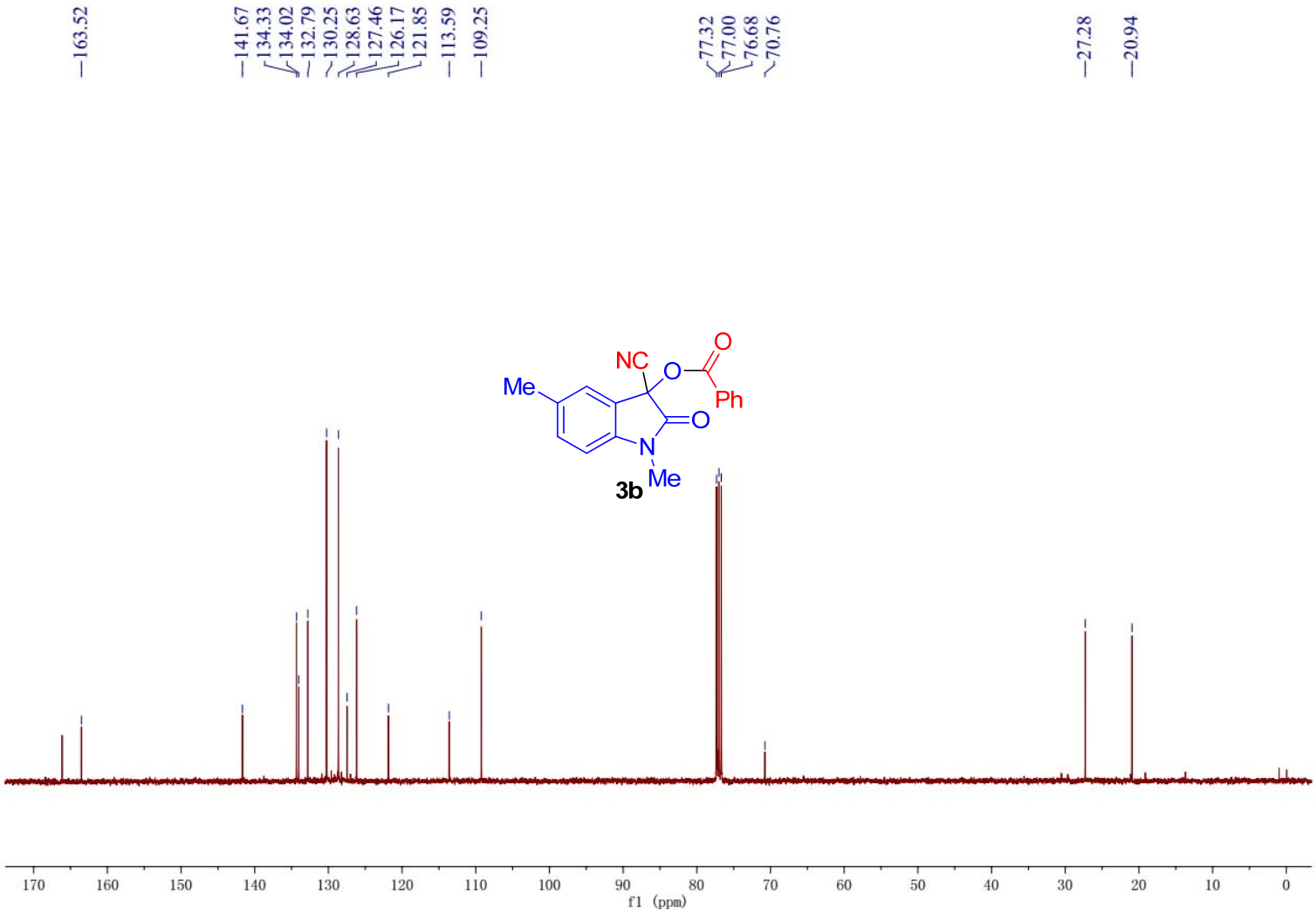
Identification code	**3f**
Empirical formula	$C_{17}\ H_{11}ClN_2O_3$
Formula weight	326.73
Temperature	113 K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P−1
Unit cell dimensions	a = 8.0653(16) Å α= 99.73(3)°
	b = 8.4613(17) Å β = 96.54(3)°
	c = 12.124(2) Å γ= 97.78(3)°
Volume	800.0(3) $Å^3$
Z, Calculated density	2, 1.356 Mg/m^3
Absorption coefficient	0.254 mm^{-1}
F(000)	336
Theta range for data collection	2.473 to 27.845°
Limiting indices	-10<=h<=10, -10<=k<=11, -15<=l<=15
Reflections collected / unique	3763 / 2581 [R(int) = 0.0356]
Completeness to the θ = 27.845°	99.3 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3763 / 0 / 210
Goodness-of-fit on F^2	1.031
Final R indices [I>2σ(I)]	R1 = 0.0398, wR2 = 0.1048
R indices (all data)	R1 = 0.0576, wR2 = 0.1140
Largest diff. peak and hole	0.242 and -0.287 e. $Å^{-3}$

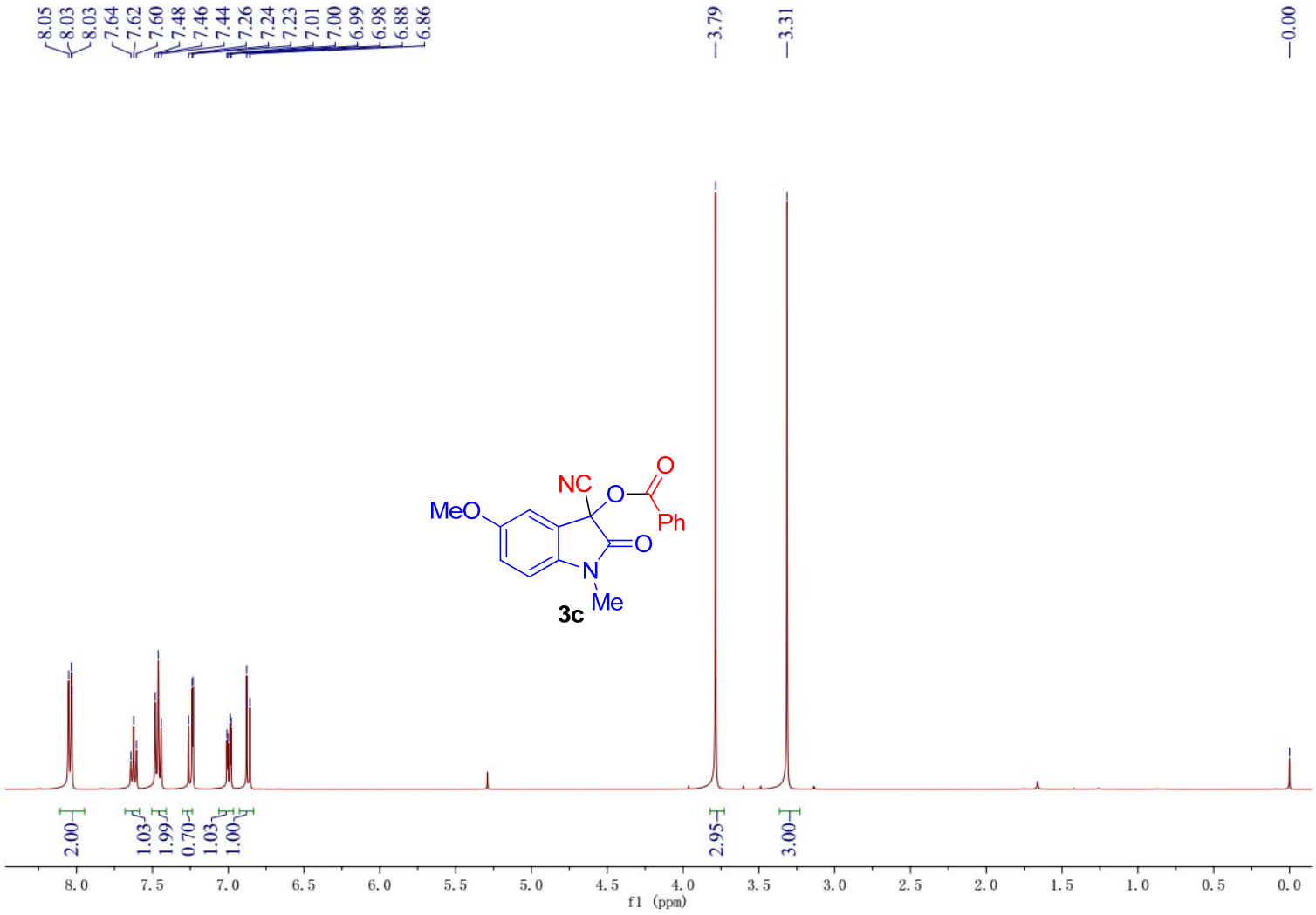
II. ^{1}H and ^{13}C NMR Spectra of Compounds 3, 4, and 6

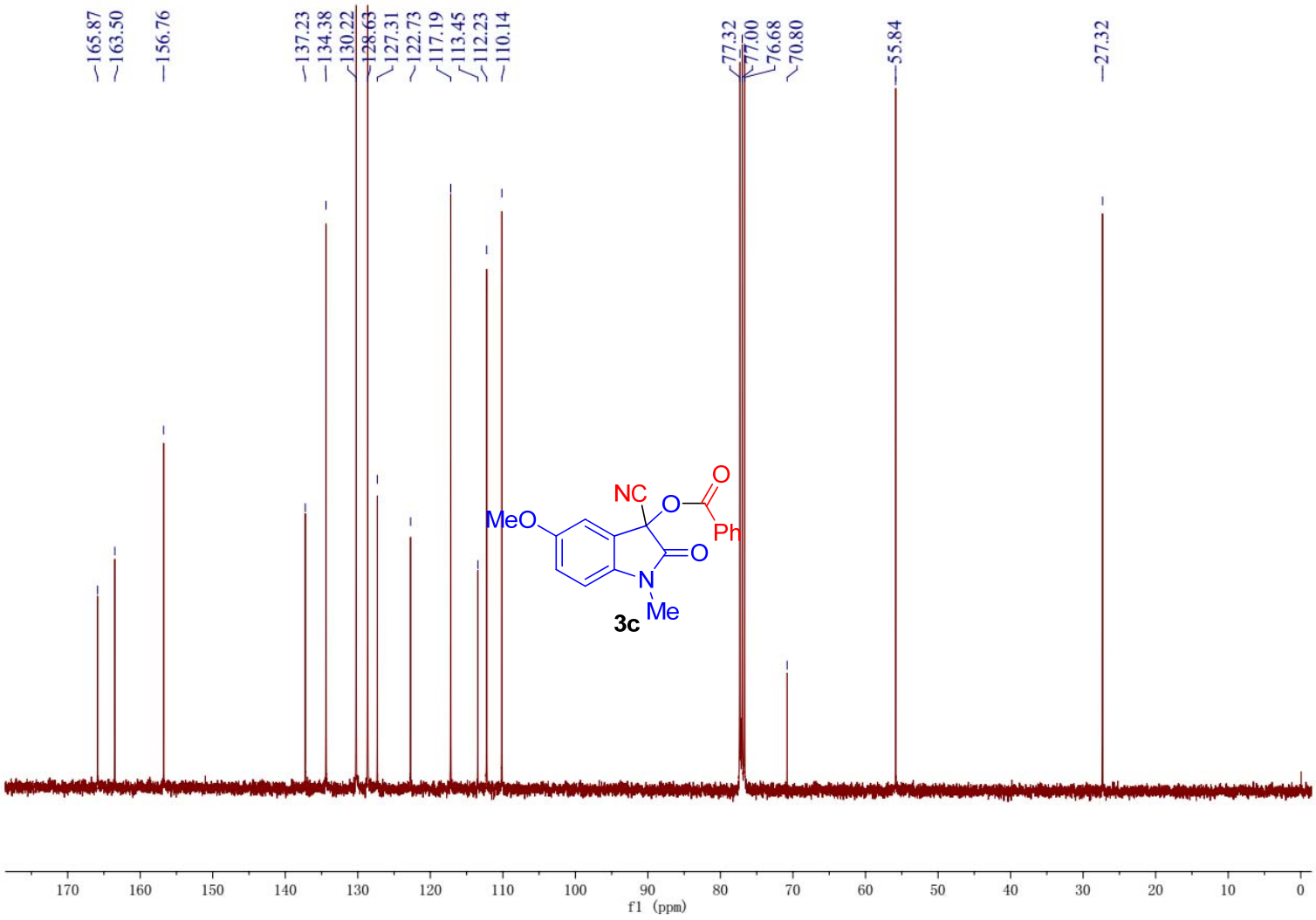


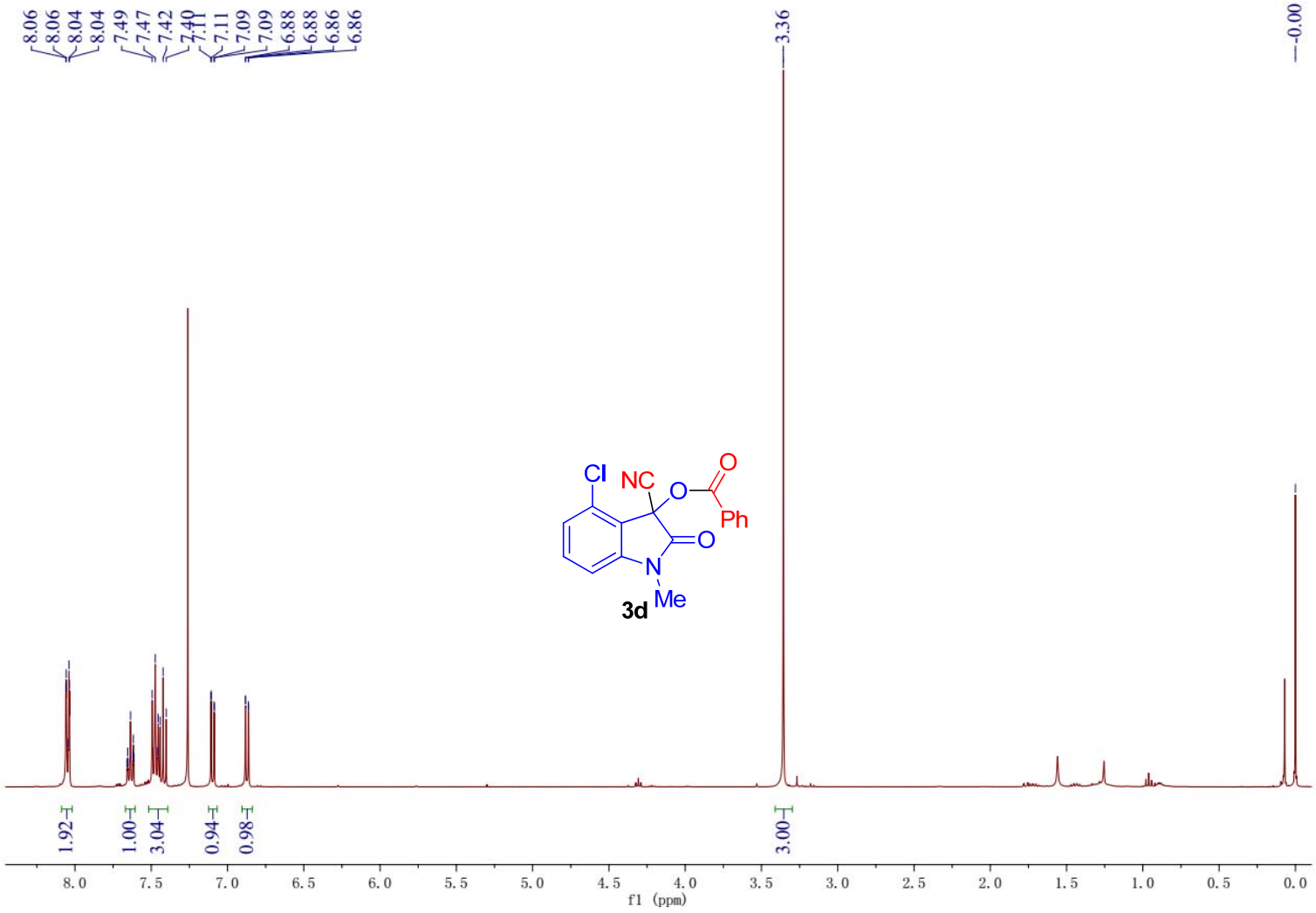

166.18
163.51
144.07
134.36
132.52
130.20
128.63
127.34
125.56
124.06
121.86
113.44
109.49
77.32
77.00
76.68
70.56
27.25
NC
O
O
Ph
O
N
Me
3a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

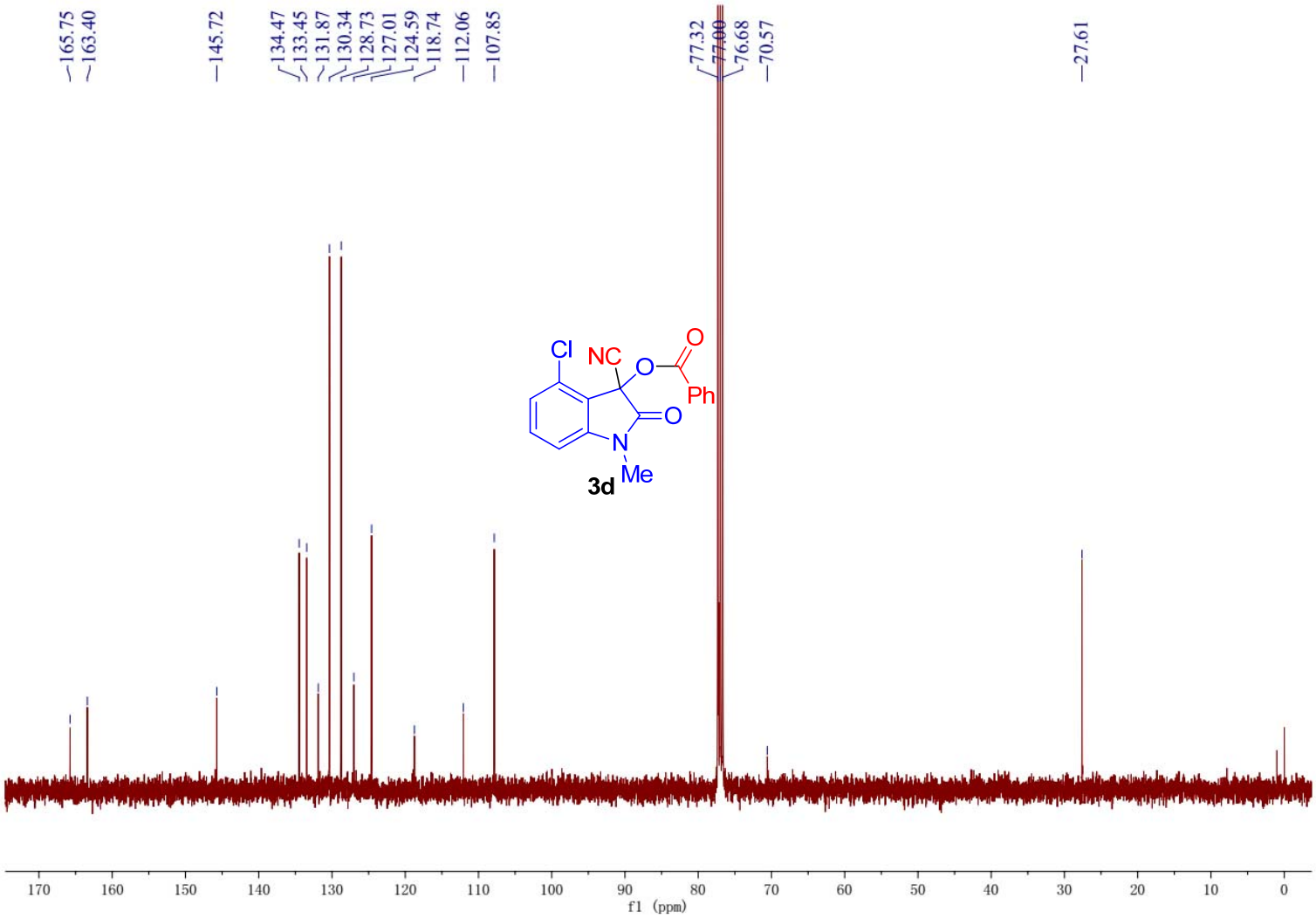

8.05
8.04
8.03
7.62
7.48
7.46
7.44
7.26
6.85
6.83
3.32
2.33
0.00
NC
O
O
Ph
Me
O
N
Me
3b
1.75
1.11
2.95
1.45
0.95
3.00
2.81
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

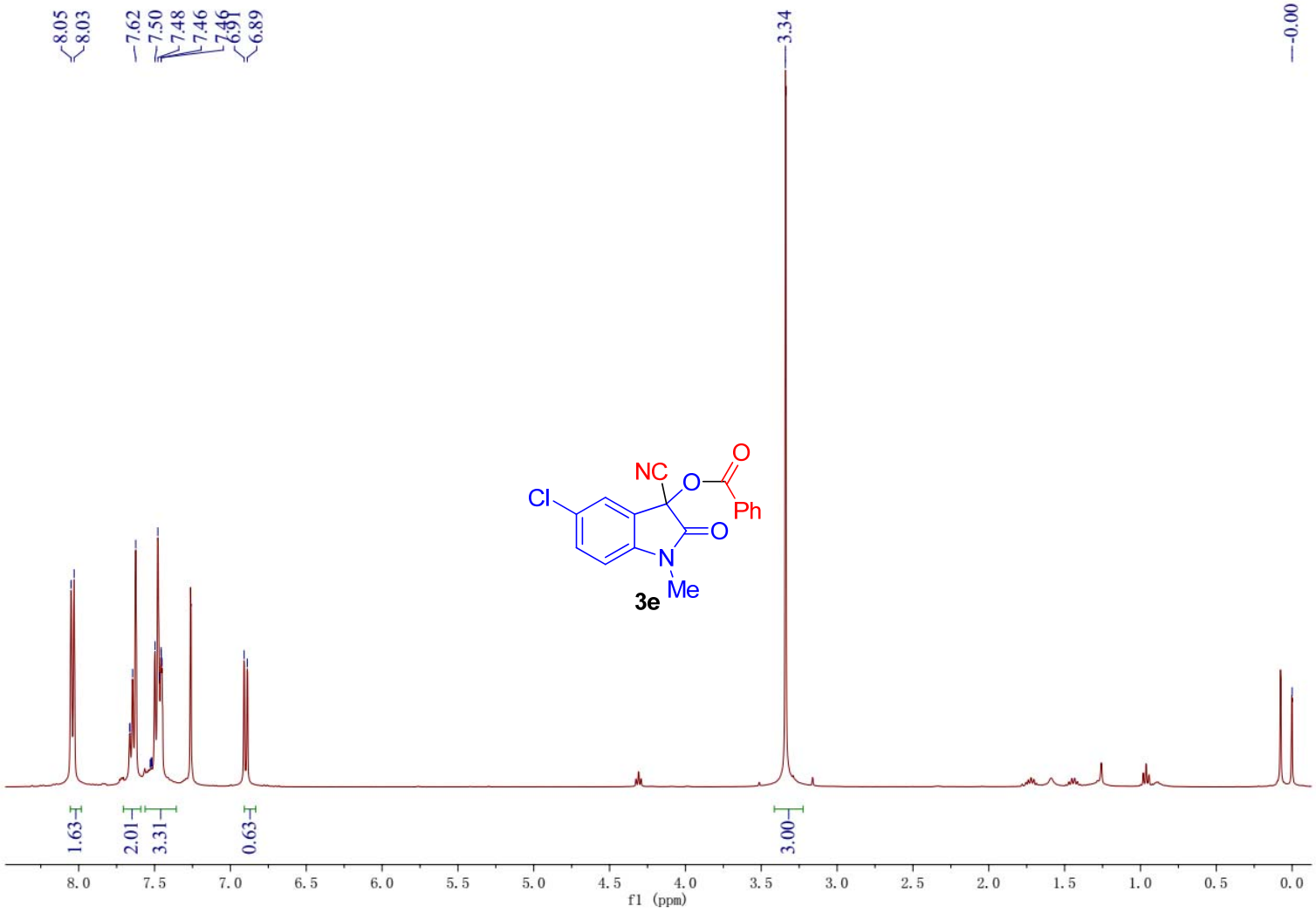

163.52
141.67
134.33
134.02
132.79
130.25
128.63
127.46
126.17
121.85
113.59
109.25
77.32
77.00
76.68
70.76
27.28
20.94
NC
O
O
Ph
Me
O
N
Me
3b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

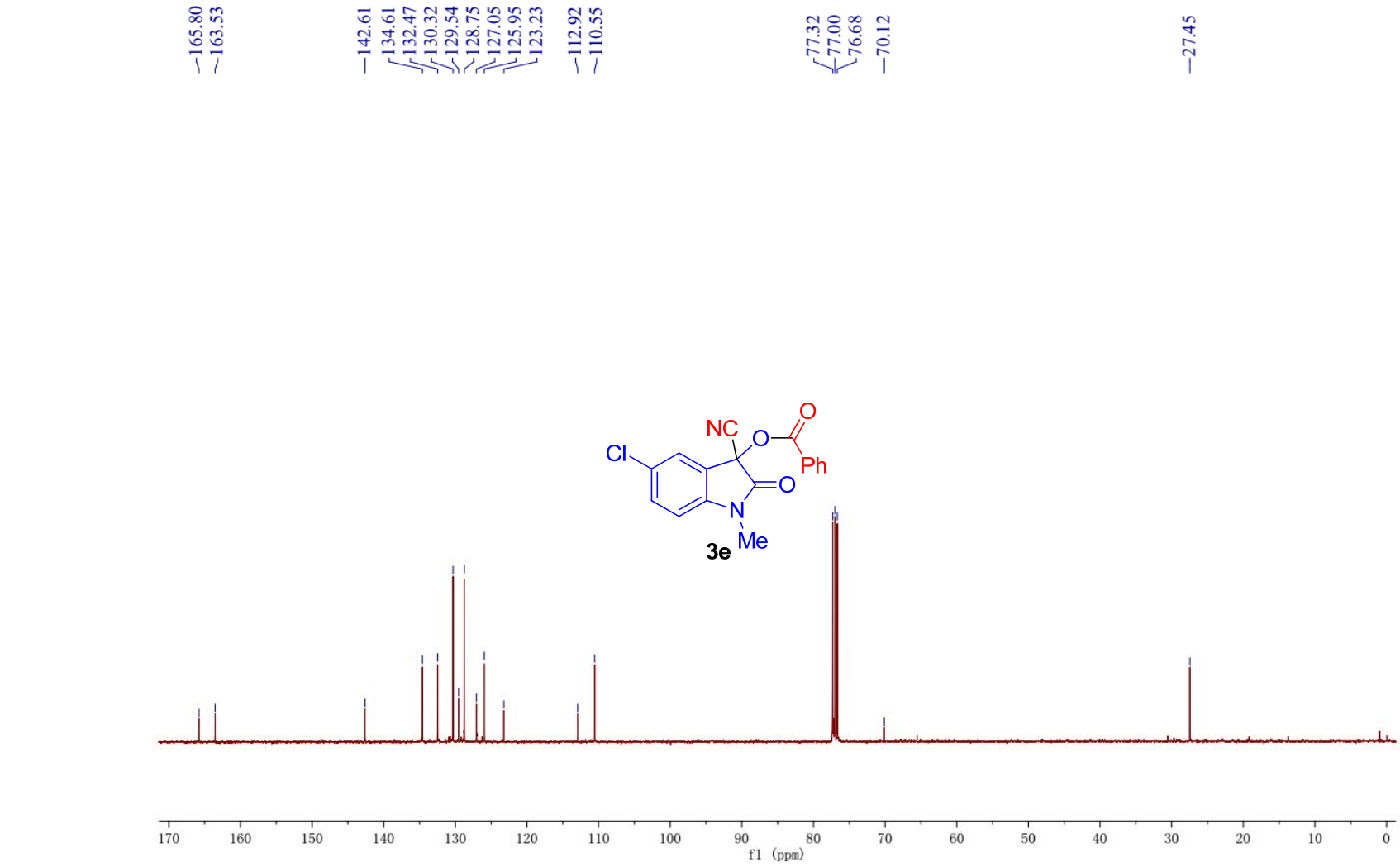

8.05
8.03
8.03
7.64
7.62
7.60
7.48
7.46
7.44
7.26
7.24
7.23
7.01
7.00
6.99
6.98
6.88
6.86
3.79
3.31
0.00
NC
O
O
Ph
MeO
O
N
Me
3c
2.00
1.03
1.99
0.70
1.03
1.00
2.95
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

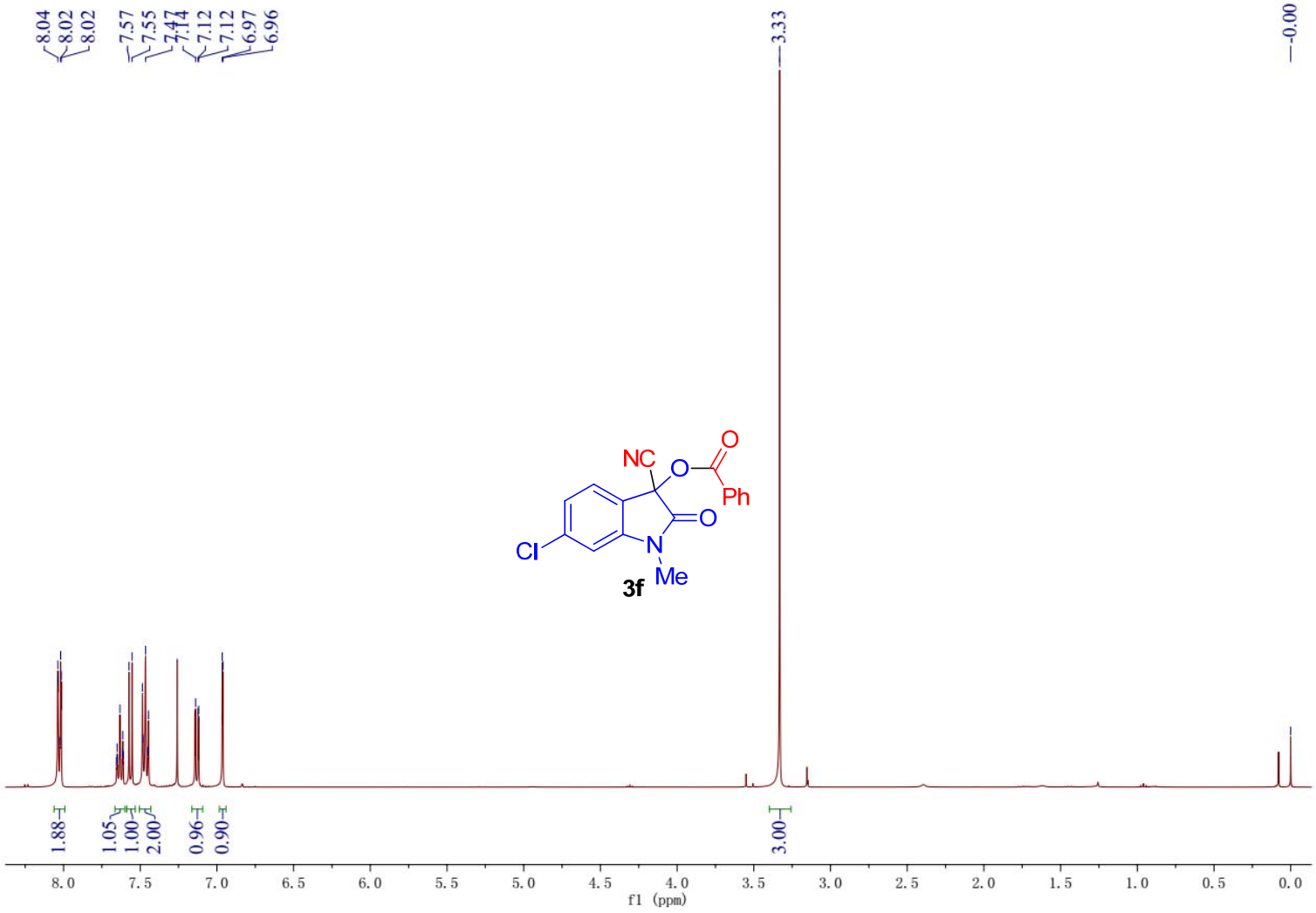

165.87
163.50
156.76
137.23
134.38
130.22
128.63
127.31
122.73
117.19
113.45
112.23
110.14
77.32
77.00
76.68
70.80
55.84
27.32
NC
O
O
Ph
MeO
O
N
Me
3c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

