Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Affording Linear Naphthalene Exclusively *via* Mild Aromatic Tetradehydro-Diels-Alder Reaction

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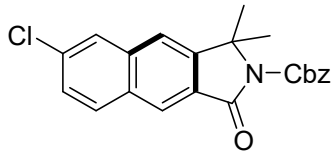
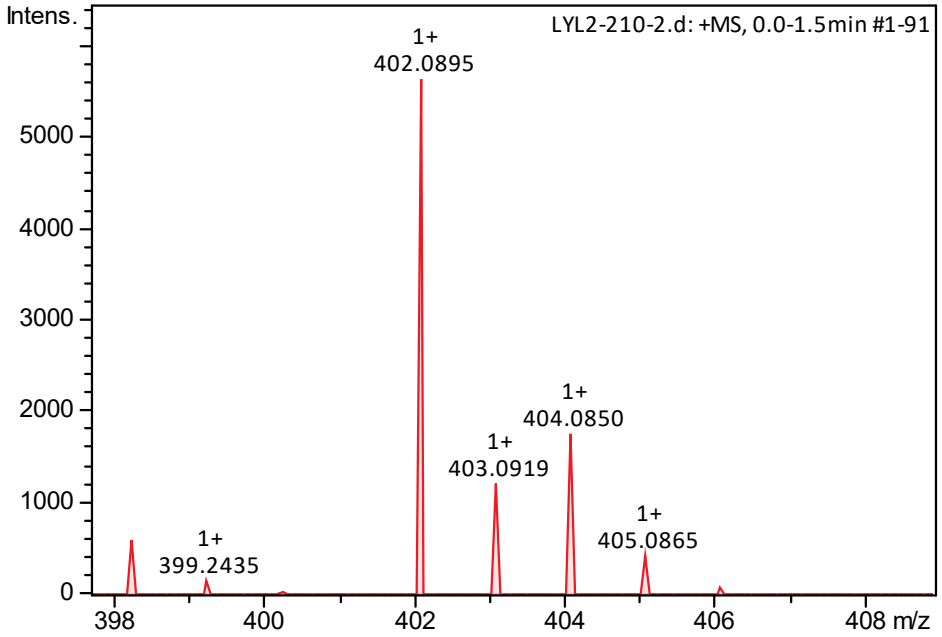
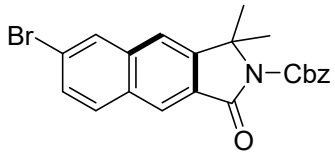
Characterization Data for Products:

The original graphics are shown below:

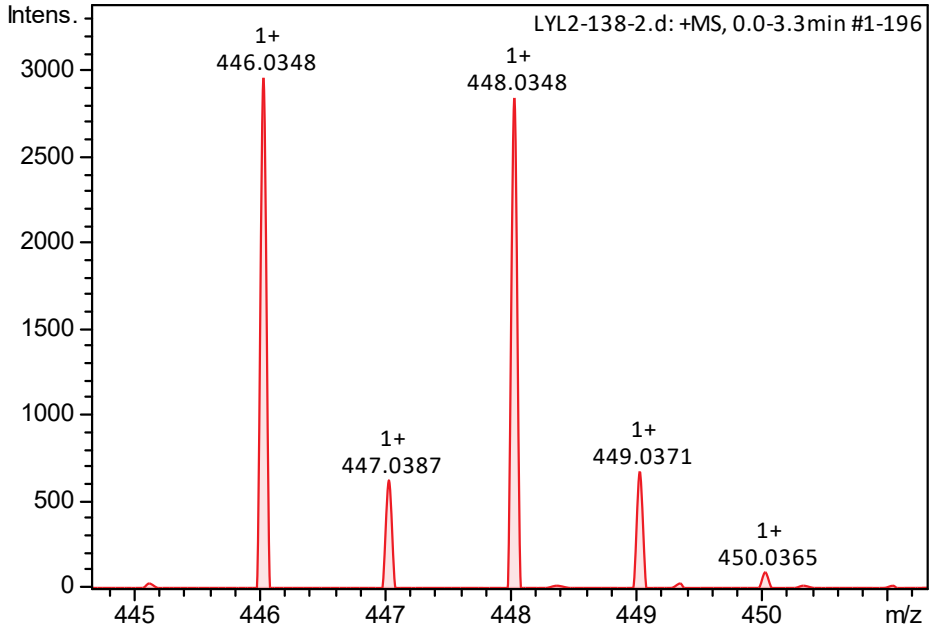


3ag

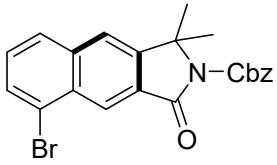


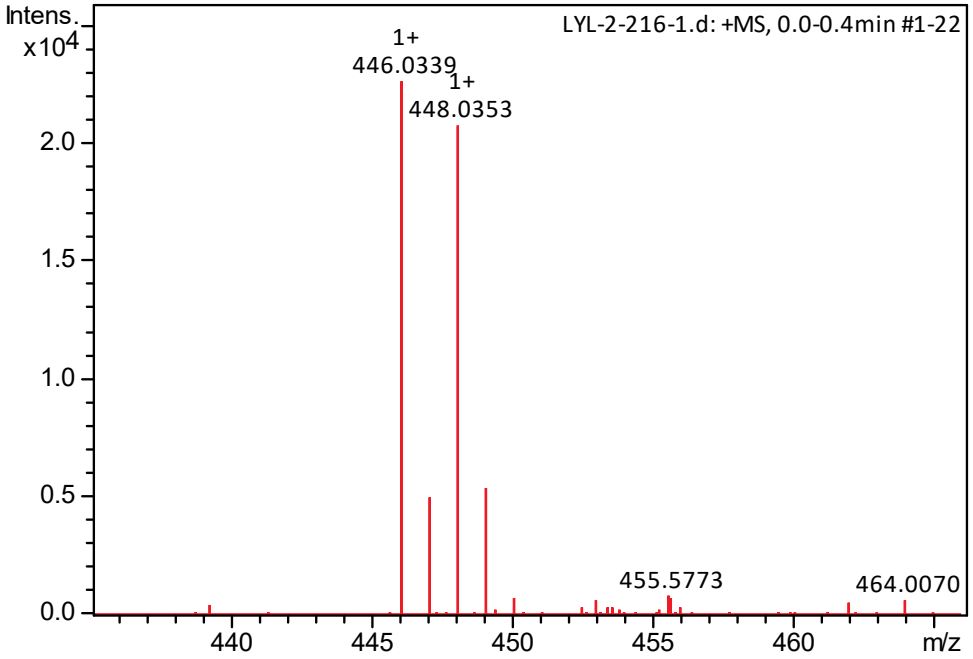


3ah



3am


N−Cbz
O
Br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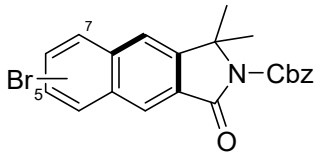
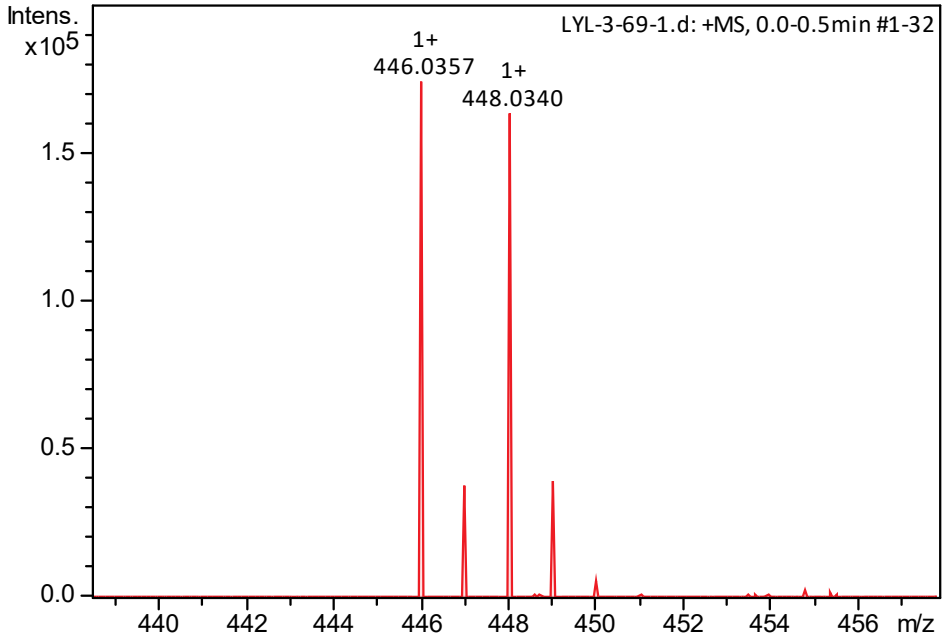
1+
448.0353
455.5773
464.0070
2.0
1.5
1.0
0.5
0.0
440
445
450
455
460
m/z

3an


7
Br
5
N−Cbz
O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1+
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1.0
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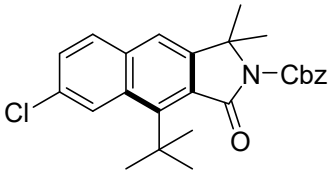
0.0
440
442
444
446
448
450
452
454
456
m/z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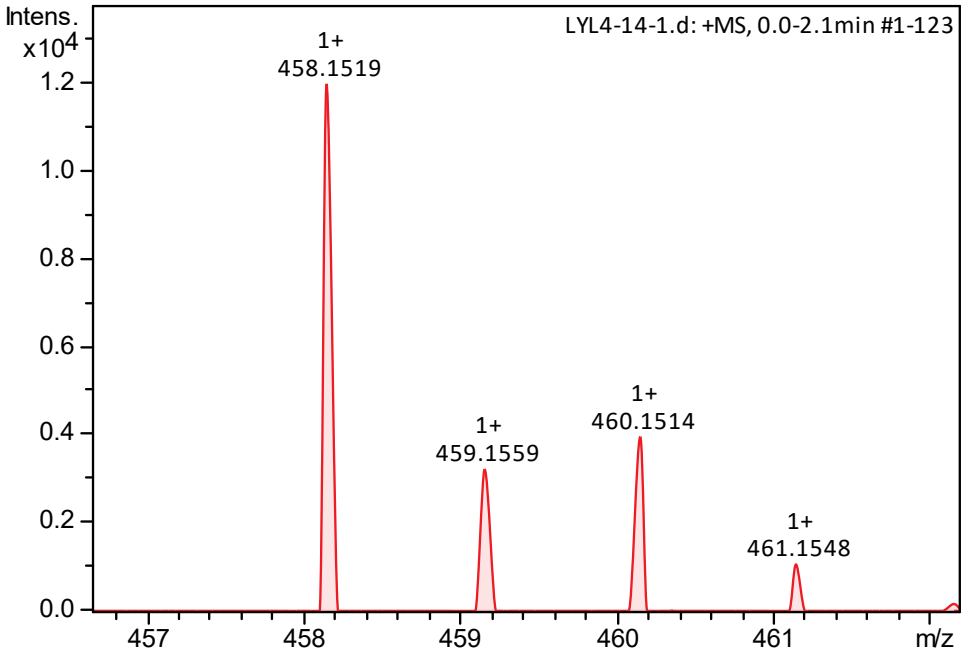
N−Cbz
O

3bd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0.6
0.4
0.2
0.0
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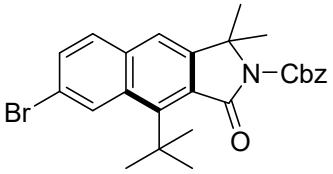
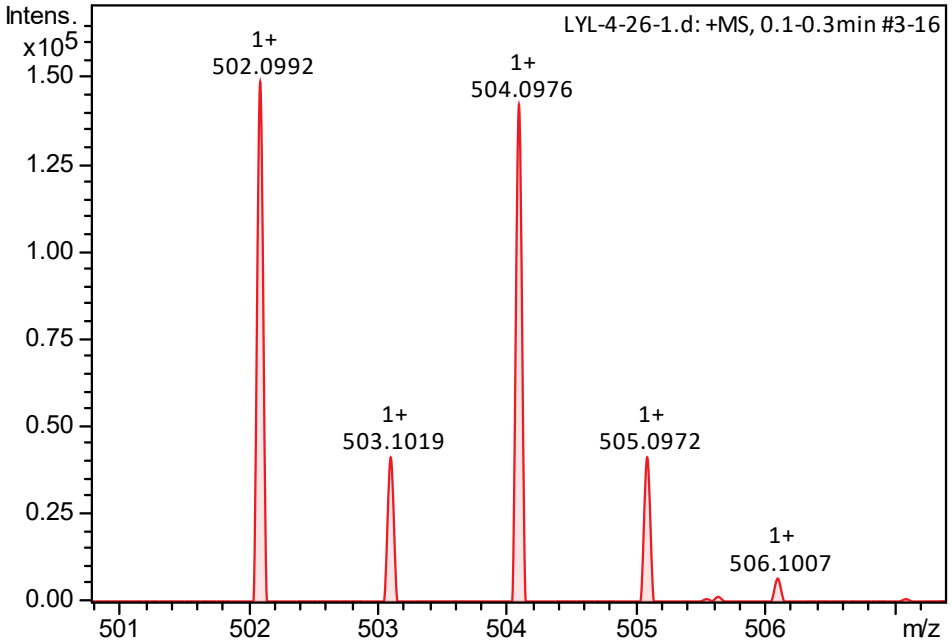
1+
459.1559
1+
460.1514
1+
461.1548
457
458
459
460
461
m/z


Br
N−Cbz
O

3be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x10^5
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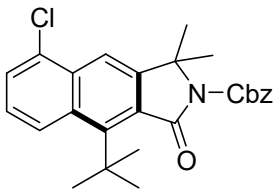
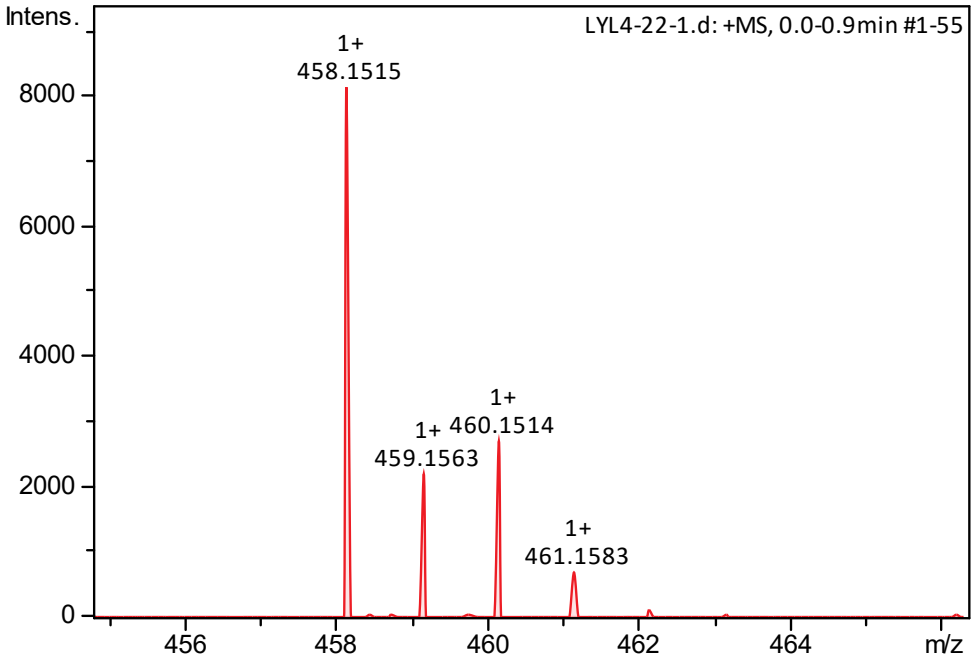
1.25
1.00
0.75
0.50
0.25
0.00
LYL-4-26-1.d: +MS, 0.1-0.3min #3-16
1+
502.0992
1+
503.1019
1+
504.0976
1+
505.0972
1+
506.1007
501
502
503
504
505
506
m/z


Cl
N−Cbz
O

3bh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LYL4-22-1.d: +MS, 0.0-0.9min #1-55
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1+
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1+
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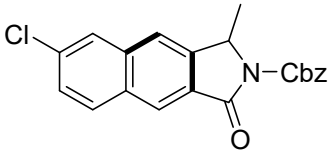
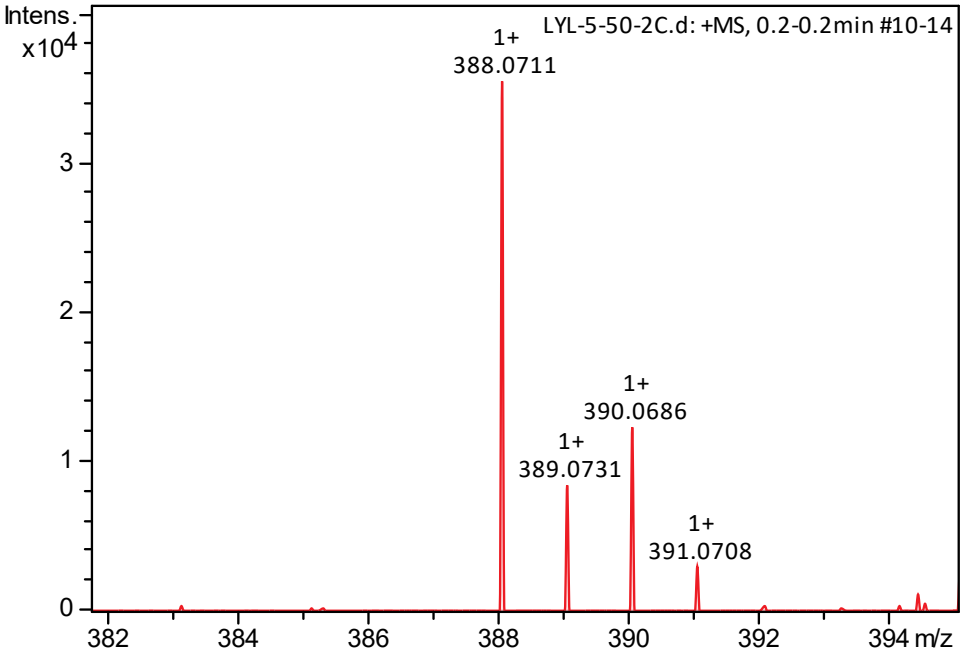
8000
6000
4000
2000
0
456
458
460
462
464
m/z


Cl
N−Cbz
O

3bw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1+
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1+
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1+
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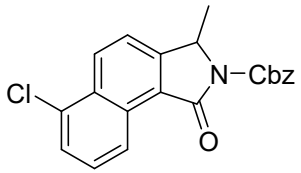
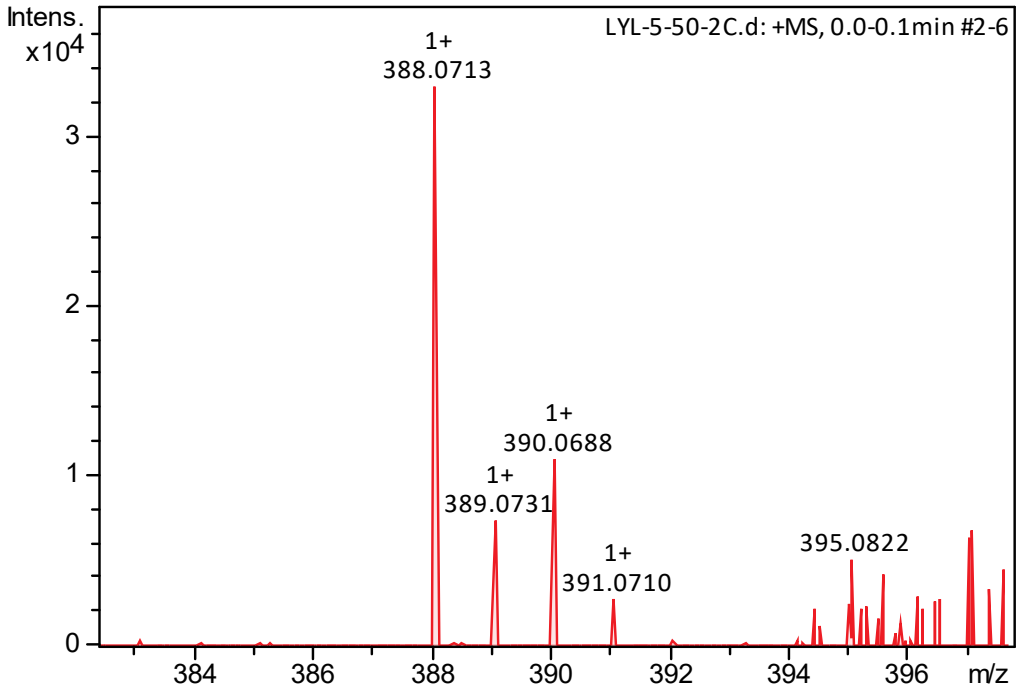
2
1
0
382
384
386
388
390
392
394 m/z