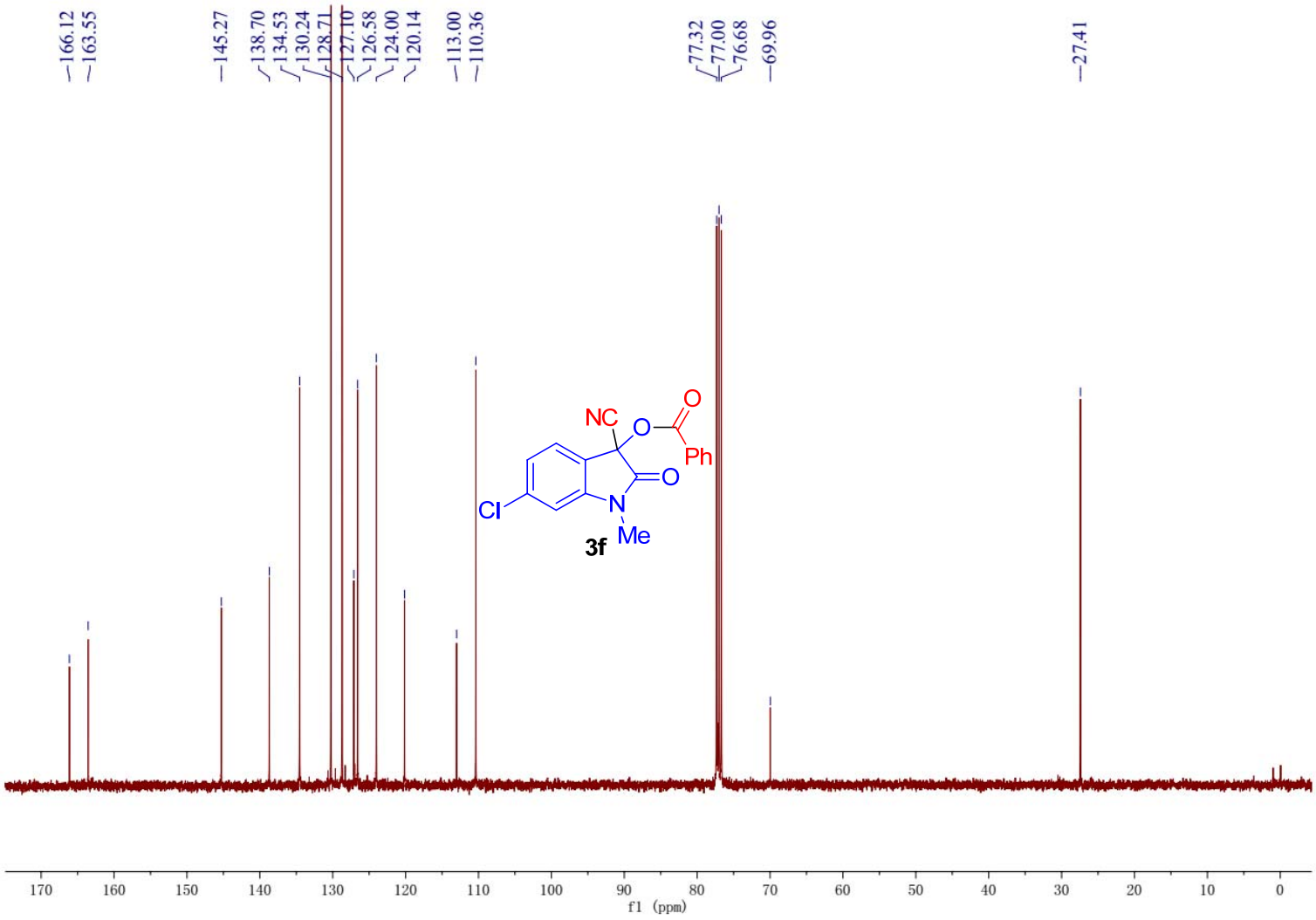

8.06
8.06
8.04
8.04
7.49
7.47
7.42
7.40
7.11
7.09
7.09
6.88
6.88
6.86
6.86
3.36
-0.00
Cl
NC
O
O
Ph
O
N
Me
3d
1.92
1.00
3.04
0.94
0.98
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

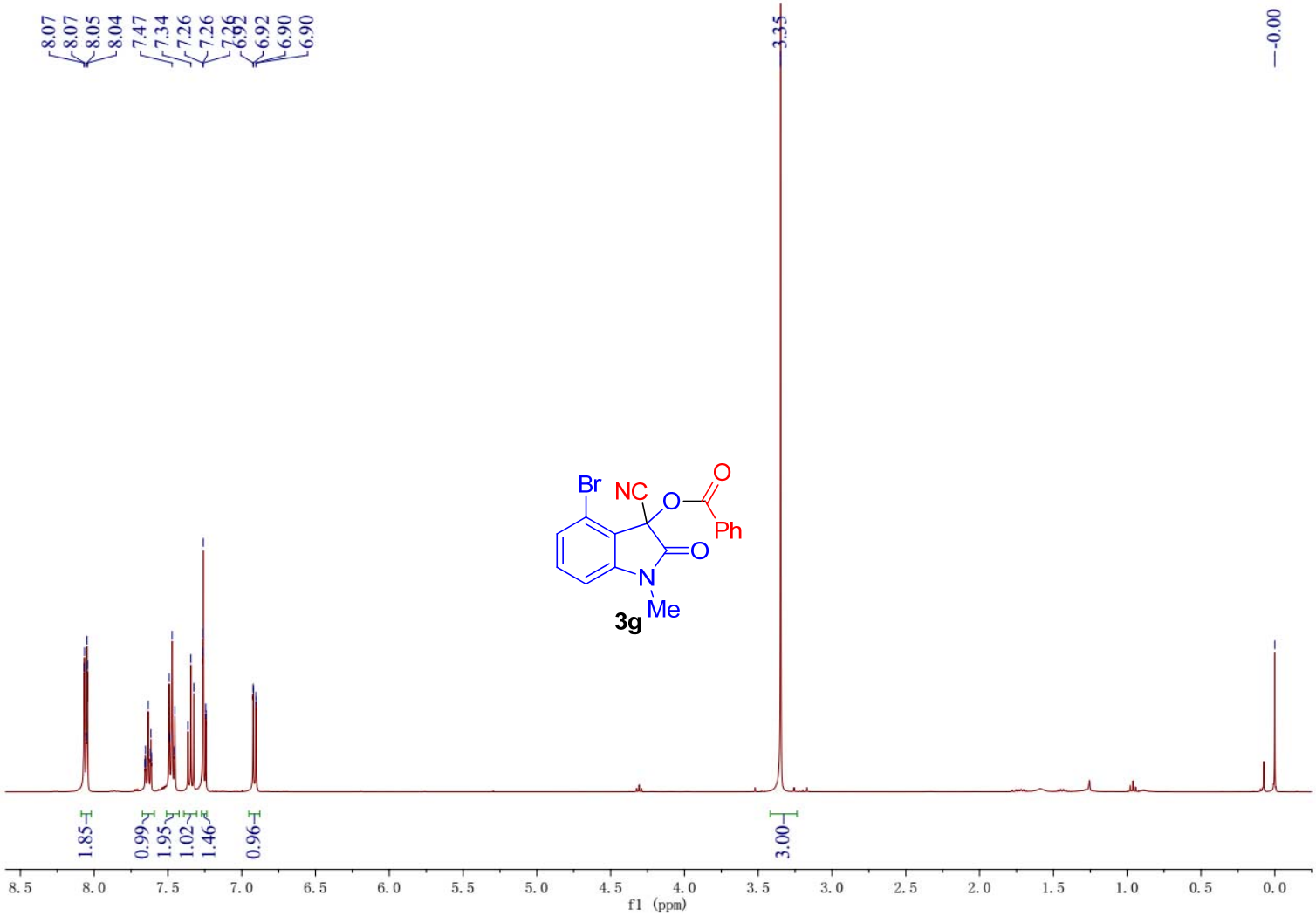

165.75
163.40
145.72
134.47
133.45
131.87
130.34
128.73
127.01
124.59
118.74
112.06
107.85
77.32
77.00
76.68
70.57
27.61
Cl
NC
O
O
Ph
O
N
Me
3d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

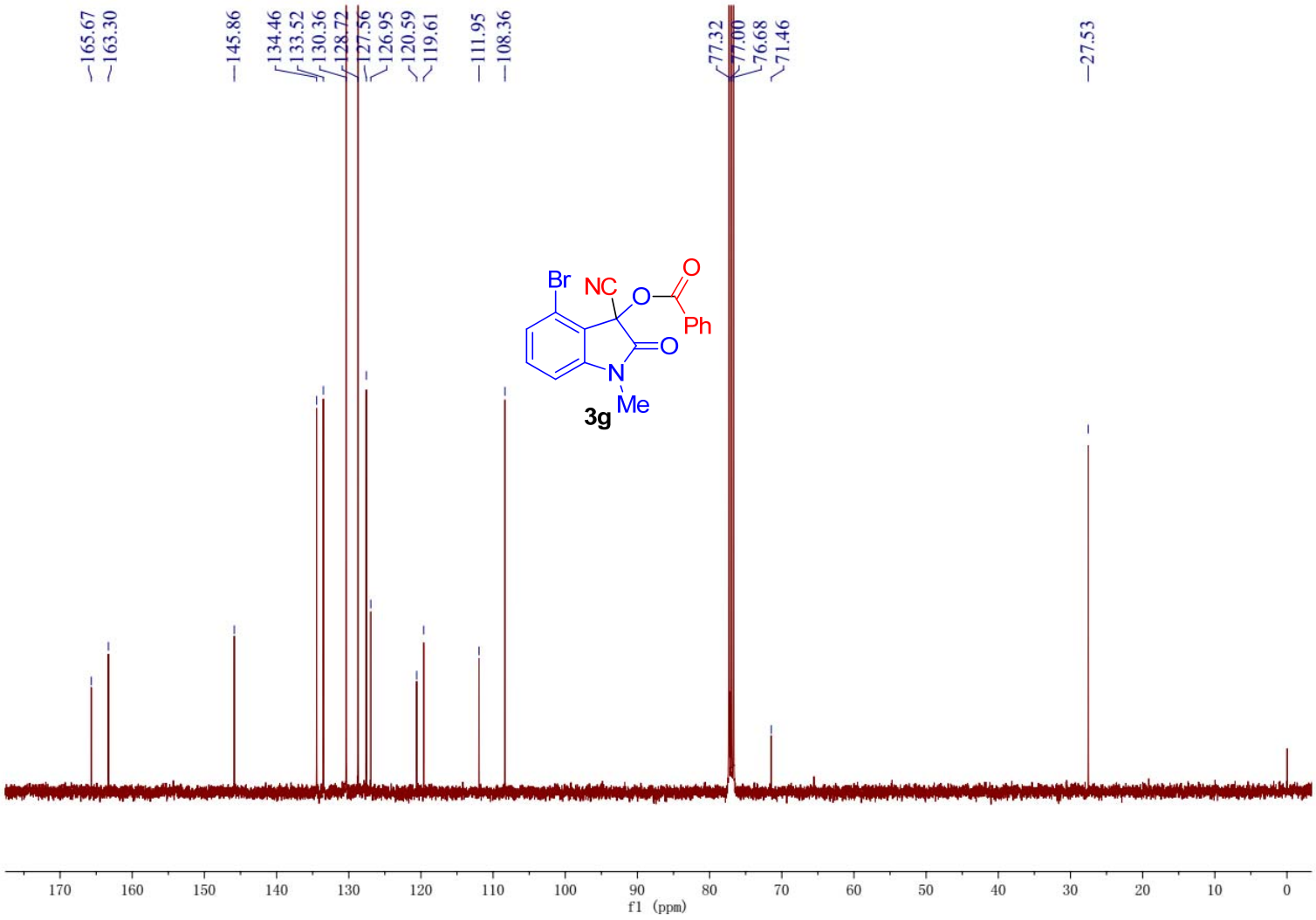

8.05
8.03
7.62
7.50
7.48
7.46
7.46
6.91
6.89
3.34
-0.00
NC
O
O
Ph
Cl
O
N
Me
3e
1.63
2.01
3.31
0.63
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

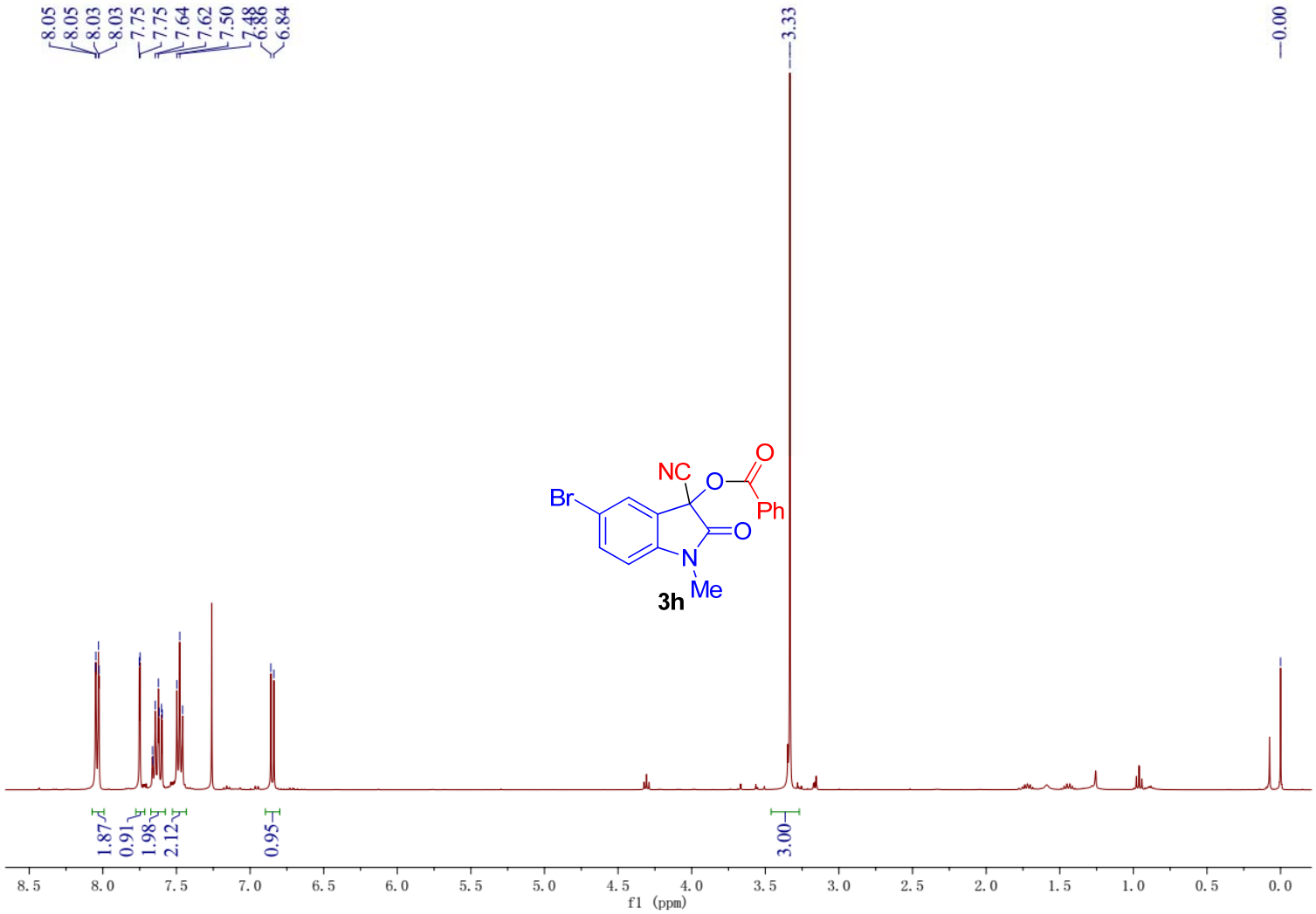

165.80
163.53
142.61
134.61
132.47
130.32
129.54
128.75
127.05
125.95
123.23
112.92
110.55
77.32
77.00
76.68
70.12
27.45
NC
O
O
Ph
Cl
O
N
Me
3e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

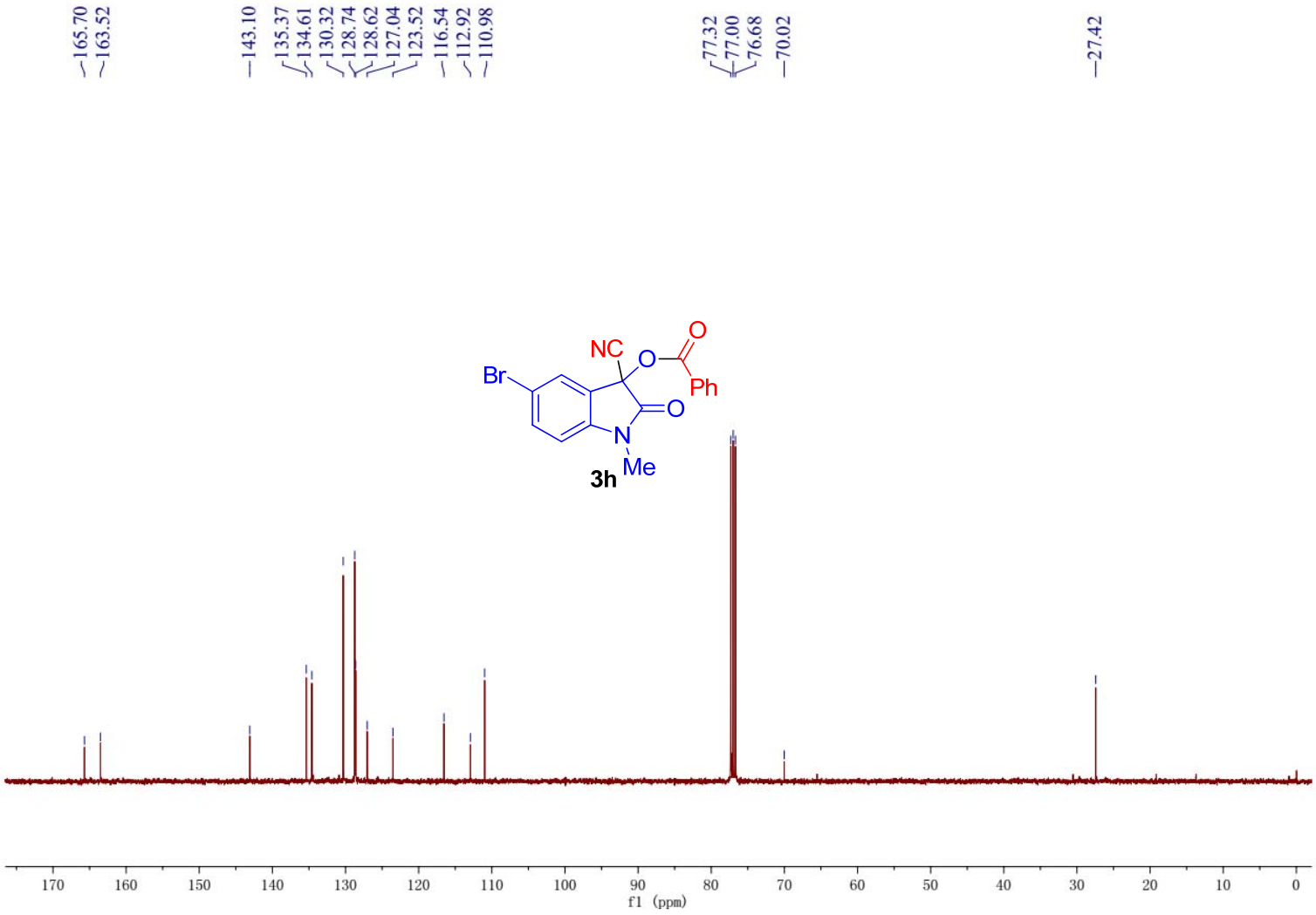

8.04
8.02
8.02
7.57
7.55
7.47
7.14
7.12
7.12
6.97
6.96
3.33
-0.00
NC
O
O
Ph
O
Cl
N
Me
3f
1.88
1.05
1.00
2.00
0.96
0.90
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

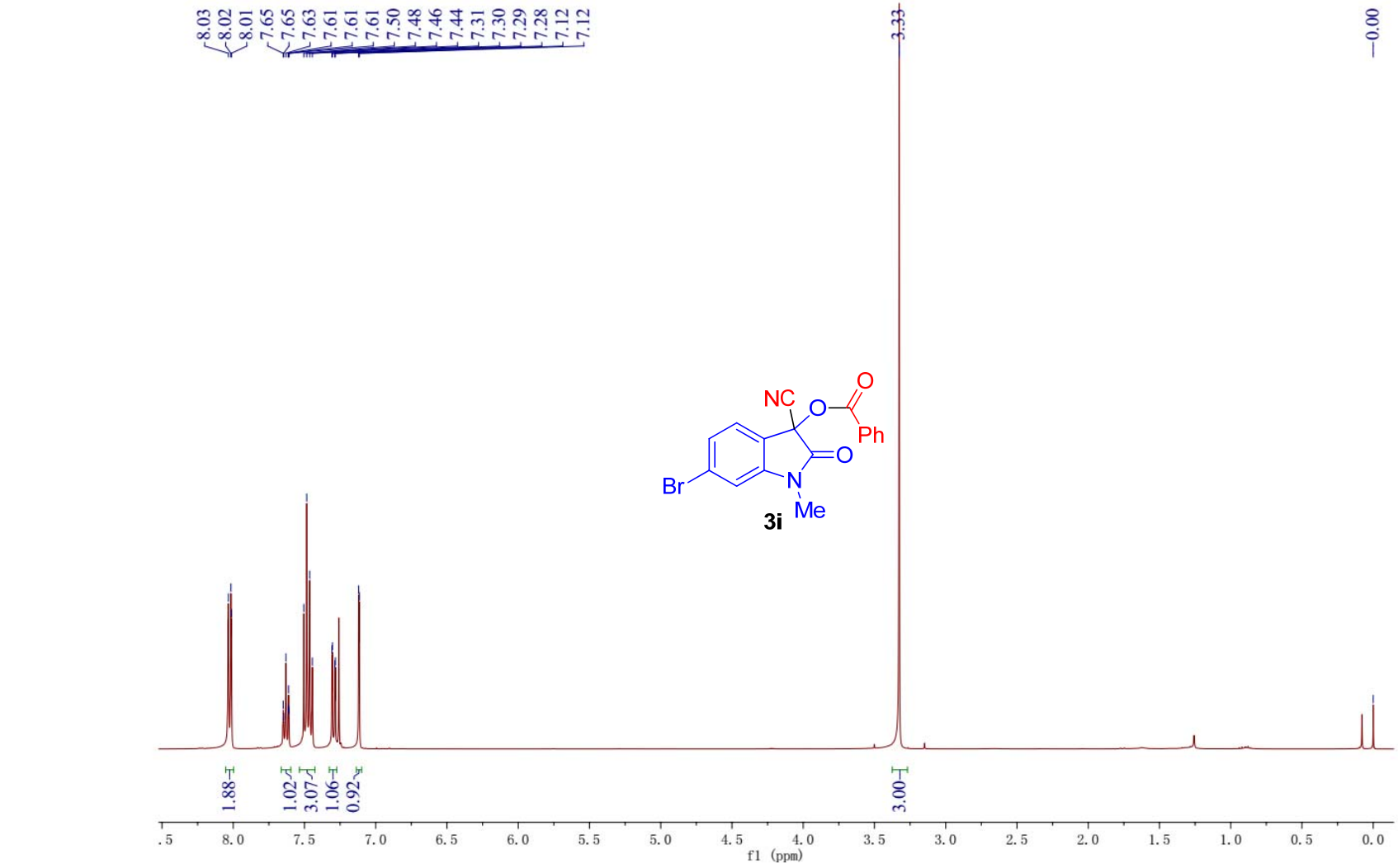

166.12
163.55
145.27
138.70
134.53
130.24
128.71
127.10
126.58
124.00
120.14
113.00
110.36
77.32
77.00
76.68
69.96
27.41
NC
O
O
Ph
O
Cl
N
Me
3f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

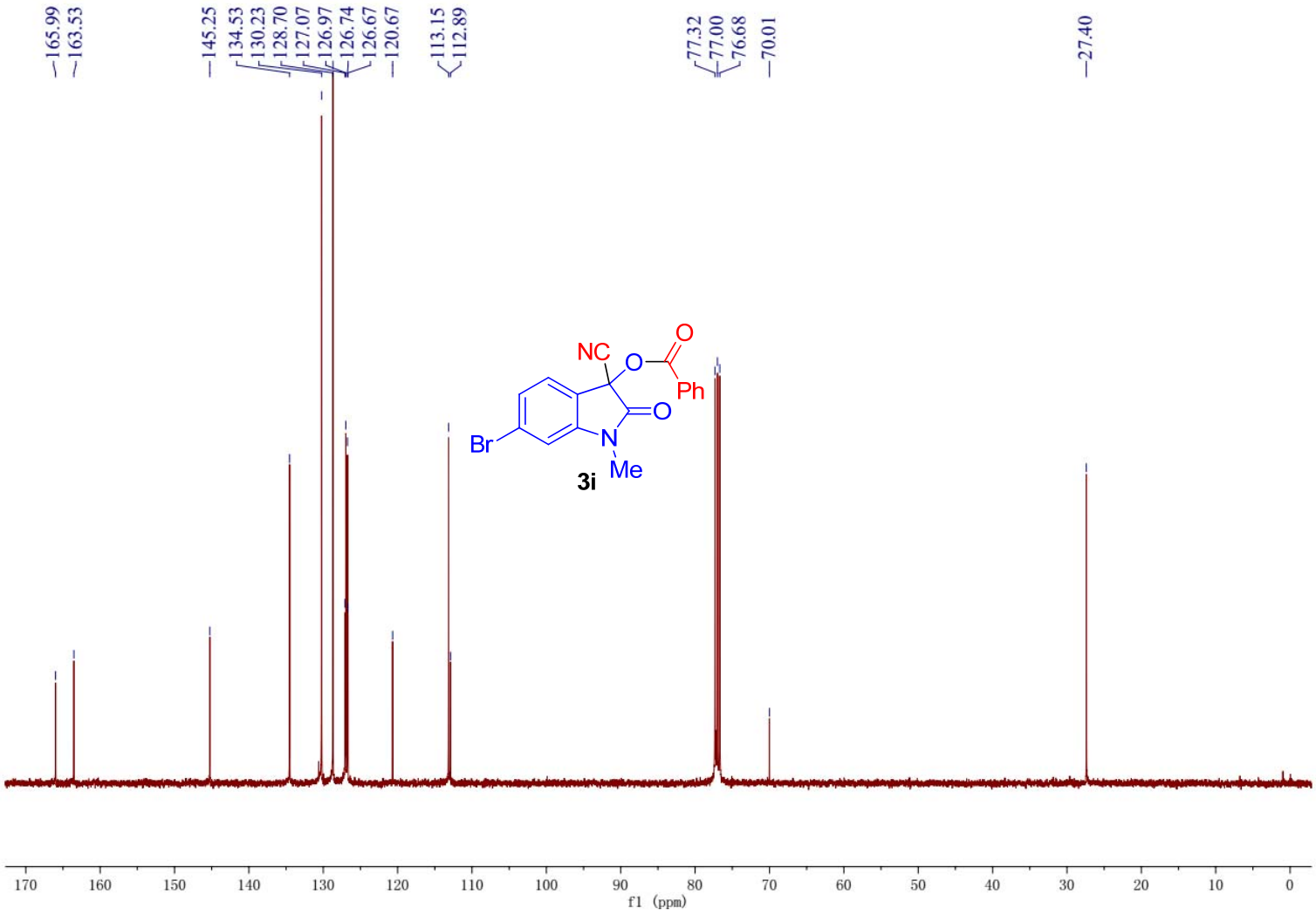

8.07
8.07
8.05
8.04
7.47
7.34
7.26
7.26
7.26
6.92
6.92
6.90
6.90
3.35
-0.00
Br
NC
O
O
Ph
O
N
Me
3g
1.85
0.99
1.95
1.02
1.46
0.96
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

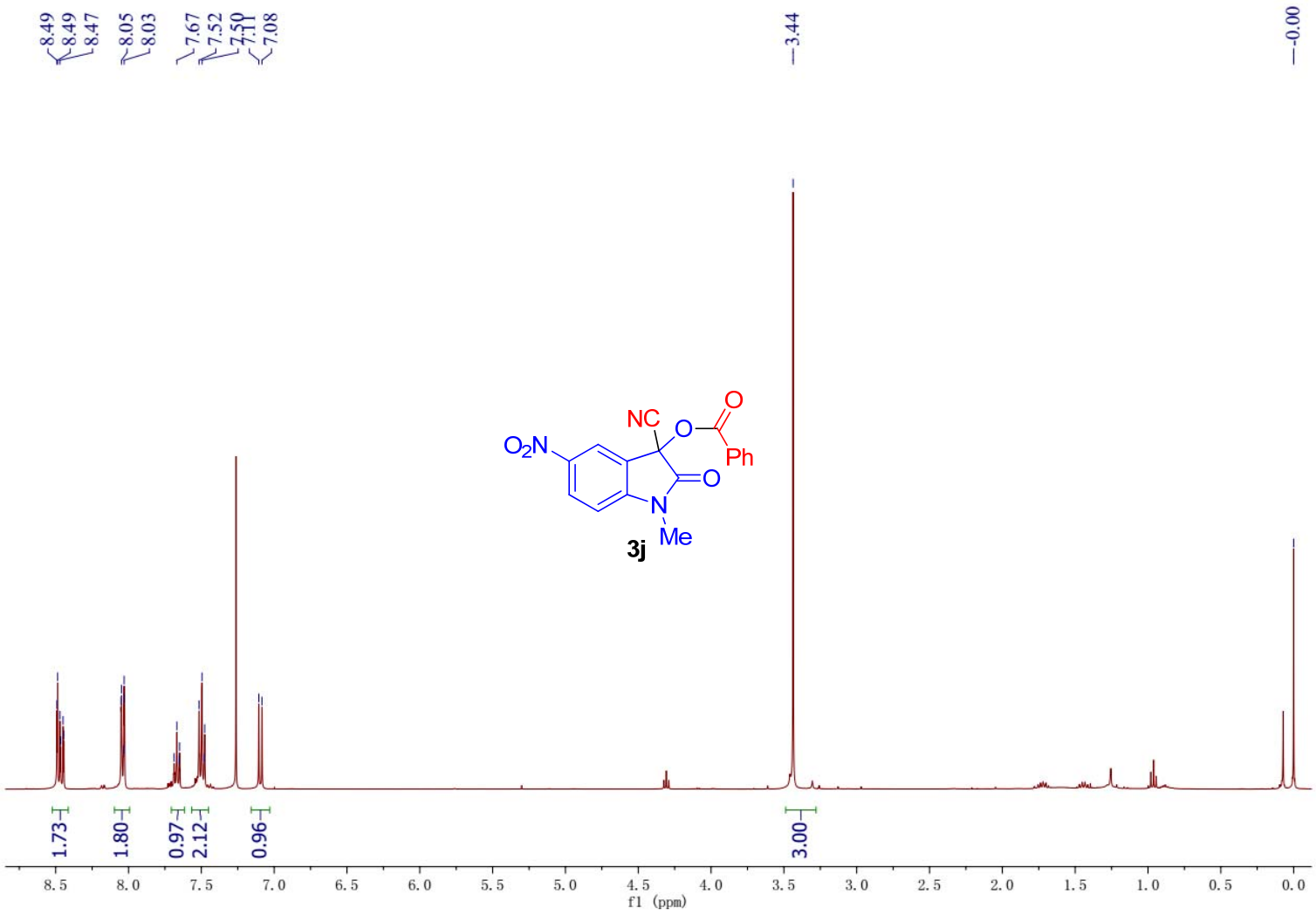

165.67
163.30
145.86
134.46
133.52
130.36
128.72
127.56
126.95
120.59
119.61
111.95
108.36
77.32
77.00
76.68
71.46
27.53
Br
NC
O
O
Ph
O
N
Me
3g
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

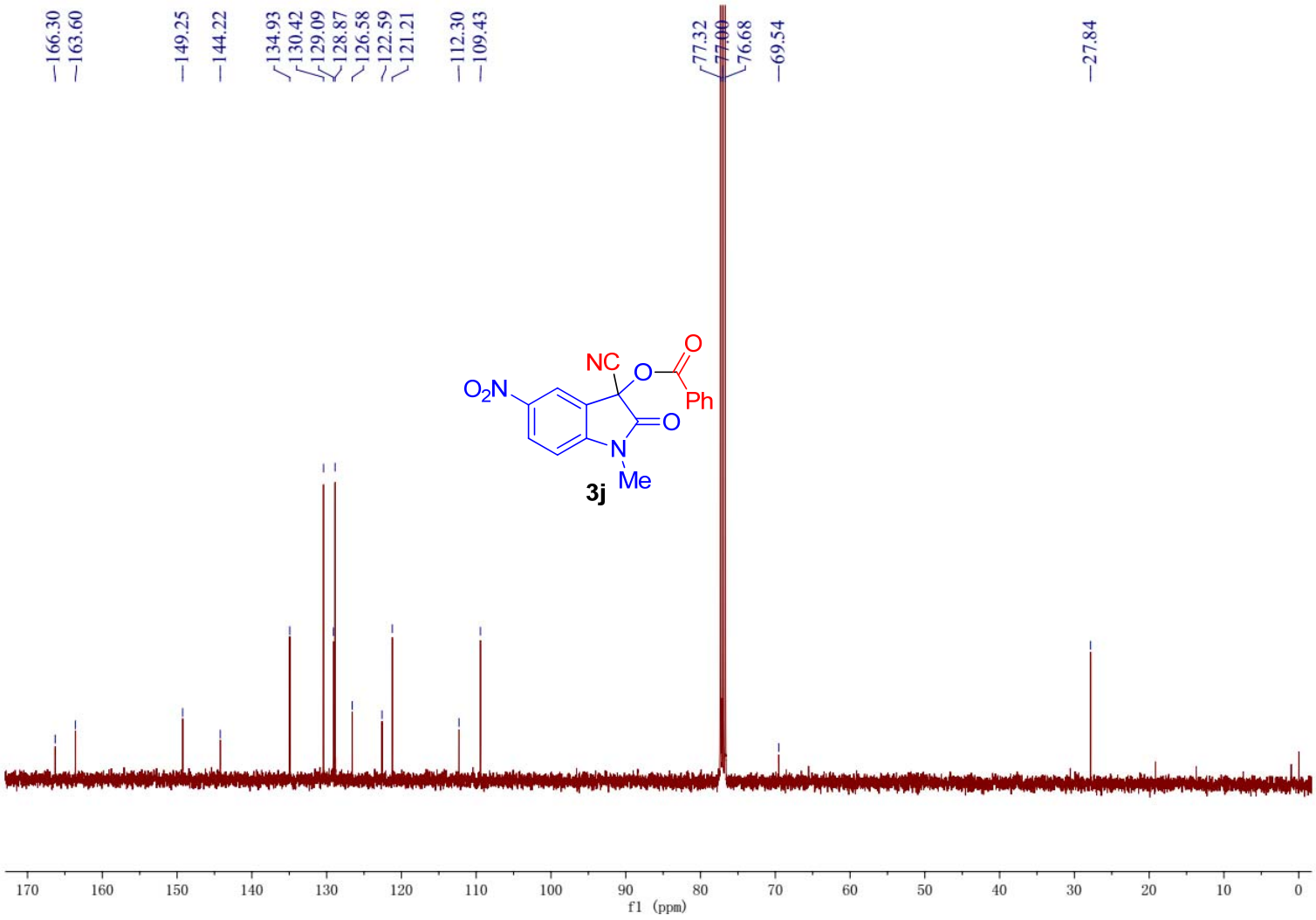

8.05
8.05
8.03
8.03
7.75
7.75
7.64
7.62
7.50
7.48
6.86
6.84
3.33
0.00
NC
O
O
Ph
Br
O
N
Me
3h
1.87
0.91
1.98
2.12
0.95
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

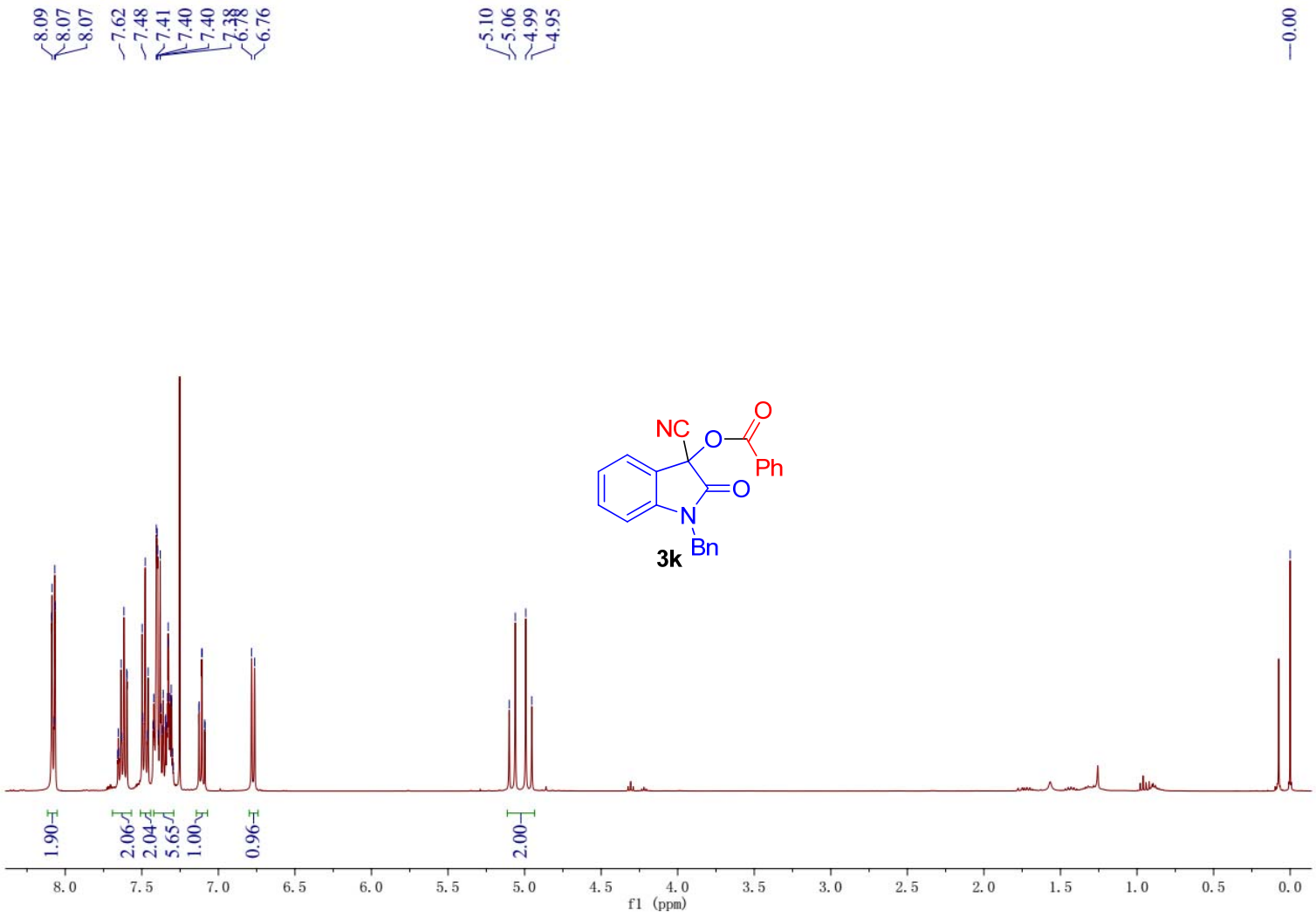

165.70
163.52
143.10
135.37
134.61
130.32
128.74
128.62
127.04
123.52
116.54
112.92
110.98
77.32
77.00
76.68
70.02
27.42
NC
O
O
Ph
Br
O
N
Me
3h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

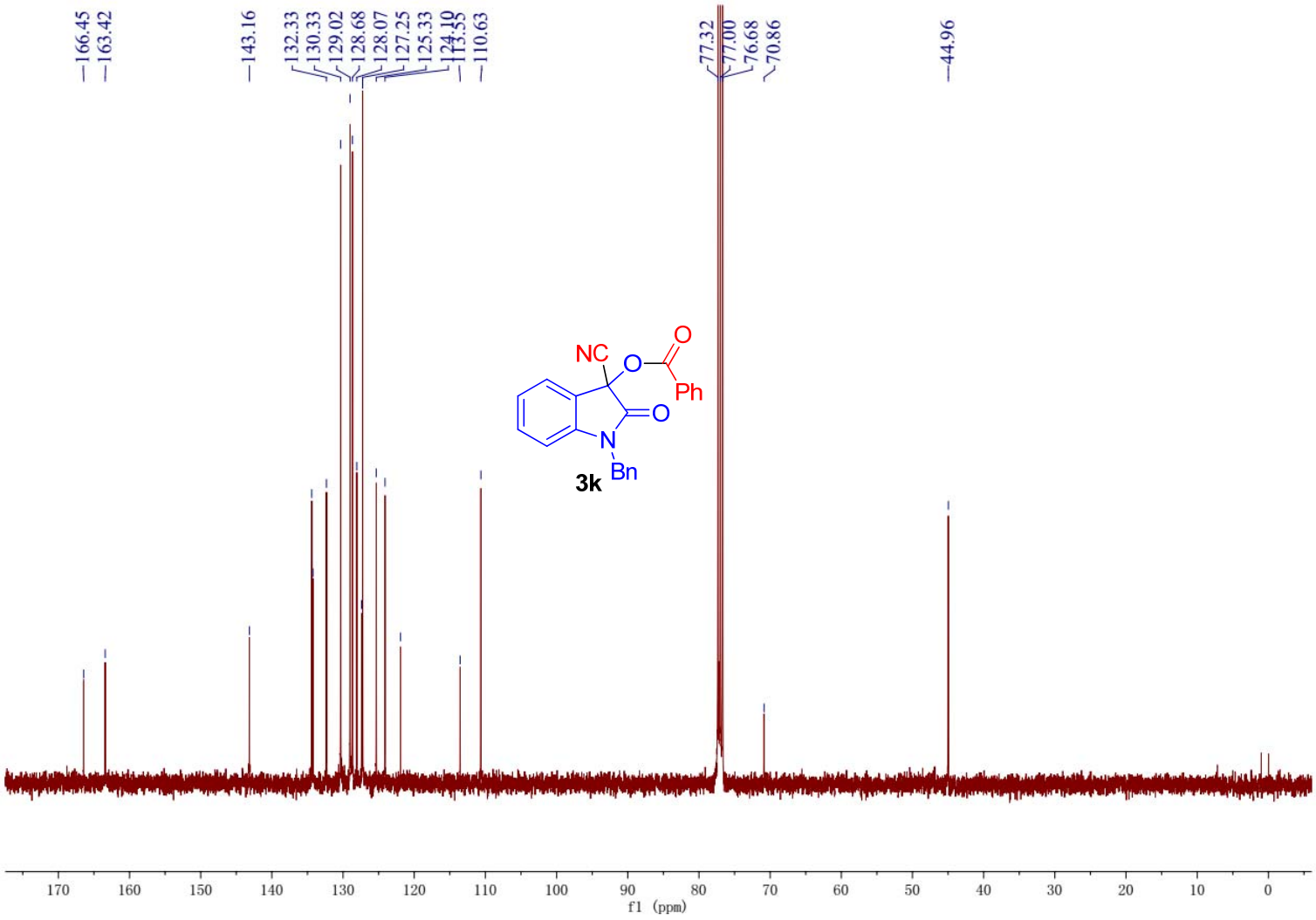

8.03
8.02
8.01
7.65
7.65
7.63
7.61
7.61
7.61
7.50
7.48
7.46
7.44
7.31
7.30
7.29
7.28
7.12
7.12
3.33
0.00
NC
O
O
Ph
O
N
Me
Br
3i
1.88
1.02
3.07
1.06
0.92
3.00
f1 (ppm)

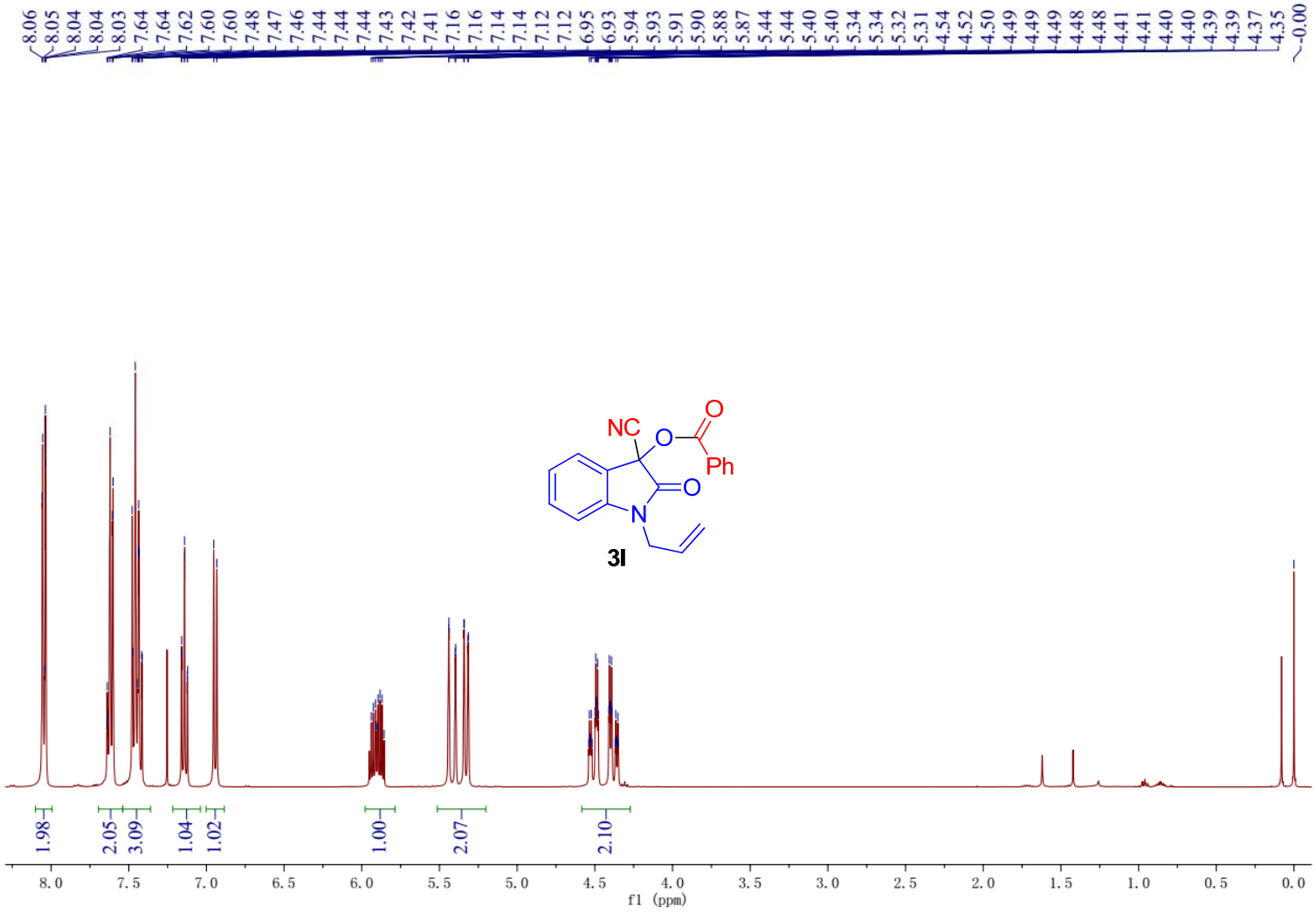

165.99
163.53
145.25
134.53
130.23
128.70
127.07
126.97
126.74
126.67
120.67
113.15
112.89
77.32
77.00
76.68
70.01
27.40
NC
O
O
Ph
O
Br
N
Me
3i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

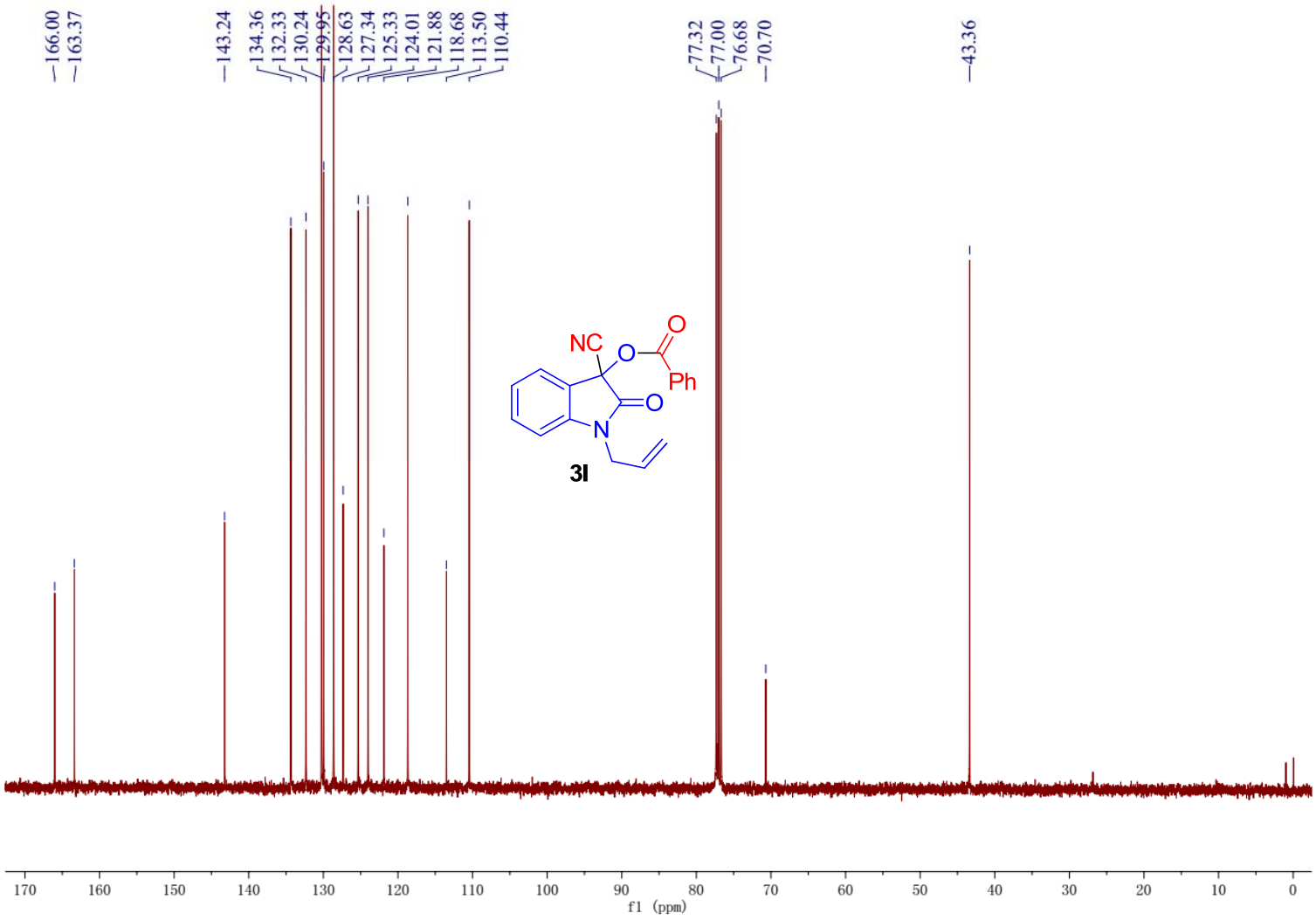

8.49
8.49
8.47
8.05
8.03
7.67
7.52
7.50
7.11
7.08
3.44
0.00
NC
O
O
Ph
O2N
O
N
Me
3j
1.73
1.80
0.97
2.12
0.96
3.00
f1 (ppm)

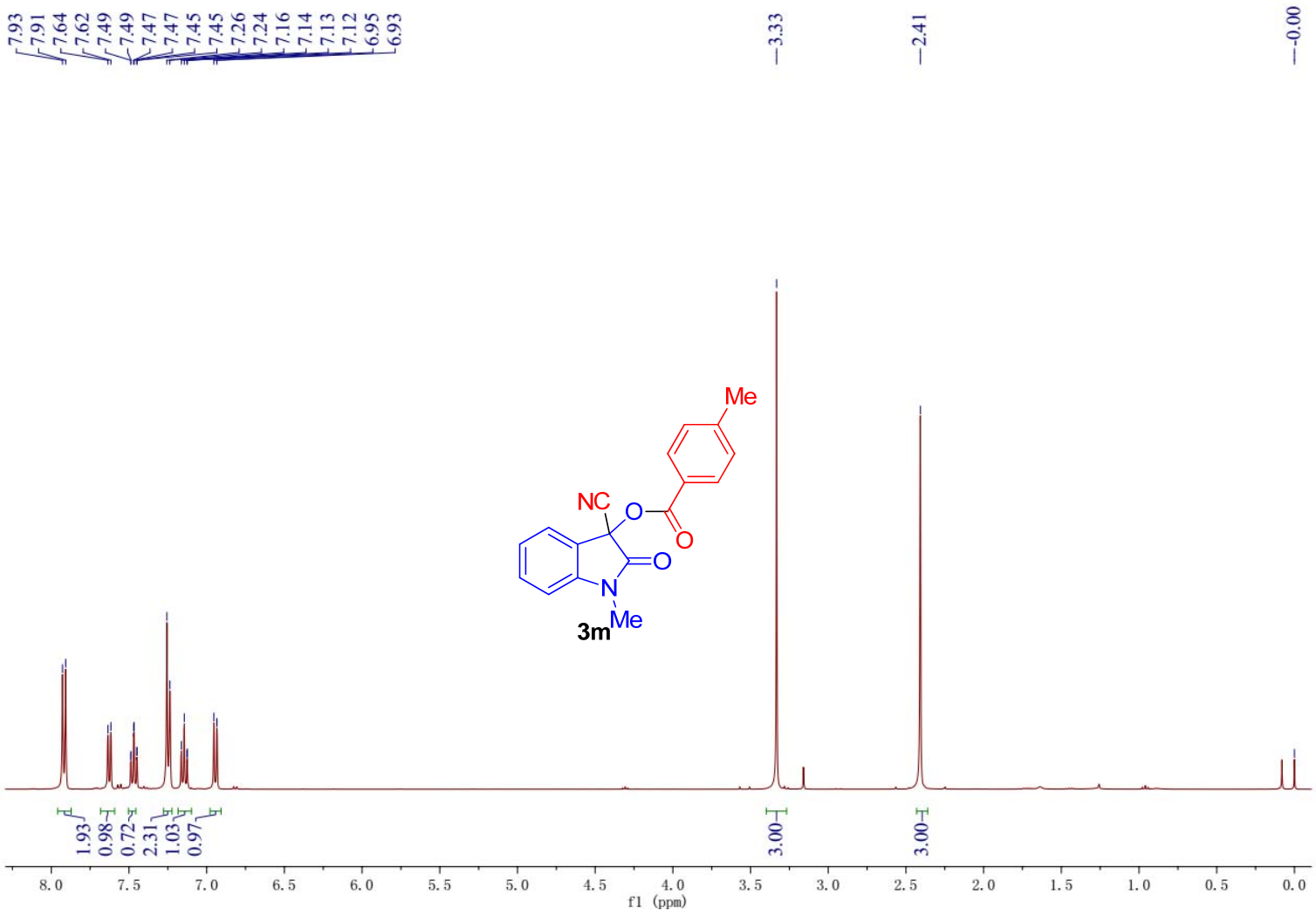

166.30
163.60
149.25
144.22
134.93
130.42
129.09
128.87
126.58
122.59
121.21
112.30
109.43
77.32
77.00
76.68
69.54
27.84
NC
O
O
Ph
O2N
O
N
Me
3j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

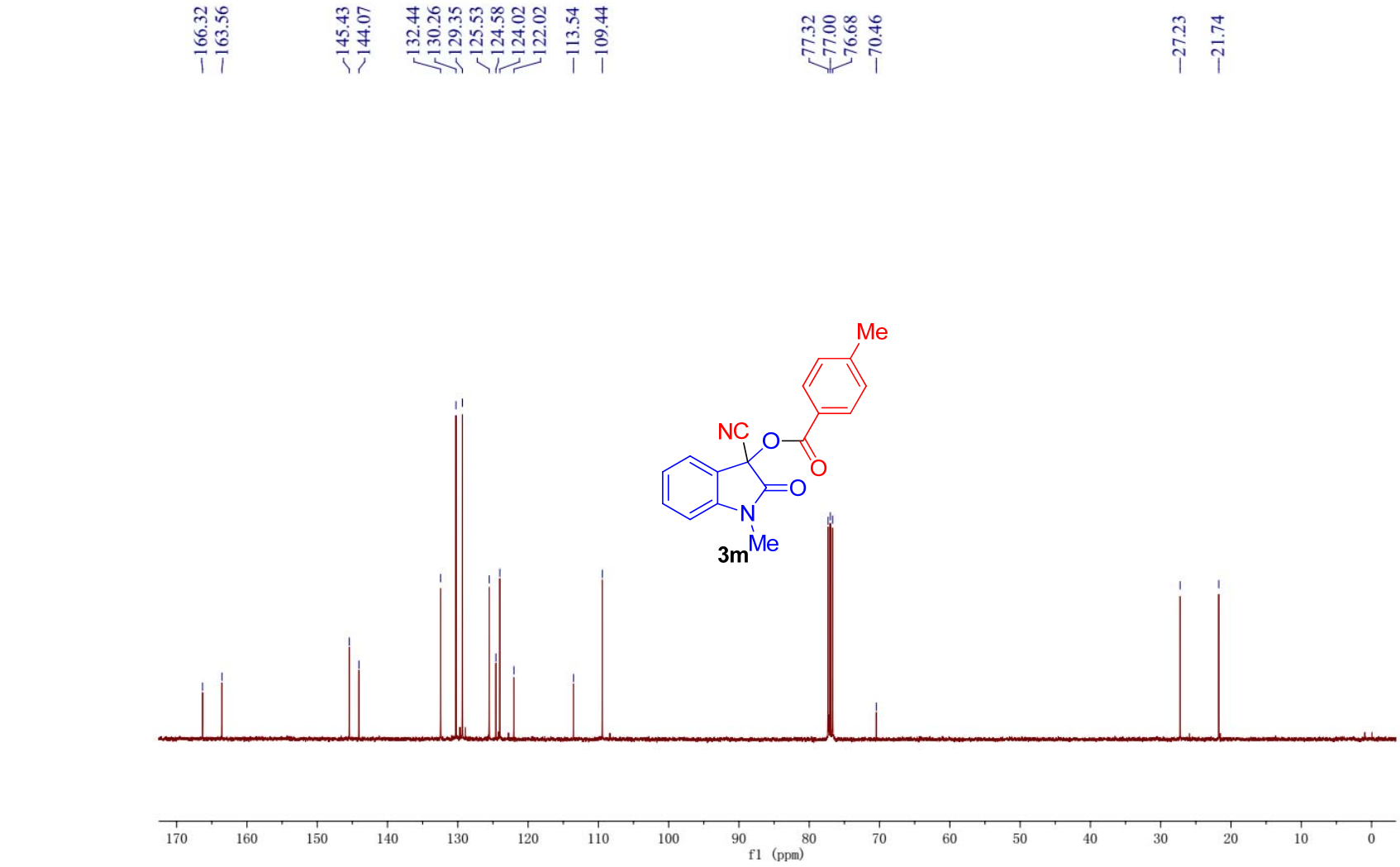

8.09
8.07
8.07
7.62
7.48
7.41
7.40
7.40
7.38
6.78
6.76
5.10
5.06
4.99
4.95
0.00
NC
O
O
Ph
O
N
Bn
3k
1.90
2.06
2.04
5.65
1.00
0.96
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

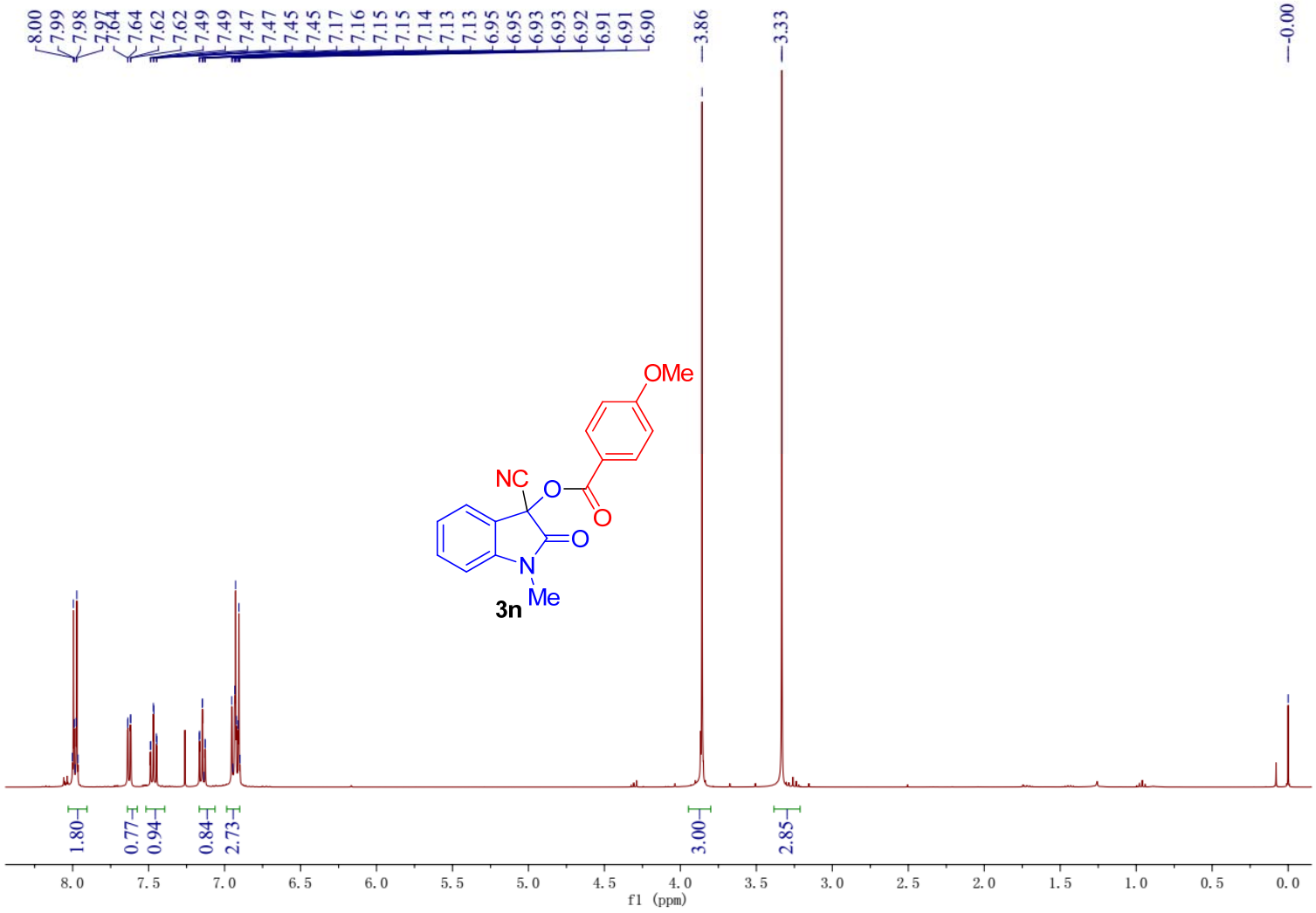

166.45
163.42
143.16
132.33
130.33
129.02
128.68
128.07
127.25
125.33
110.63
77.32
77.00
76.68
70.86
44.96
NC
O
O
Ph
O
N
Bn
3k
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