Cl
N−Cbz
O

3bw'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x10^4
LYL-5-50-2C.d: +MS, 0.0-0.1min #2-6
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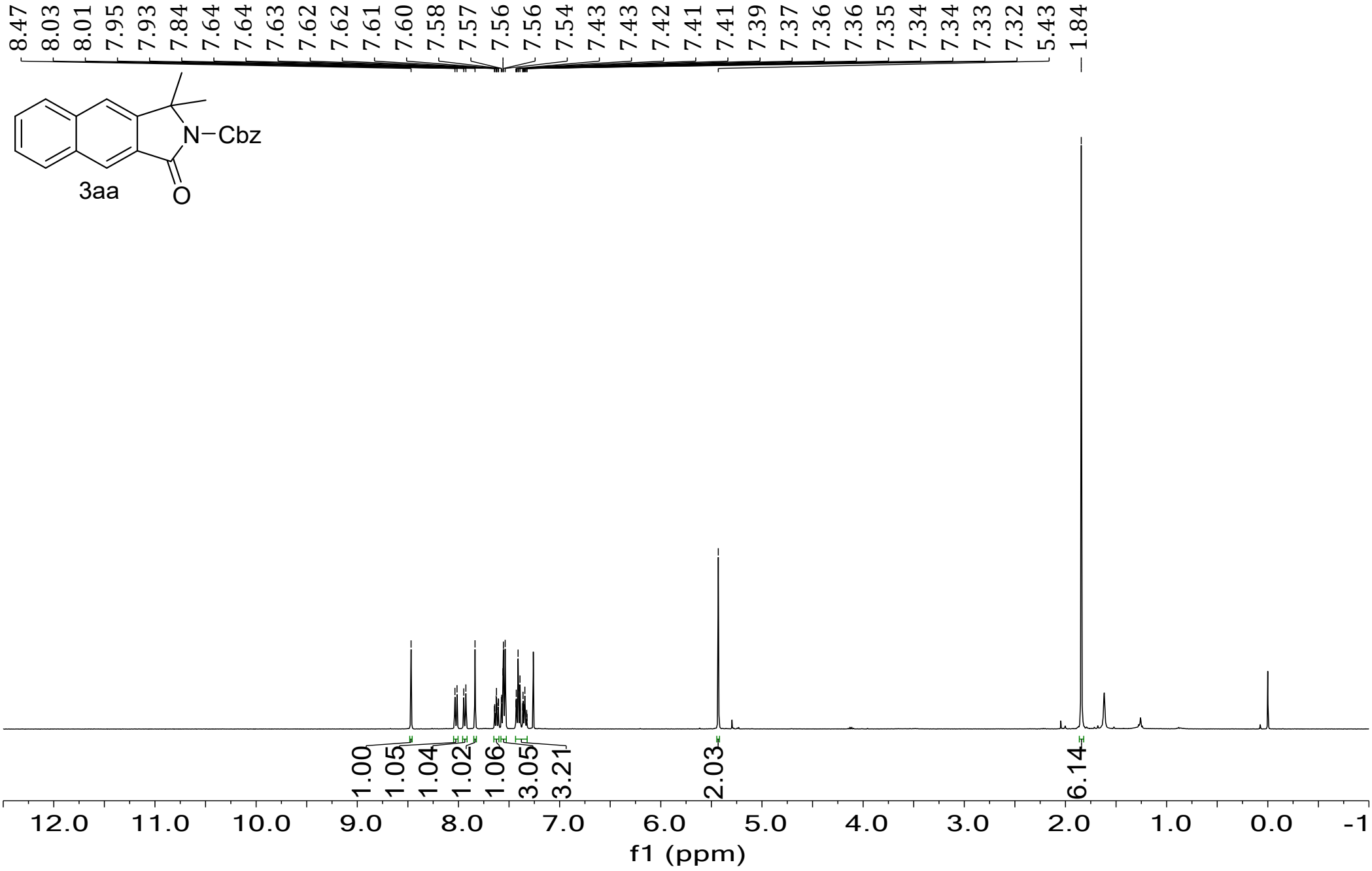
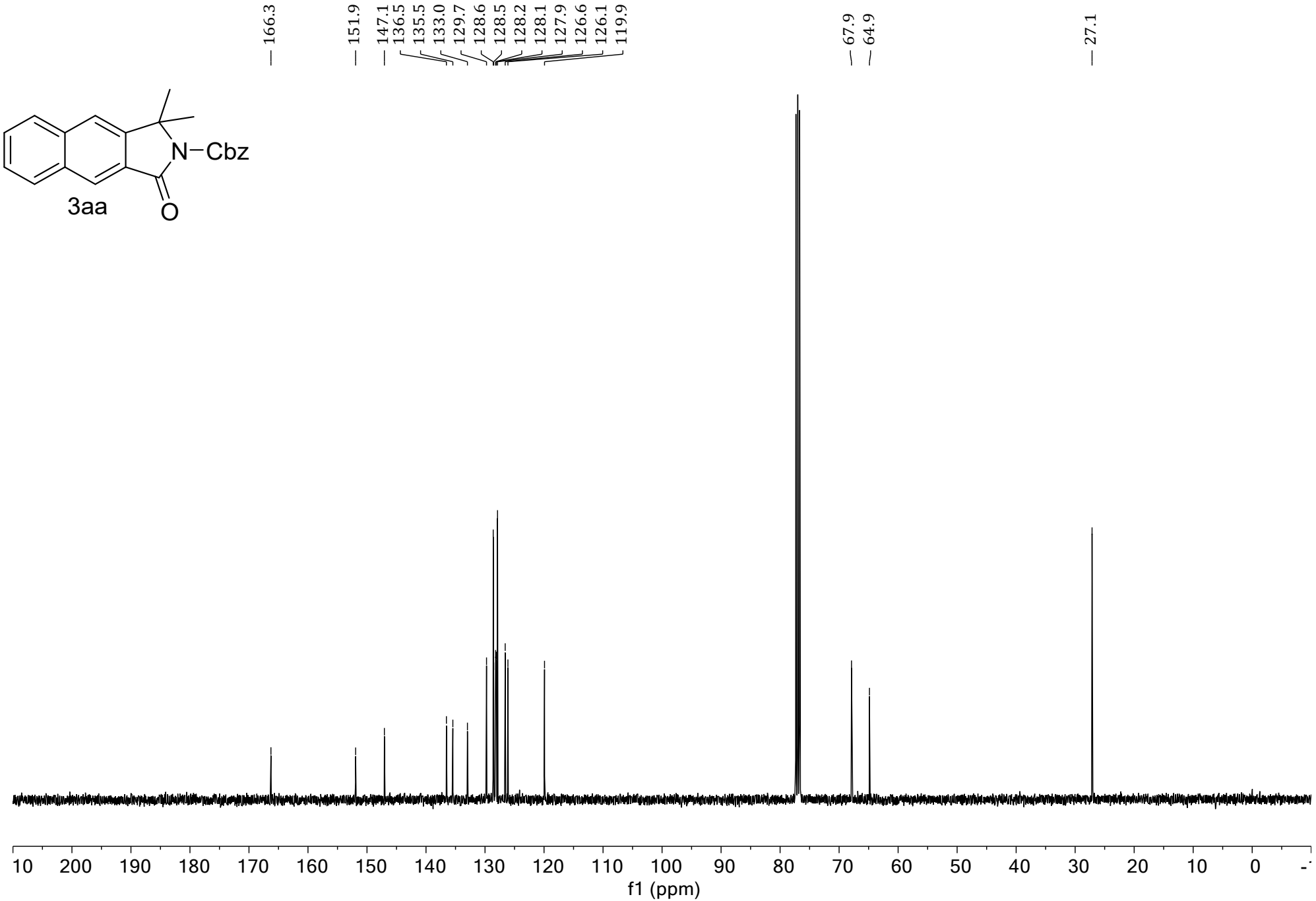
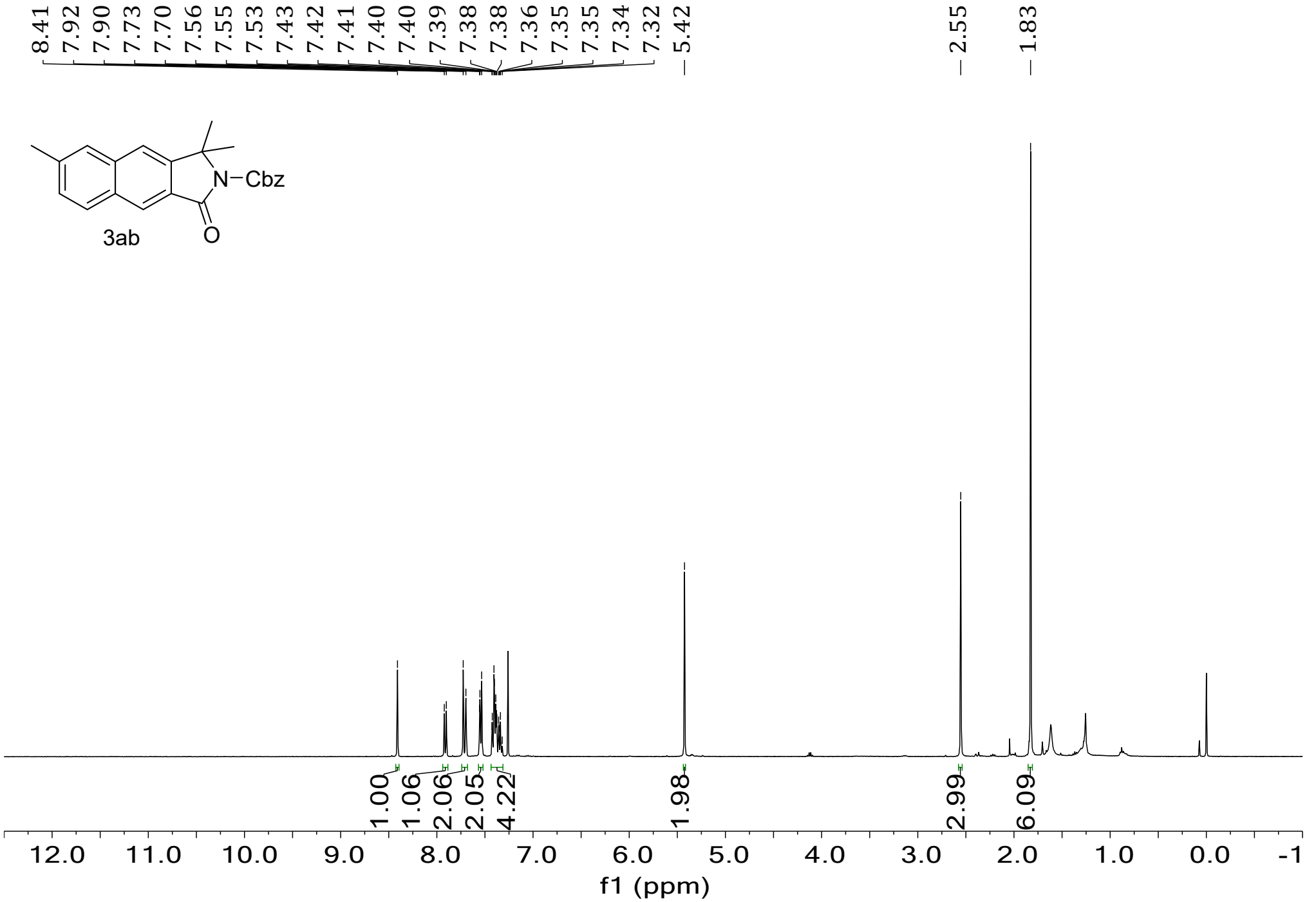
388.0713
1+
390.0688
1+
389.0731
1+
391.0710
395.0822
0
1
2
3
384
386
388
390
392
394
396
m/z



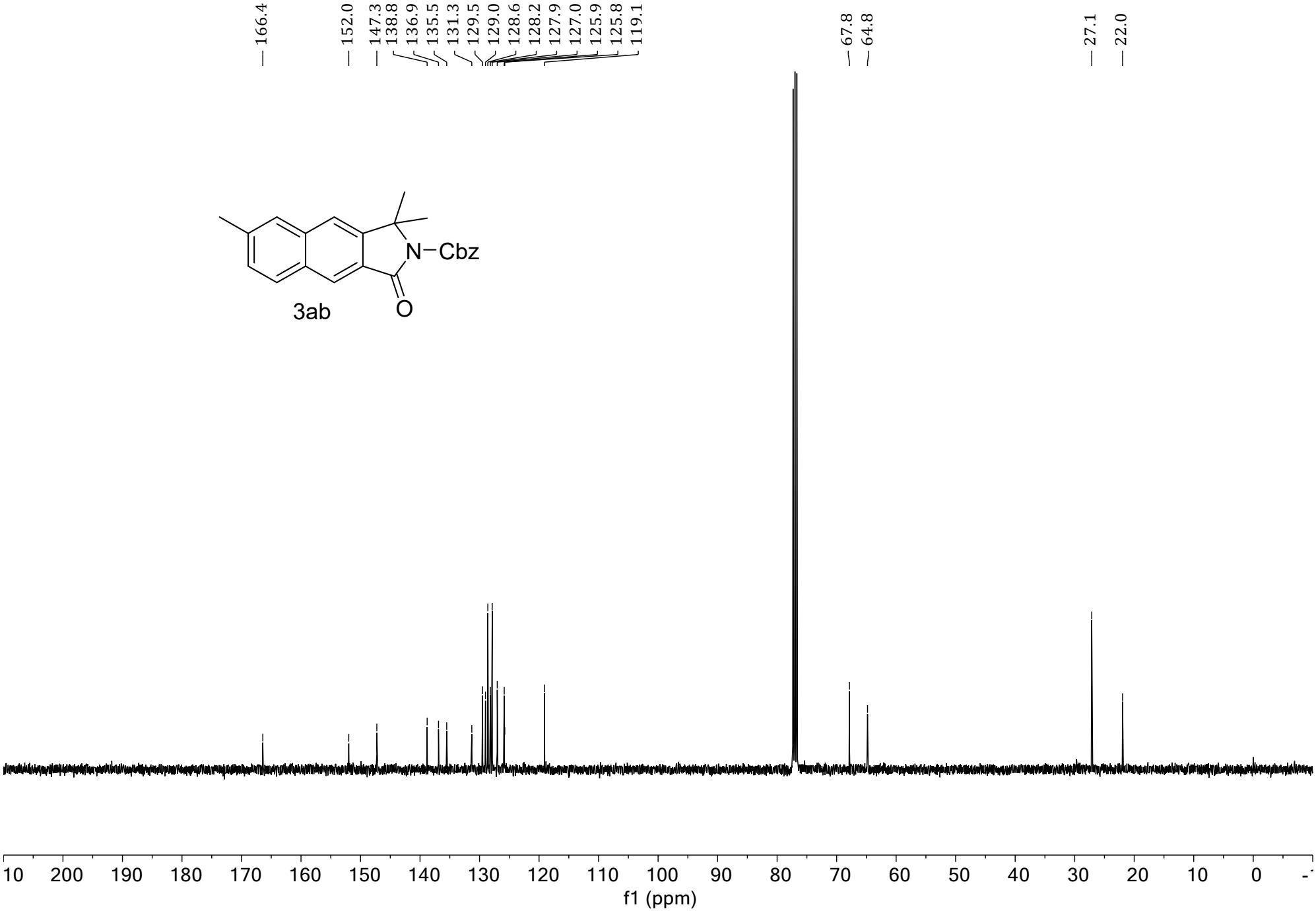
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3aa**



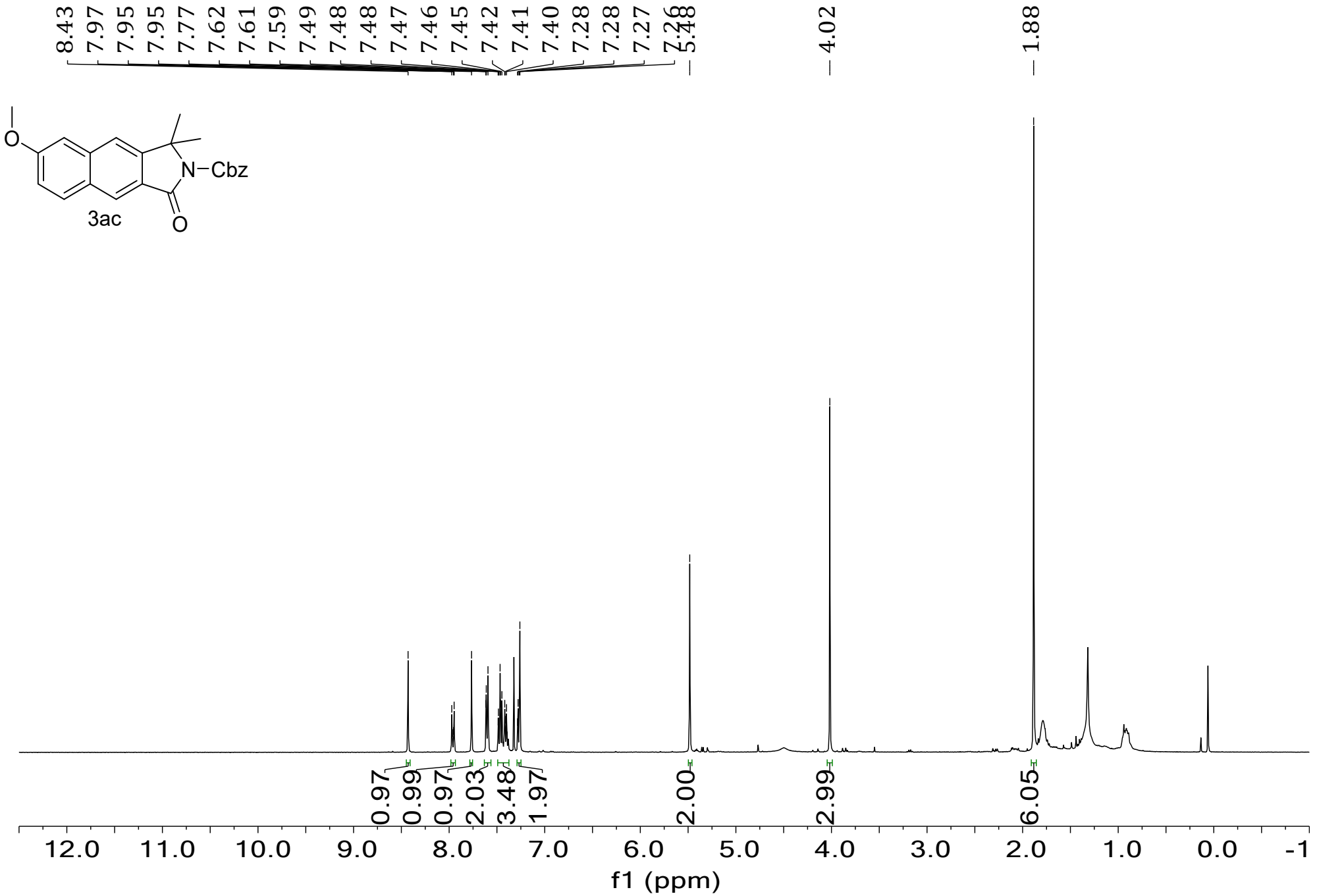
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3aa**