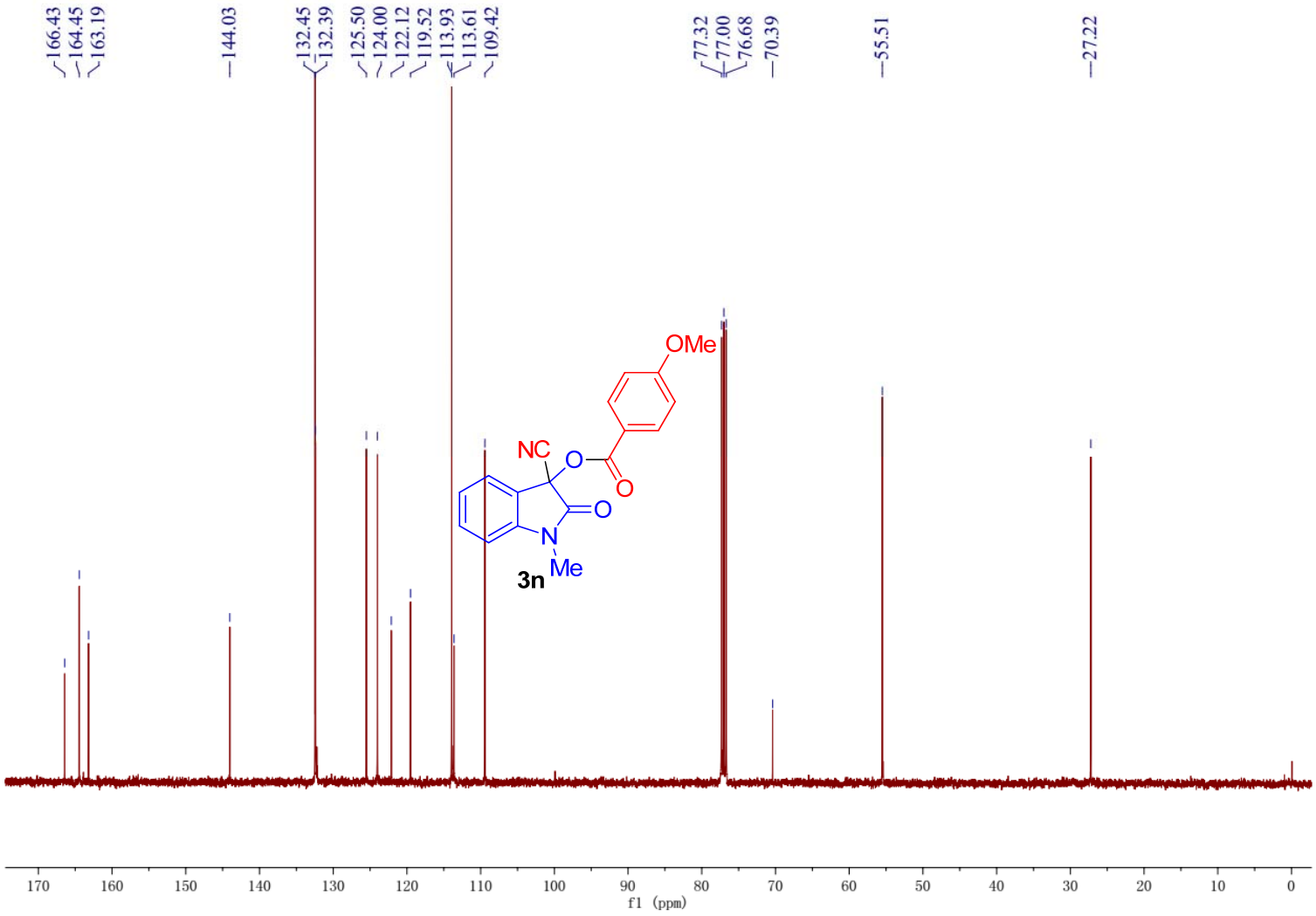

8.06
8.05
8.04
8.04
8.03
7.64
7.64
7.62
7.60
7.60
7.48
7.47
7.46
7.44
7.44
7.44
7.43
7.42
7.41
7.16
7.16
7.14
7.14
7.12
7.12
6.95
6.93
5.94
5.93
5.91
5.90
5.88
5.87
5.44
5.44
5.40
5.40
5.34
5.34
5.32
5.31
4.54
4.52
4.50
4.49
4.49
4.49
4.48
4.48
4.41
4.41
4.40
4.40
4.39
4.39
4.37
4.35
-0.00
NC
O
O
Ph
O
N
3l
1.98
2.05
3.09
1.04
1.02
1.00
2.07
2.10
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)

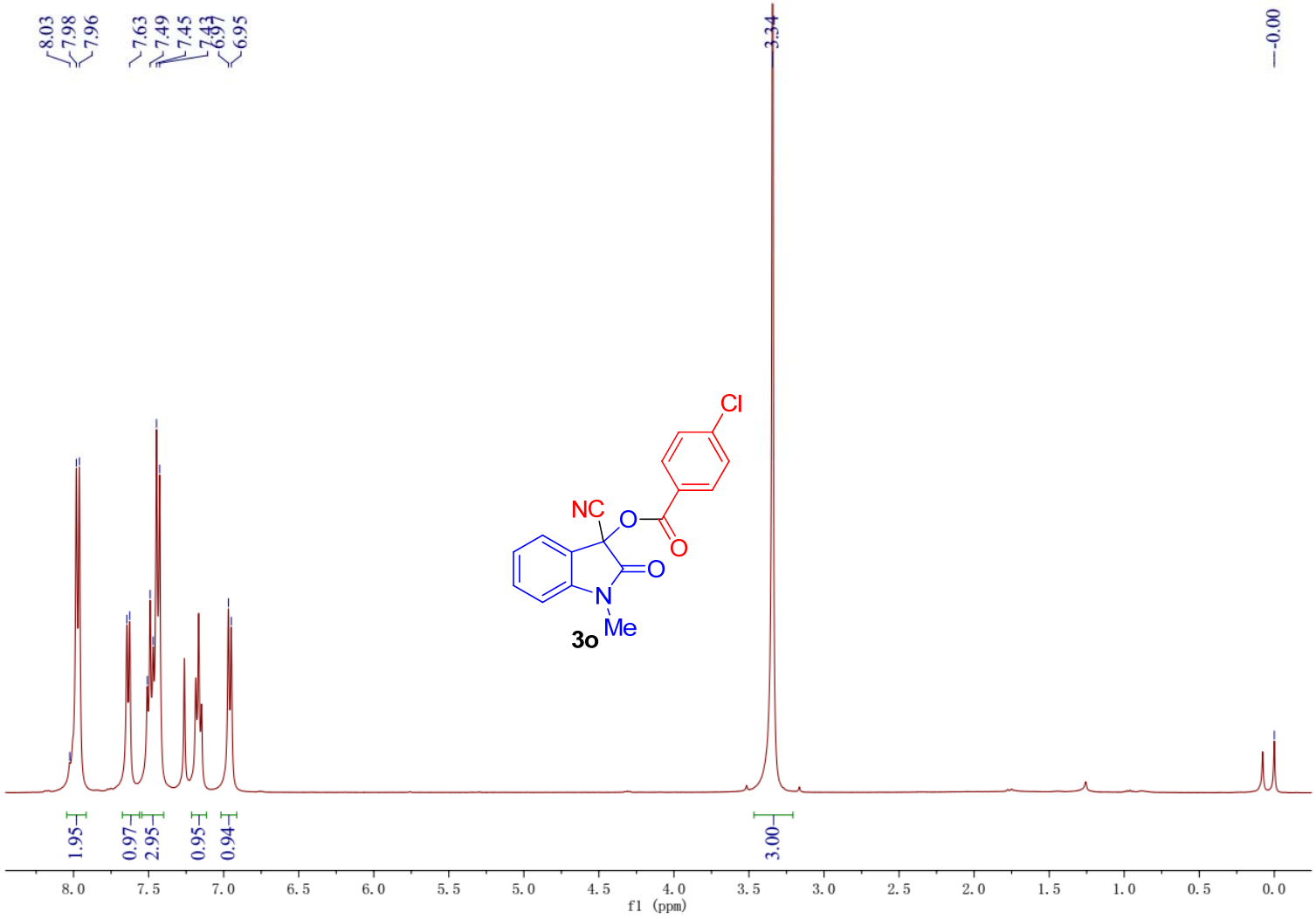

166.00
163.37
143.24
134.36
132.33
130.24
129.95
128.63
127.34
125.33
124.01
121.88
118.68
113.50
110.44
77.32
77.00
76.68
70.70
43.36
NC
O
O
Ph
O
N
3l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

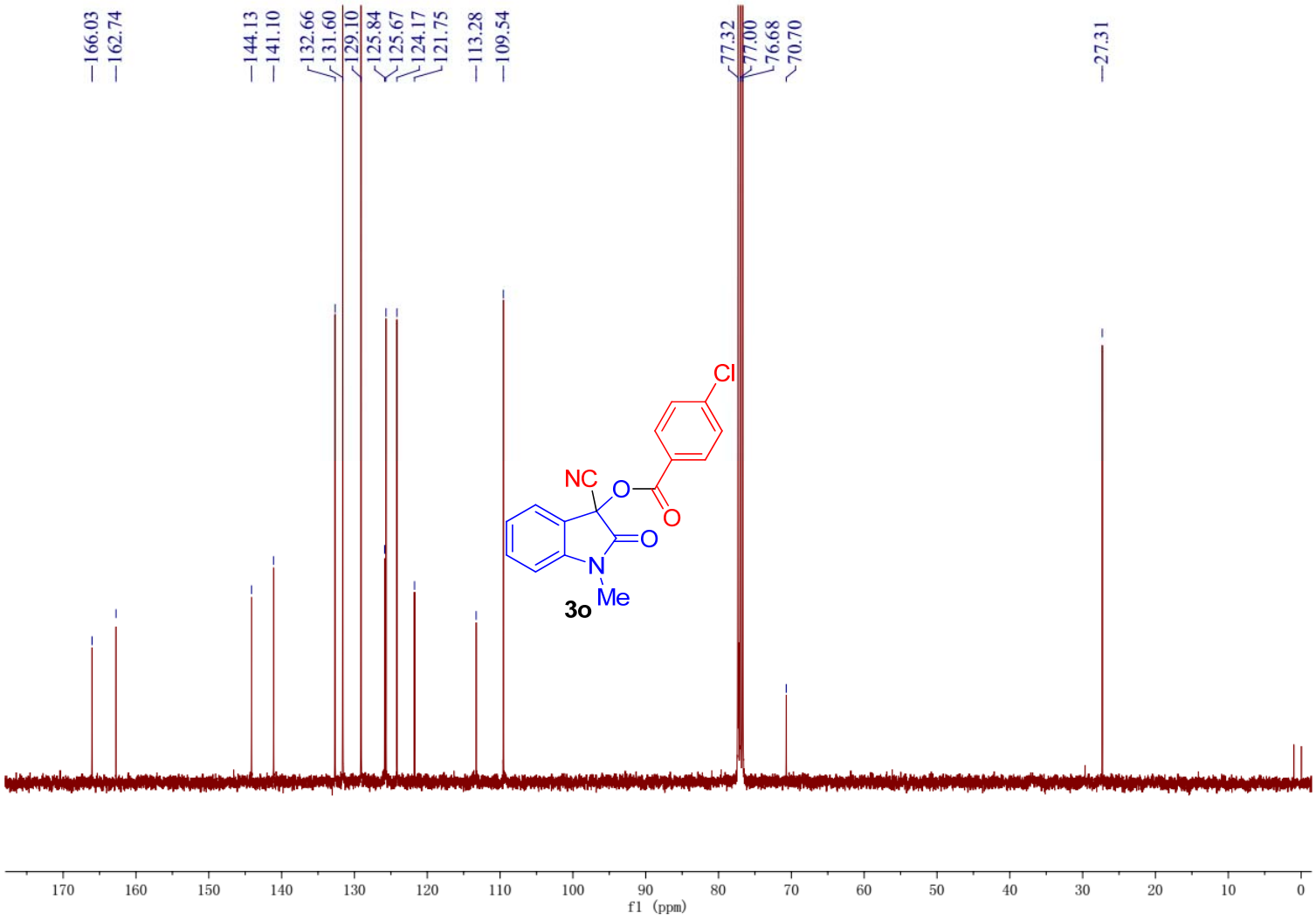

7.93
7.91
7.64
7.62
7.49
7.49
7.47
7.47
7.45
7.45
7.26
7.24
7.16
7.14
7.13
7.12
6.95
6.93
3.33
2.41
0.00
Me
NC
O
O
O
N
Me
3m
1.93
0.98
0.72
2.31
1.03
0.97
3.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

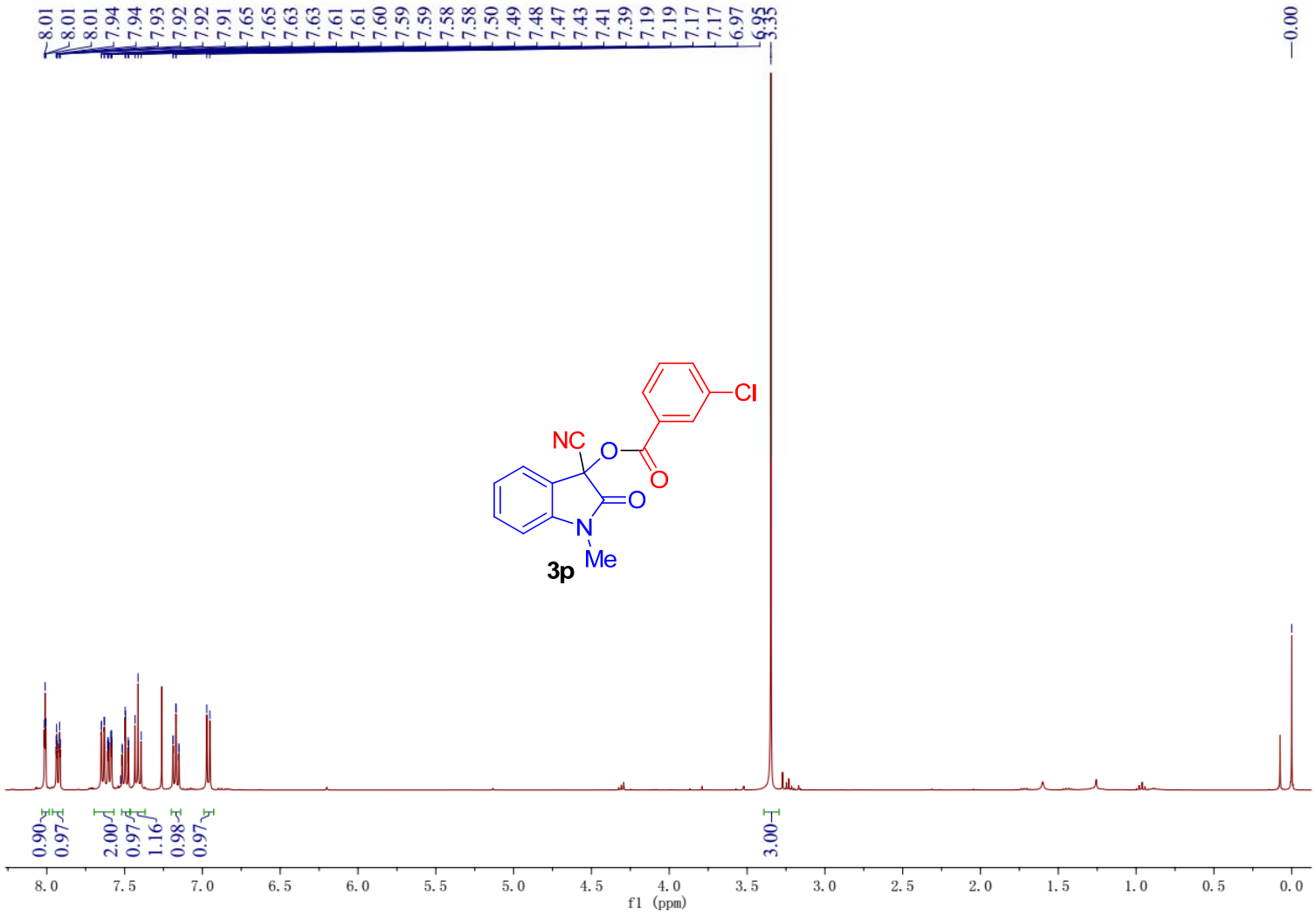

166.32
163.56
145.43
144.07
132.44
130.26
129.35
125.53
124.58
124.02
122.02
113.54
109.44
77.32
77.00
76.68
70.46
27.23
21.74
Me
NC
O
O
O
N
Me
3m
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

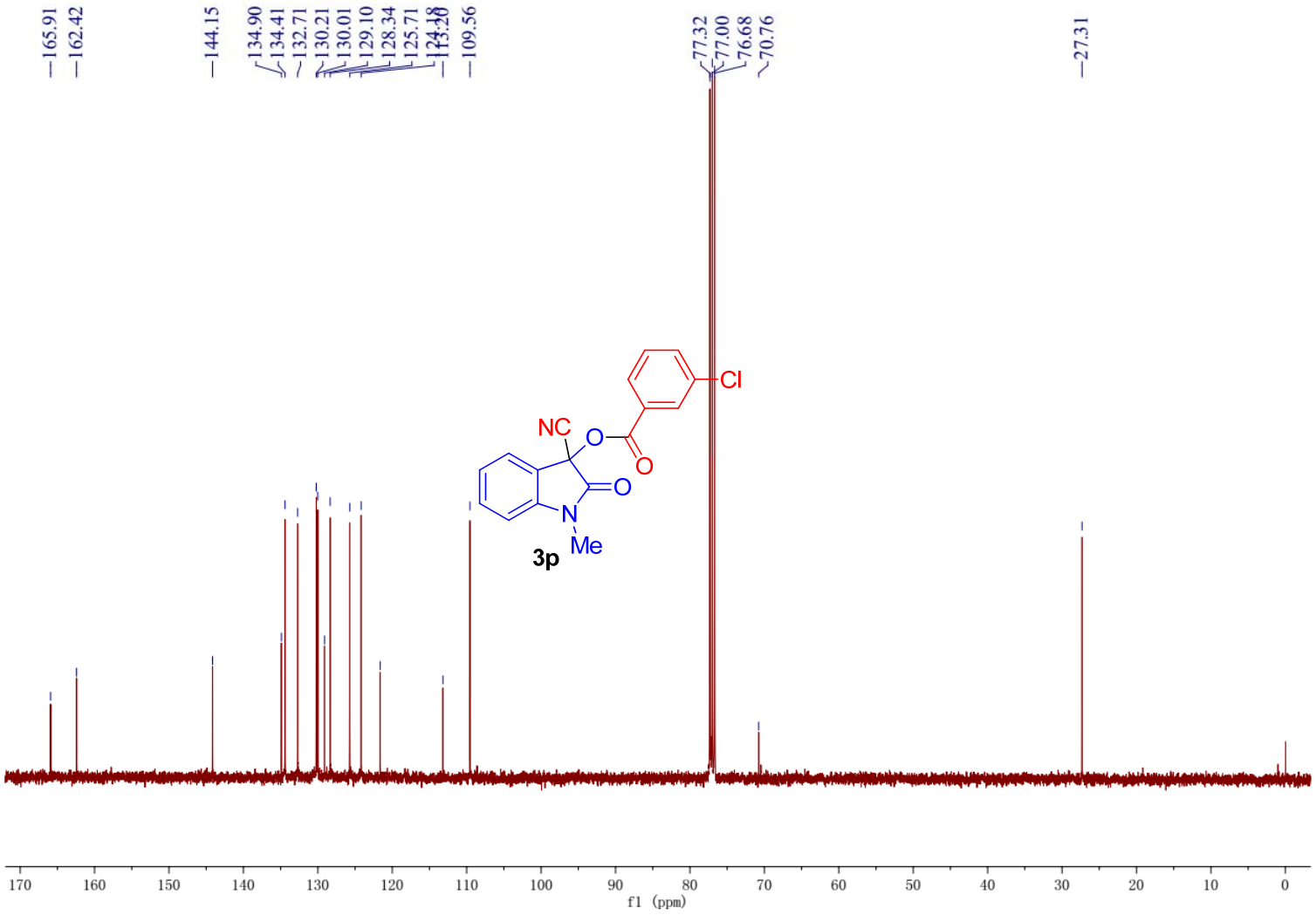

8.00
7.99
7.98
7.97
7.64
7.64
7.62
7.62
7.49
7.49
7.47
7.47
7.45
7.45
7.17
7.16
7.15
7.15
7.14
7.13
7.13
6.95
6.95
6.93
6.93
6.92
6.91
6.91
6.90
3.86
3.33
-0.00
OMe
NC
O
O
O
N
Me
3n
1.80
0.77
0.94
0.84
2.73
3.00
2.85
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

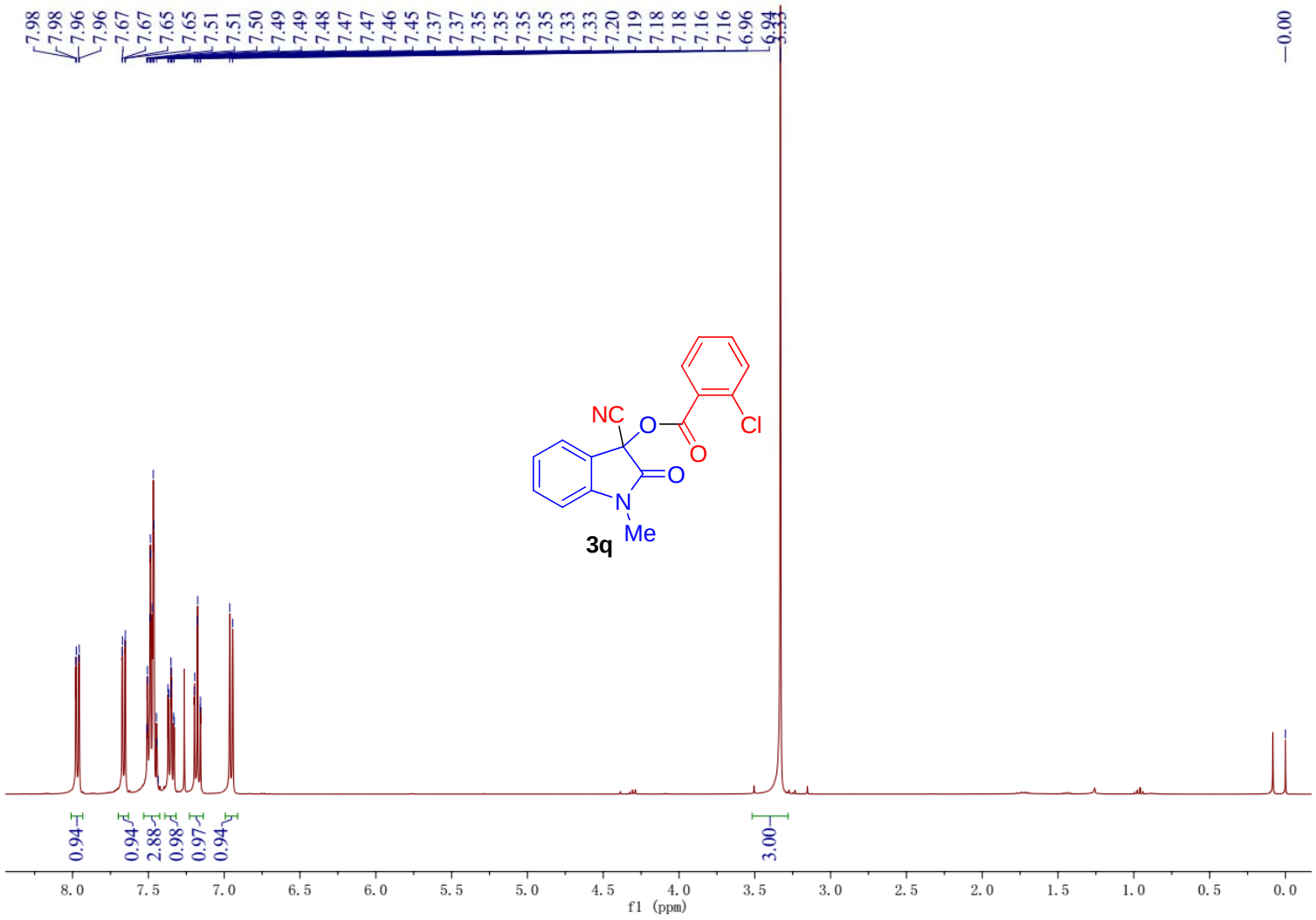

166.43
164.45
163.19
144.03
132.45
132.39
125.50
124.00
122.12
119.52
113.93
113.61
109.42
77.32
77.00
76.68
70.39
55.51
27.22
OMe
NC
O
O
O
N
Me
3n
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

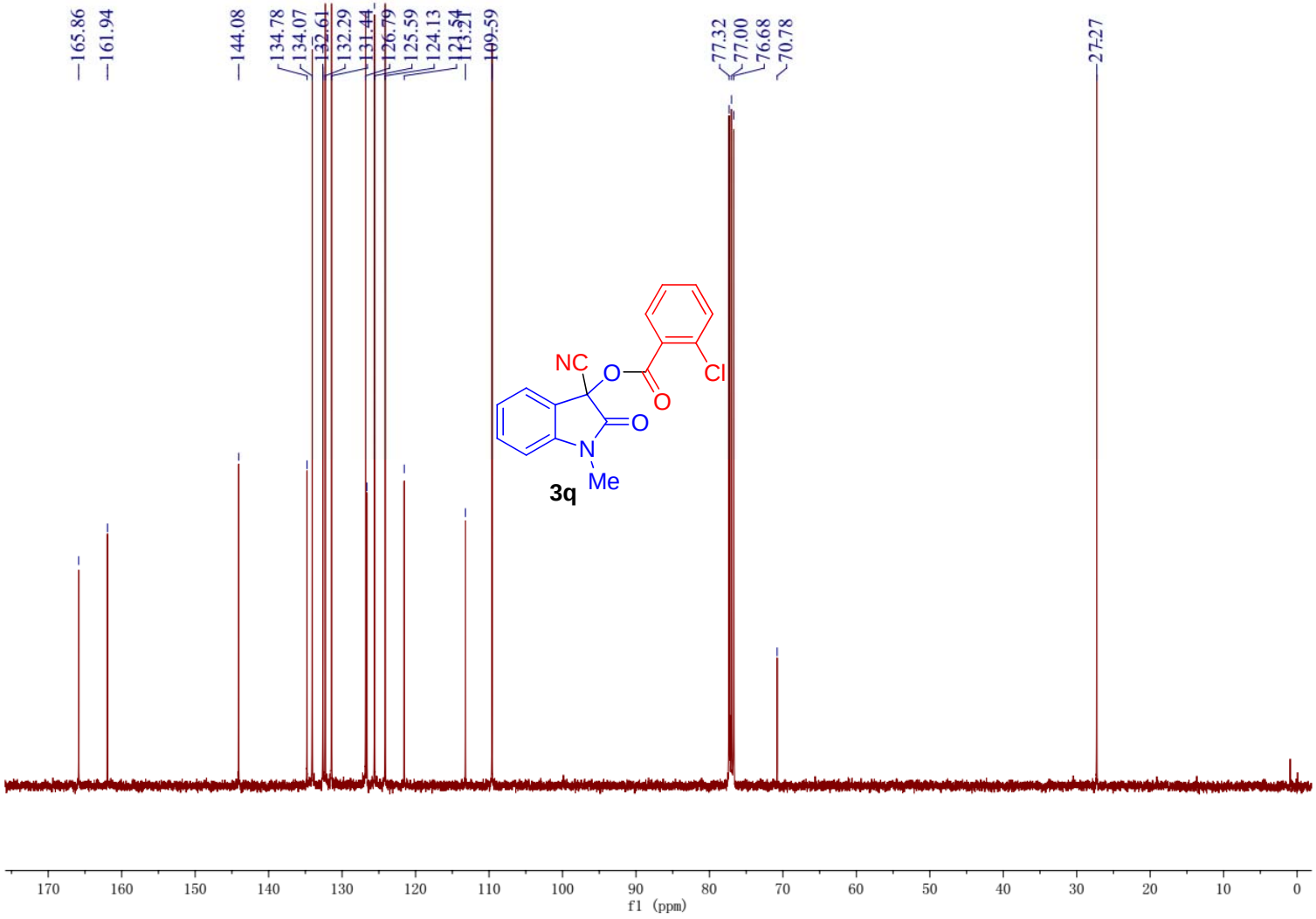

8.03
7.98
7.96
7.63
7.49
7.45
7.43
6.97
6.95
3.34
-0.00
Cl
NC
O
O
O
N
Me
3o
1.95
0.97
2.95
0.95
0.94
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

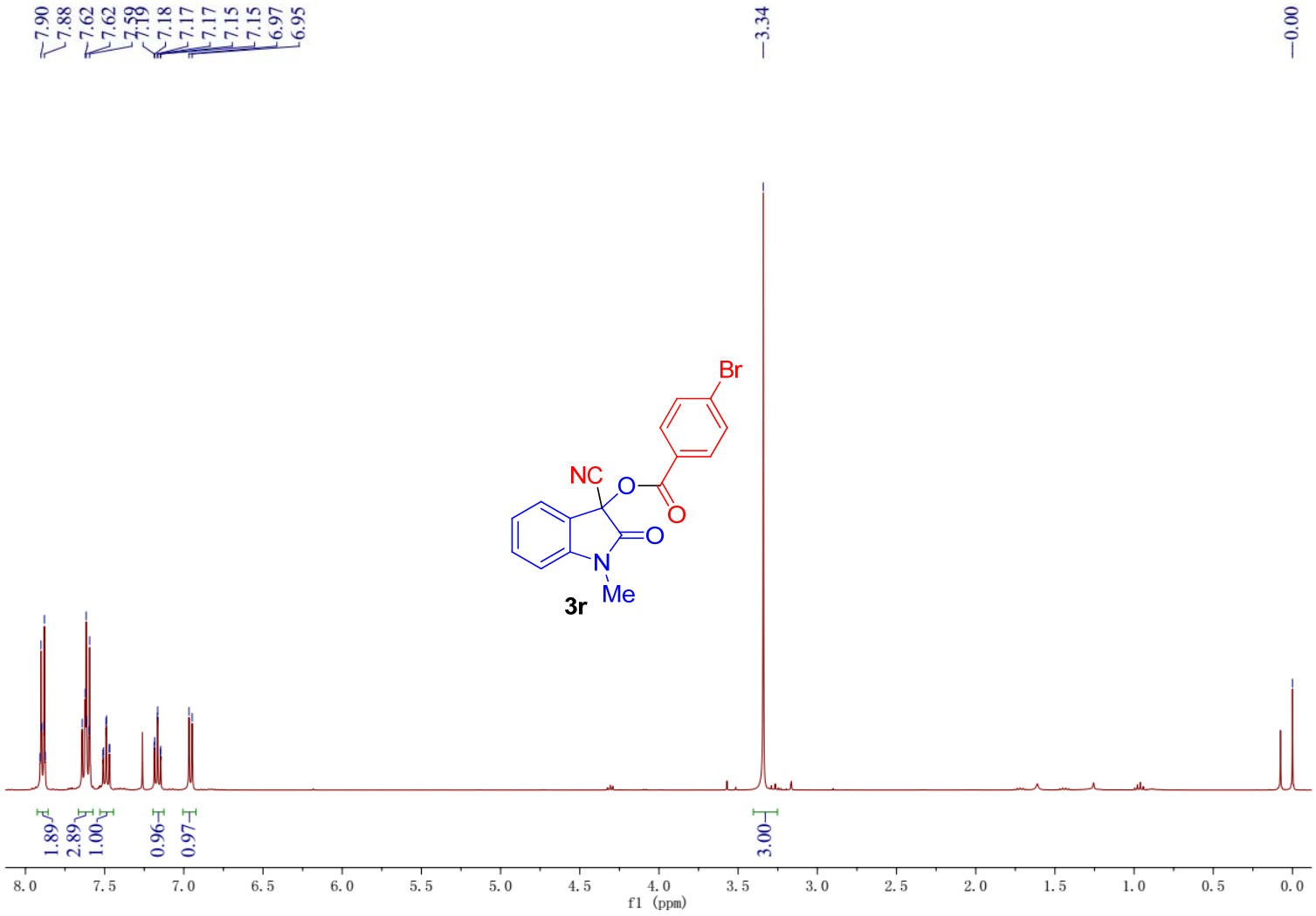

166.03
162.74
144.13
141.10
132.66
131.60
129.10
125.84
125.67
124.17
121.75
113.28
109.54
77.32
77.00
76.68
70.70
27.31
Cl
NC
O
O
O
N
Me
3o
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