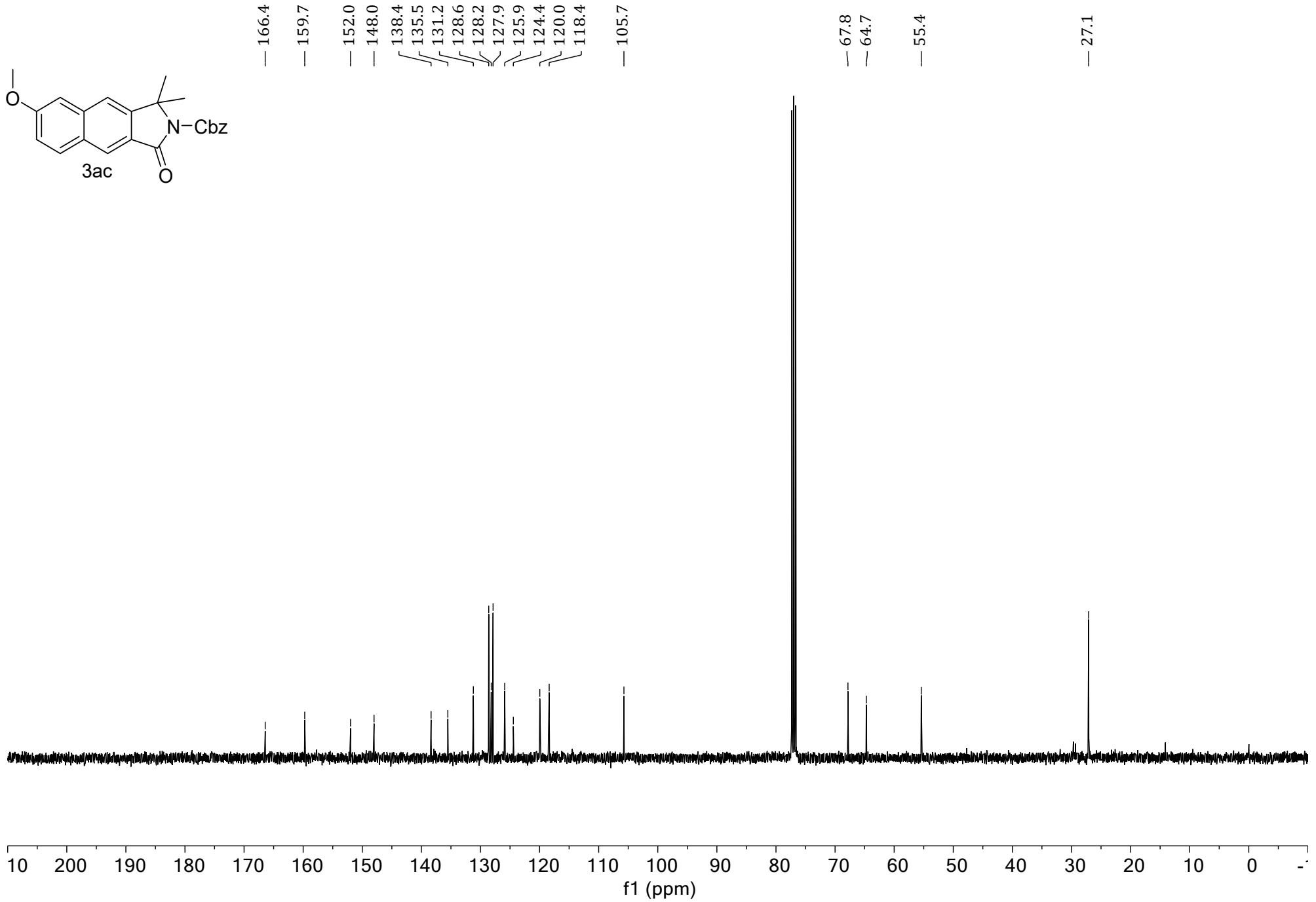
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ab**.



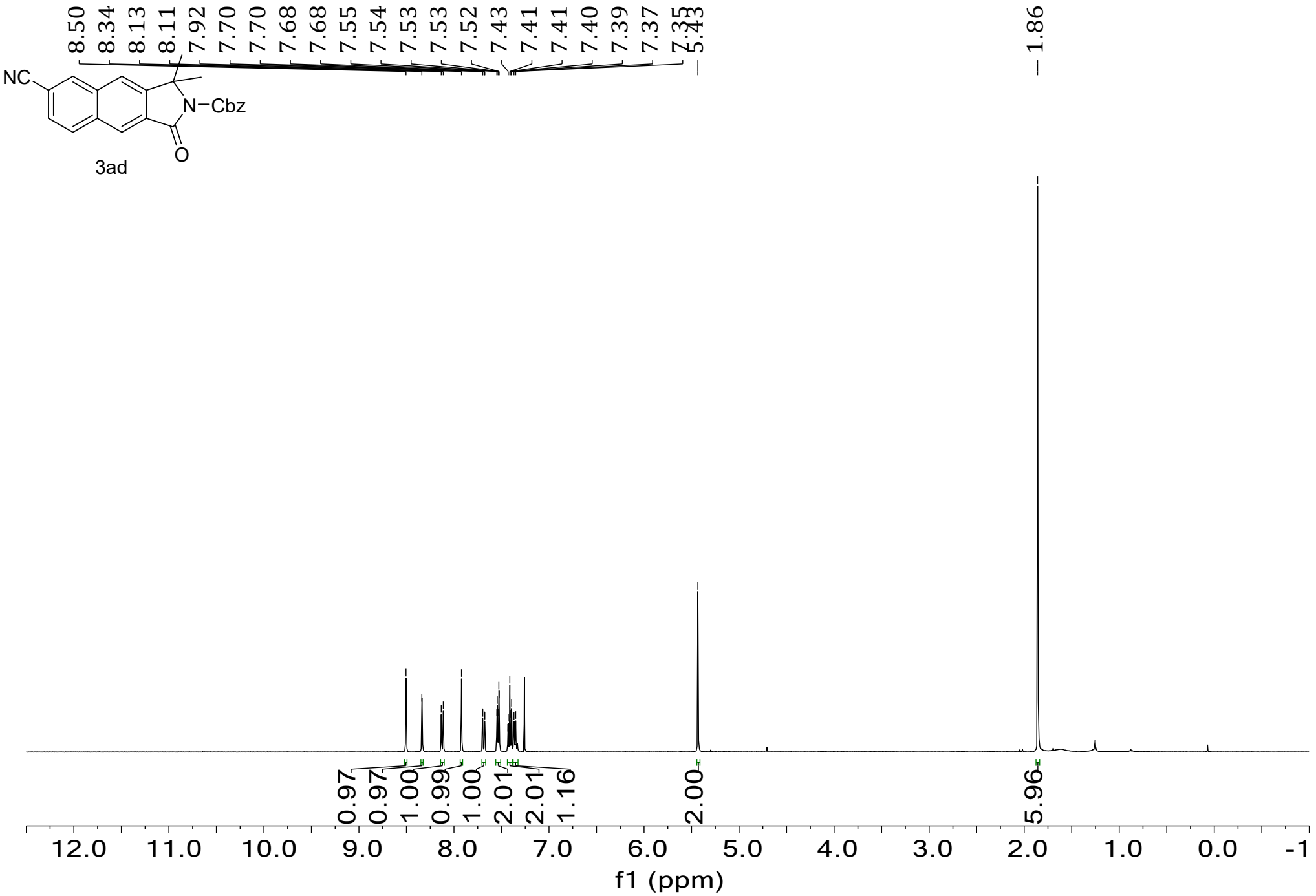
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ab**.



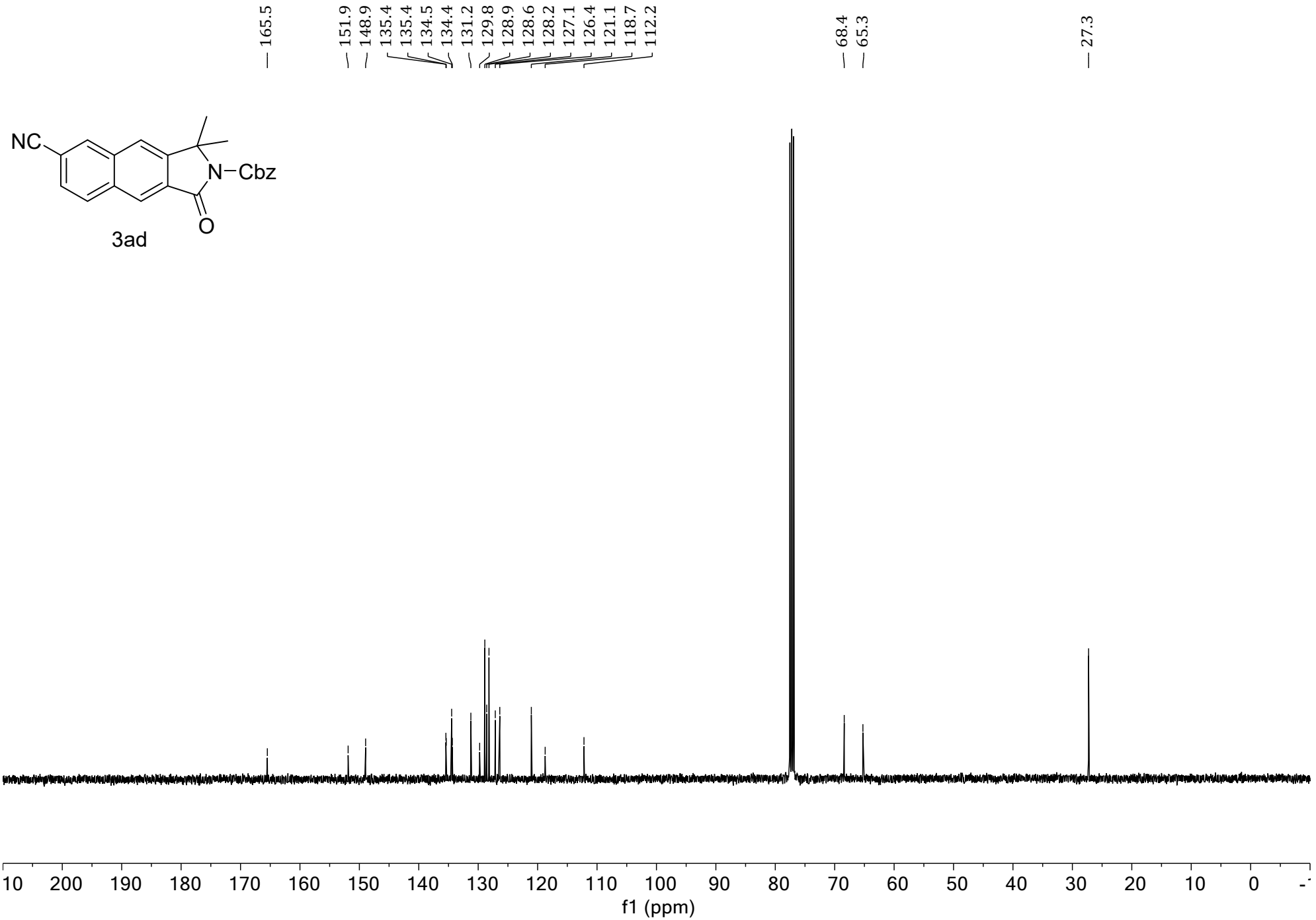
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ac**



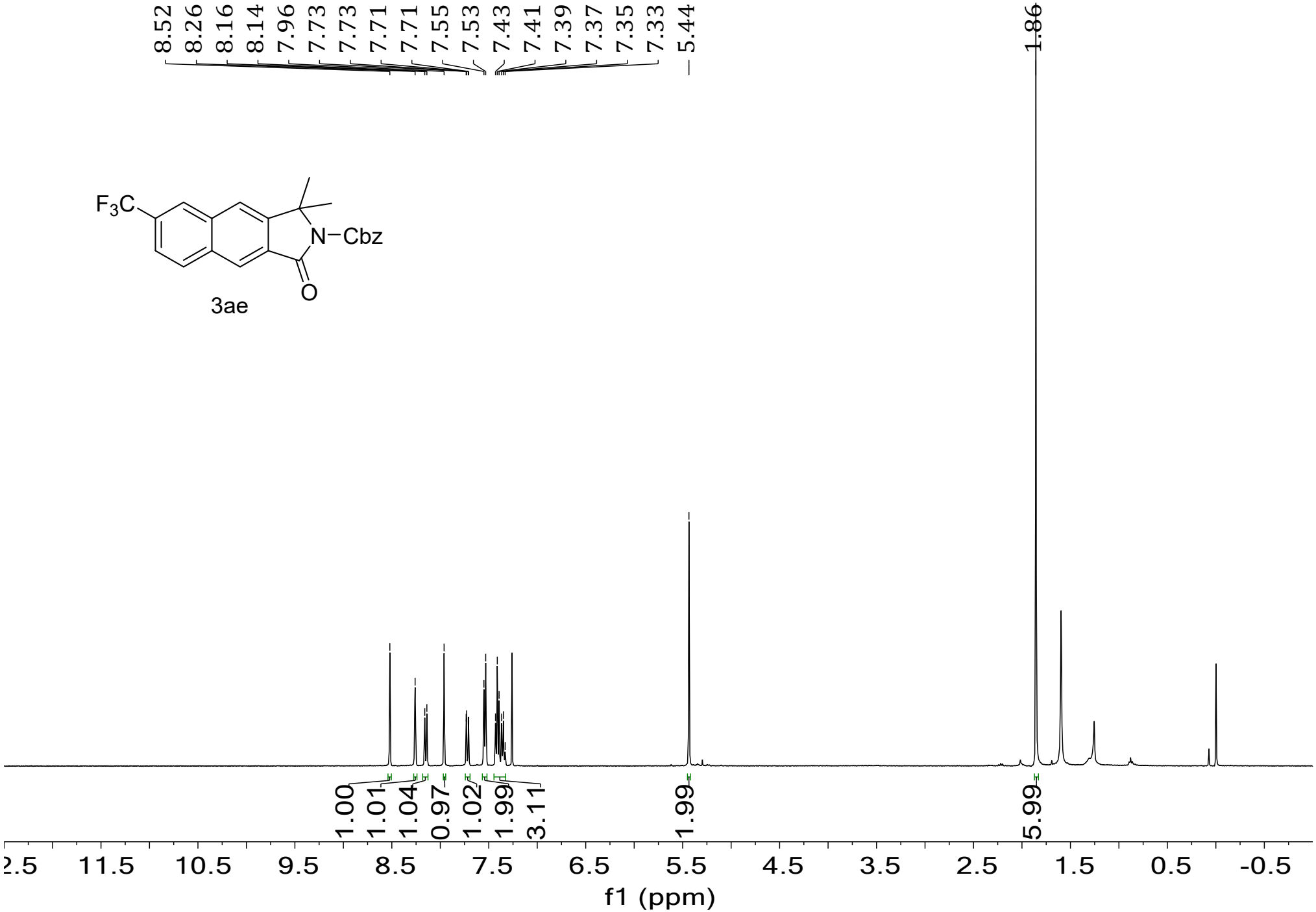
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ac**.



^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ad**



^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ad**.



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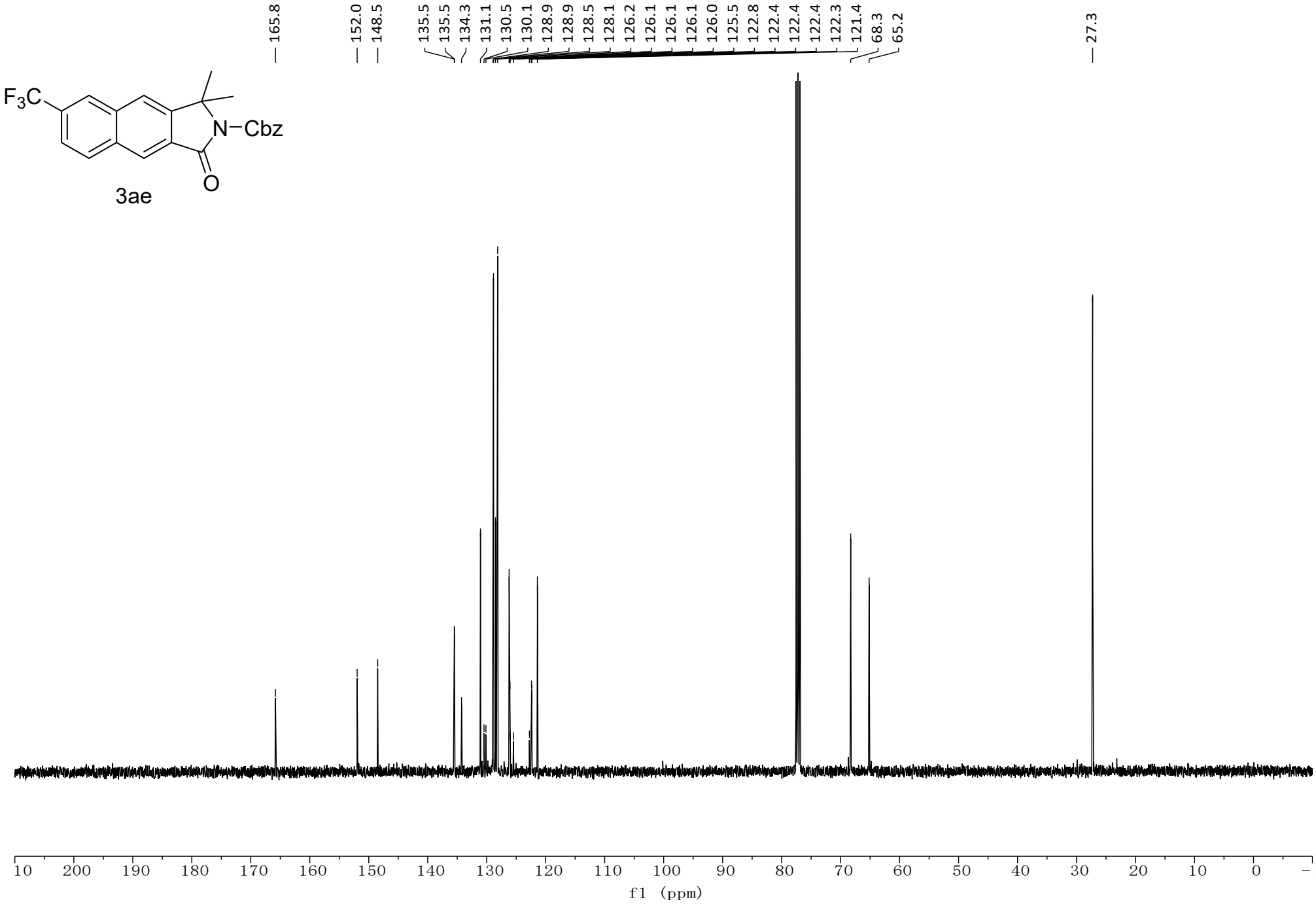
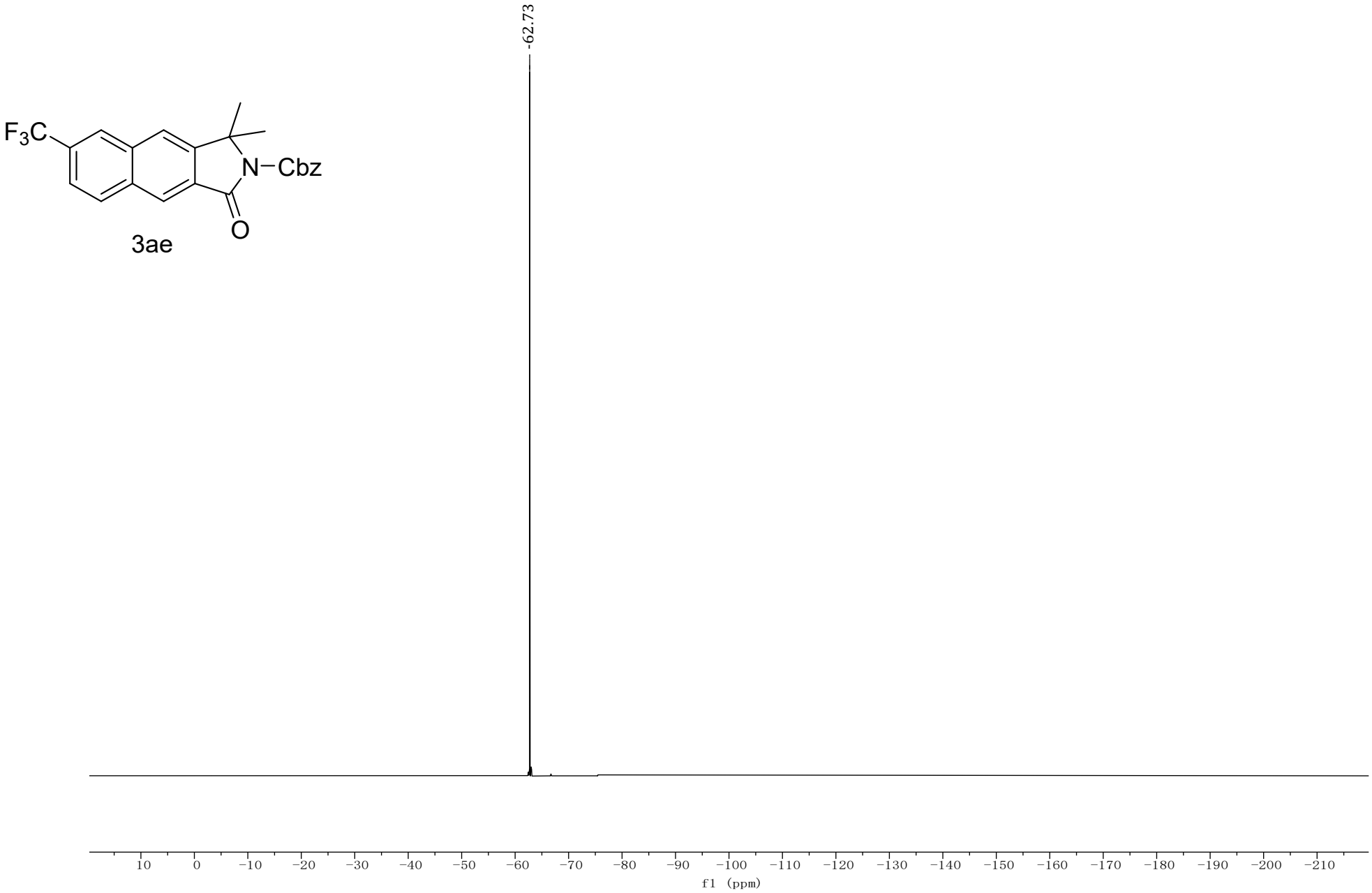
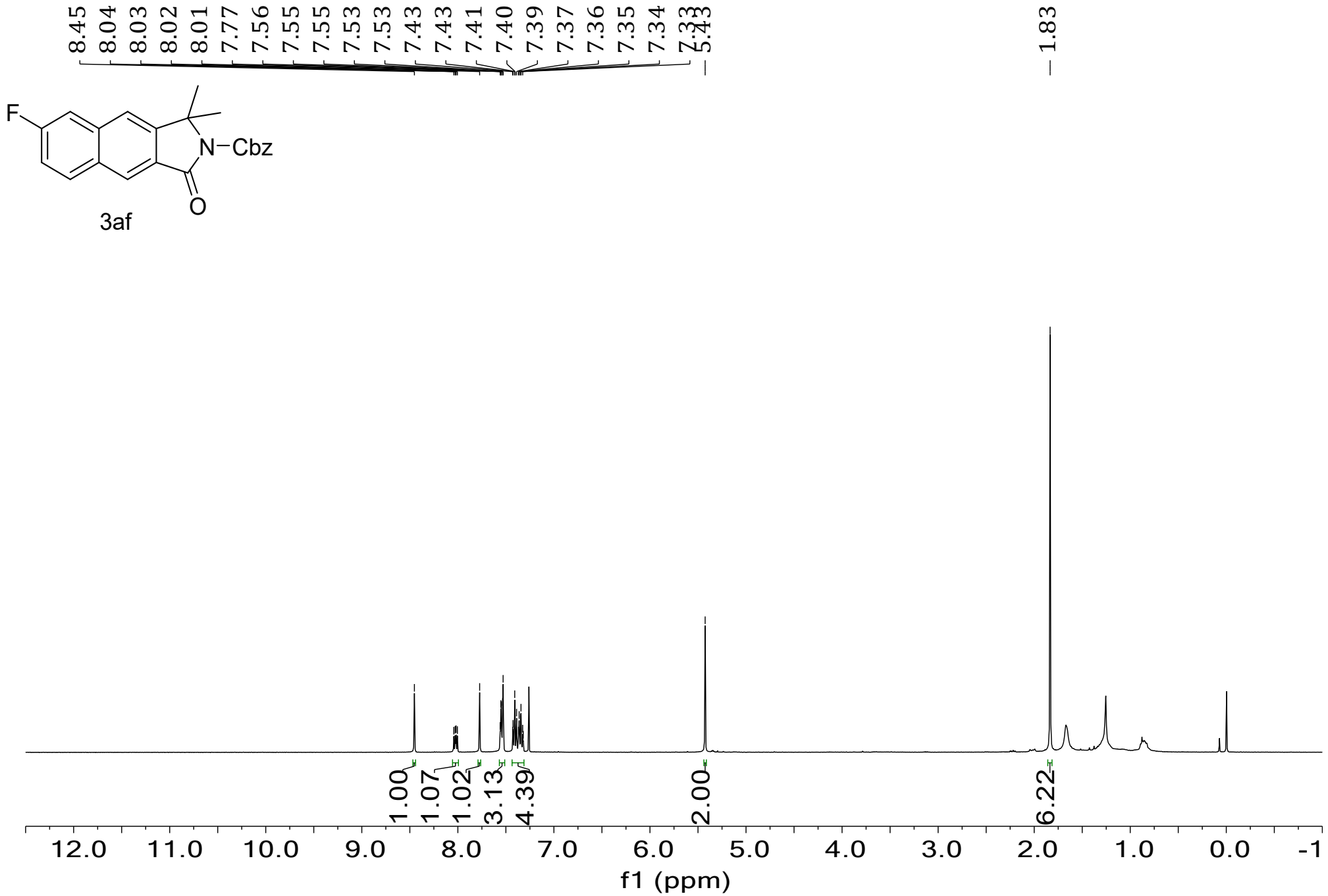


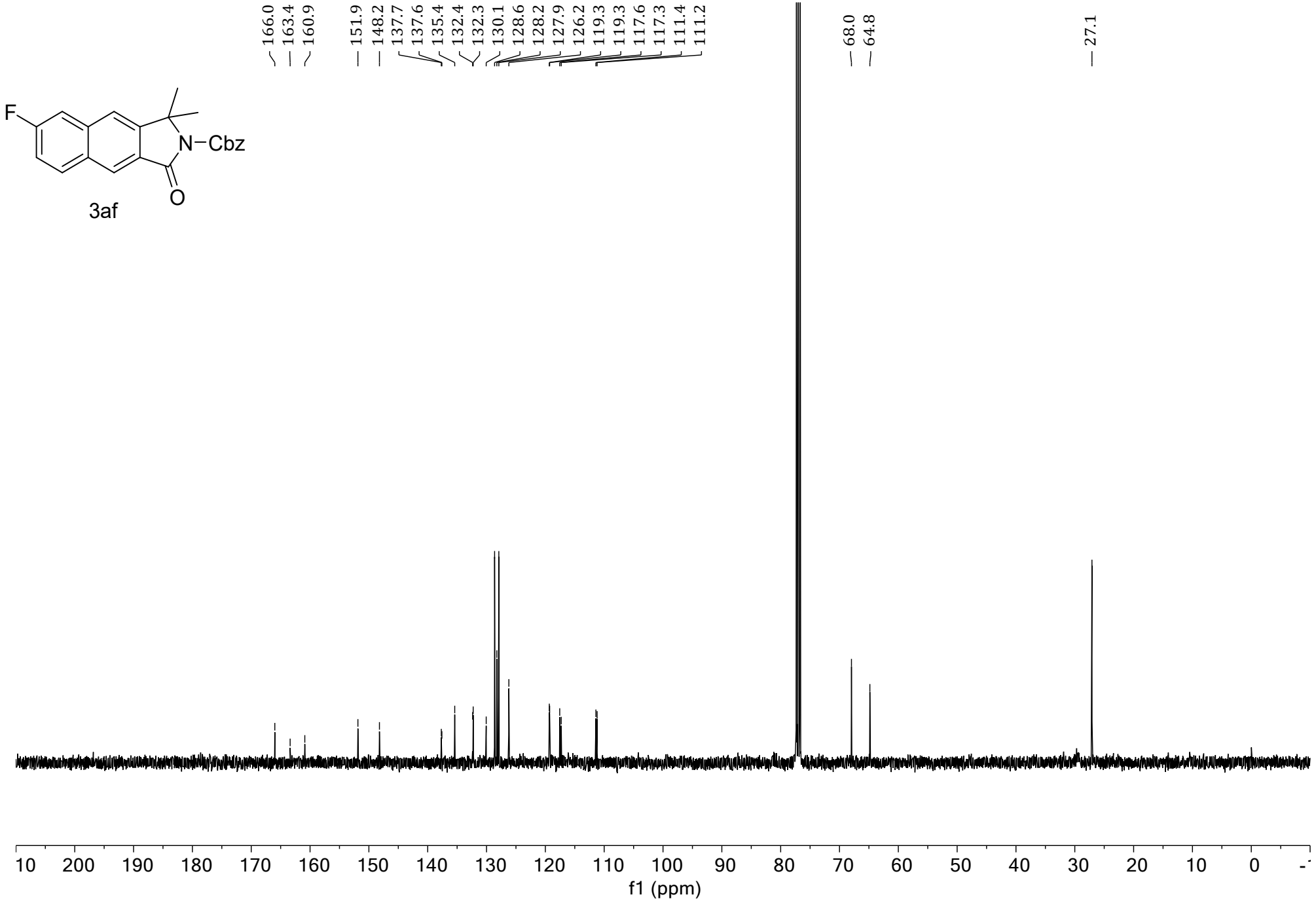
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ae**.



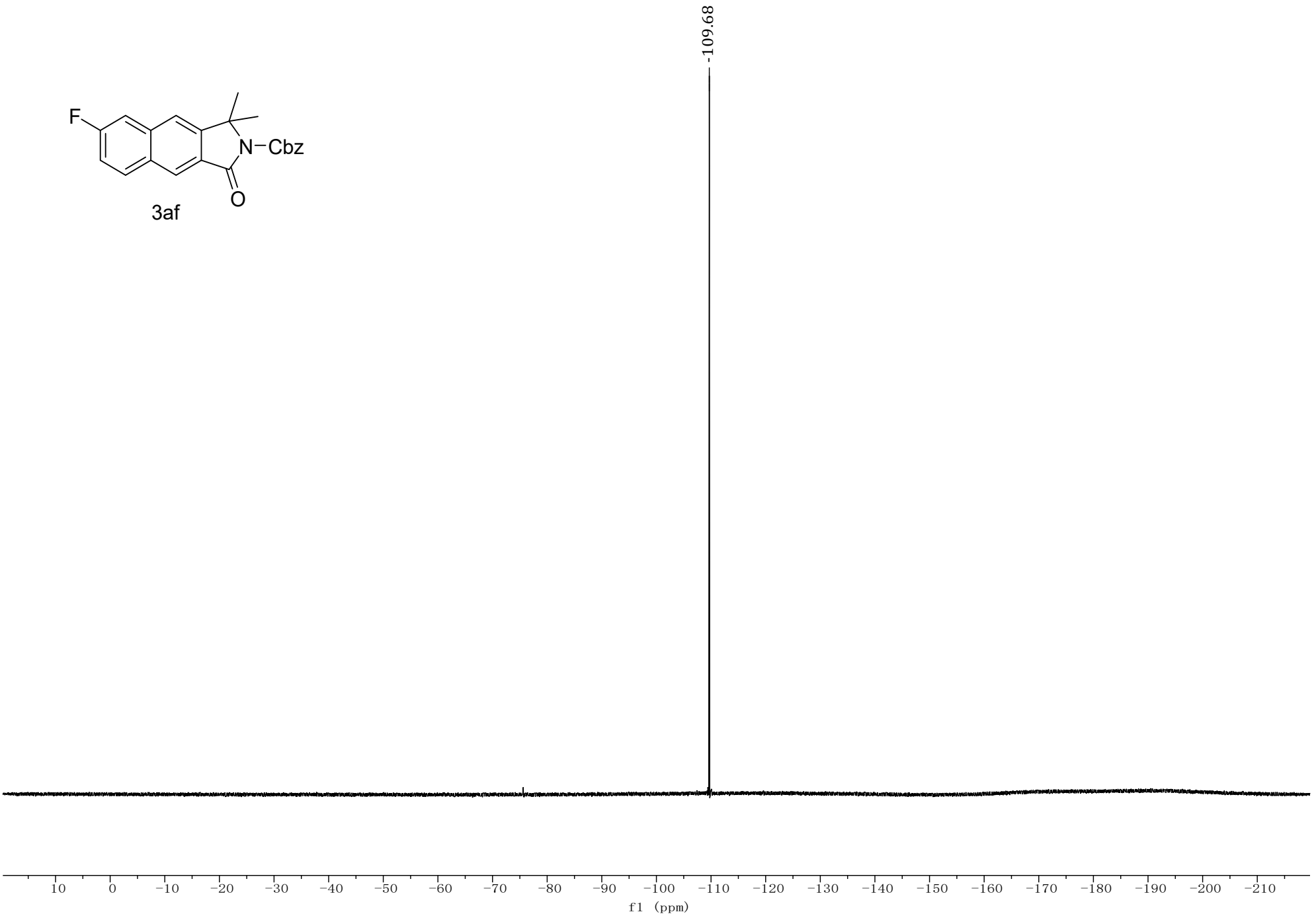
^{19}F NMR (400 MHz, $CDCl_3$) spectra of **3ae**.



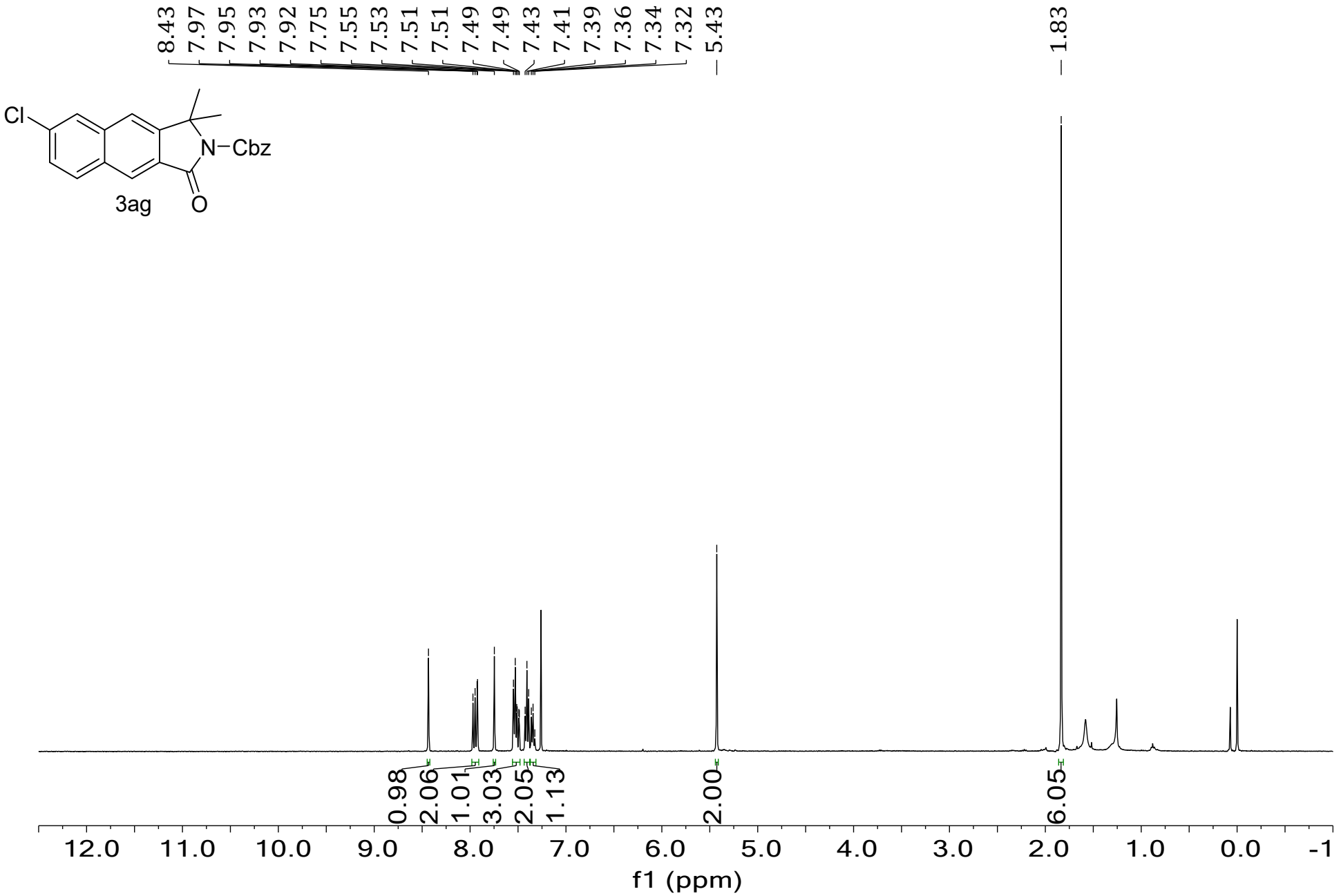
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3af**.



^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3af**.



^{19}F NMR (400 MHz, $CDCl_3$) spectra of **3af**.