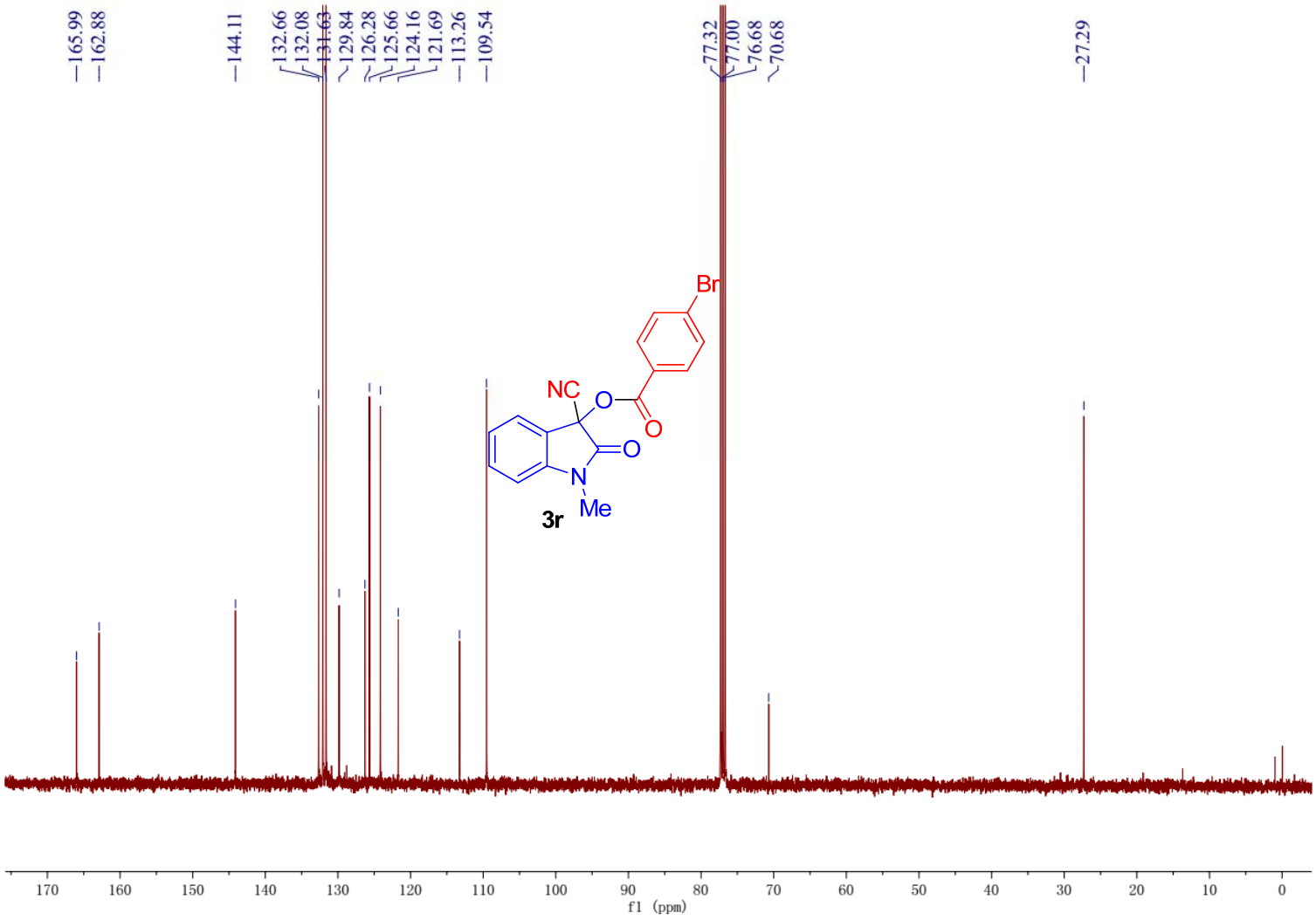

8.01
8.01
8.01
7.94
7.94
7.93
7.92
7.92
7.91
7.65
7.65
7.63
7.63
7.61
7.61
7.60
7.59
7.59
7.58
7.58
7.50
7.49
7.48
7.47
7.43
7.41
7.39
7.19
7.19
7.17
7.17
6.97
6.95
3.35
0.00
Cl
NC
O
O
O
N
Me
3p
0.90
0.97
2.00
0.97
1.16
0.98
0.97
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

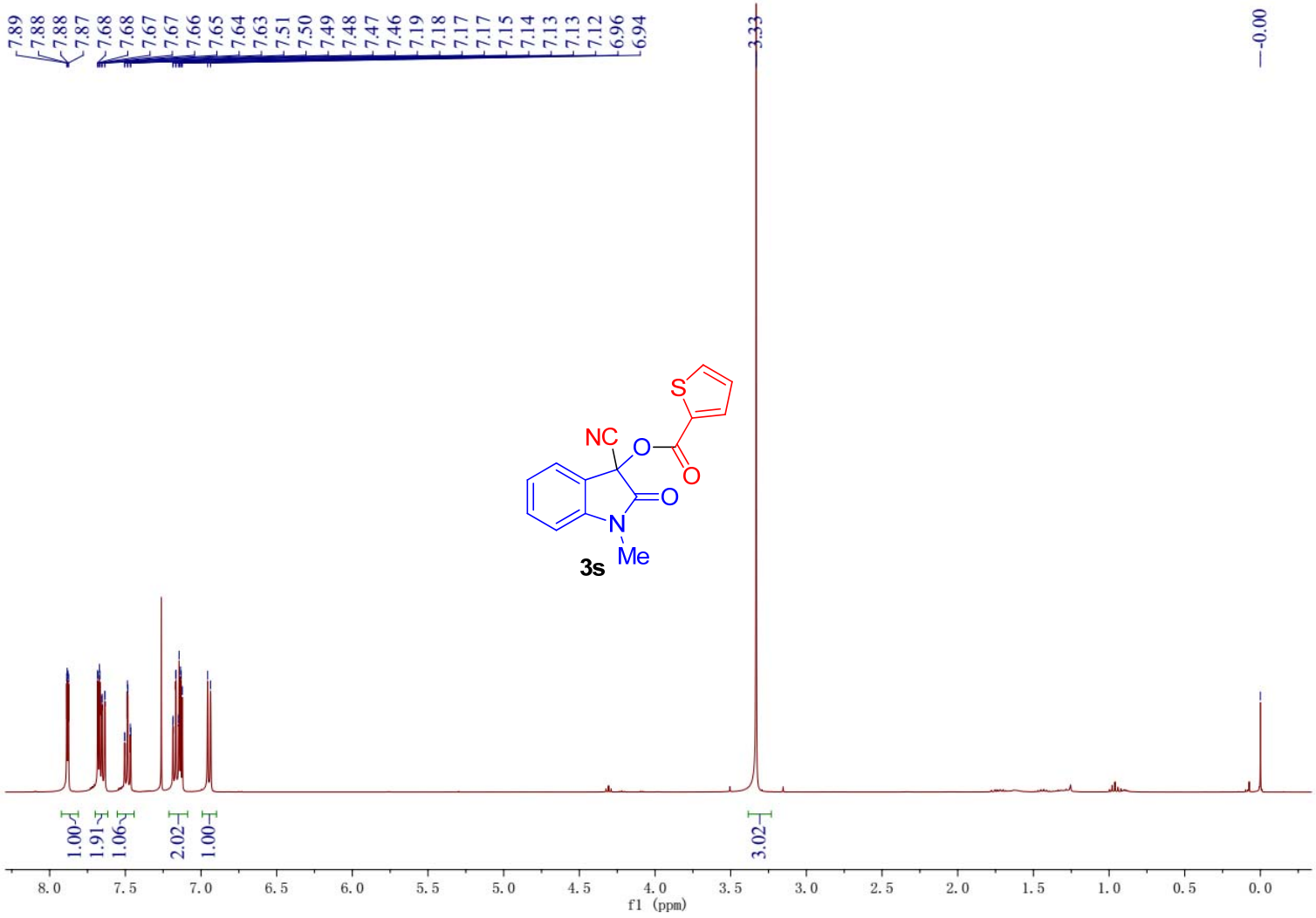

165.91
162.42
144.15
134.90
134.41
132.71
130.21
130.01
129.10
128.34
125.71
109.56
77.32
77.00
76.68
70.76
27.31
Cl
NC
O
O
O
N
Me
3p
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

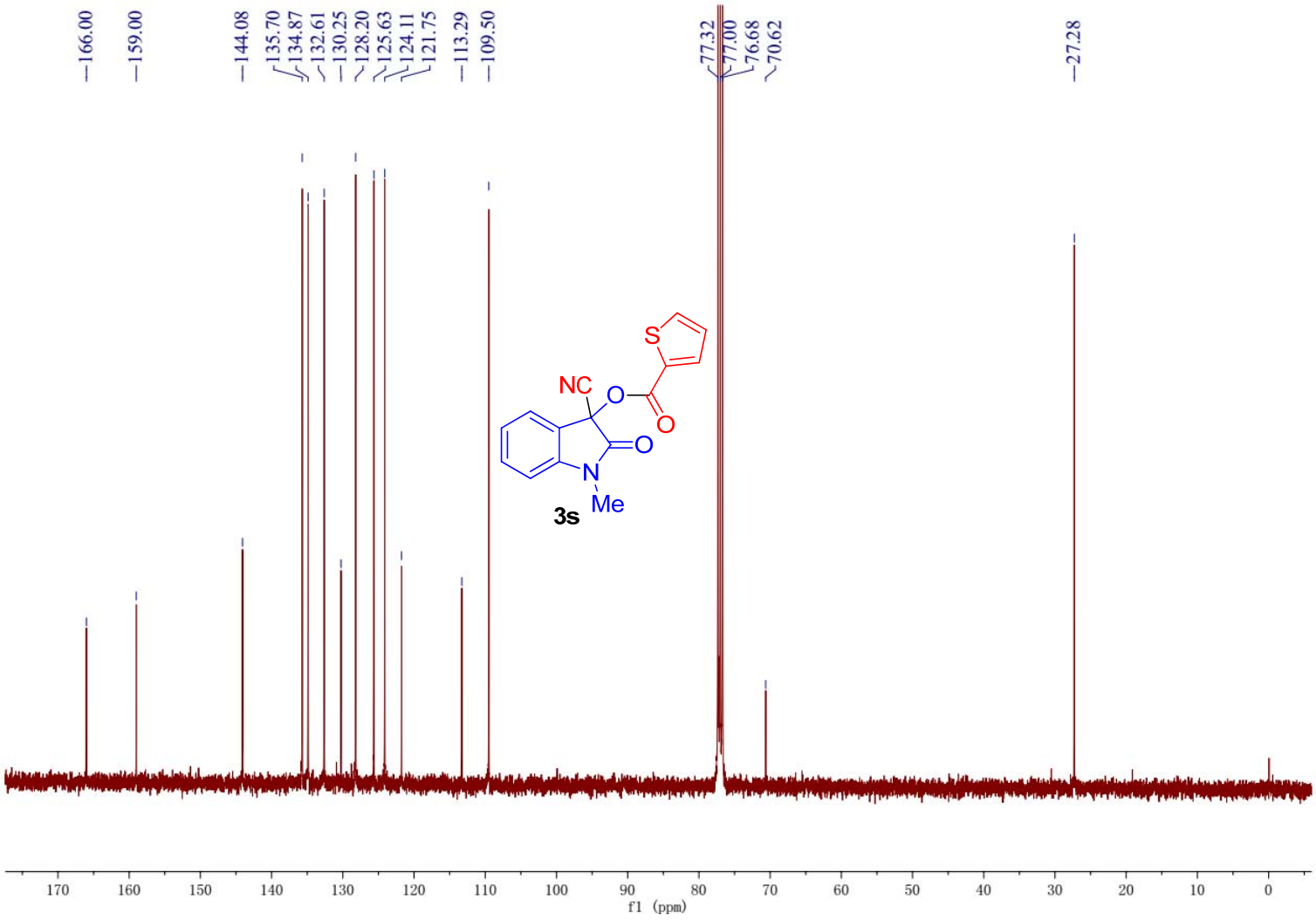

7.98
7.98
7.96
7.96
7.67
7.67
7.65
7.65
7.51
7.51
7.50
7.49
7.49
7.48
7.47
7.47
7.46
7.45
7.37
7.37
7.35
7.35
7.35
7.35
7.33
7.33
7.20
7.19
7.18
7.18
7.16
7.16
6.96
6.94
3.33
0.00
NC
O
O
Cl
O
N
Me
3q
0.94
0.94
2.88
0.98
0.97
0.94
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

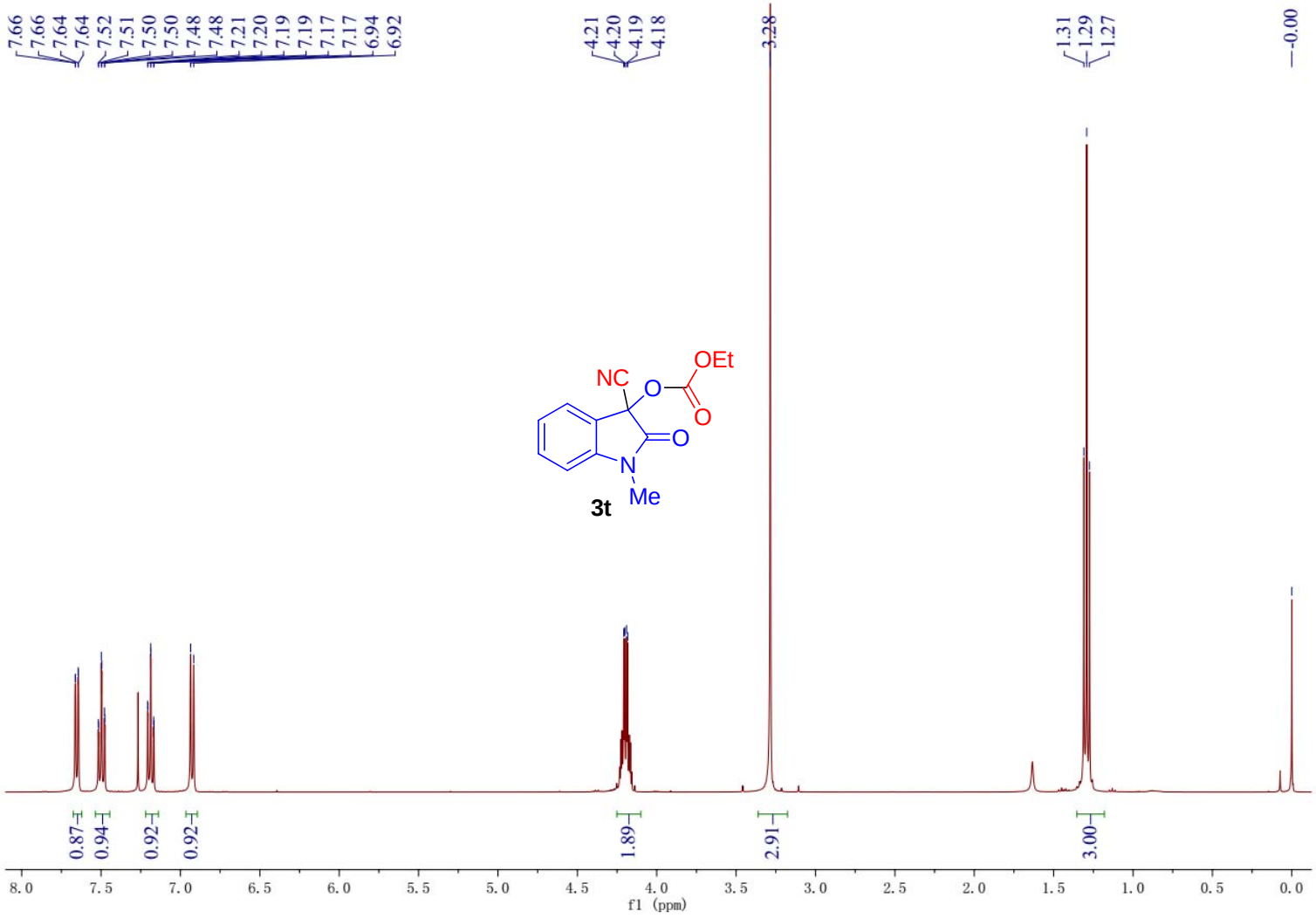

165.86
161.94
144.08
134.78
134.07
132.61
132.29
131.44
126.79
125.59
124.13
121.54
121.21
109.59
77.32
77.00
76.68
70.78
27.27
NC
O
O
Cl
O
N
Me
3q
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

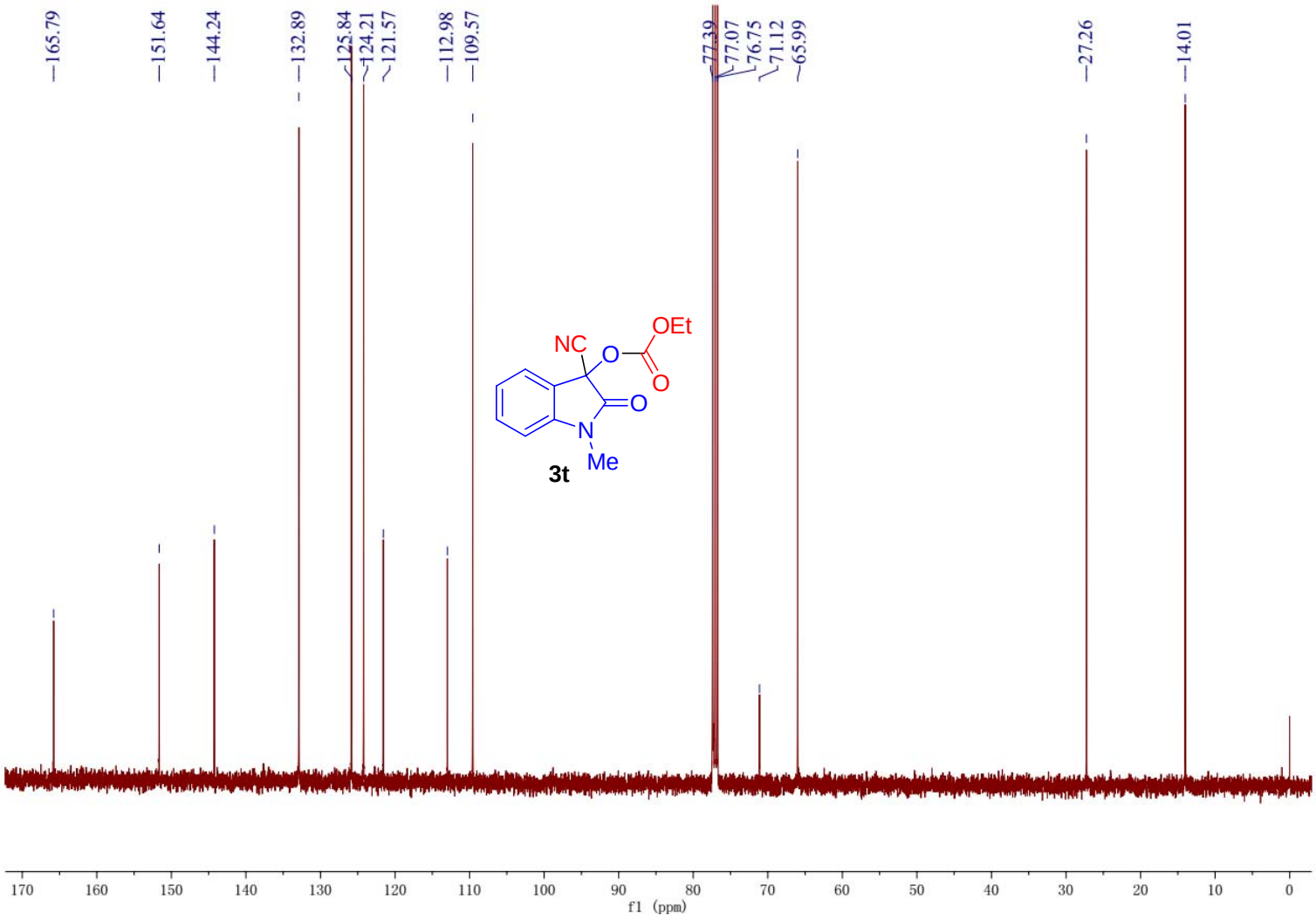

7.90
7.88
7.62
7.62
7.59
7.19
7.18
7.17
7.17
7.15
7.15
6.97
6.95
3.34
0.00
Br
NC
O
O
O
N
Me
3r
1.89
2.89
1.00
0.96
0.97
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

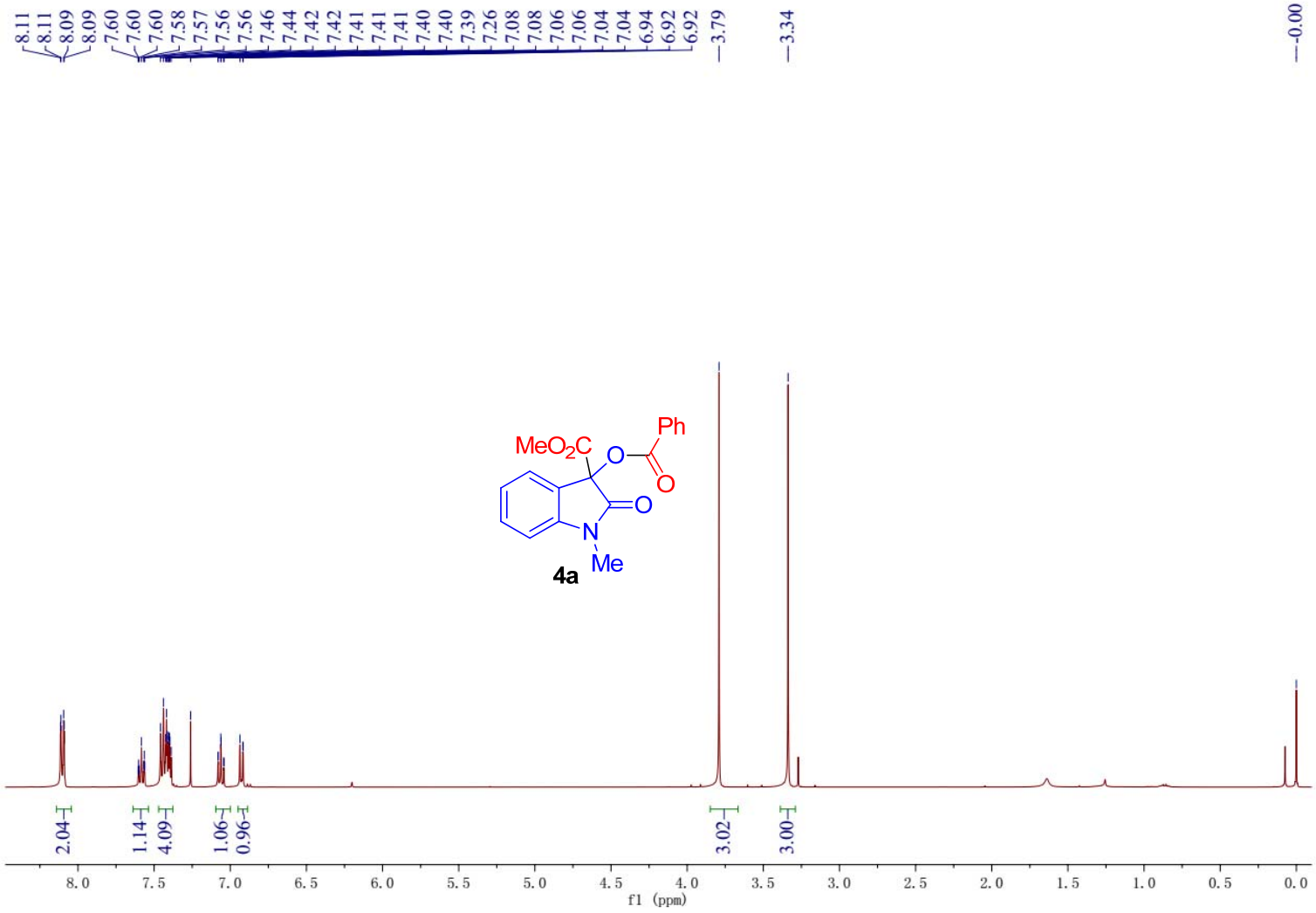

165.99
162.88
144.11
132.66
132.08
131.63
129.84
126.28
125.66
124.16
121.69
113.26
109.54
77.32
77.00
76.68
70.68
27.29
Br
NC
O
O
O
N
Me
3r
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

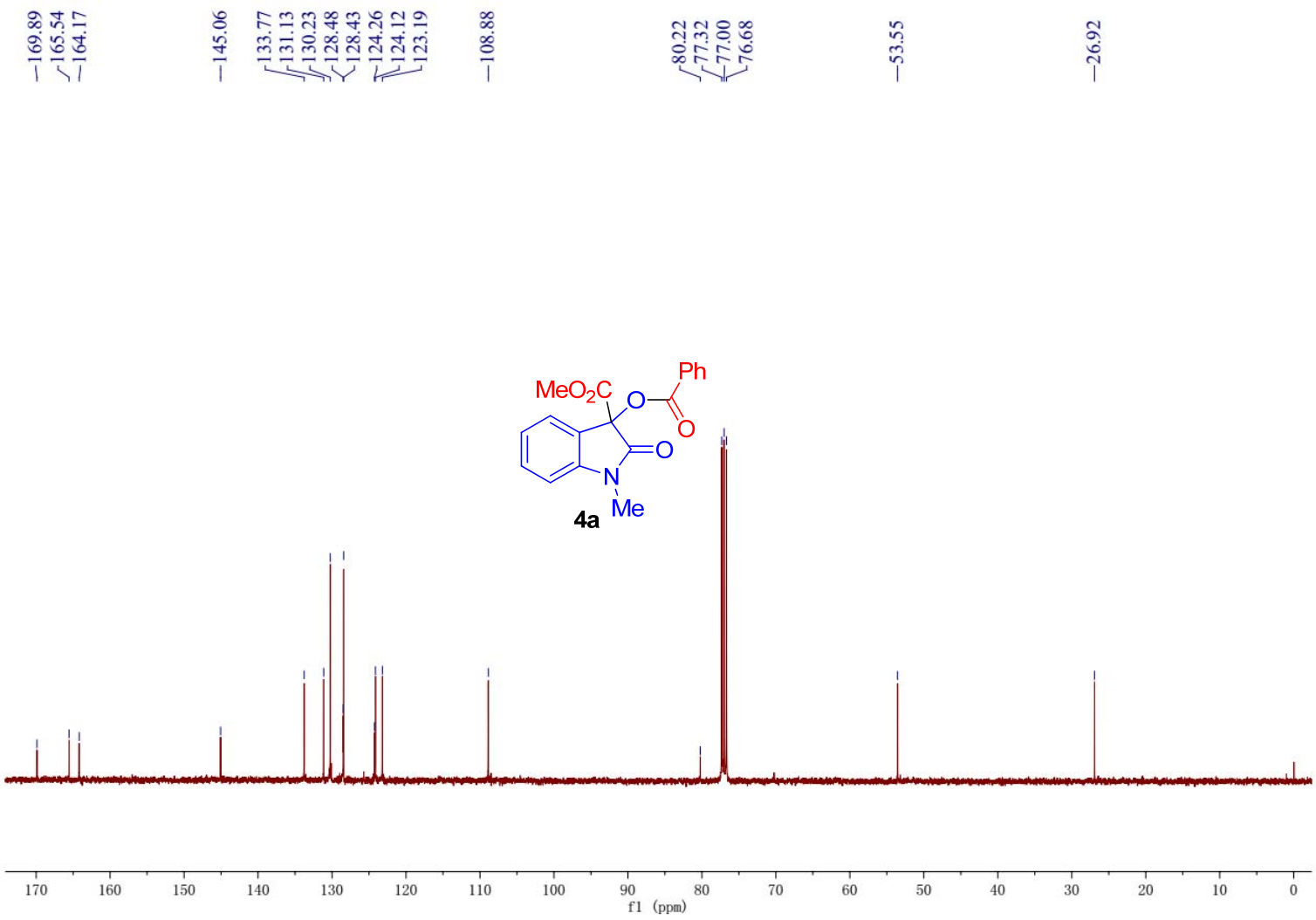

7.89
7.88
7.88
7.87
7.68
7.68
7.67
7.67
7.66
7.65
7.64
7.63
7.51
7.50
7.49
7.48
7.47
7.46
7.19
7.18
7.17
7.17
7.15
7.14
7.13
7.13
7.12
6.96
6.94
3.33
-0.00
S
NC
O
O
O
N
Me
3s
1.00
1.91
1.06
2.02
1.00
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

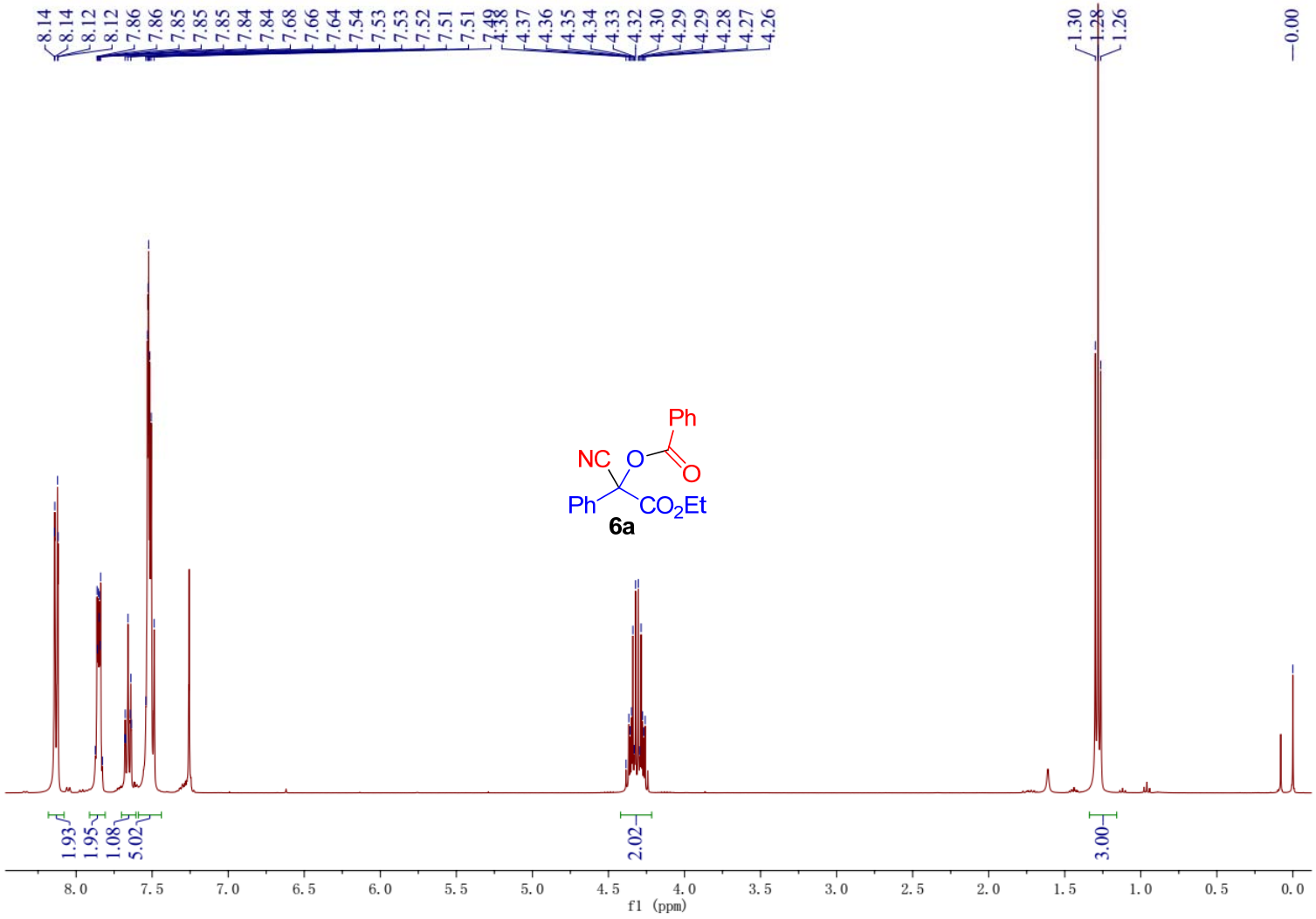

166.00
159.00
144.08
135.70
134.87
132.61
130.25
128.20
125.63
124.11
121.75
113.29
109.50
77.32
77.00
76.68
70.62
27.28
NC
O
O
O
S
N
Me
3s
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