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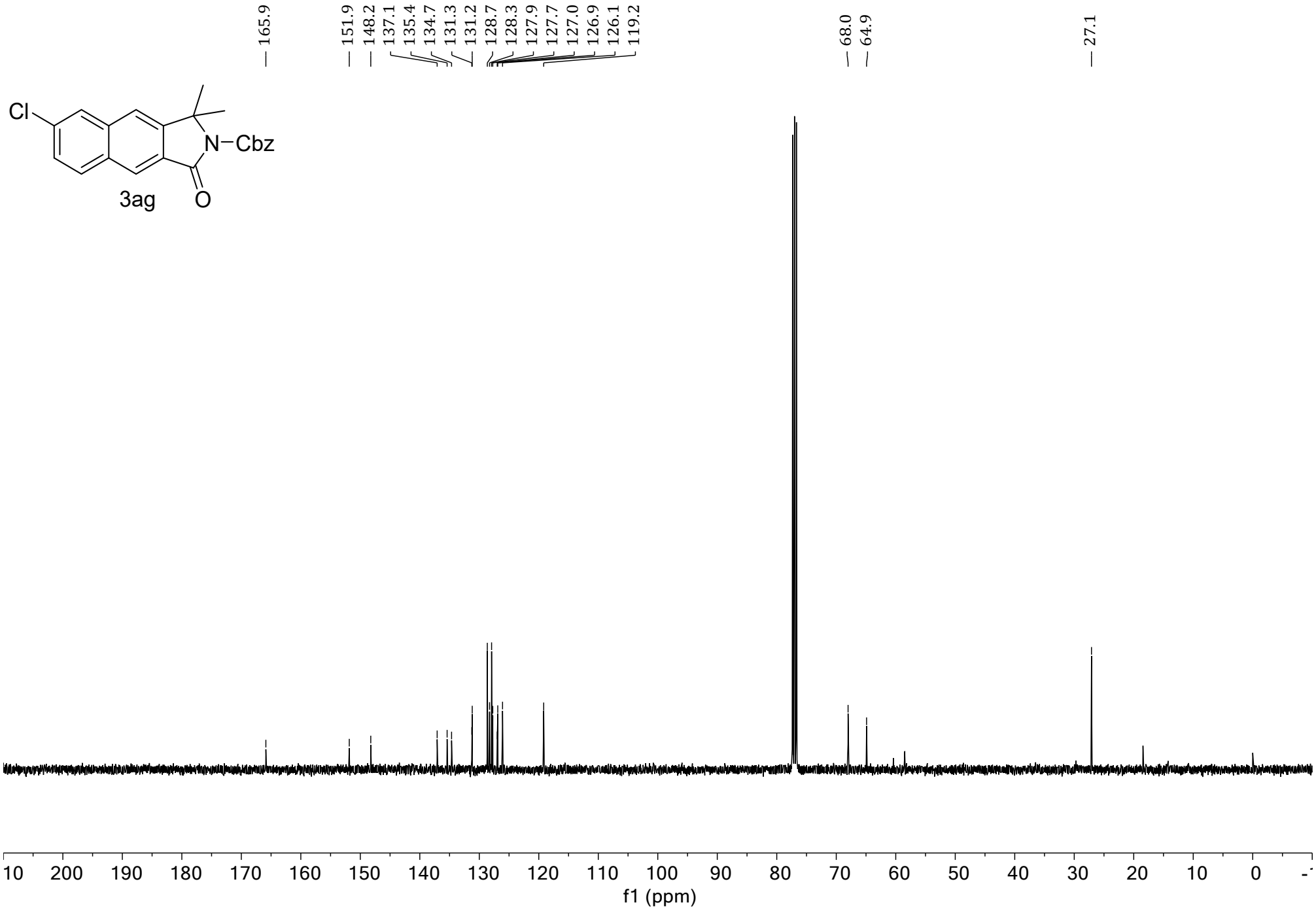
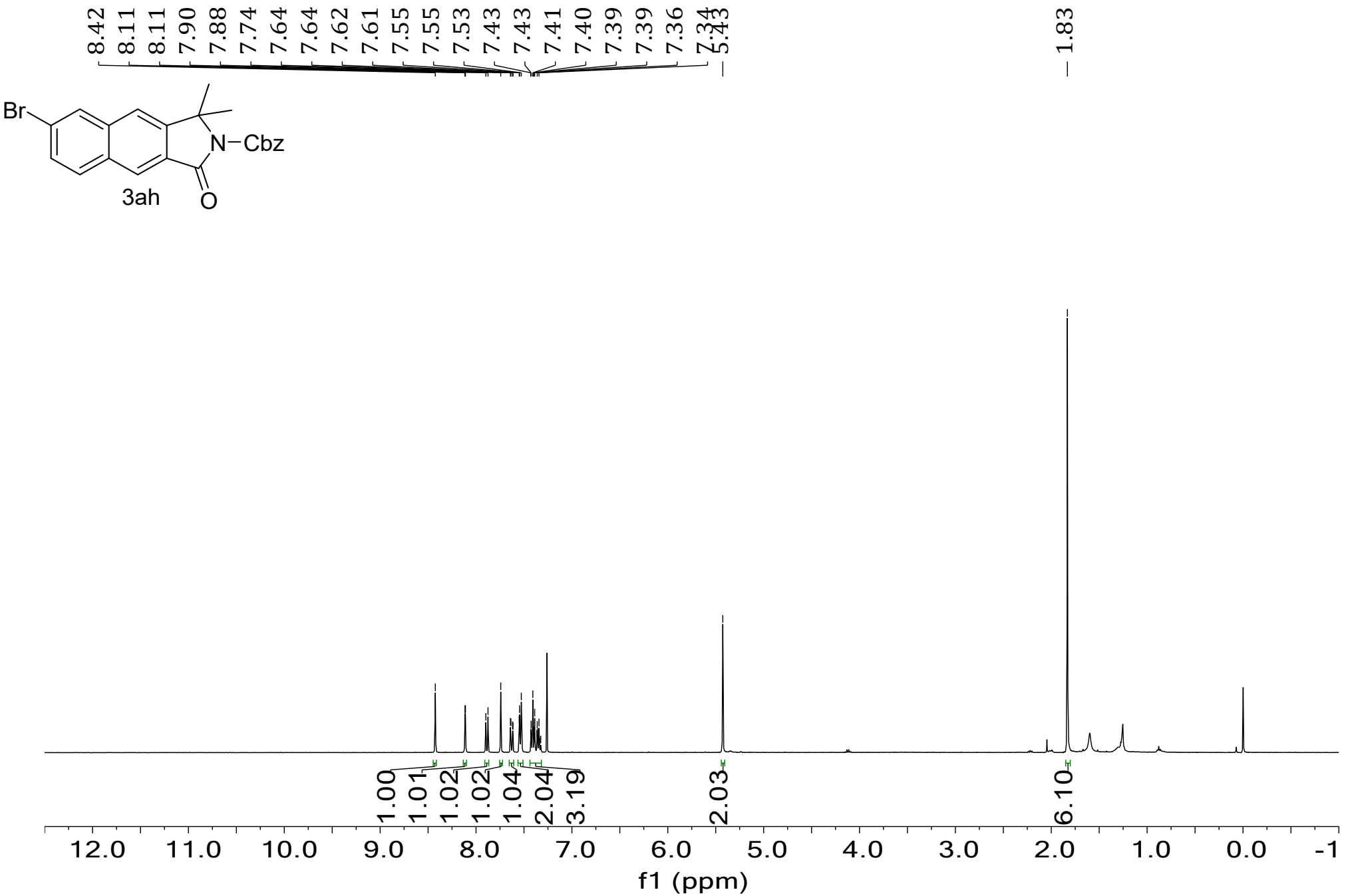
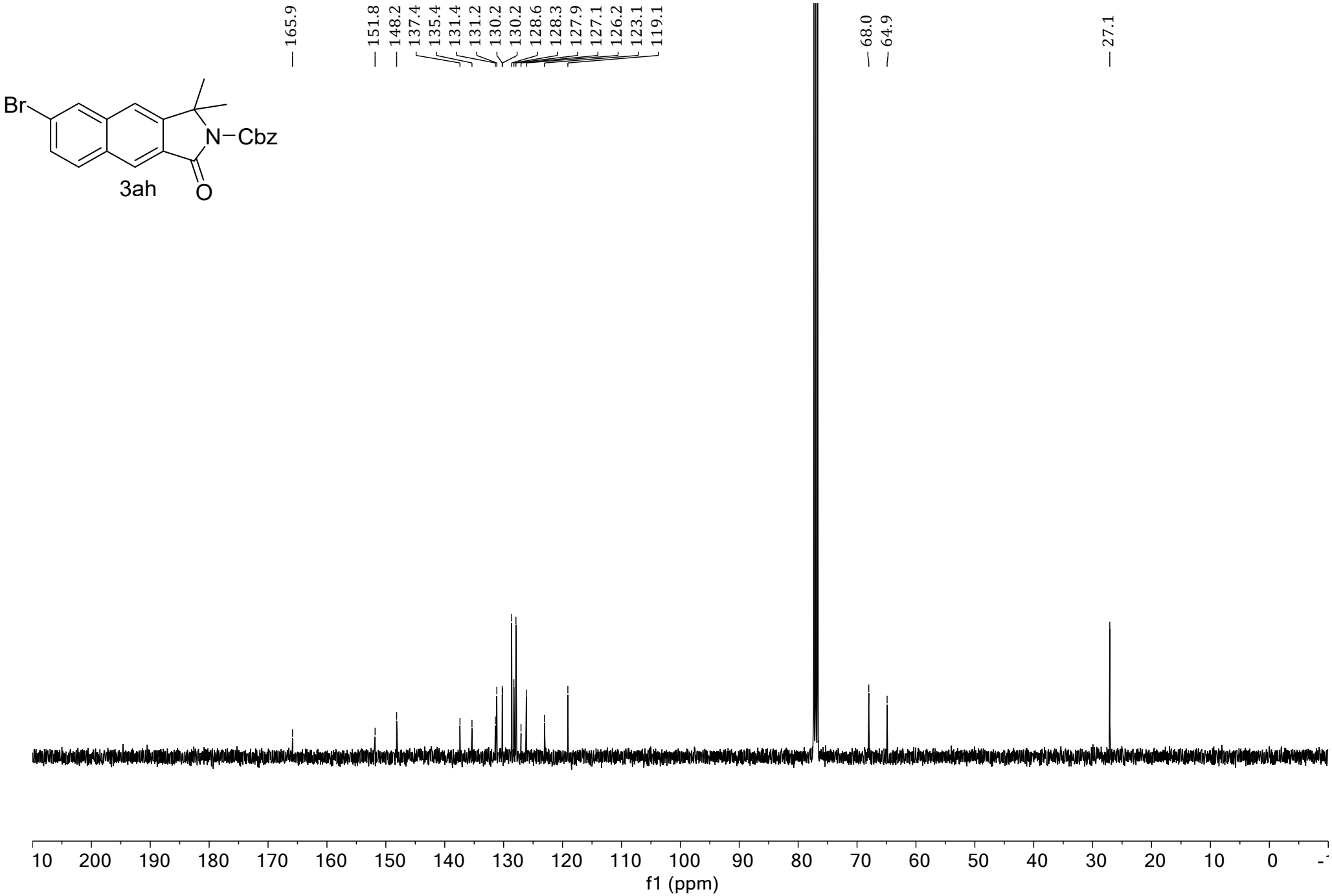


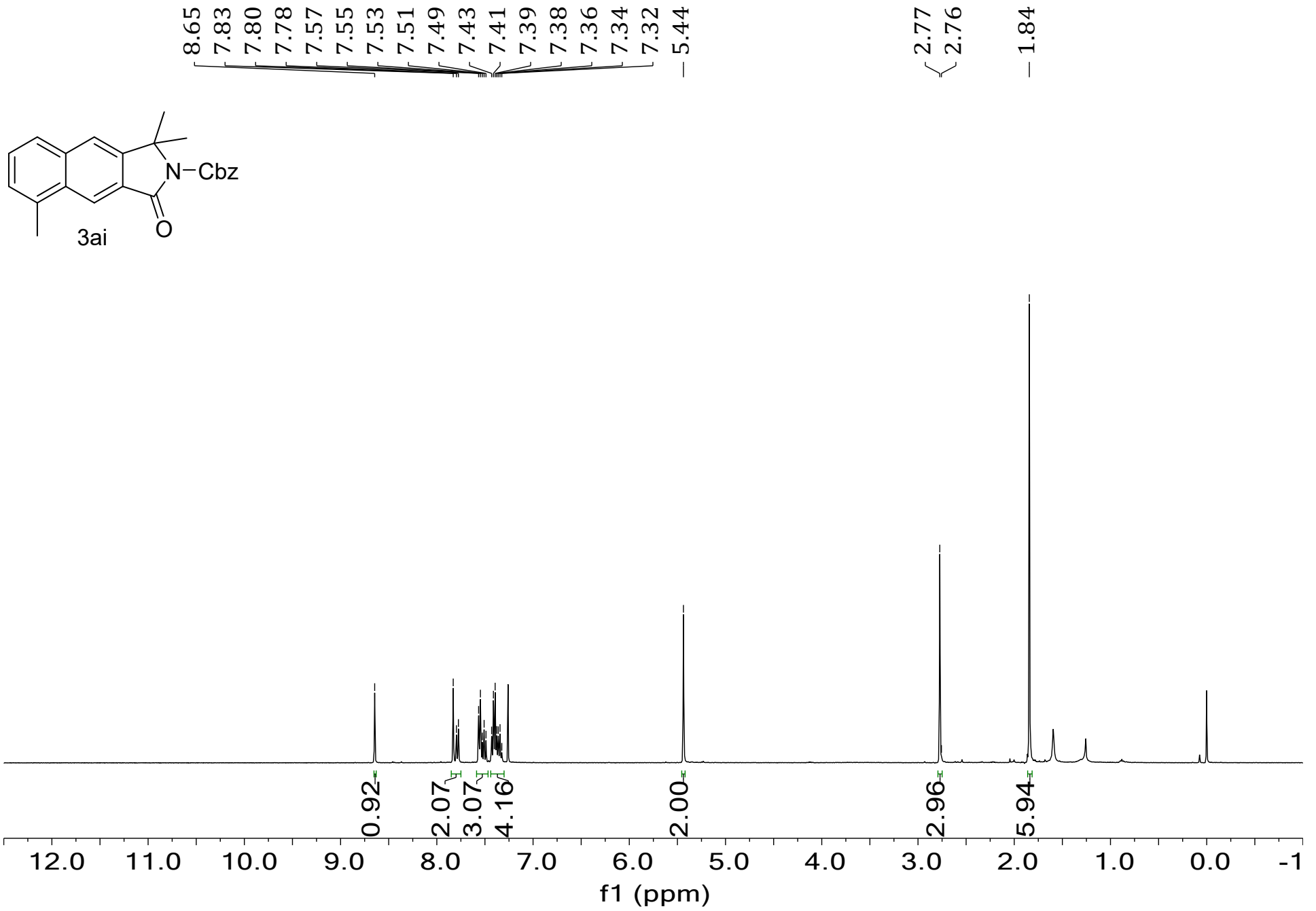
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ag**.



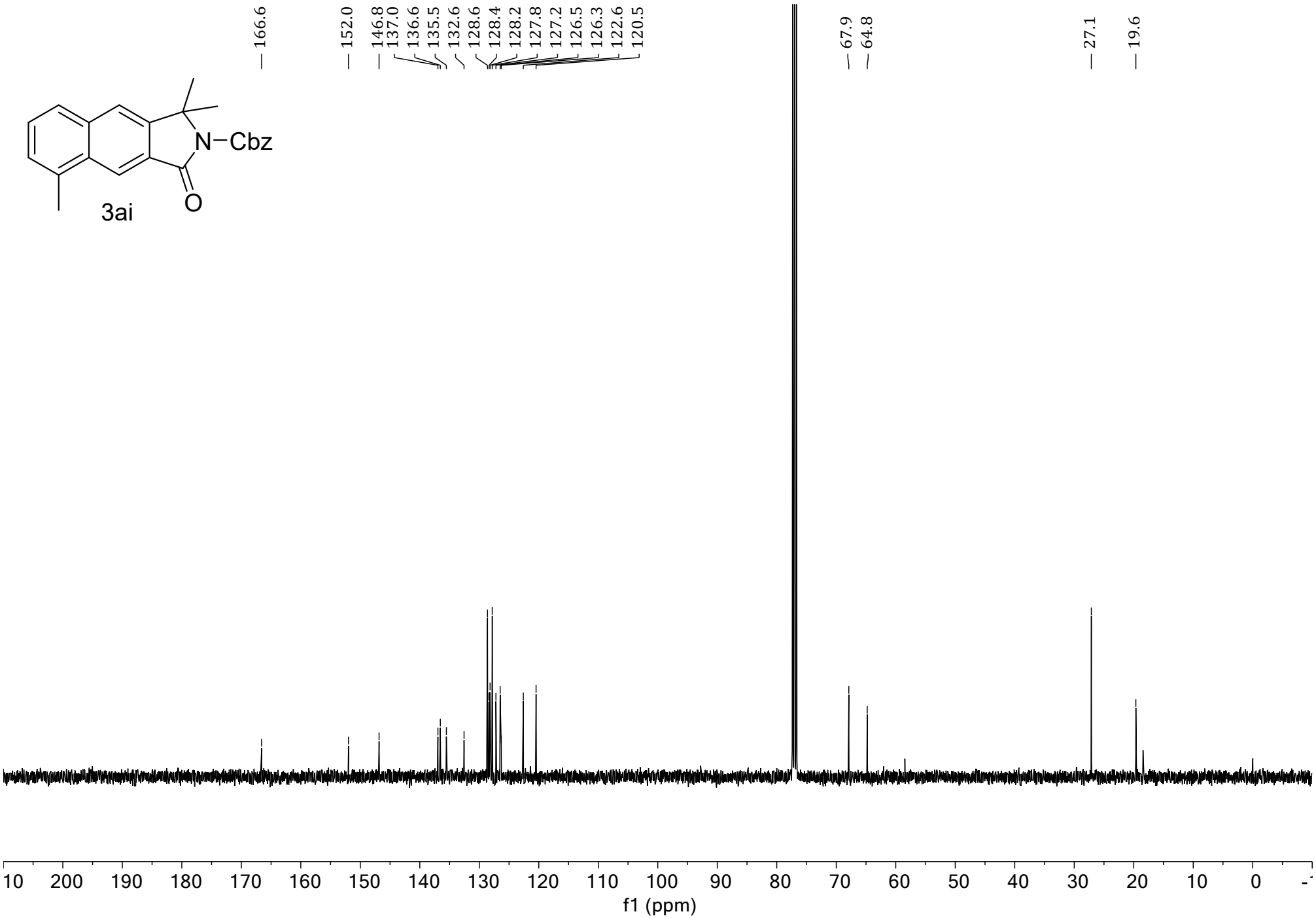
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ah**.



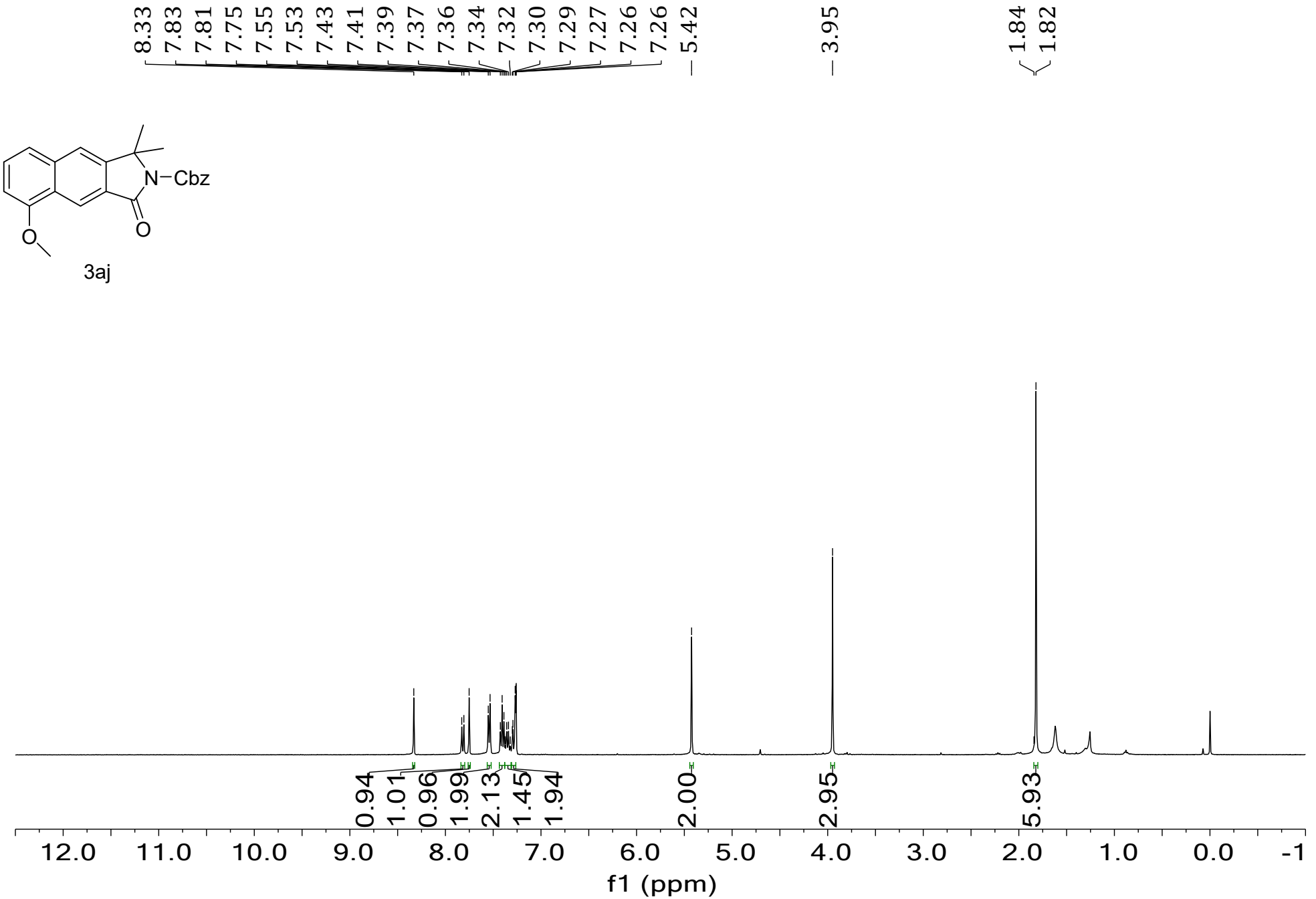
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ah**.



^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ai**.

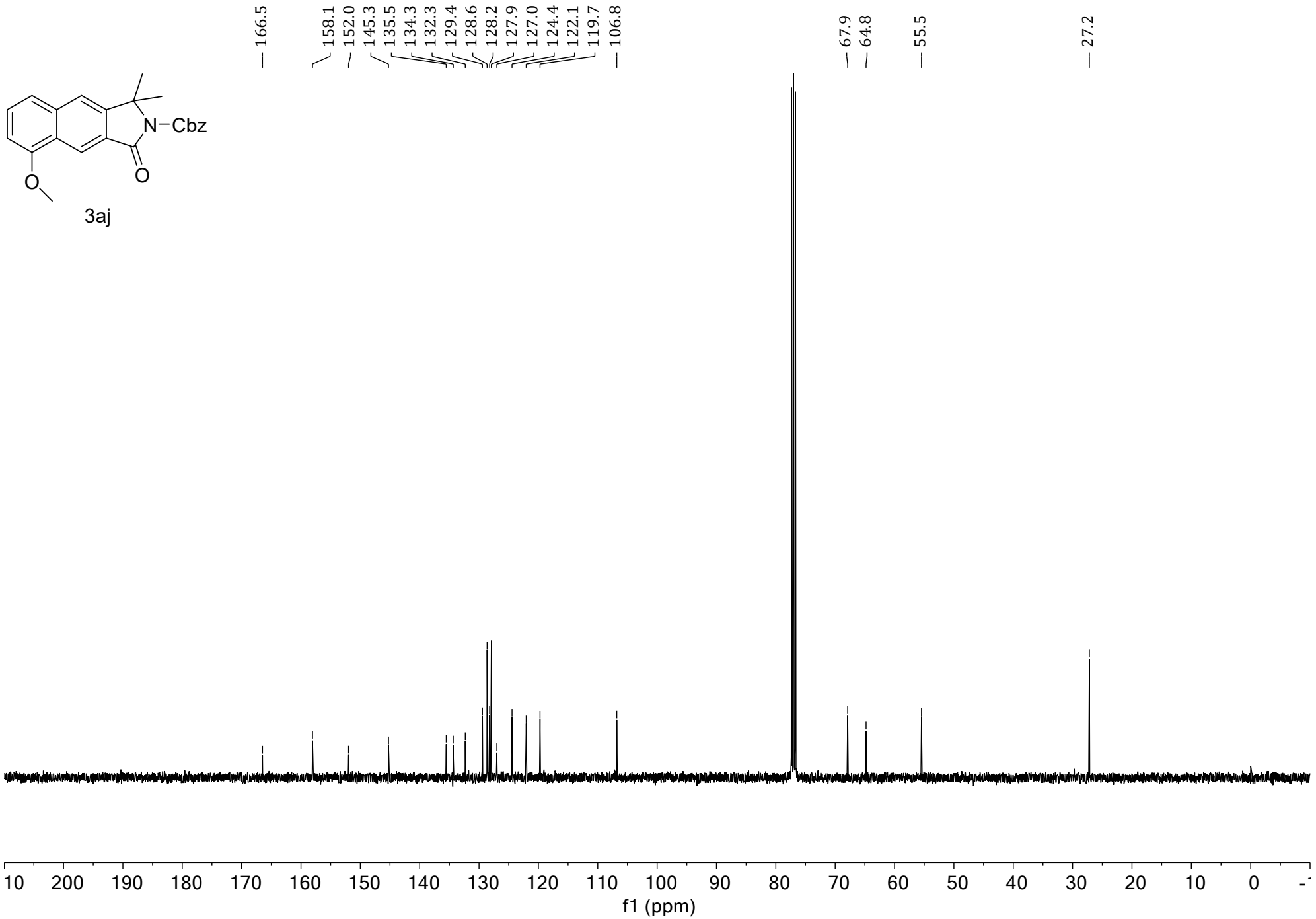


^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ai**.

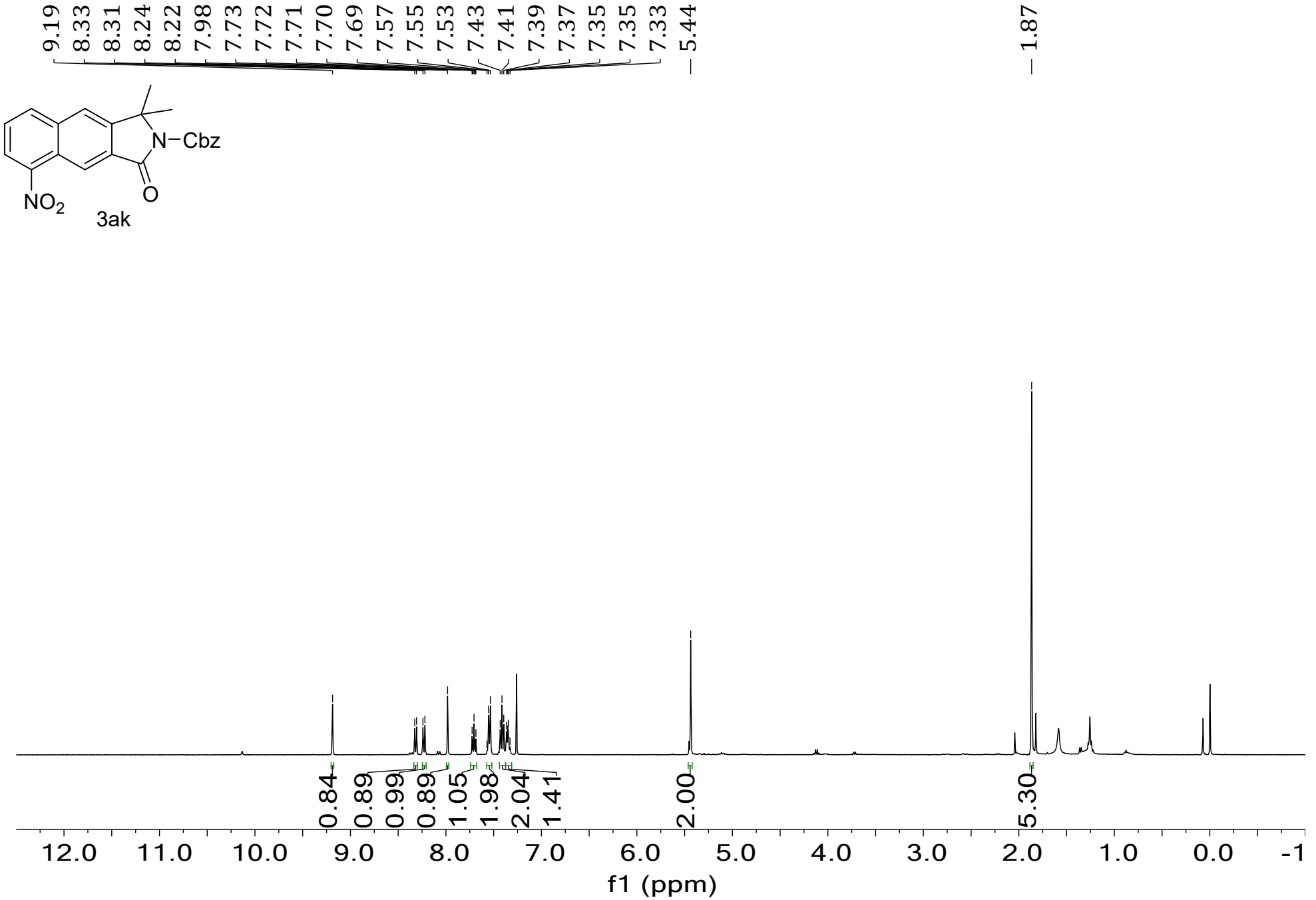


3aj

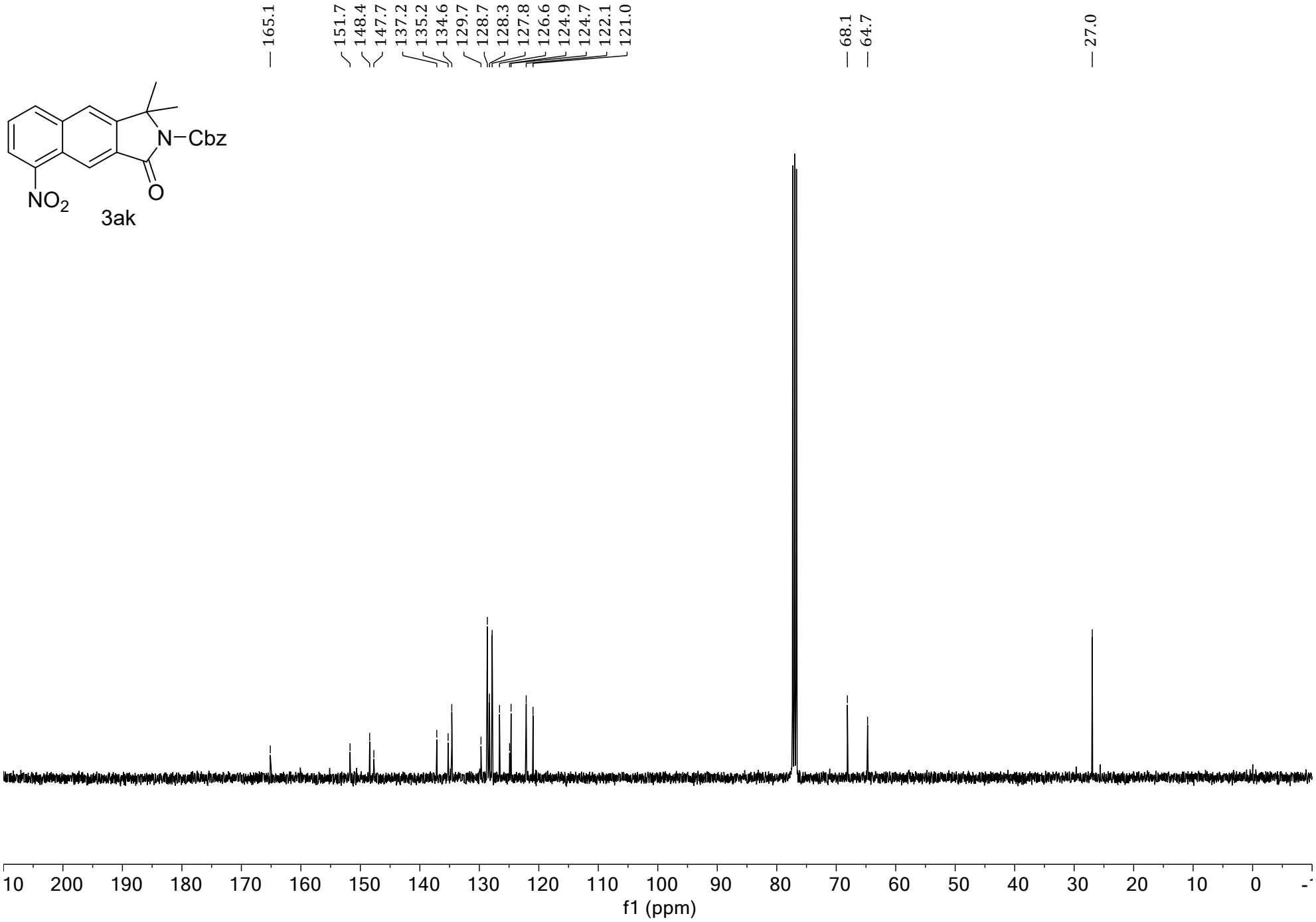
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3aj**.



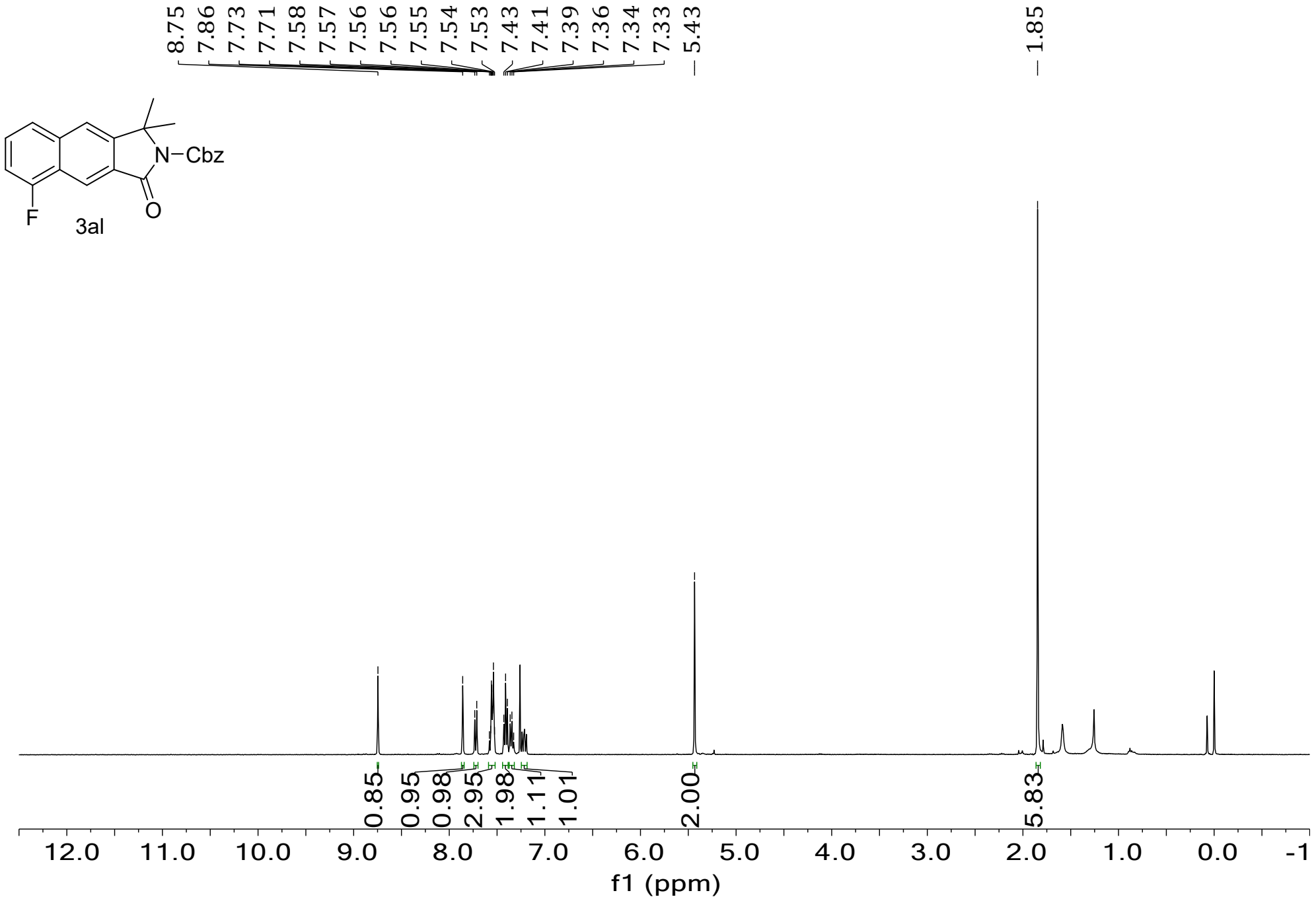
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3aj**.



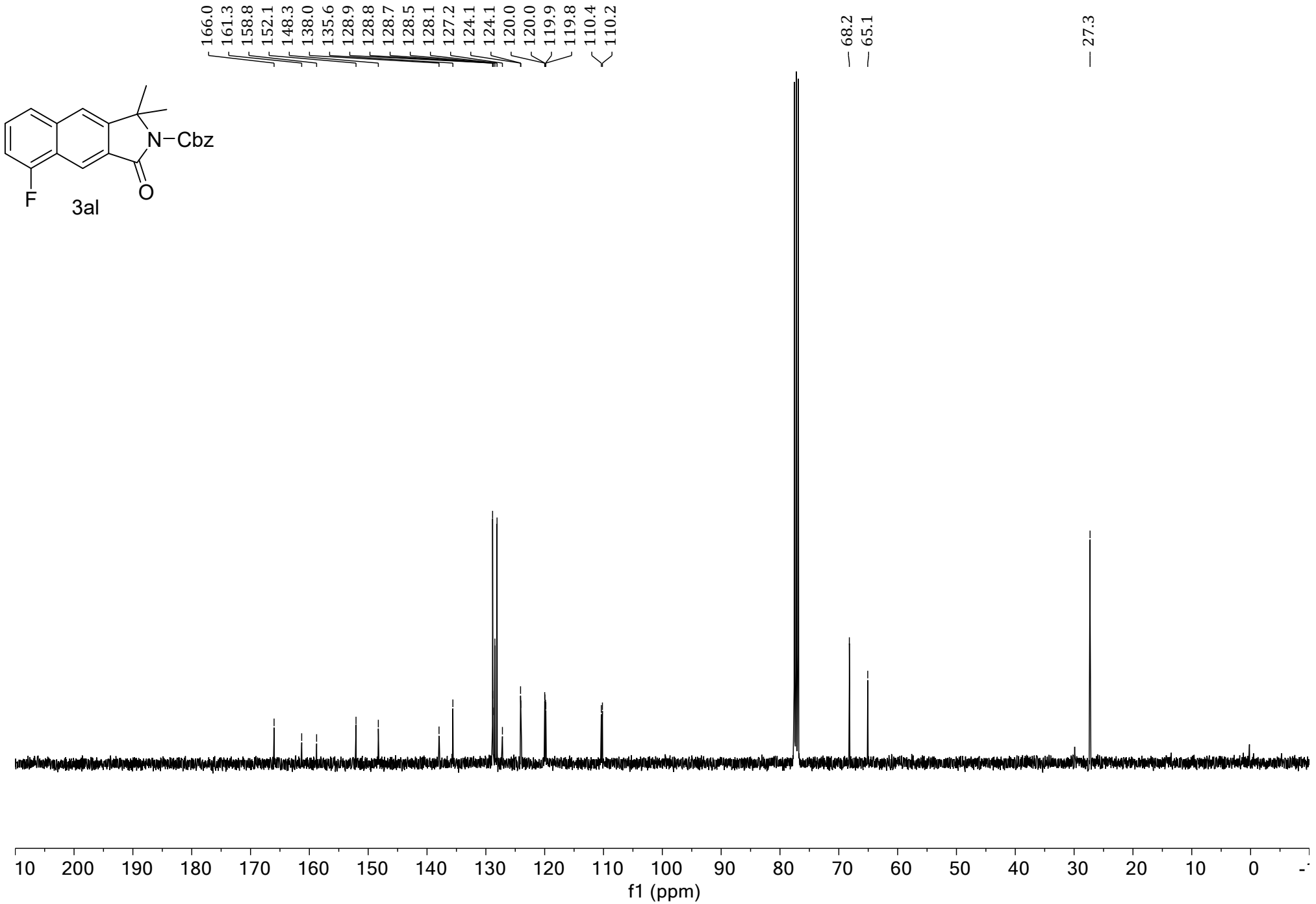
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ak**.