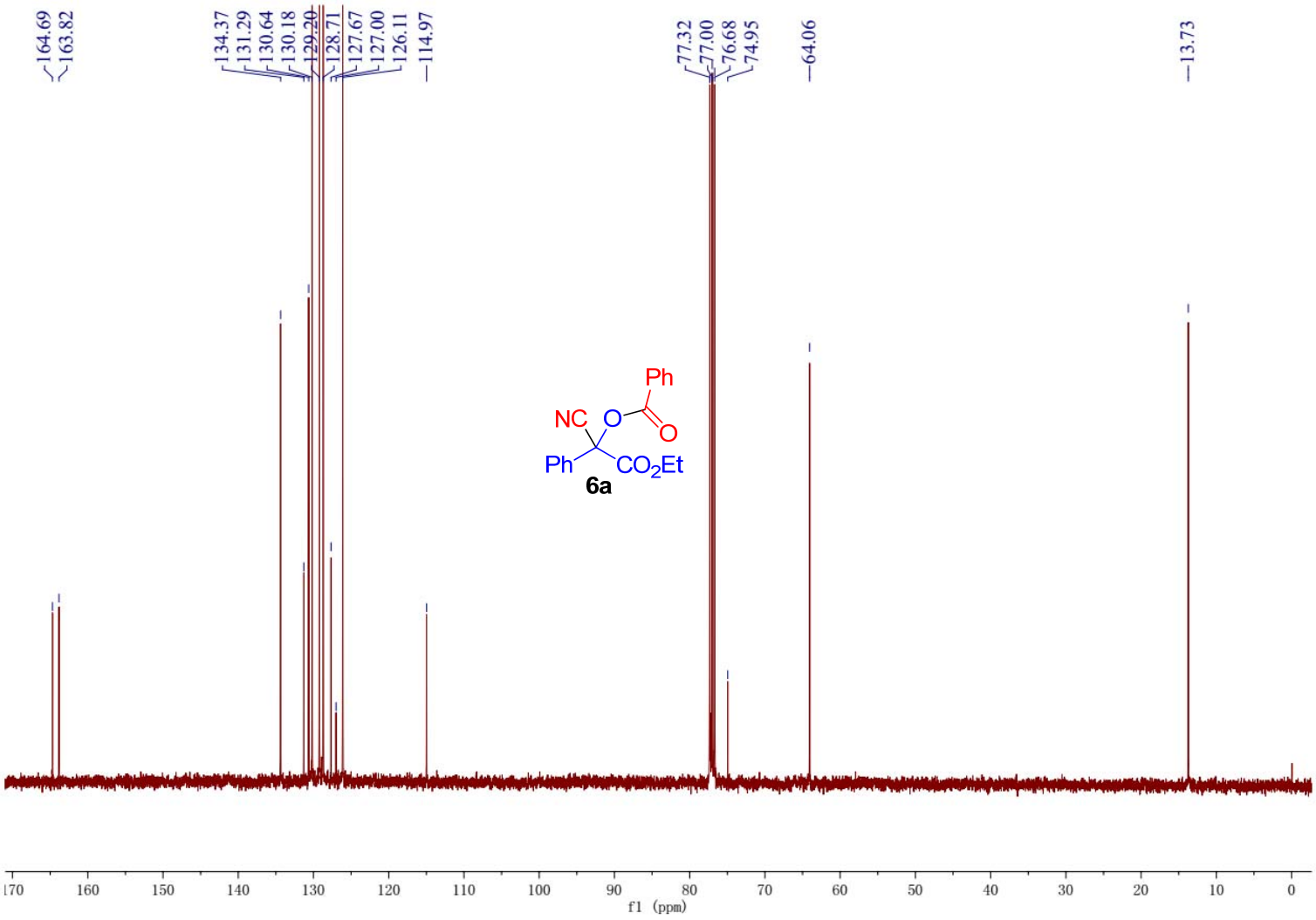

7.66
7.66
7.64
7.64
7.52
7.51
7.50
7.50
7.48
7.48
7.21
7.20
7.19
7.19
7.17
7.17
6.94
6.92
4.21
4.20
4.19
4.18
3.28
1.31
1.29
1.27
0.00
NC
O
OEt
O
O
N
Me
3t
0.87
0.94
0.92
0.92
1.89
2.91
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

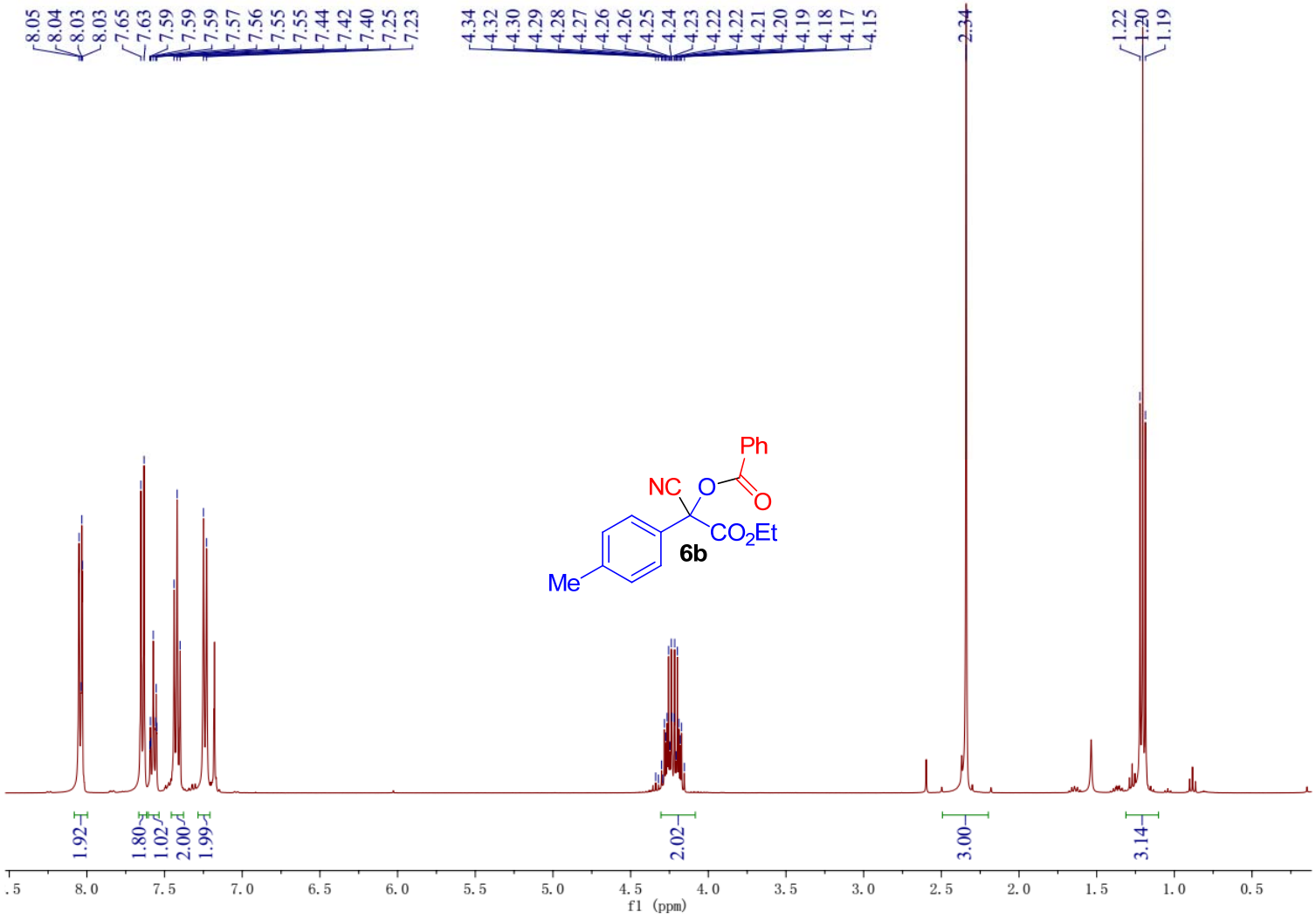

165.79
151.64
144.24
132.89
125.84
124.21
121.57
112.98
109.57
77.39
77.07
76.75
71.12
65.99
27.26
14.01
NC
O
OEt
O
O
N
Me
3t
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

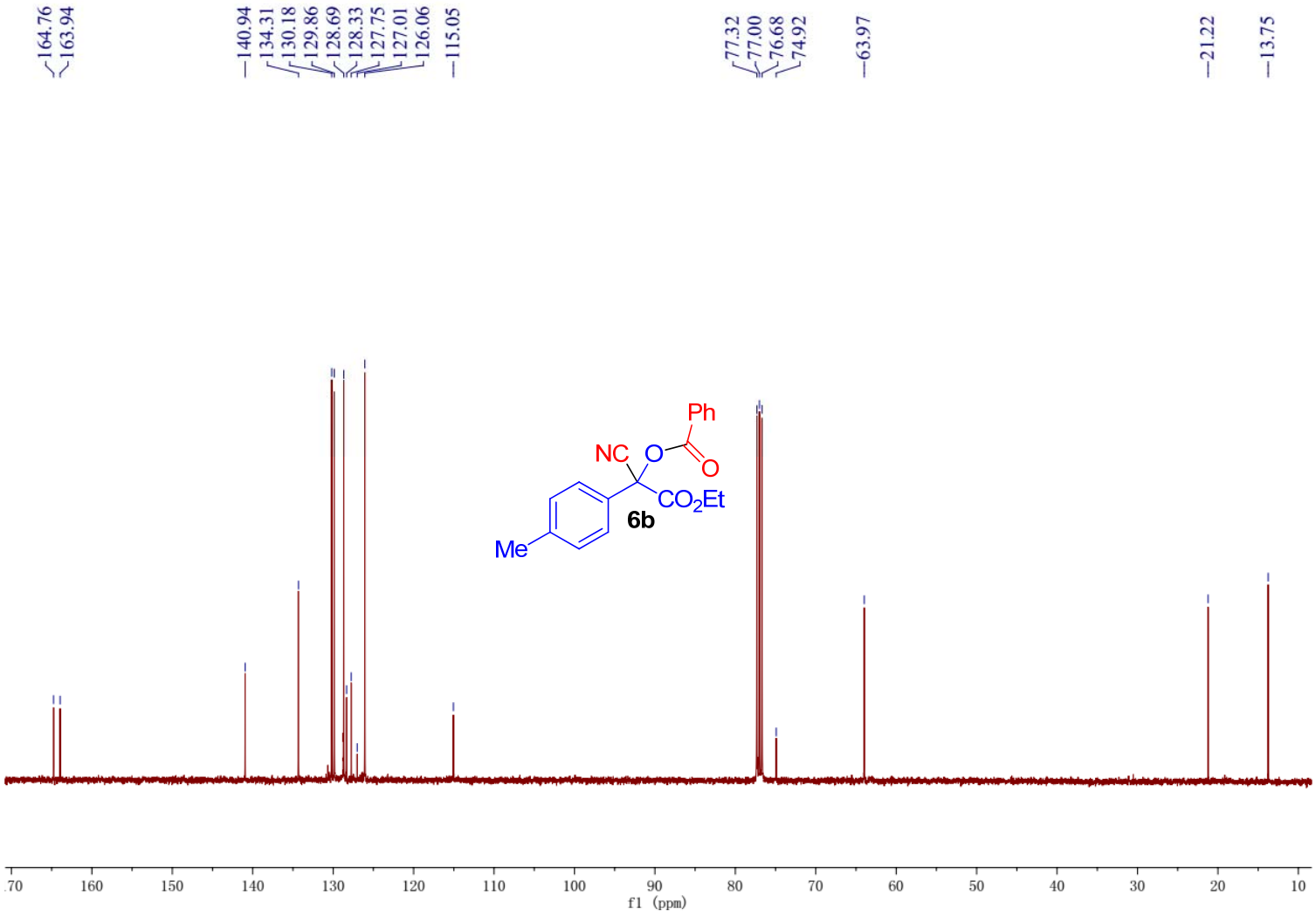

8.11
8.11
8.09
8.09
7.60
7.60
7.60
7.58
7.57
7.56
7.56
7.46
7.44
7.42
7.42
7.41
7.41
7.41
7.40
7.40
7.39
7.26
7.08
7.08
7.06
7.06
7.04
7.04
6.94
6.92
6.92
3.79
3.34
0.00
MeO2C
O
Ph
O
O
N
Me
4a
2.04
1.14
4.09
1.06
0.96
3.02
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

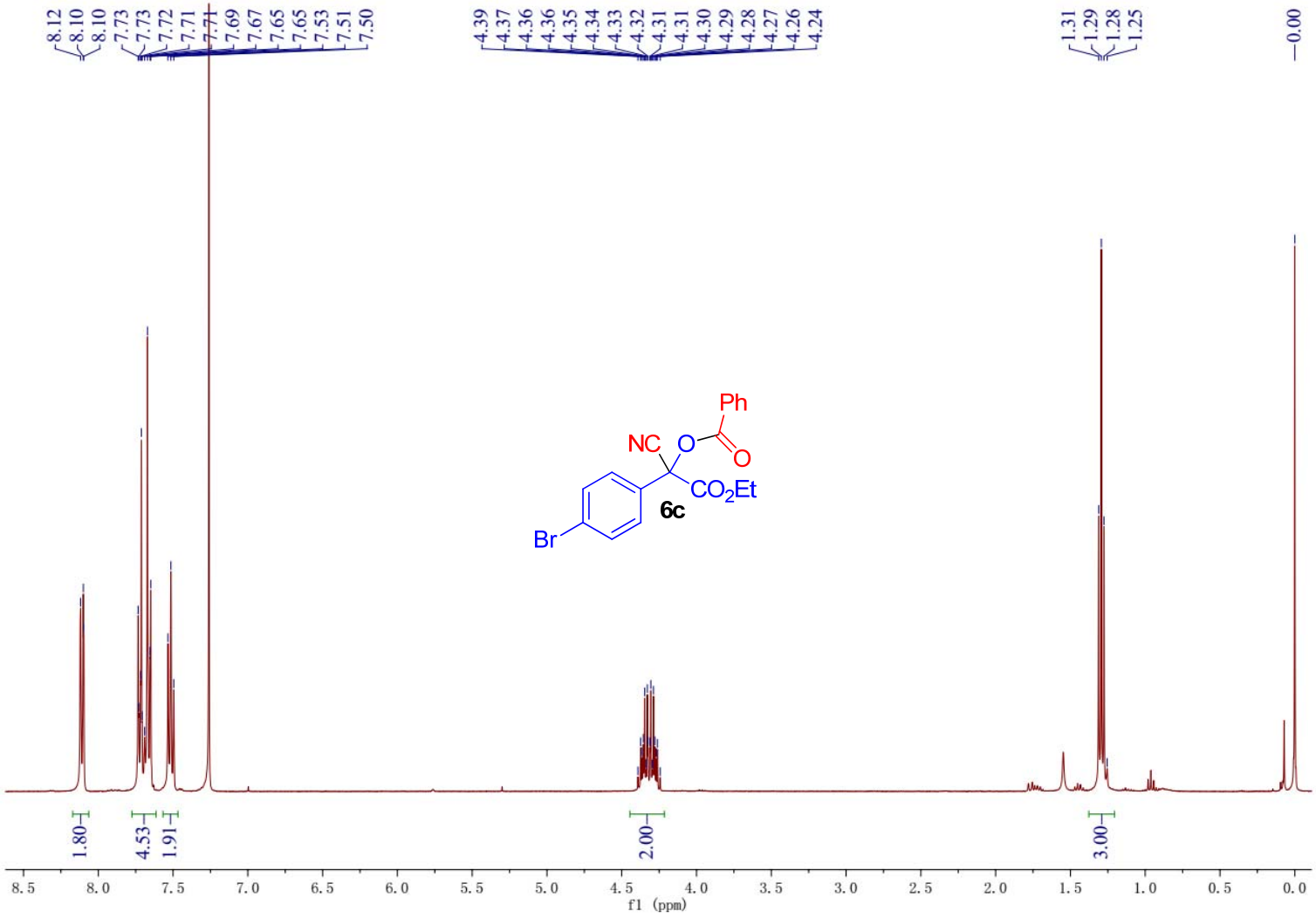

169.89
165.54
164.17
145.06
133.77
131.13
130.23
128.48
128.43
124.26
124.12
123.19
108.88
80.22
77.32
77.00
76.68
53.55
26.92
MeO2C
O
Ph
O
O
N
Me
4a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

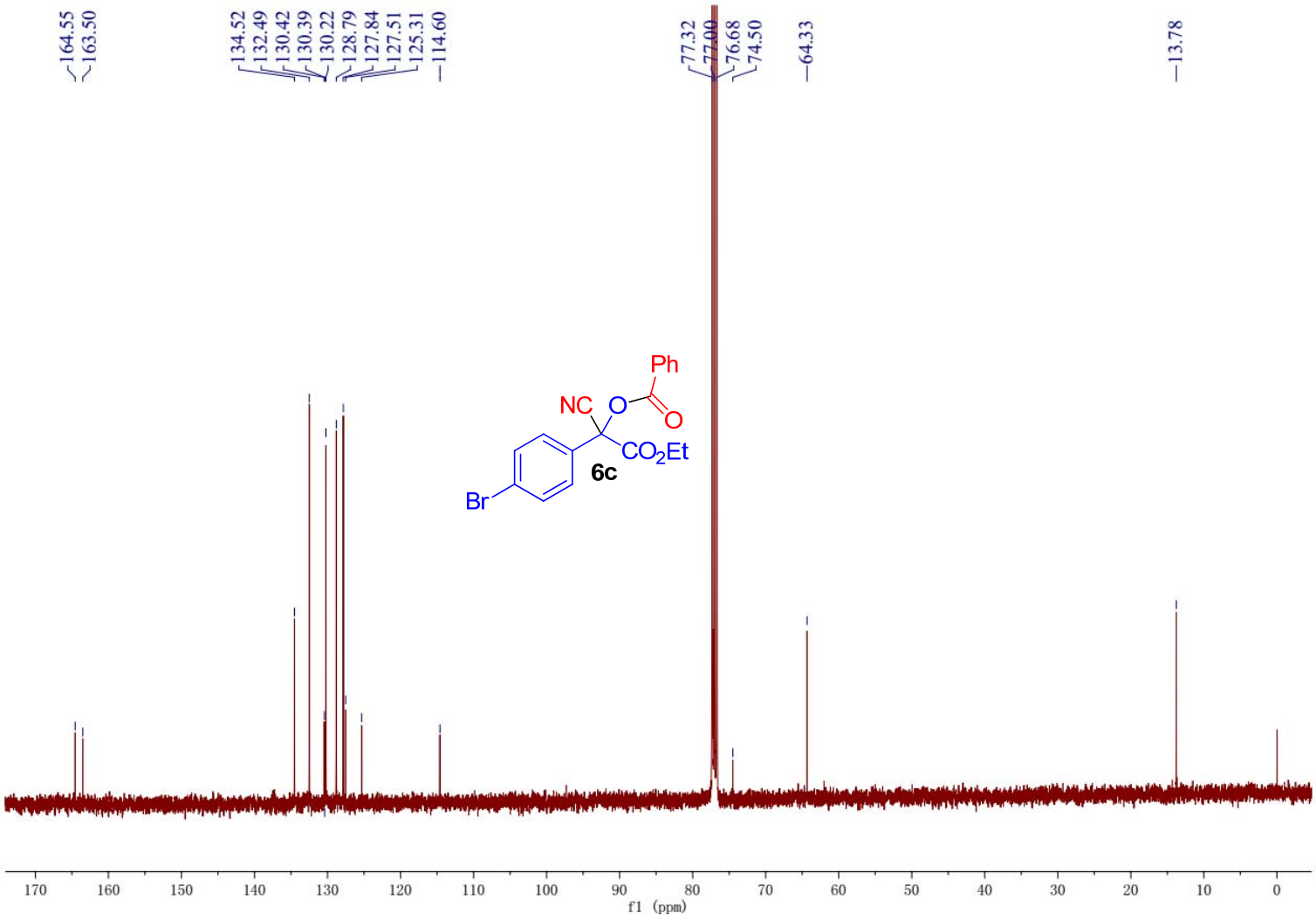

8.14
8.14
8.12
8.12
7.86
7.86
7.85
7.85
7.85
7.84
7.84
7.68
7.66
7.64
7.54
7.53
7.53
7.52
7.51
7.51
7.49
4.38
4.37
4.36
4.35
4.34
4.33
4.32
4.30
4.29
4.29
4.28
4.27
4.26
1.30
1.28
1.26
0.00
Ph
NC
O
O
Ph
CO2Et
6a
1.93
1.95
1.08
5.02
2.02
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

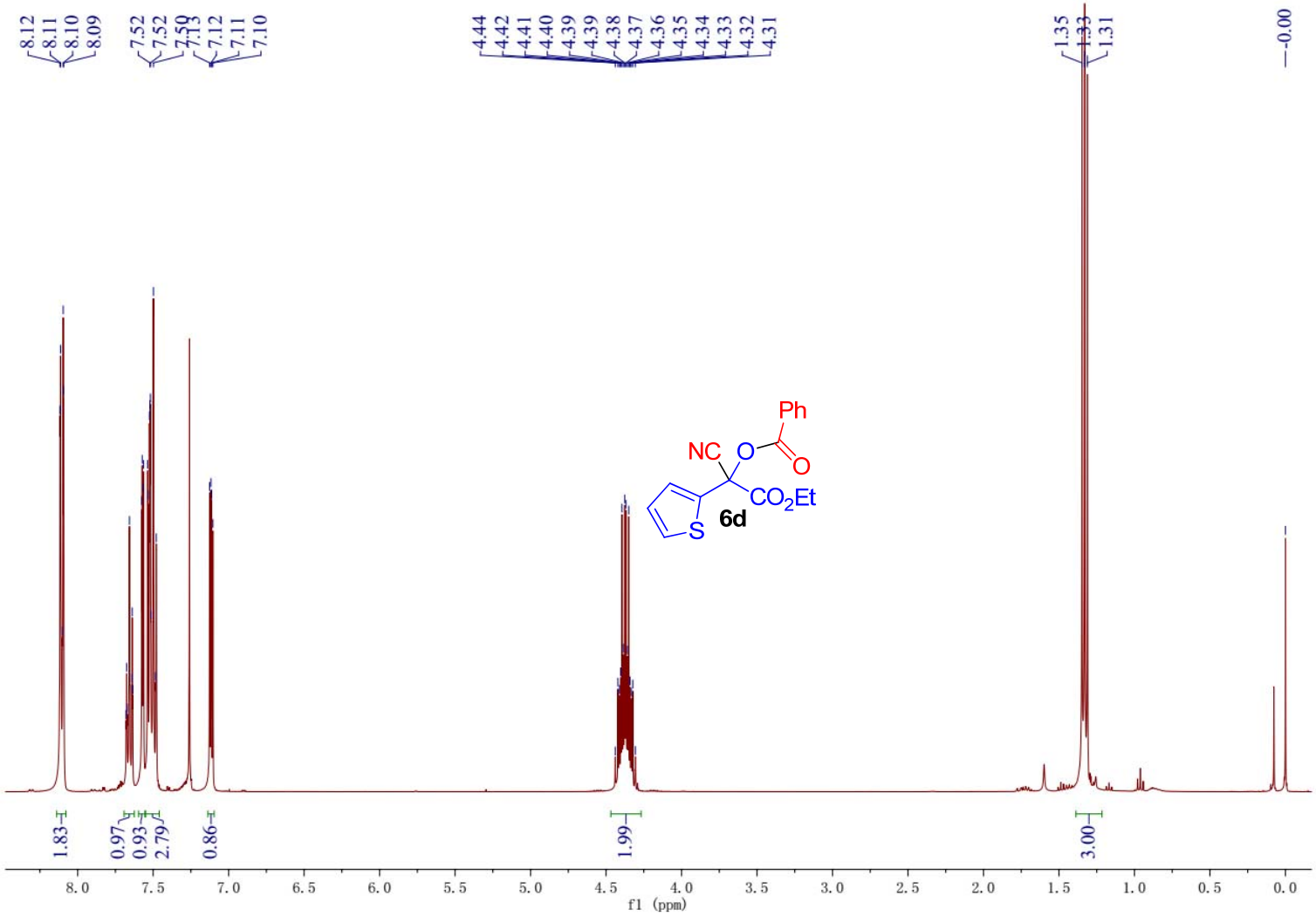

164.69
163.82
134.37
131.29
130.64
130.18
129.20
128.71
127.67
127.00
126.11
114.97
77.32
77.00
76.68
74.95
64.06
13.73
Ph
NC
O
O
Ph
CO2Et
6a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

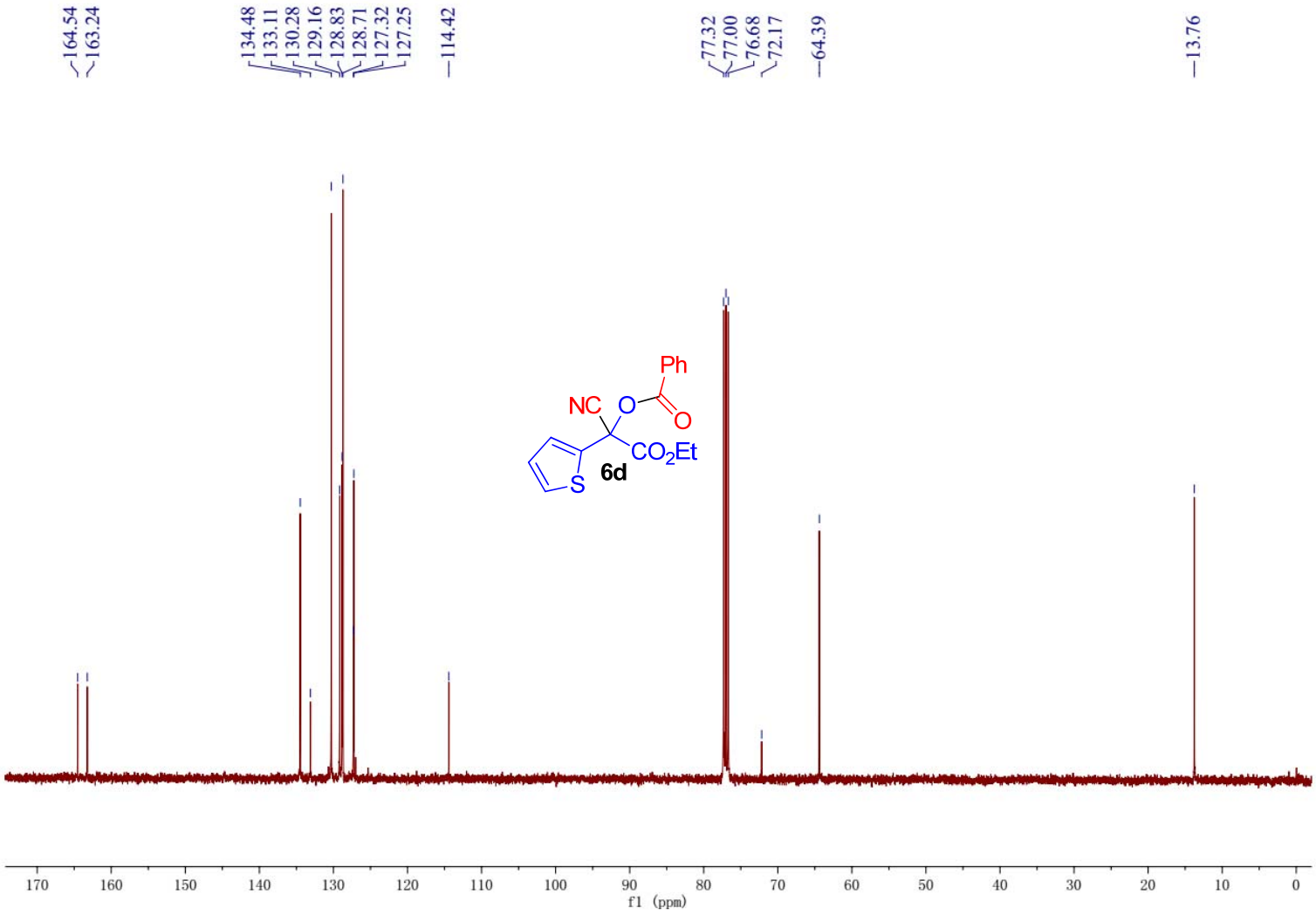

8.05
8.04
8.03
8.03
7.65
7.63
7.59
7.59
7.59
7.57
7.56
7.55
7.55
7.44
7.42
7.40
7.25
7.23
4.34
4.32
4.30
4.29
4.28
4.27
4.26
4.26
4.25
4.24
4.23
4.22
4.22
4.21
4.20
4.19
4.18
4.17
4.15
2.34
1.22
1.20
1.19
Ph
NC
O
O
CO2Et
6b
Me
1.92
1.80
1.02
2.00
1.99
2.02
3.00
3.14
f1 (ppm)

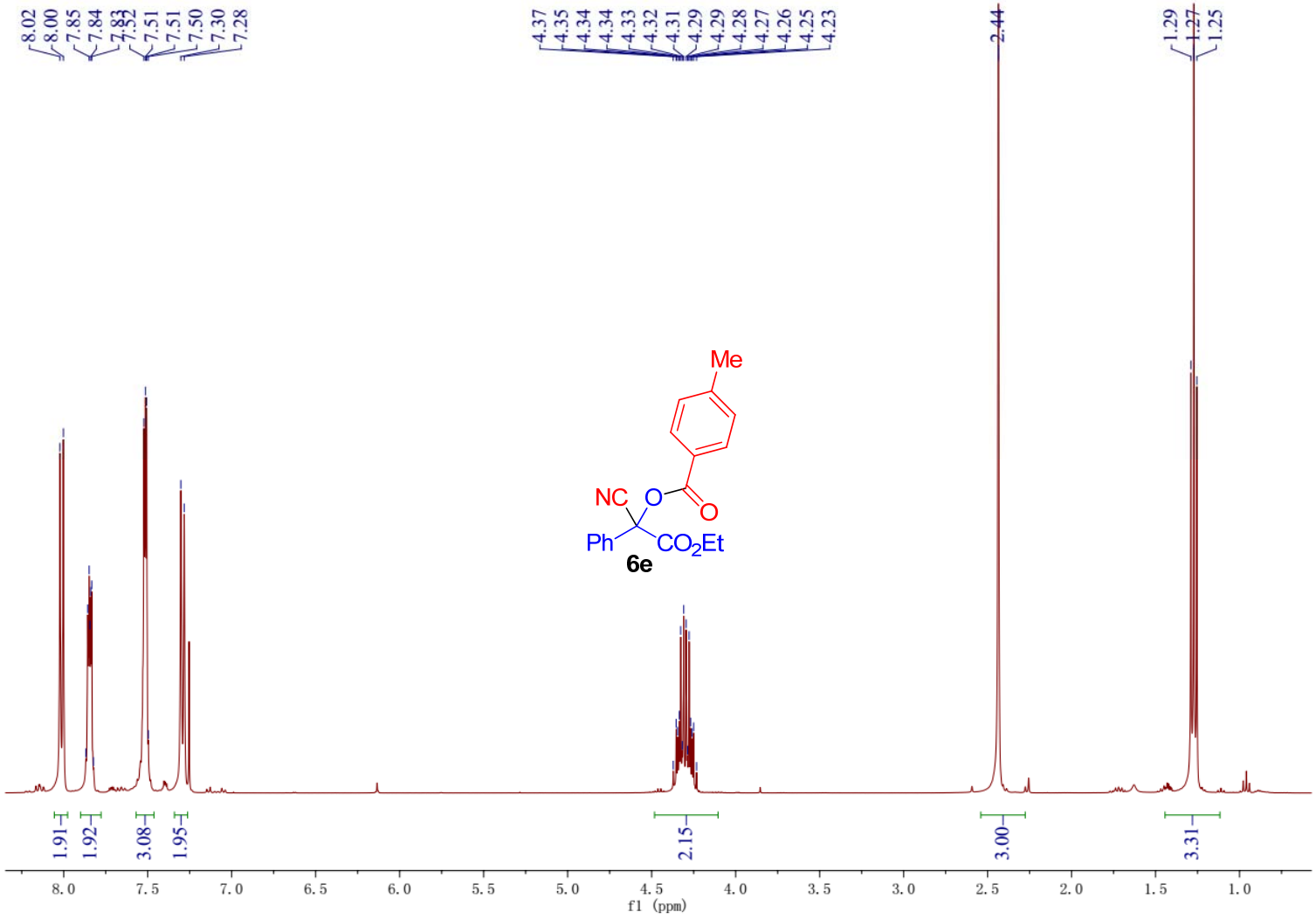

164.76
163.94
140.94
134.31
130.18
129.86
128.69
128.33
127.75
127.01
126.06
115.05
77.32
77.00
76.68
74.92
63.97
21.22
13.75
Ph
NC
O
O
CO2Et
6b
Me
f1 (ppm)