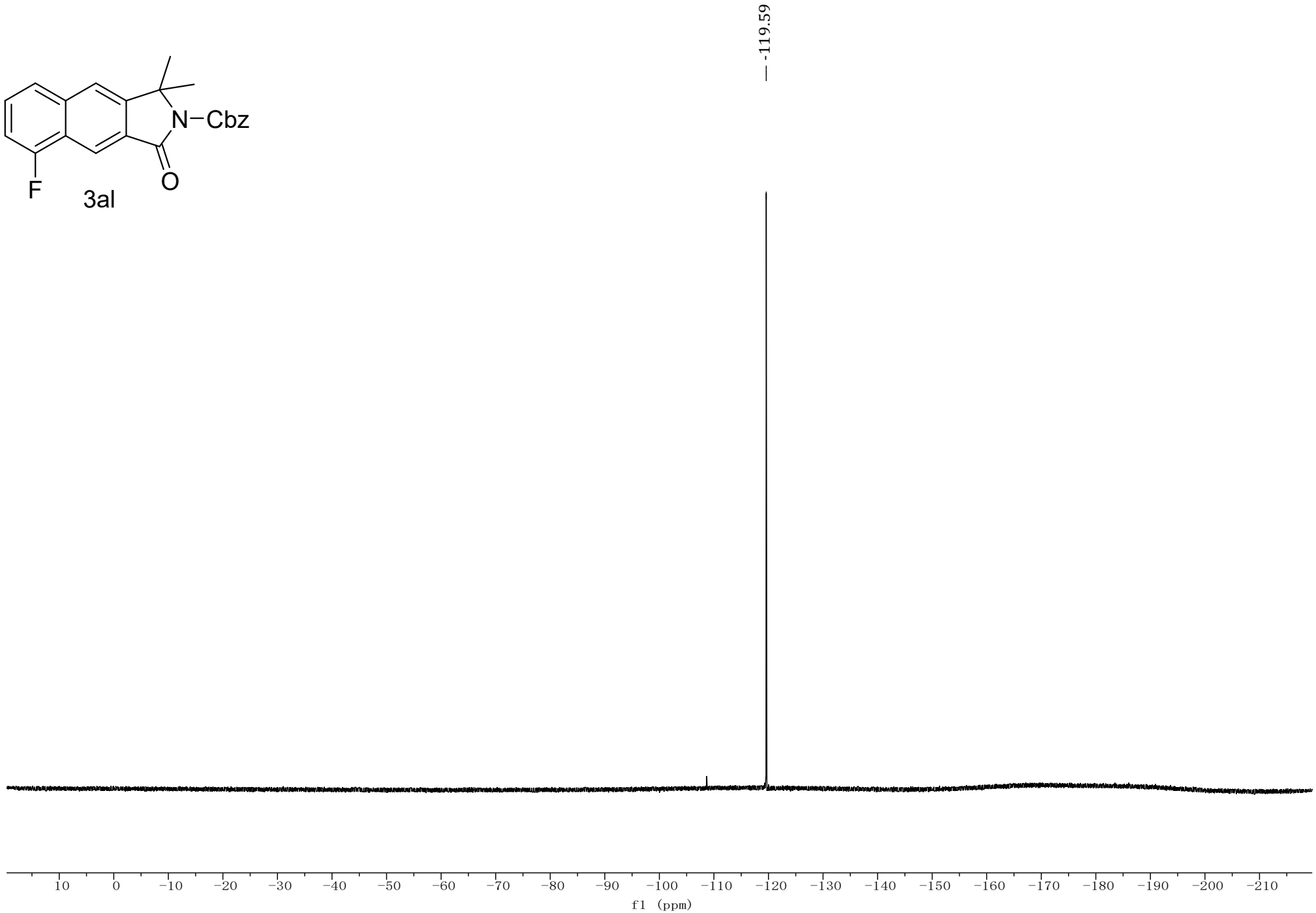
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ak**.



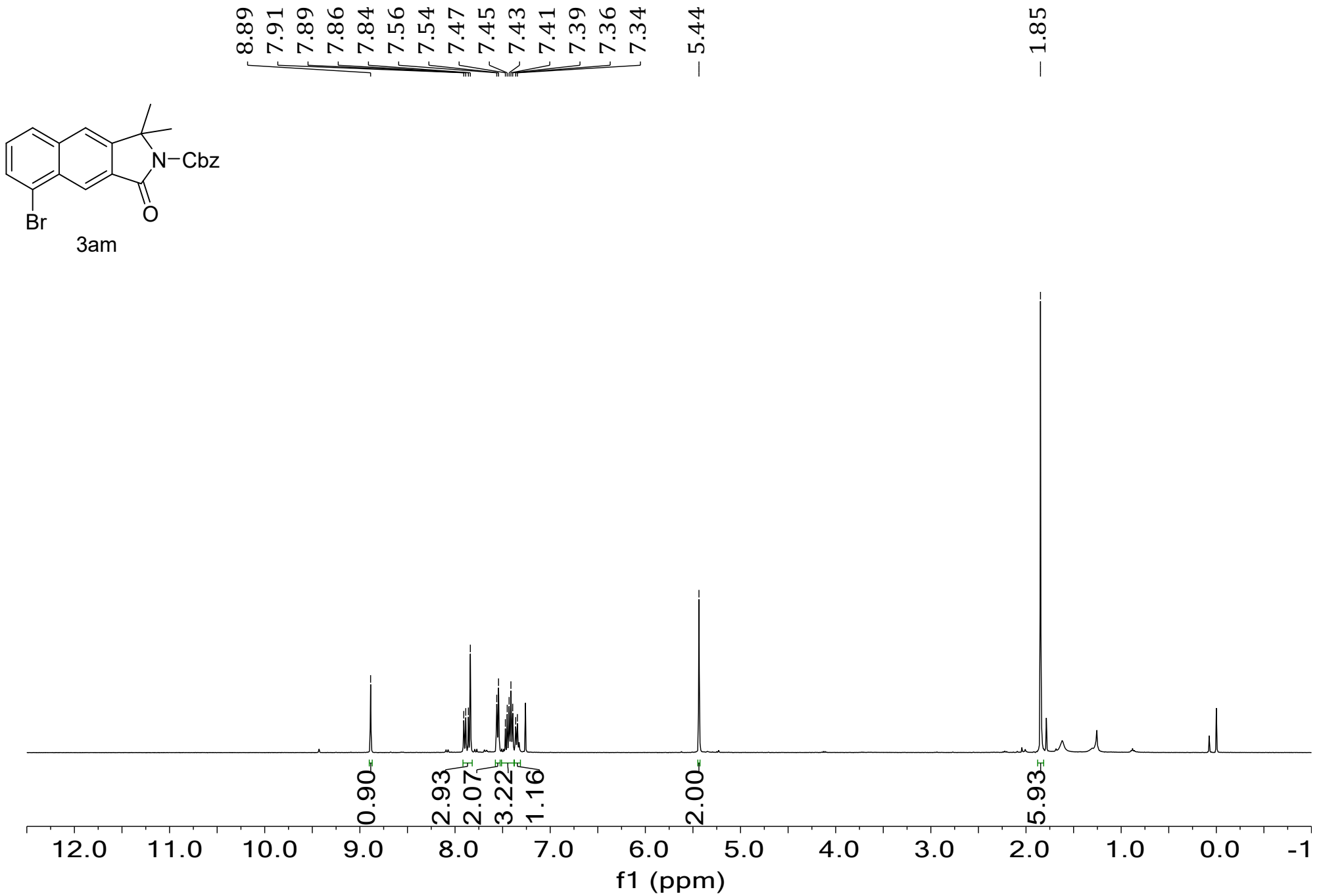
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3al**.



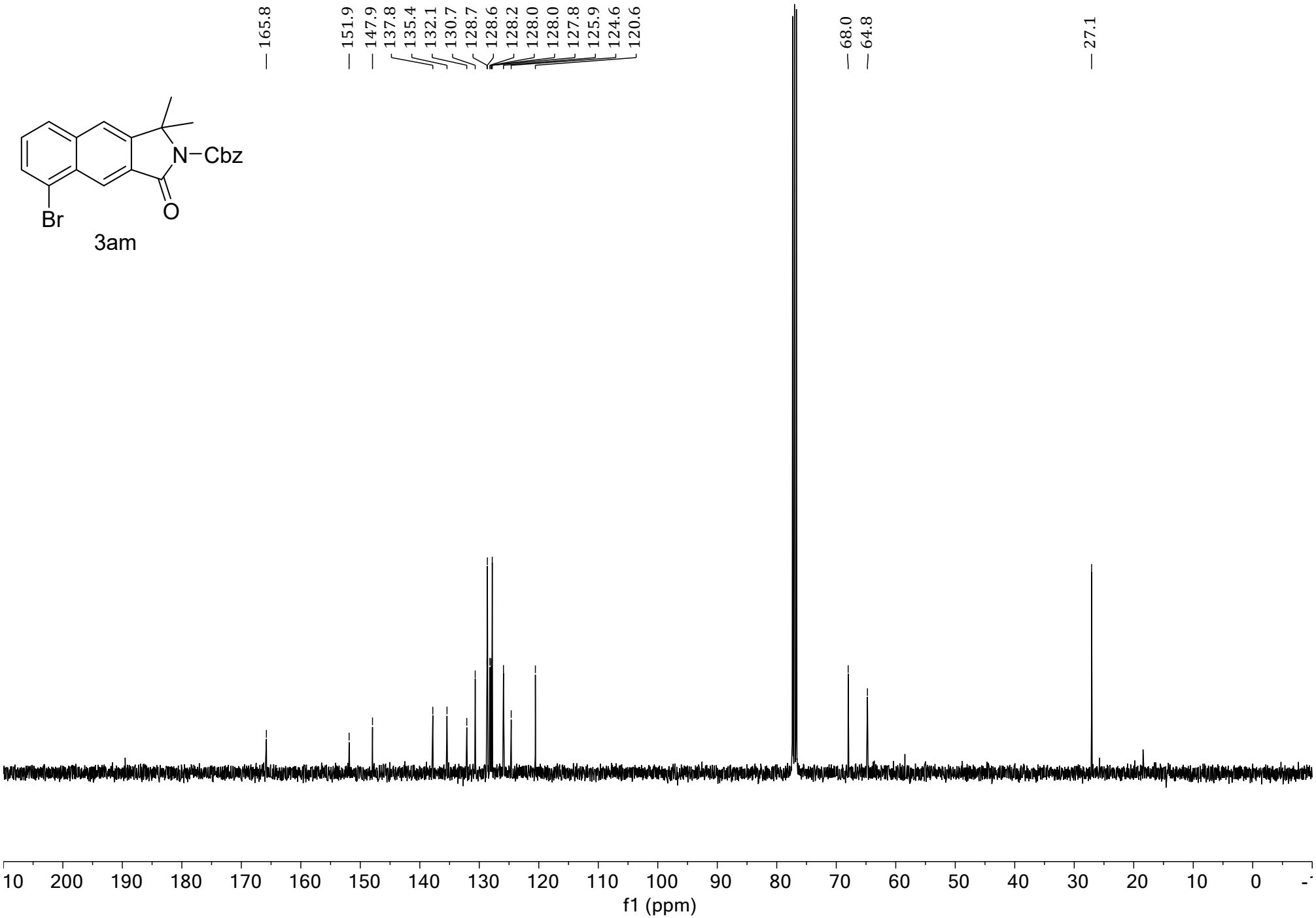
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3al**.



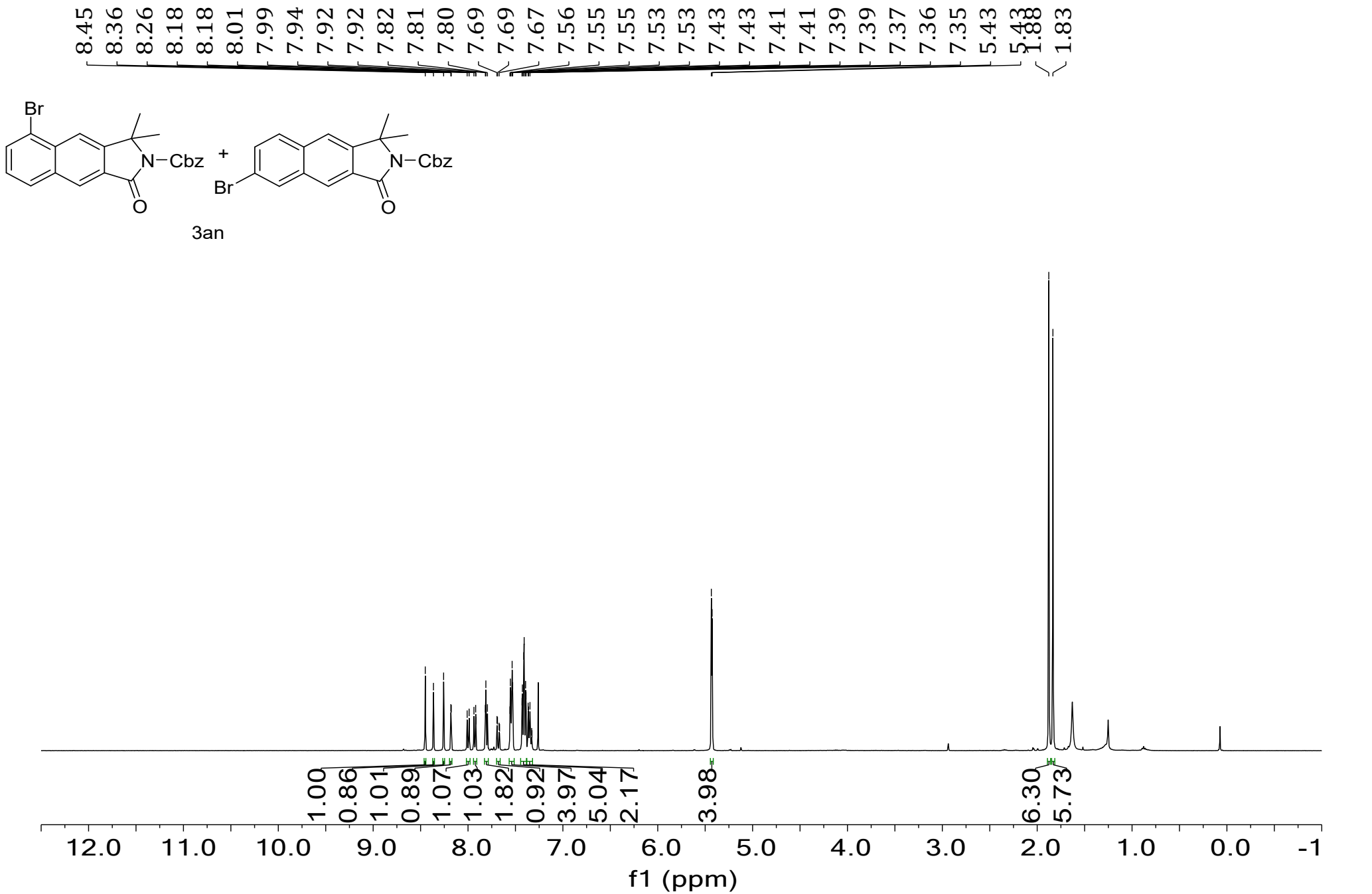
^{19}F NMR (400 MHz, $CDCl_3$) spectra of **3al**.



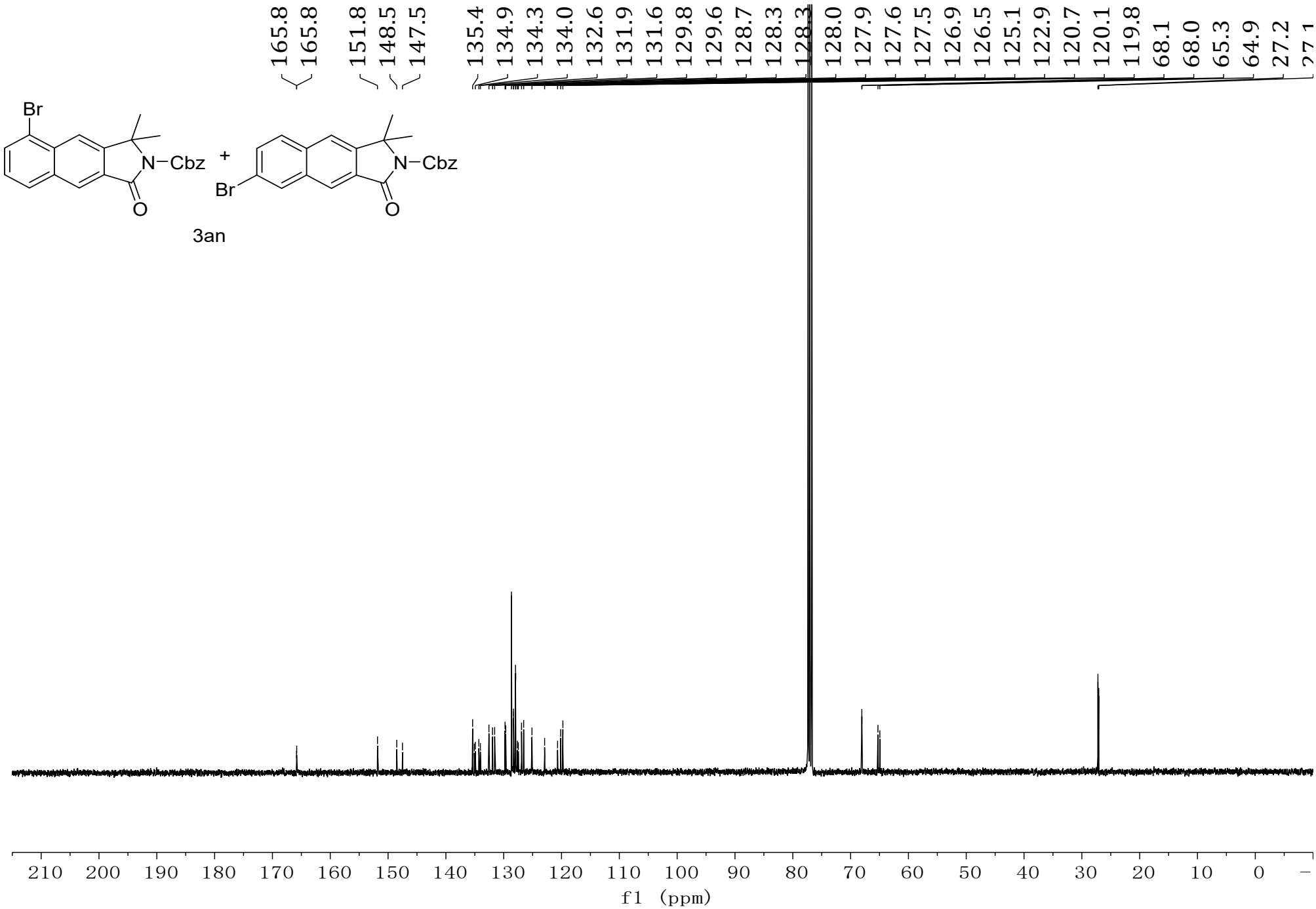
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3am**.



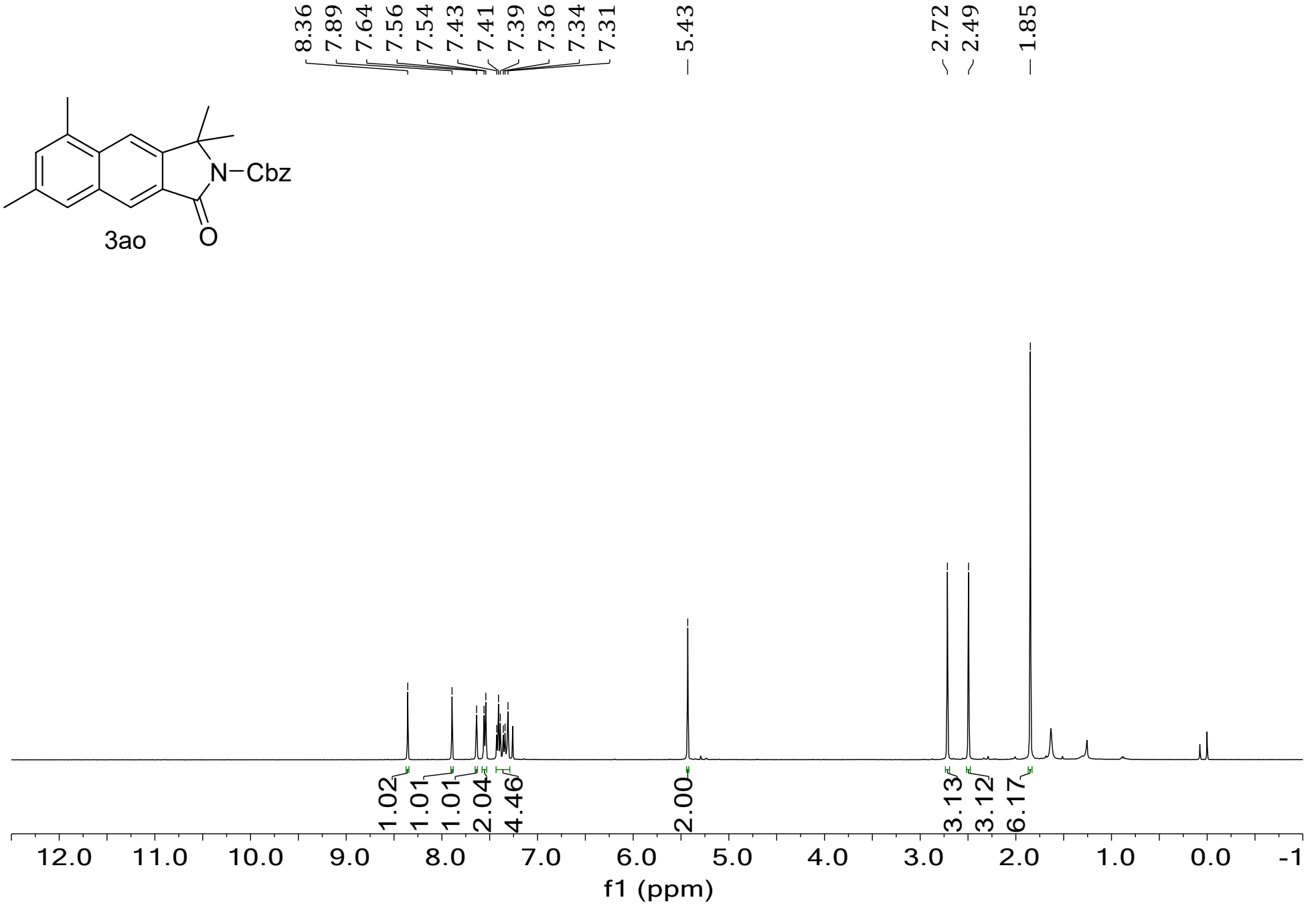
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3am**.