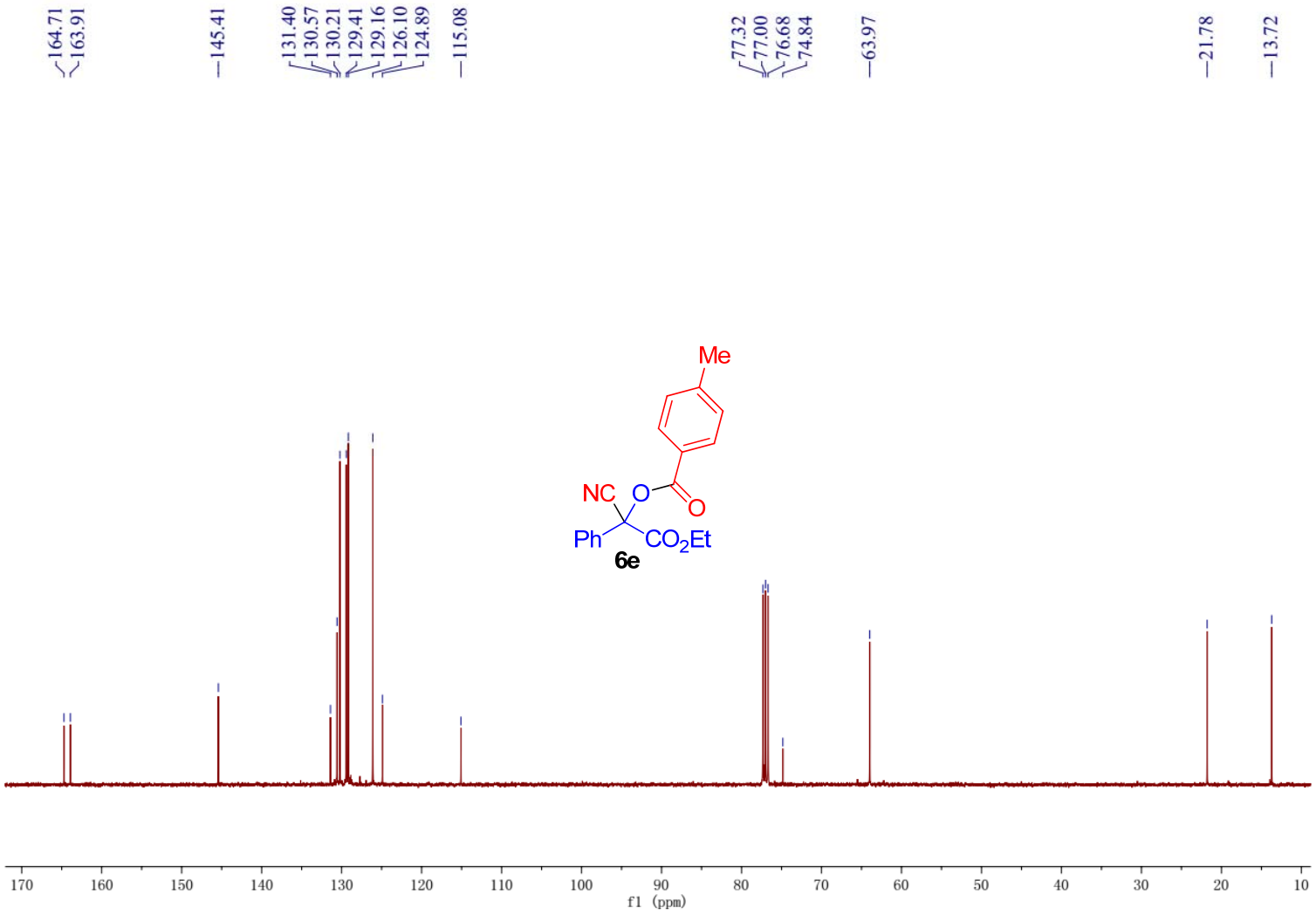

8.12
8.10
8.10
7.73
7.73
7.72
7.71
7.71
7.69
7.67
7.65
7.65
7.53
7.51
7.50
4.39
4.37
4.36
4.36
4.35
4.34
4.33
4.32
4.31
4.31
4.30
4.29
4.28
4.27
4.26
4.24
1.31
1.29
1.28
1.25
0.00
Ph
NC
O
O
CO2Et
6c
Br
1.80
4.53
1.91
2.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

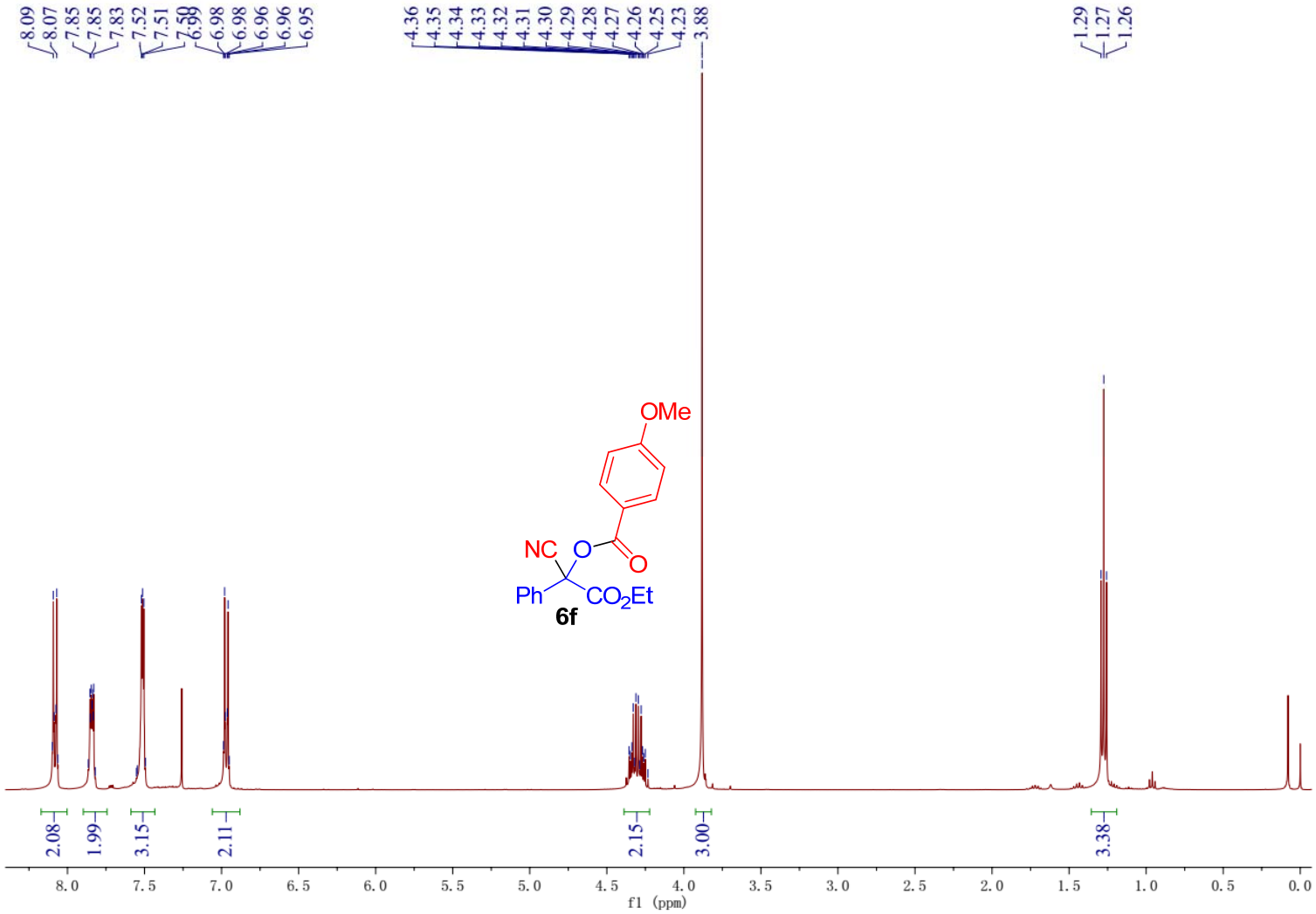

164.55
163.50
134.52
132.49
130.42
130.39
130.22
128.79
127.84
127.51
125.31
114.60
77.32
77.00
76.68
74.50
64.33
13.78
Ph
NC
O
O
CO2Et
6c
Br
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

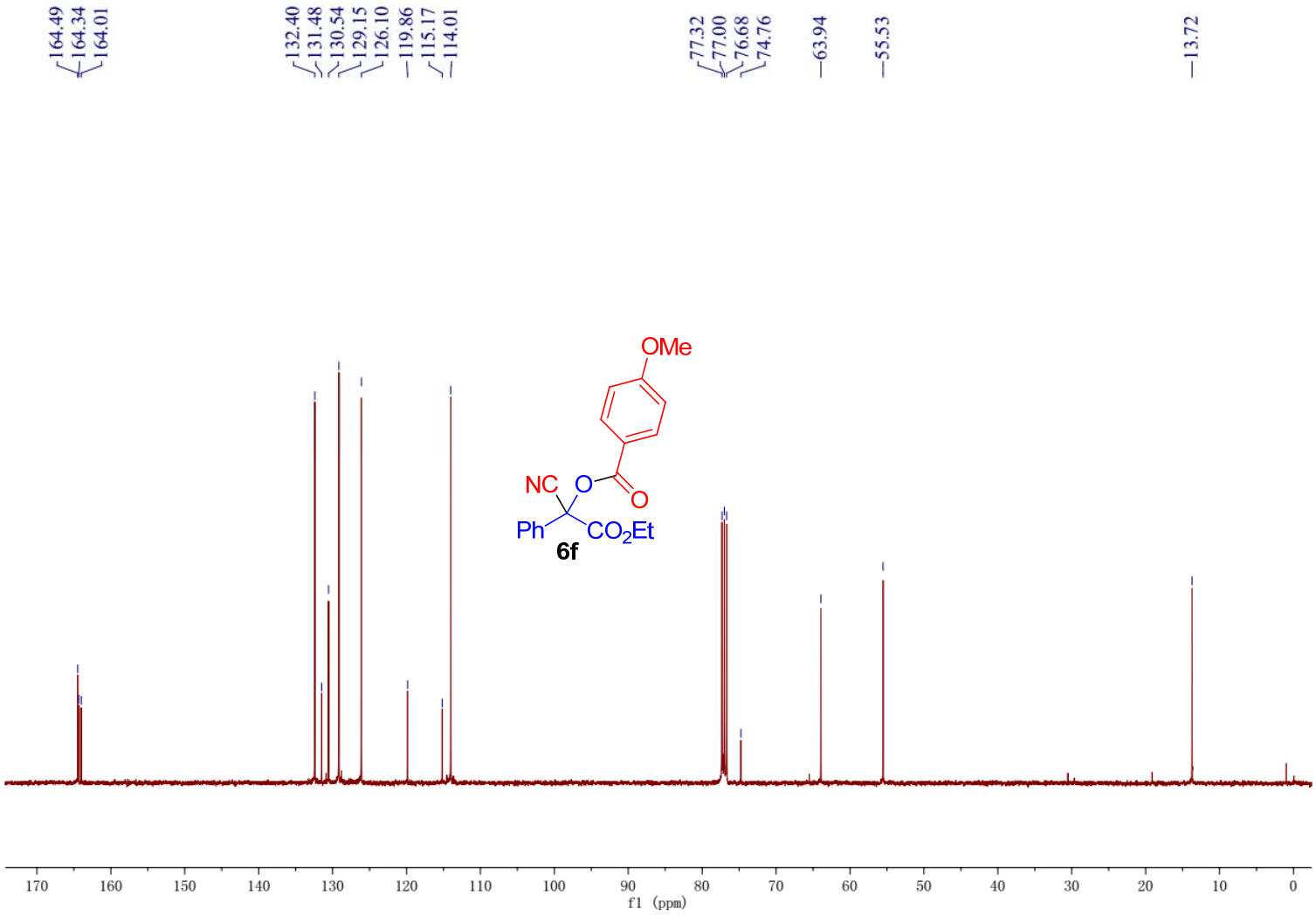

8.12
8.11
8.10
8.09
7.52
7.52
7.50
7.13
7.12
7.11
7.10
4.44
4.42
4.41
4.40
4.39
4.39
4.38
4.37
4.36
4.35
4.34
4.33
4.32
4.31
1.35
1.33
1.31
0.00
Ph
NC
O
O
CO2Et
S
6d
1.83
0.97
0.93
2.79
0.86
1.99
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

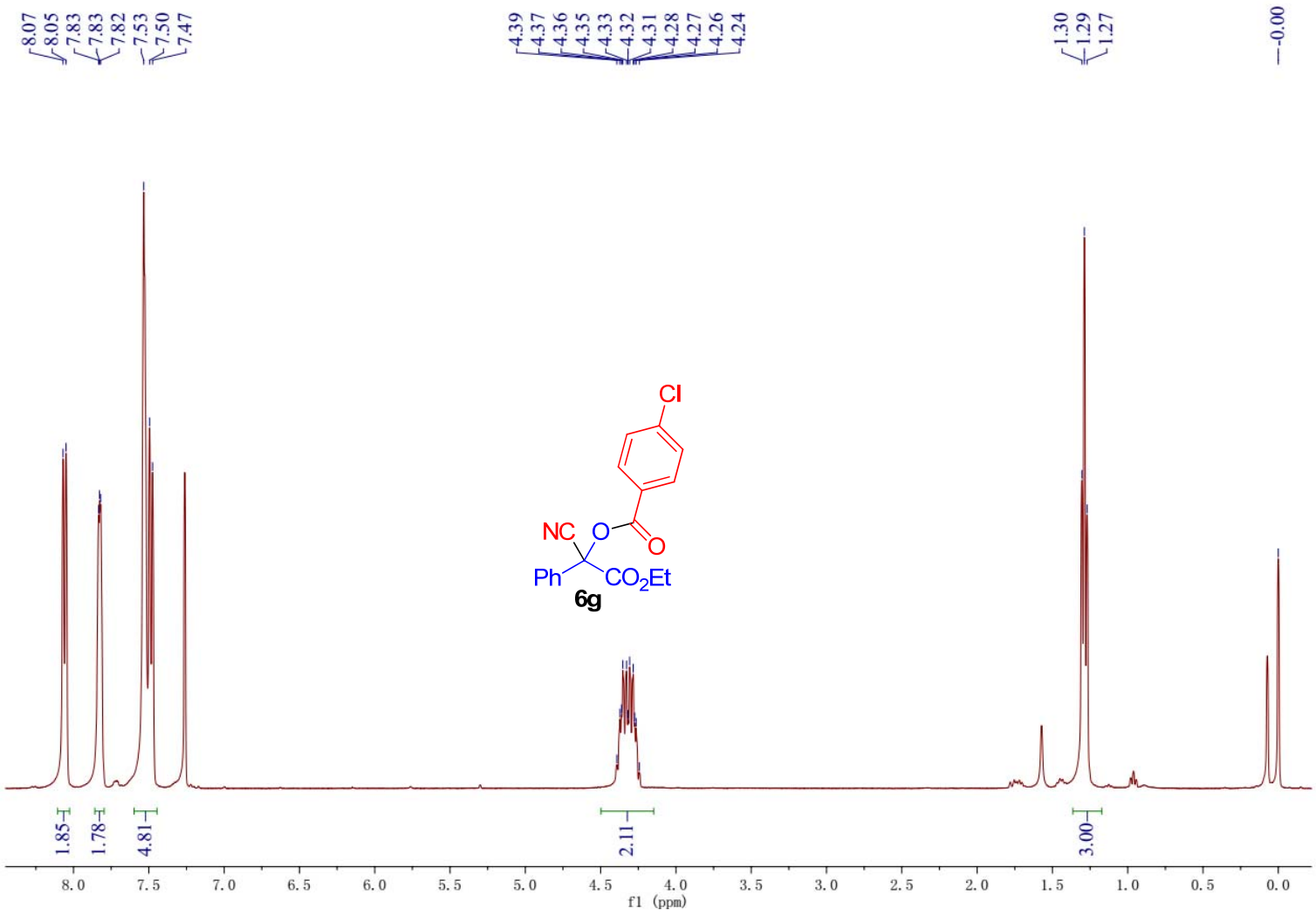

164.54
163.24
134.48
133.11
130.28
129.16
128.83
128.71
127.32
127.25
114.42
77.32
77.00
76.68
72.17
64.39
13.76
Ph
NC
O
O
CO2Et
S
6d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

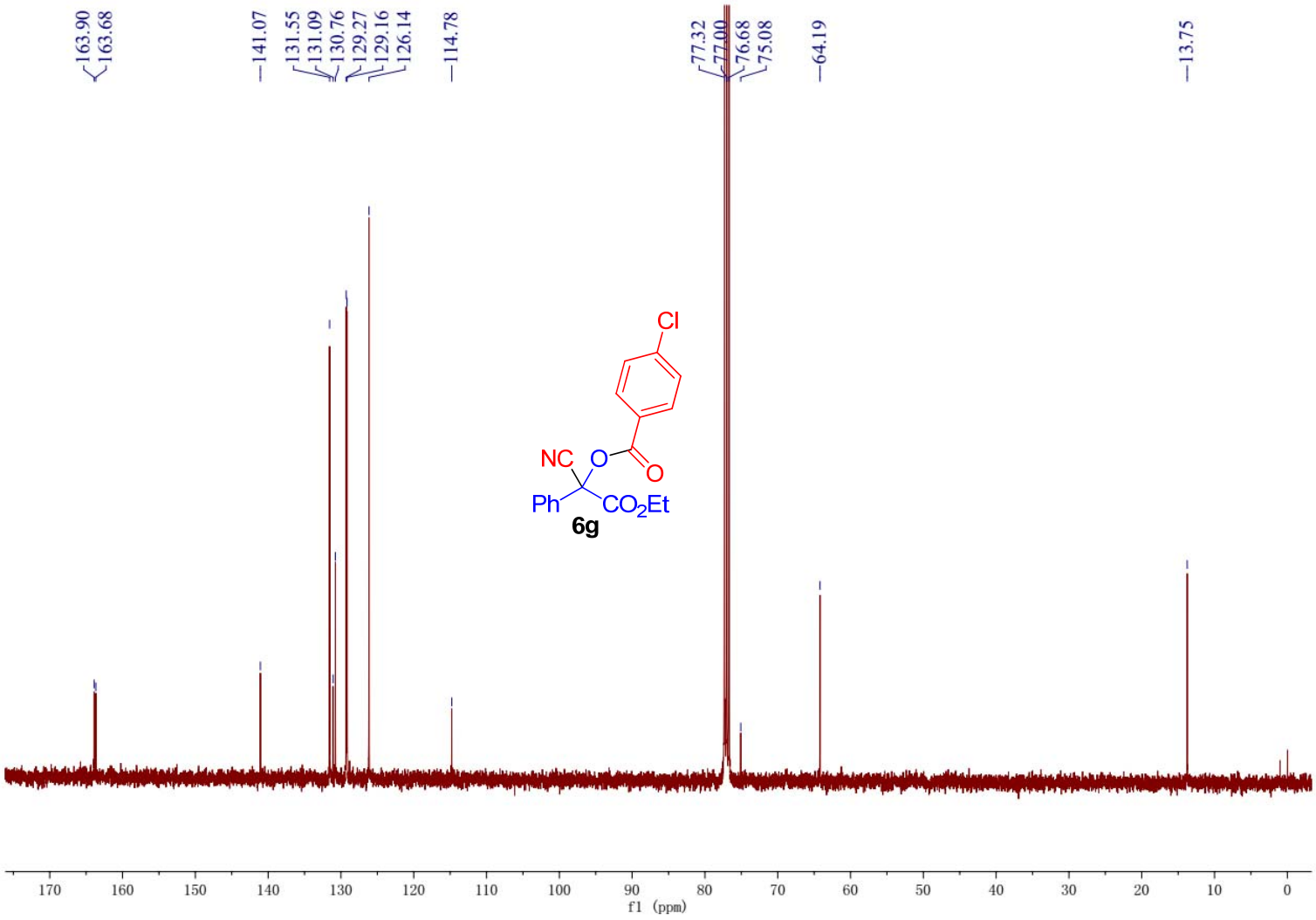

8.02
8.00
7.85
7.84
7.83
7.52
7.51
7.51
7.50
7.30
7.28
4.37
4.35
4.34
4.34
4.33
4.32
4.31
4.29
4.29
4.28
4.27
4.26
4.25
4.23
2.44
1.29
1.27
1.25
Me
NC
O
O
Ph
CO2Et
6e
1.91
1.92
3.08
1.95
2.15
3.00
3.31
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

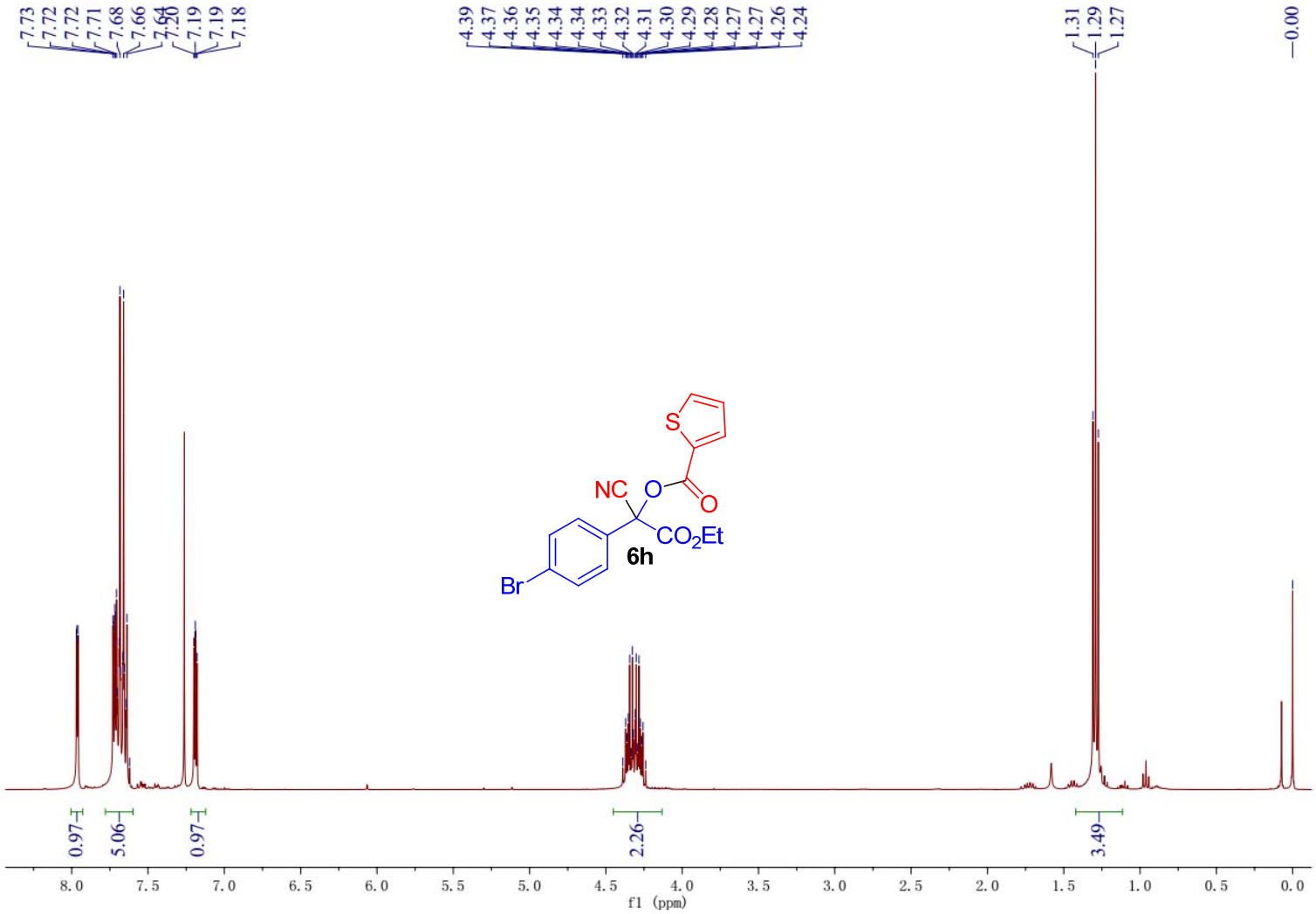

164.71
163.91
145.41
131.40
130.57
130.21
129.41
129.16
126.10
124.89
115.08
77.32
77.00
76.68
74.84
63.97
21.78
13.72
Me
NC
O
O
Ph
CO2Et
6e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

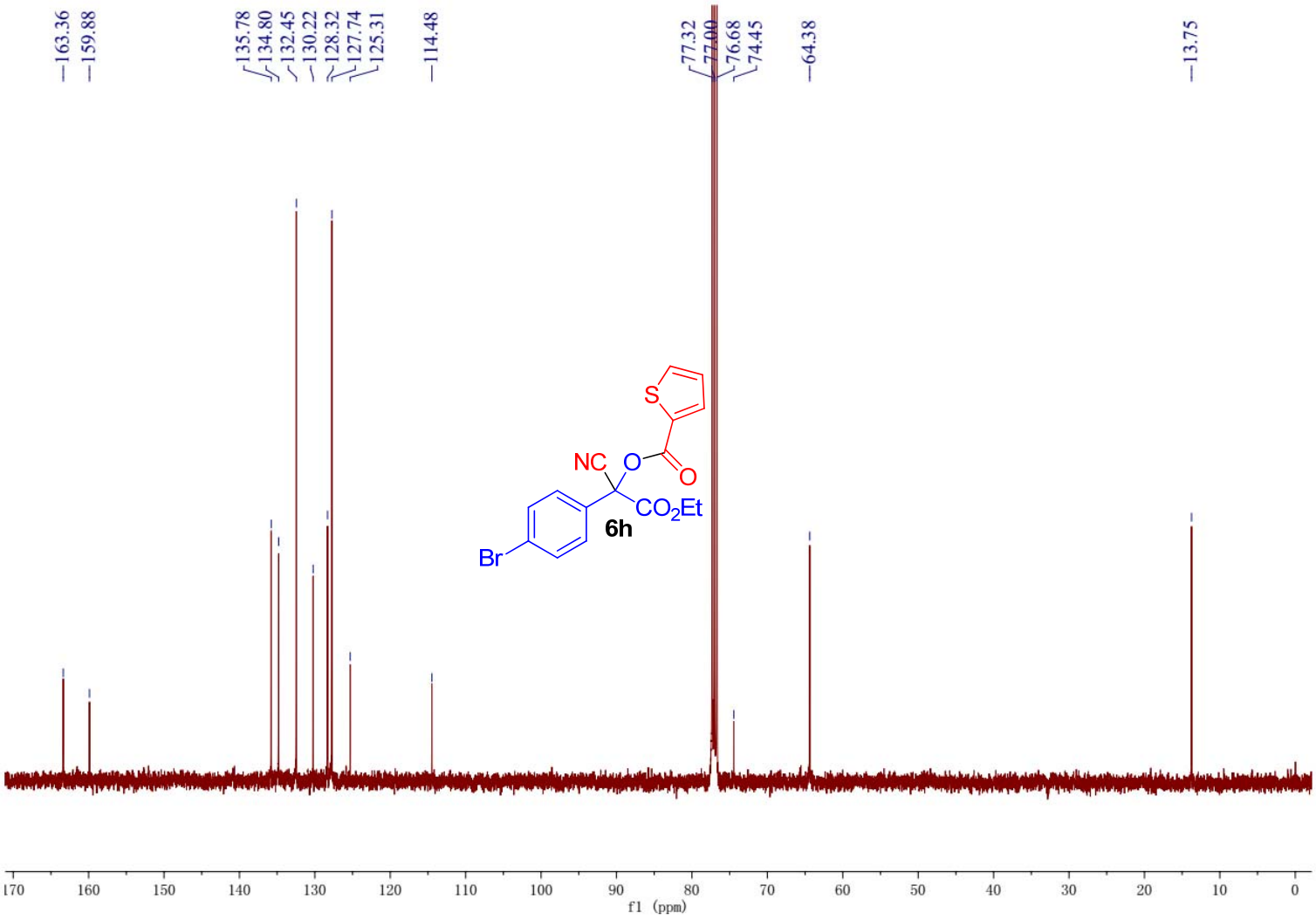

8.09
8.07
7.85
7.85
7.83
7.52
7.51
6.98
6.98
6.96
6.96
6.95
4.36
4.35
4.34
4.33
4.32
4.31
4.30
4.29
4.28
4.27
4.26
4.25
4.23
3.88
1.29
1.27
1.26
OMe
NC
O
O
Ph
CO2Et
6f
2.08
1.99
3.15
2.11
2.15
3.00
3.38
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

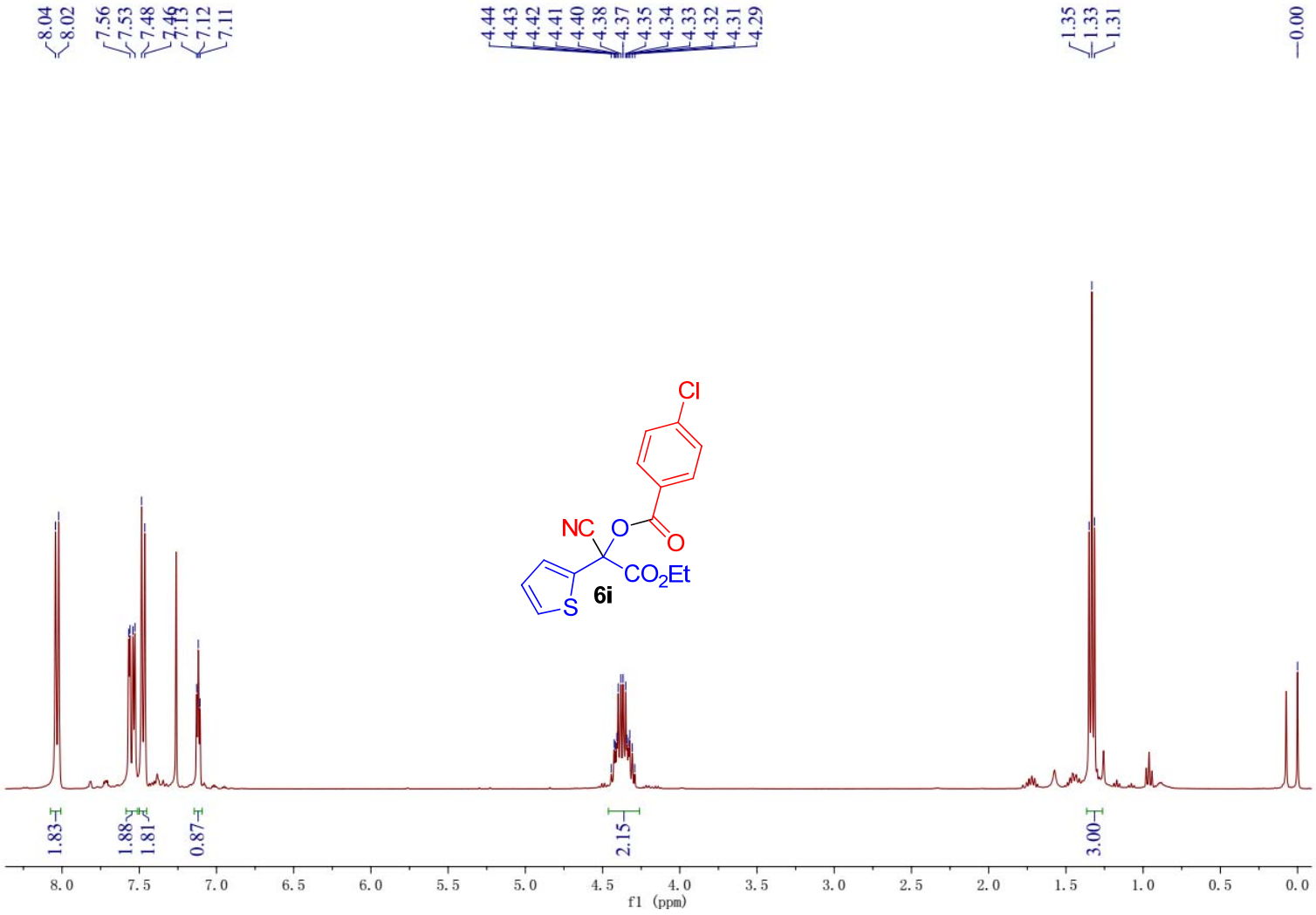

164.49
164.34
164.01
132.40
131.48
130.54
129.15
126.10
119.86
115.17
114.01
77.32
77.00
76.68
74.76
63.94
55.53
13.72
OMe
NC
O
O
Ph
CO2Et
6f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

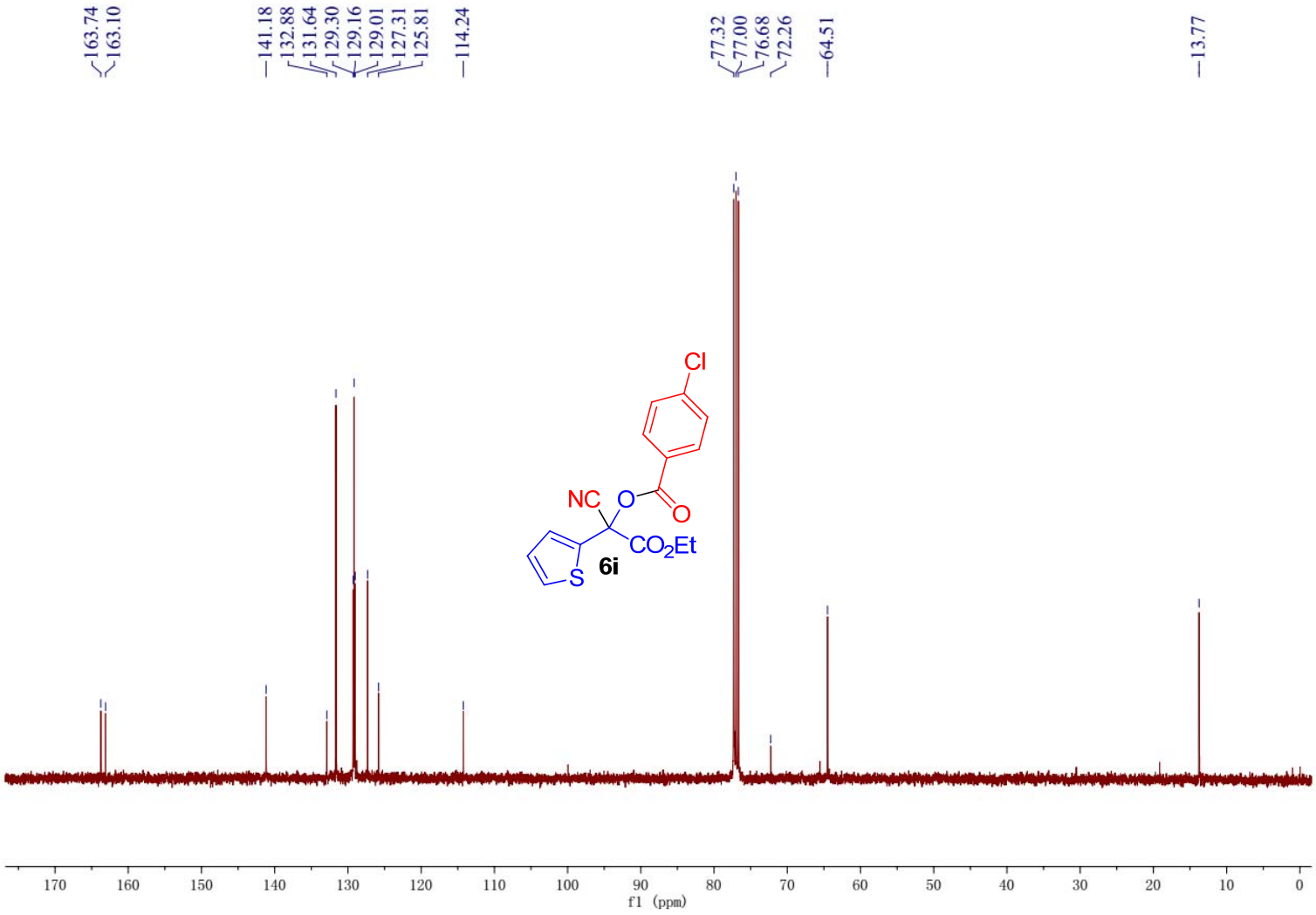

8.07
8.05
7.83
7.83
7.82
7.53
7.50
7.47
4.39
4.37
4.36
4.35
4.33
4.32
4.31
4.28
4.27
4.26
4.24
1.30
1.29
1.27
0.00
Cl
NC
O
O
Ph
CO2Et
6g
1.85
1.78
4.81
2.11
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

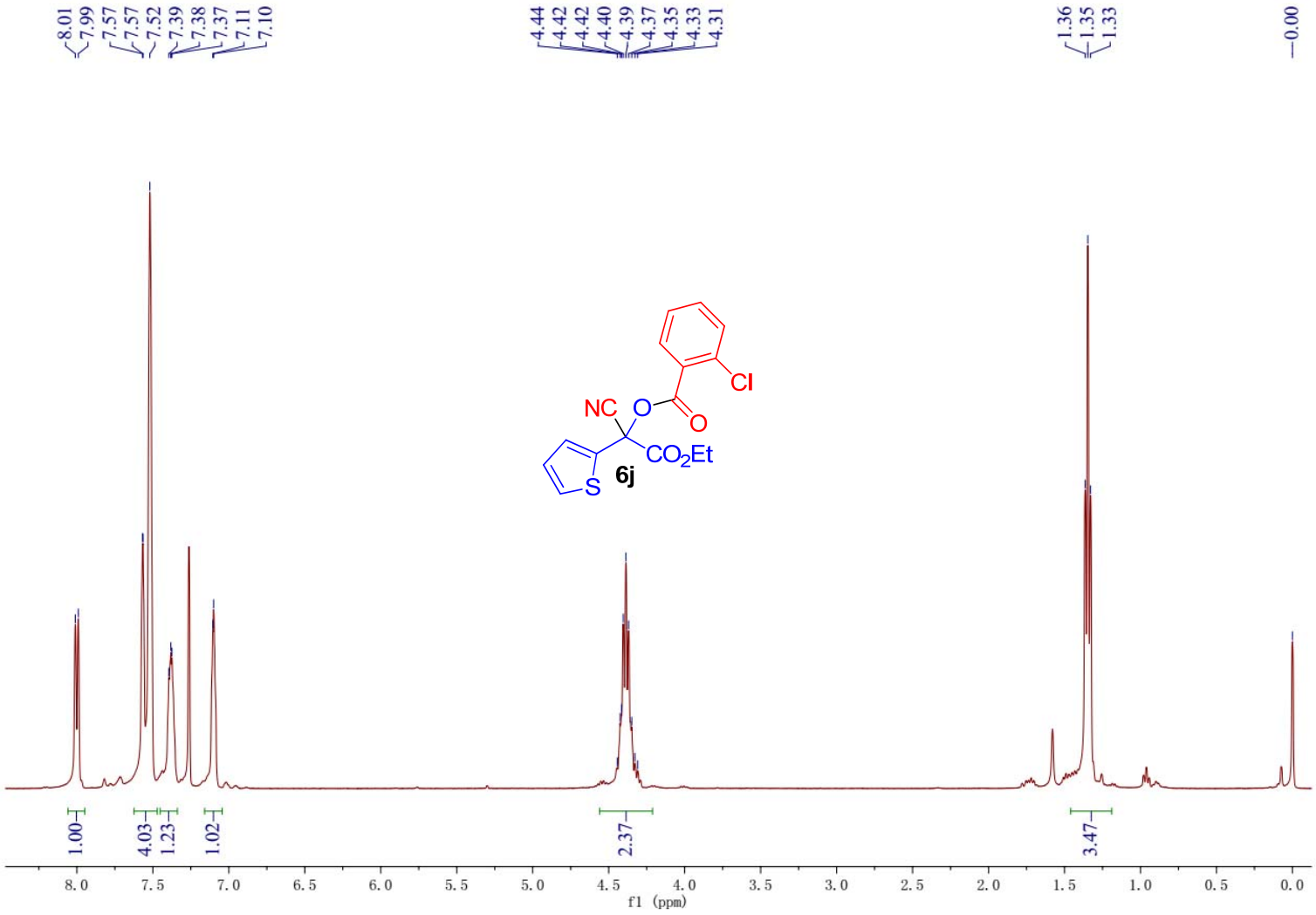

163.90
163.68
141.07
131.55
131.09
130.76
129.27
129.16
126.14
114.78
77.32
77.00
76.68
75.08
64.19
13.75
Cl
NC
O
O
Ph
CO2Et
6g
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

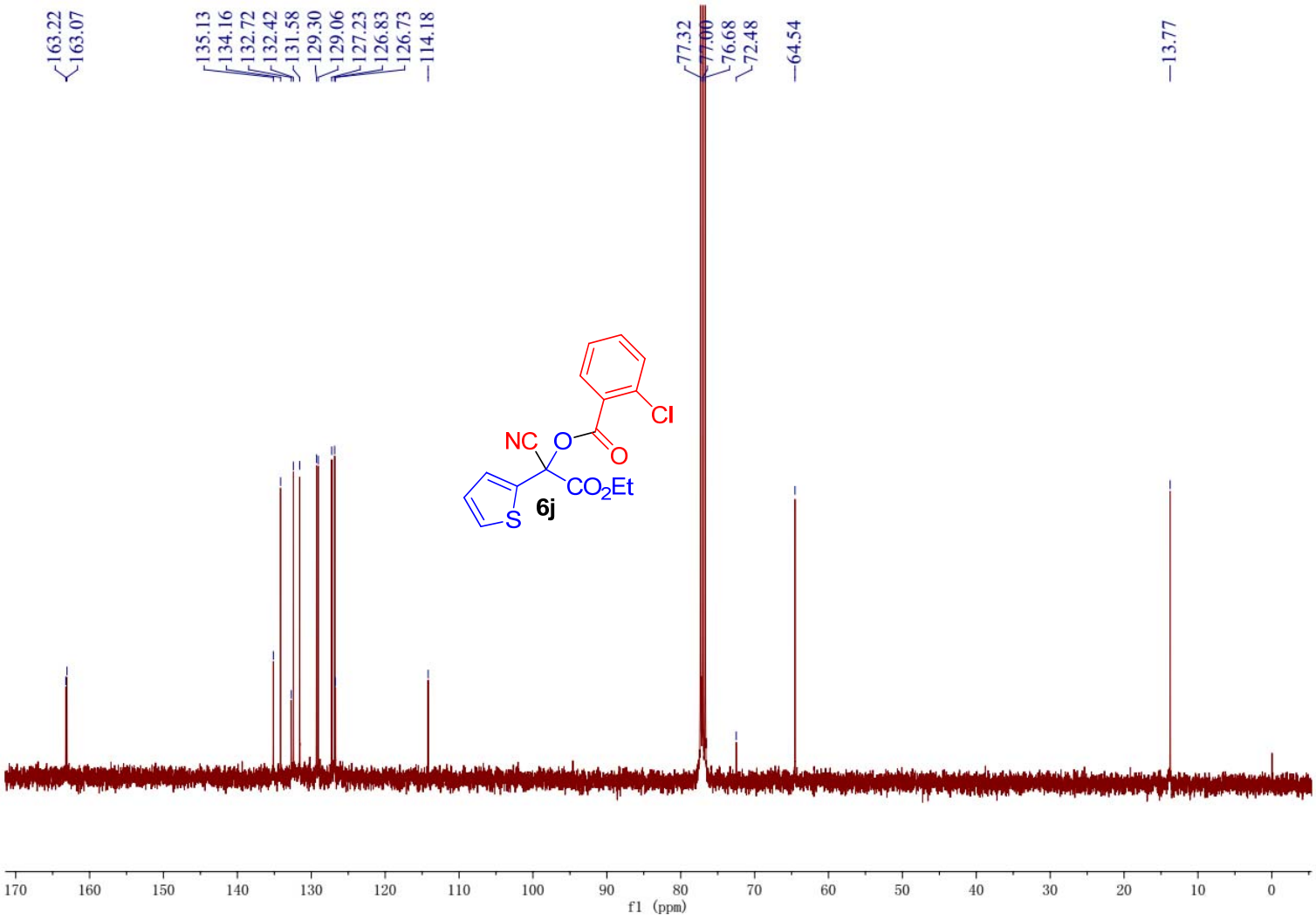

7.73
7.72
7.72
7.71
7.68
7.66
7.19
7.19
7.18
4.39
4.37
4.36
4.35
4.34
4.34
4.33
4.32
4.31
4.30
4.29
4.28
4.27
4.27
4.26
4.24
1.31
1.29
1.27
0.00
S
NC
O
O
CO2Et
Br
6h
0.97
5.06
0.97
2.26
3.49
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

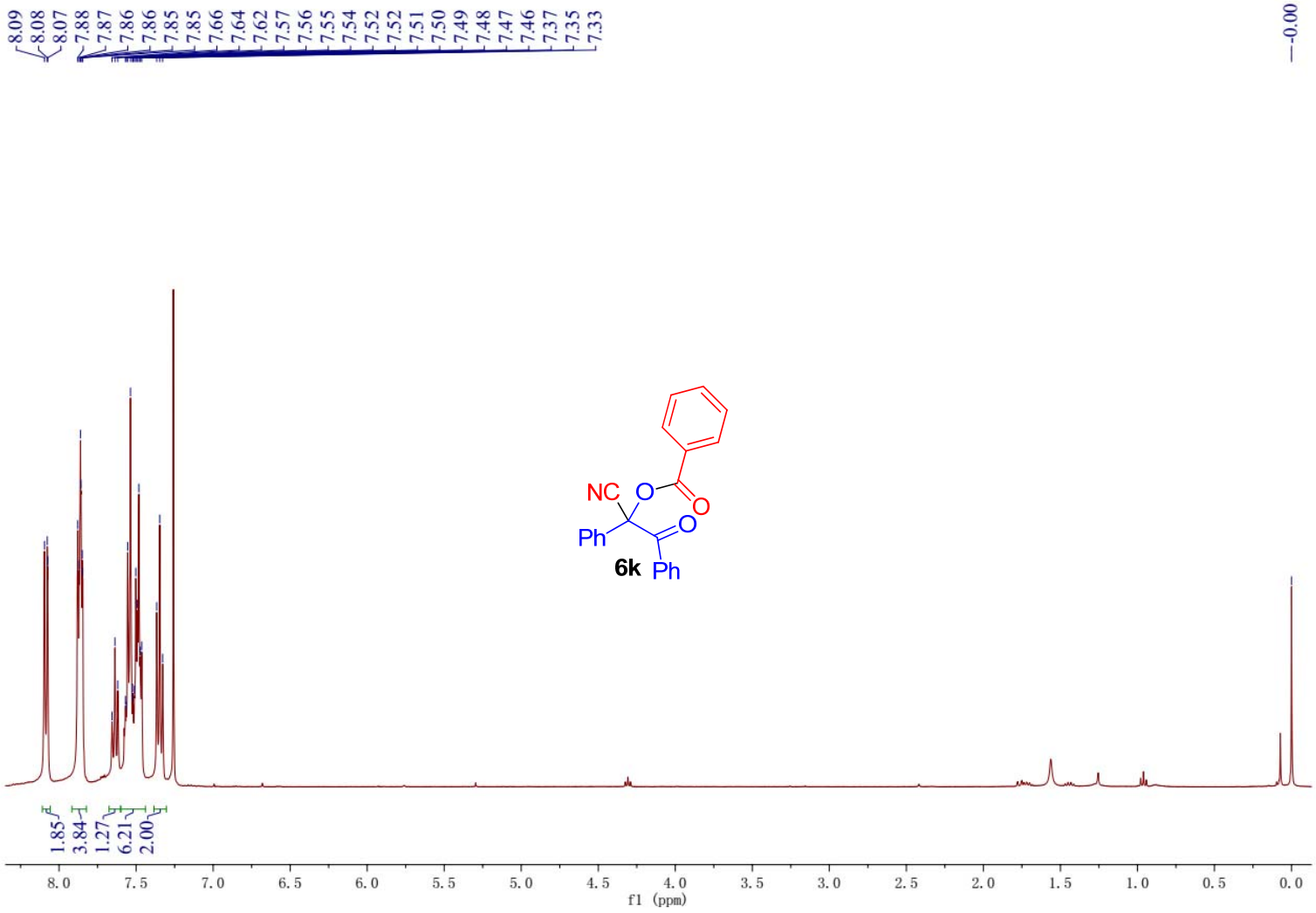

163.36
159.88
135.78
134.80
132.45
130.22
128.32
127.74
125.31
114.48
77.32
77.00
76.68
74.45
64.38
13.75
S
NC
O
O
CO2Et
Br
6h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

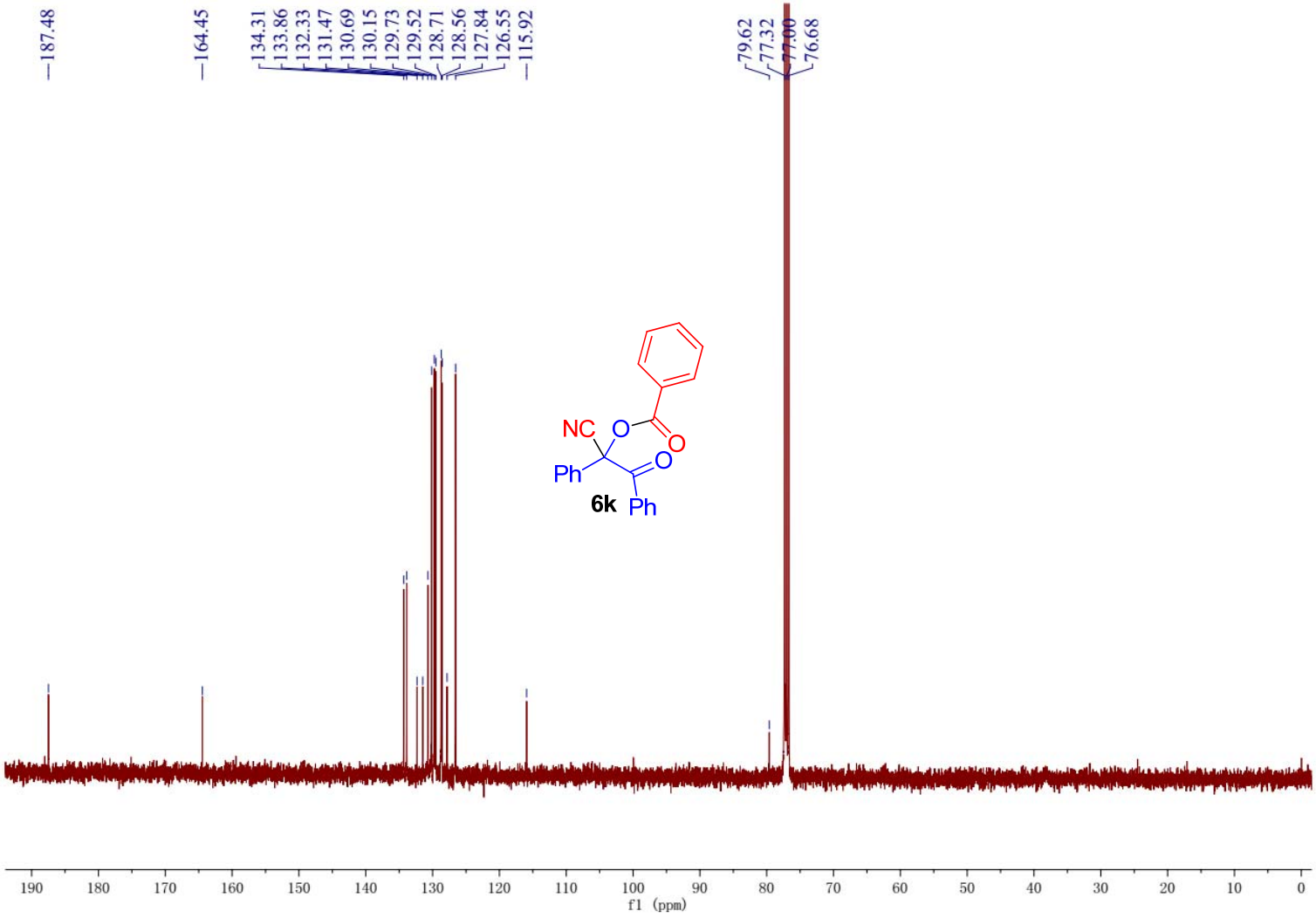

8.04
8.02
7.56
7.53
7.48
7.46
7.13
7.12
7.11
4.44
4.43
4.42
4.41
4.40
4.38
4.37
4.35
4.34
4.33
4.32
4.31
4.29
1.35
1.33
1.31
0.00
Cl
NC
O
O
CO2Et
S
6i
1.83
1.88
1.81
0.87
2.15
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

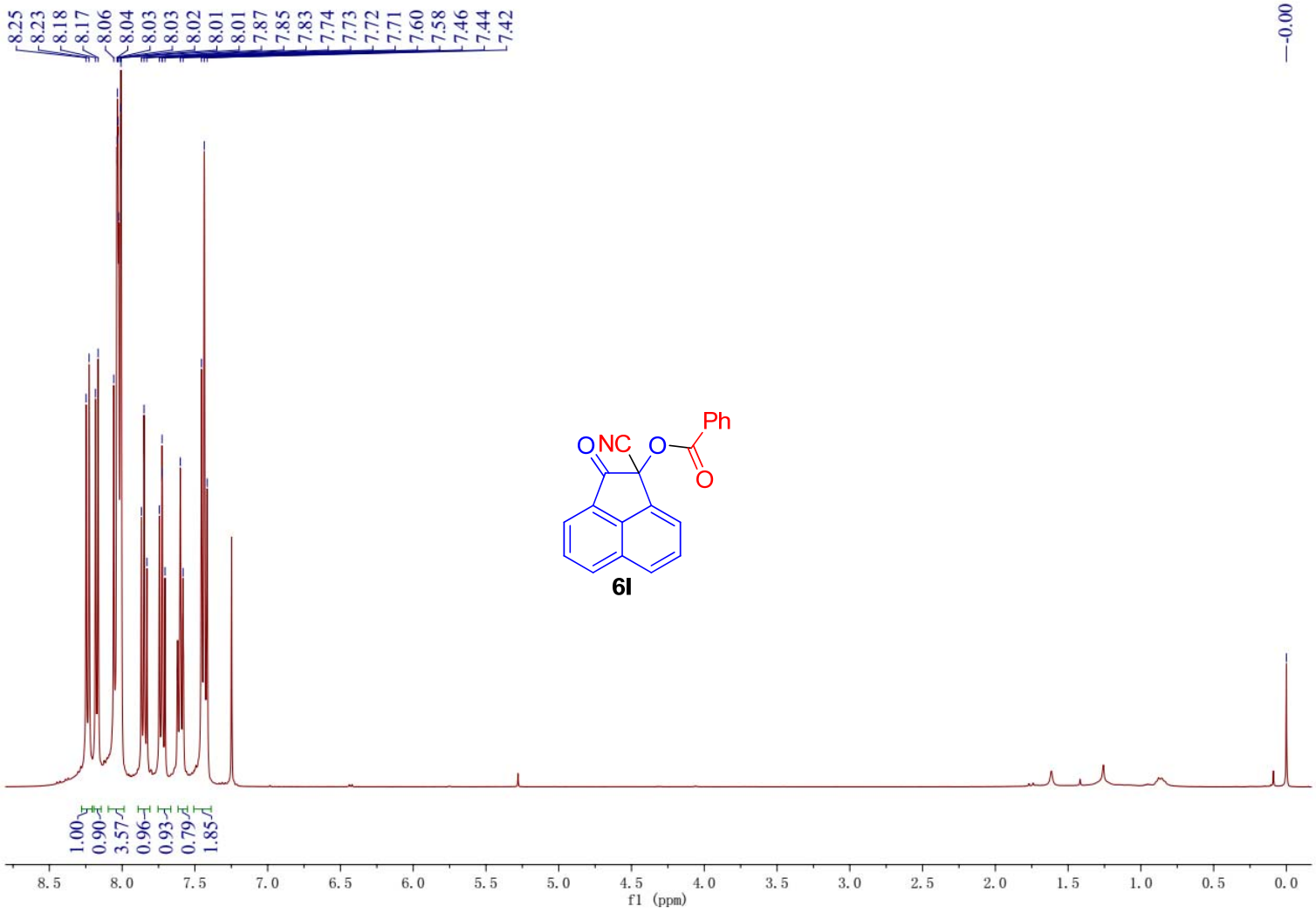

163.74
163.10
141.18
132.88
131.64
129.30
129.16
129.01
127.31
125.81
114.24
77.32
77.00
76.68
72.26
64.51
13.77
Cl
NC
O
O
CO2Et
S
6i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

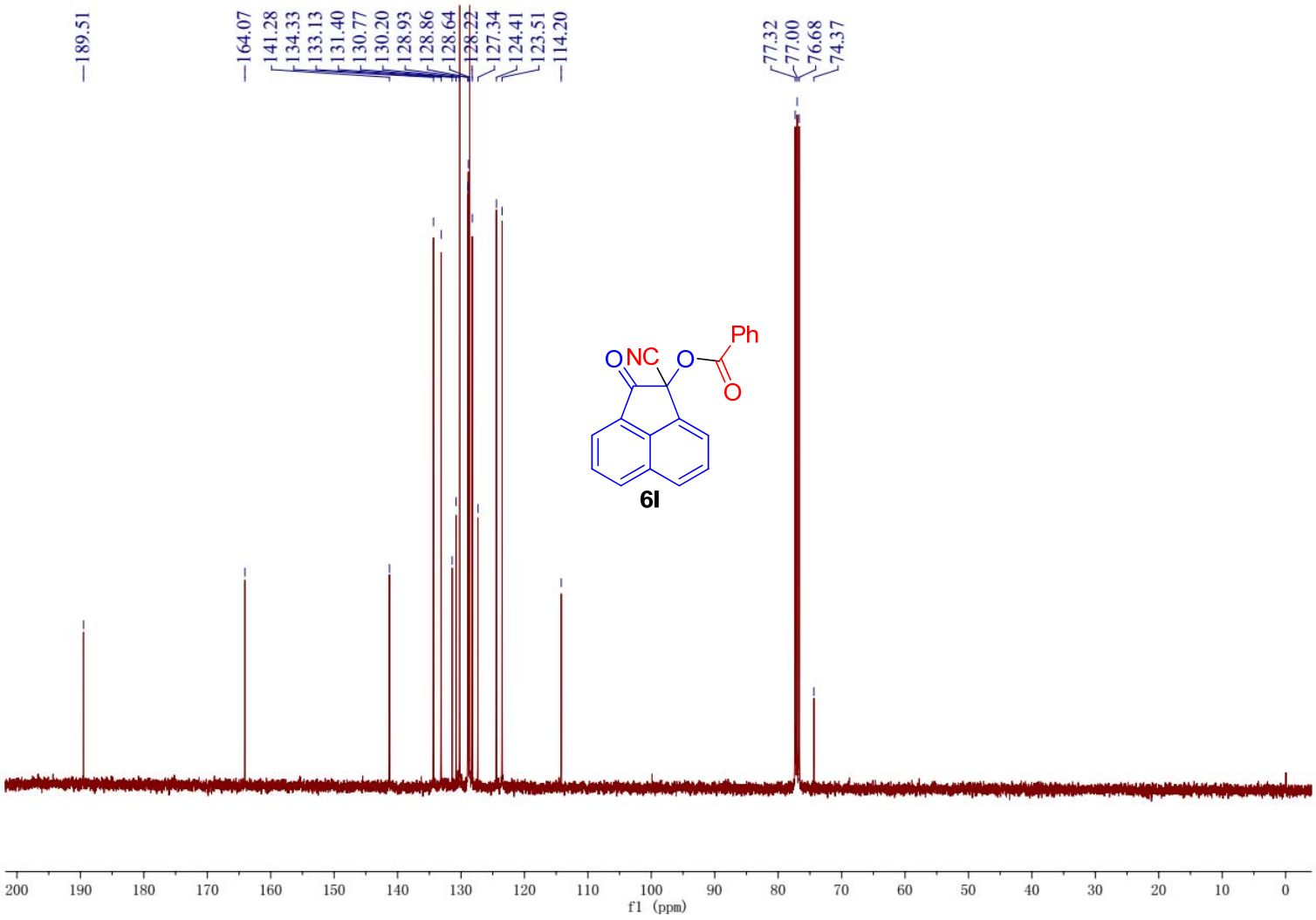

8.01
7.99
7.57
7.57
7.52
7.39
7.38
7.37
7.11
7.10
4.44
4.42
4.42
4.40
4.39
4.37
4.35
4.33
4.31
1.36
1.35
1.33
0.00
NC
O
O
Cl
CO2Et
S
6j
1.00
4.03
1.23
1.02
2.37
3.47
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


163.22
163.07
135.13
134.16
132.72
132.42
131.58
129.30
129.06
127.23
126.83
126.73
114.18
77.32
77.00
76.68
72.48
64.54
13.77
NC
O
O
Cl
CO2Et
S
6j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.09
8.08
8.07
7.88
7.87
7.86
7.86
7.85
7.85
7.66
7.64
7.62
7.57
7.56
7.55
7.54
7.52
7.52
7.51
7.50
7.49
7.48
7.47
7.46
7.37
7.35
7.33
-0.00
NC
O
O
O
Ph
6k
Ph
1.85
3.84
1.27
6.21
2.00
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)


187.48
164.45
134.31
133.86
132.33
131.47
130.69
130.15
129.73
129.52
128.71
128.56
127.84
126.55
115.92
79.62
77.32
77.00
76.68
NC
O
O
O
Ph
6k
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.25
8.23
8.18
8.17
8.06
8.04
8.03
8.03
8.02
8.01
8.01
7.87
7.85
7.83
7.74
7.73
7.72
7.71
7.60
7.58
7.46
7.44
7.42
-0.00
O
NC
O
Ph
O
6l
1.00
0.90
3.57
0.96
0.93
0.79
1.85
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)


189.51
164.07
141.28
134.33
133.13
131.40
130.77
130.20
128.93
128.86
128.64
128.22
127.34
124.41
123.51
114.20
77.32
77.00
76.68
74.37
O
NC
O
Ph
O
6l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)