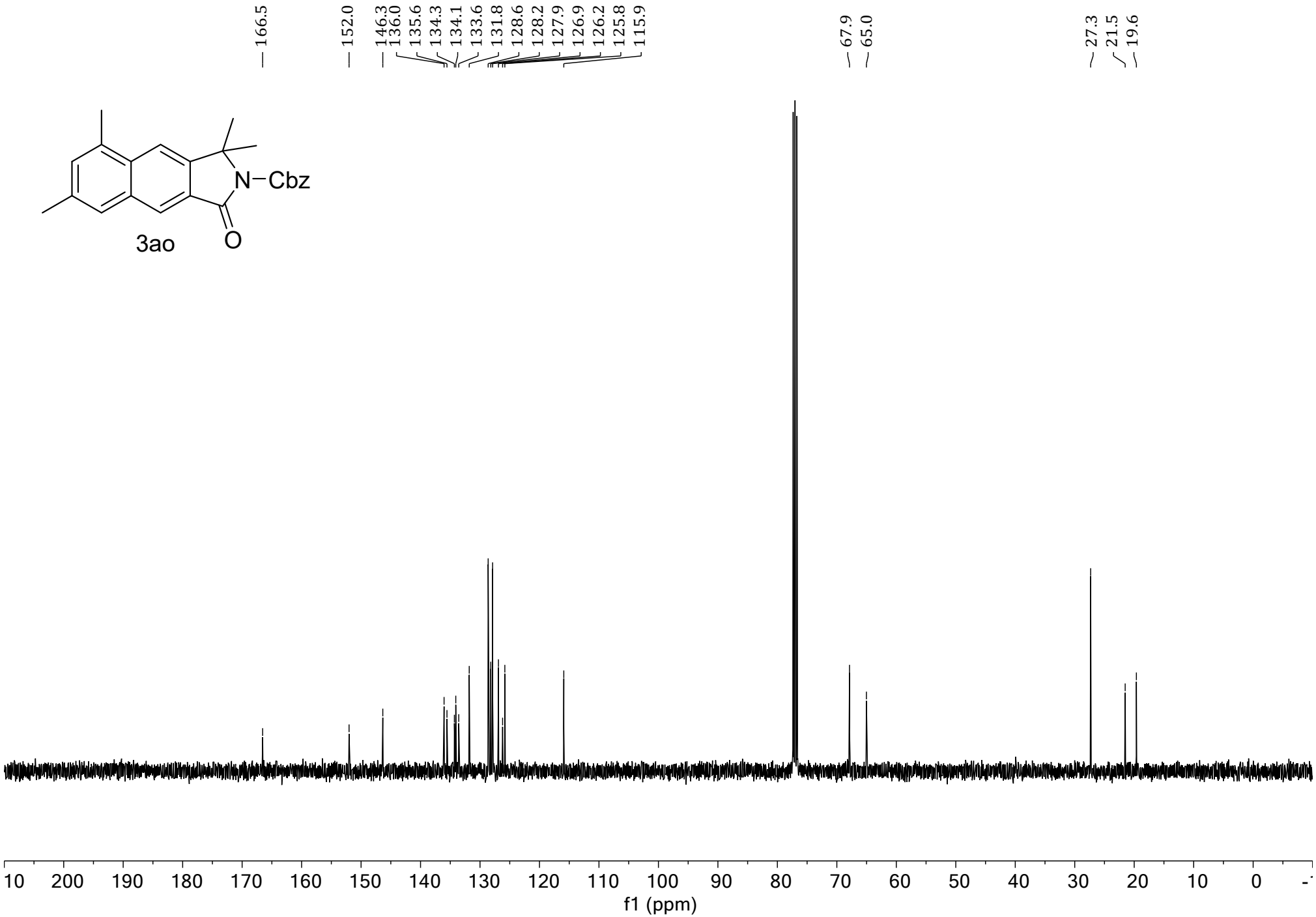
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3an**.



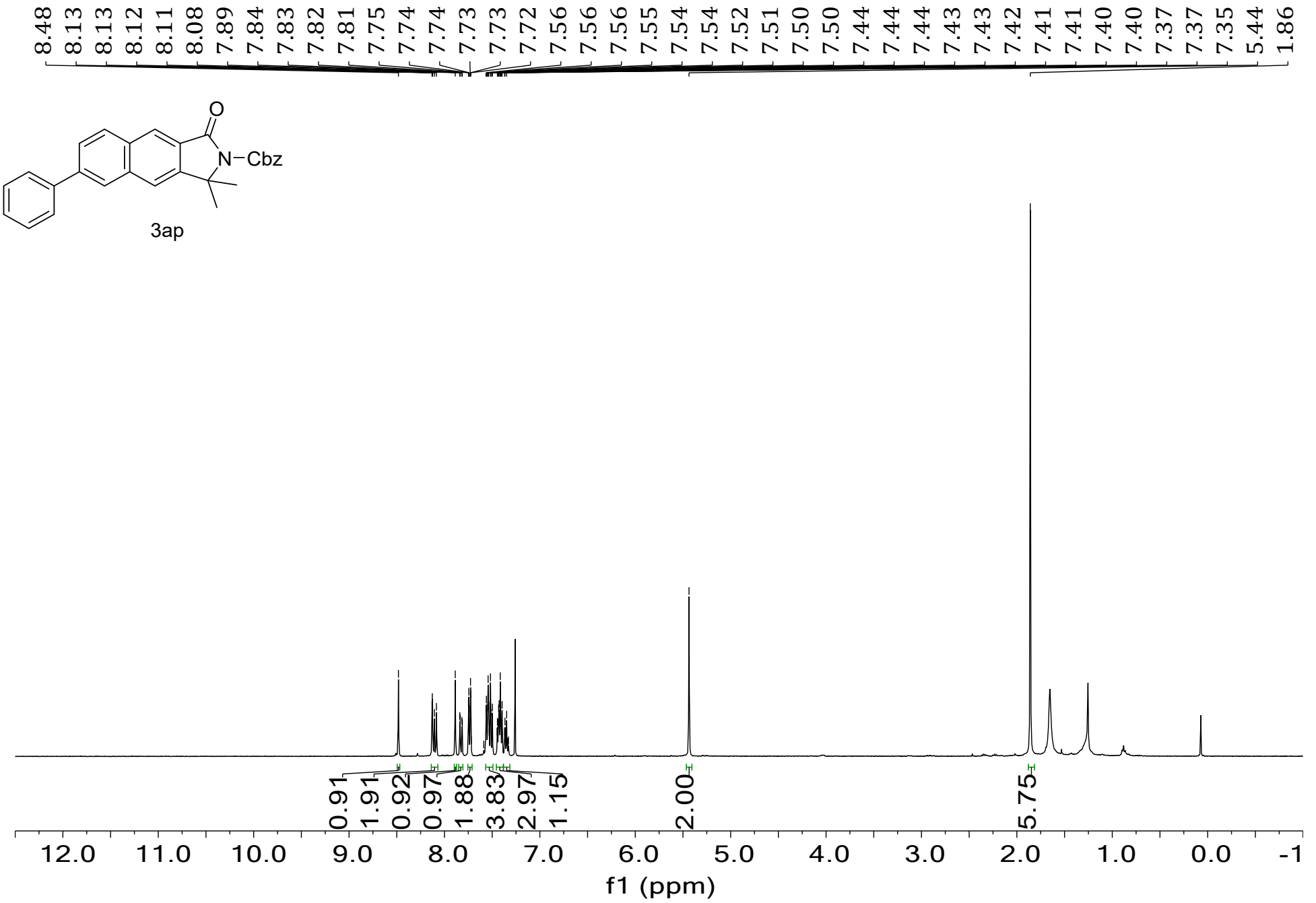
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3an**.



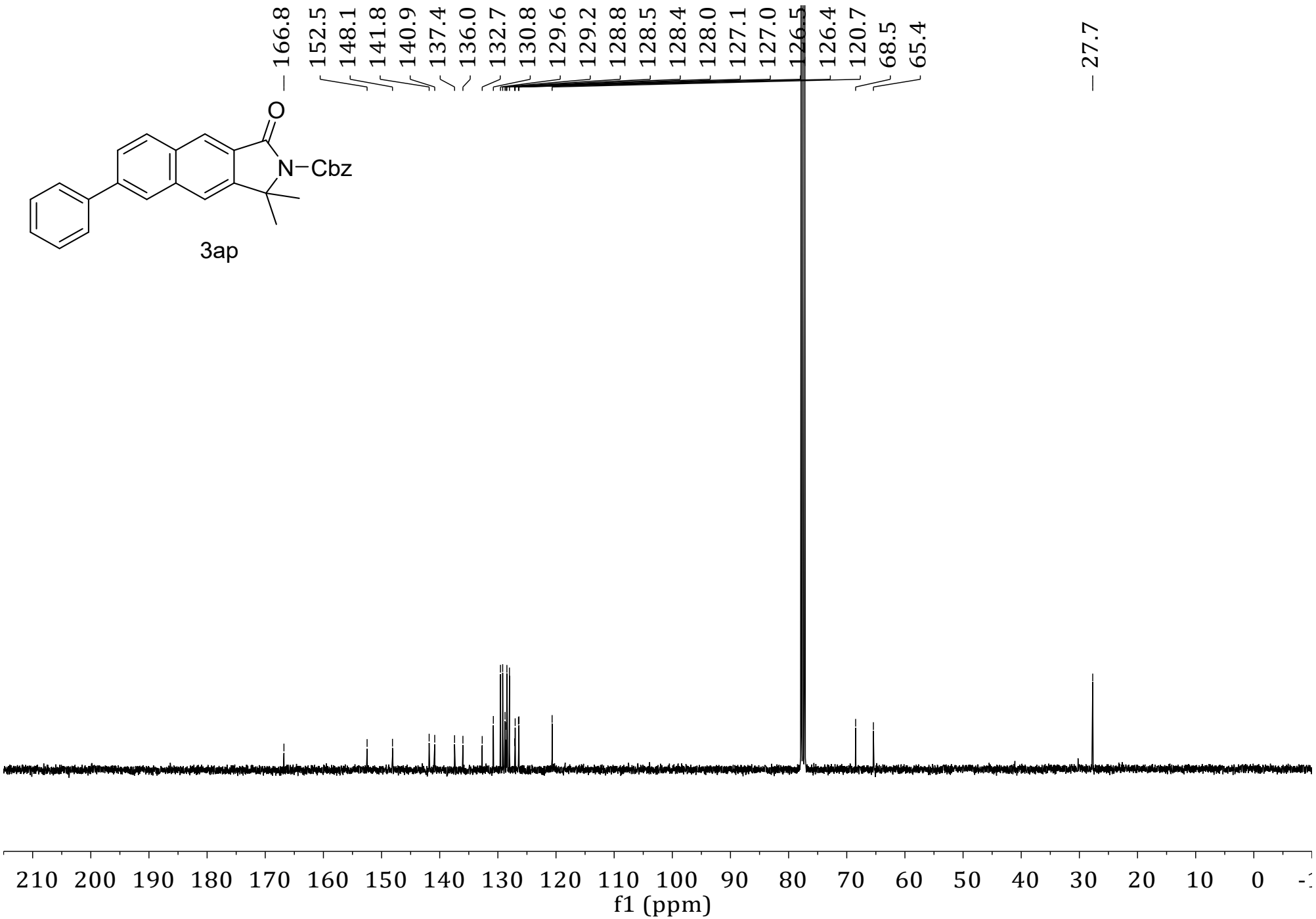
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ao**.



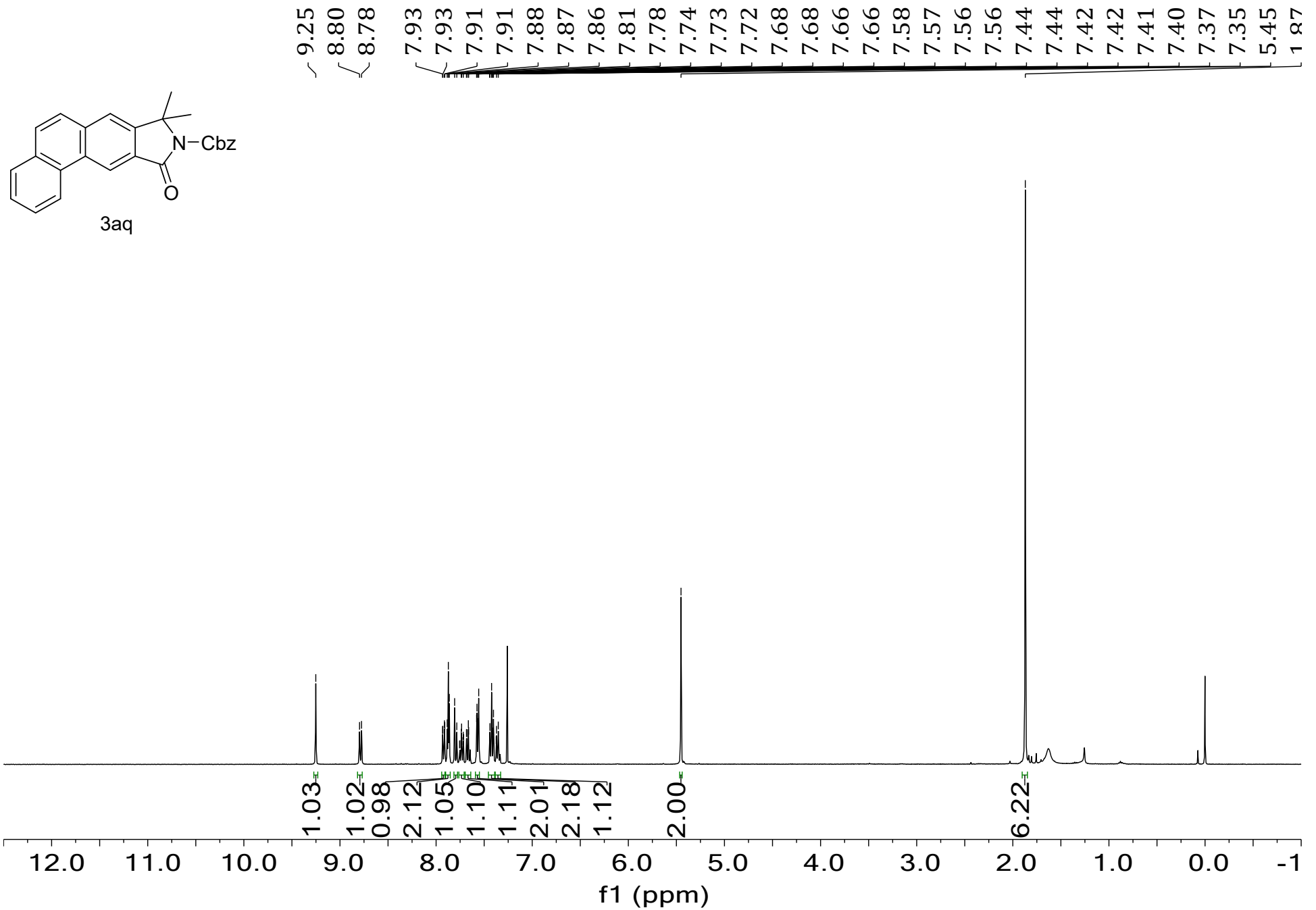
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ao**.



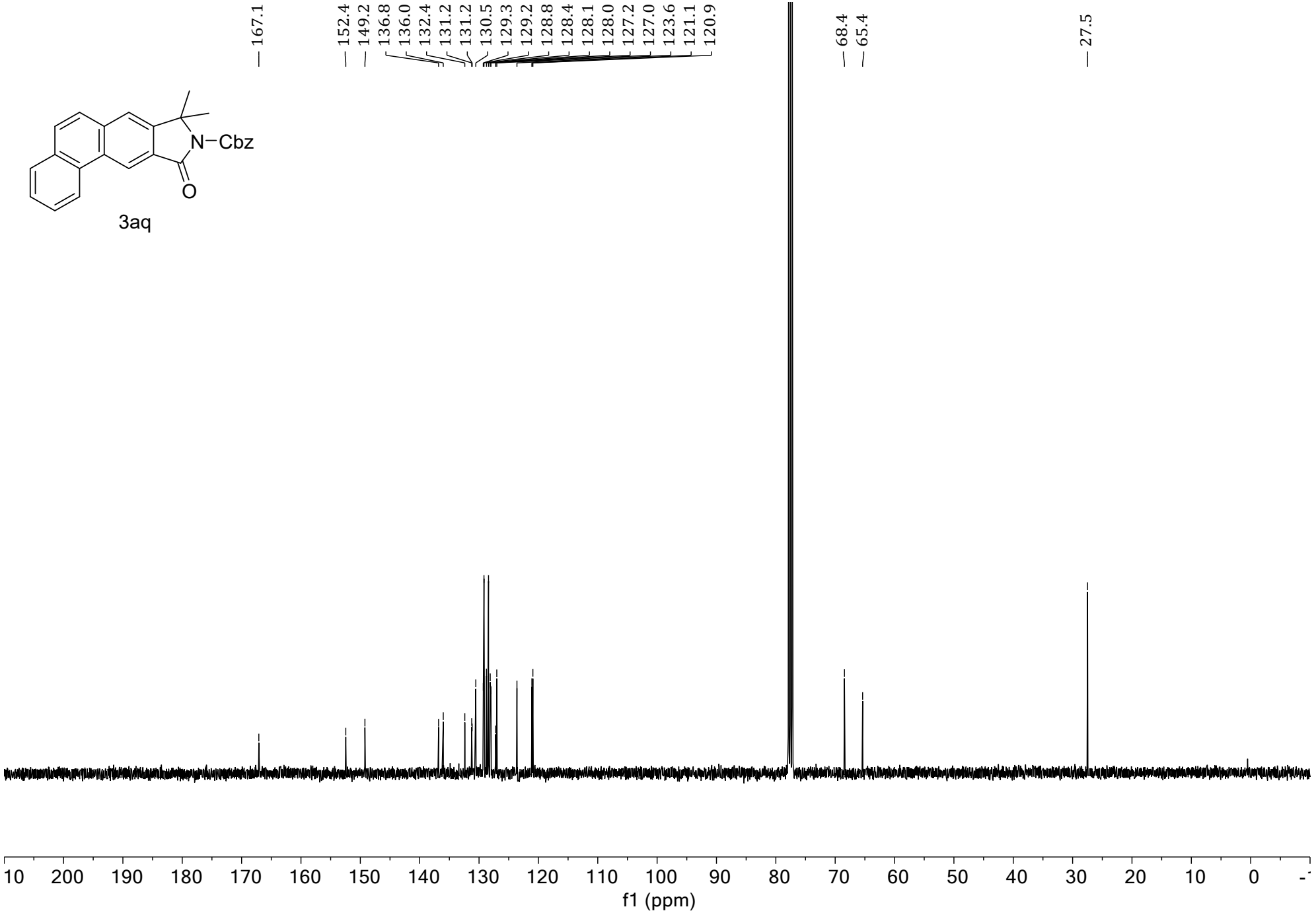
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ap**.



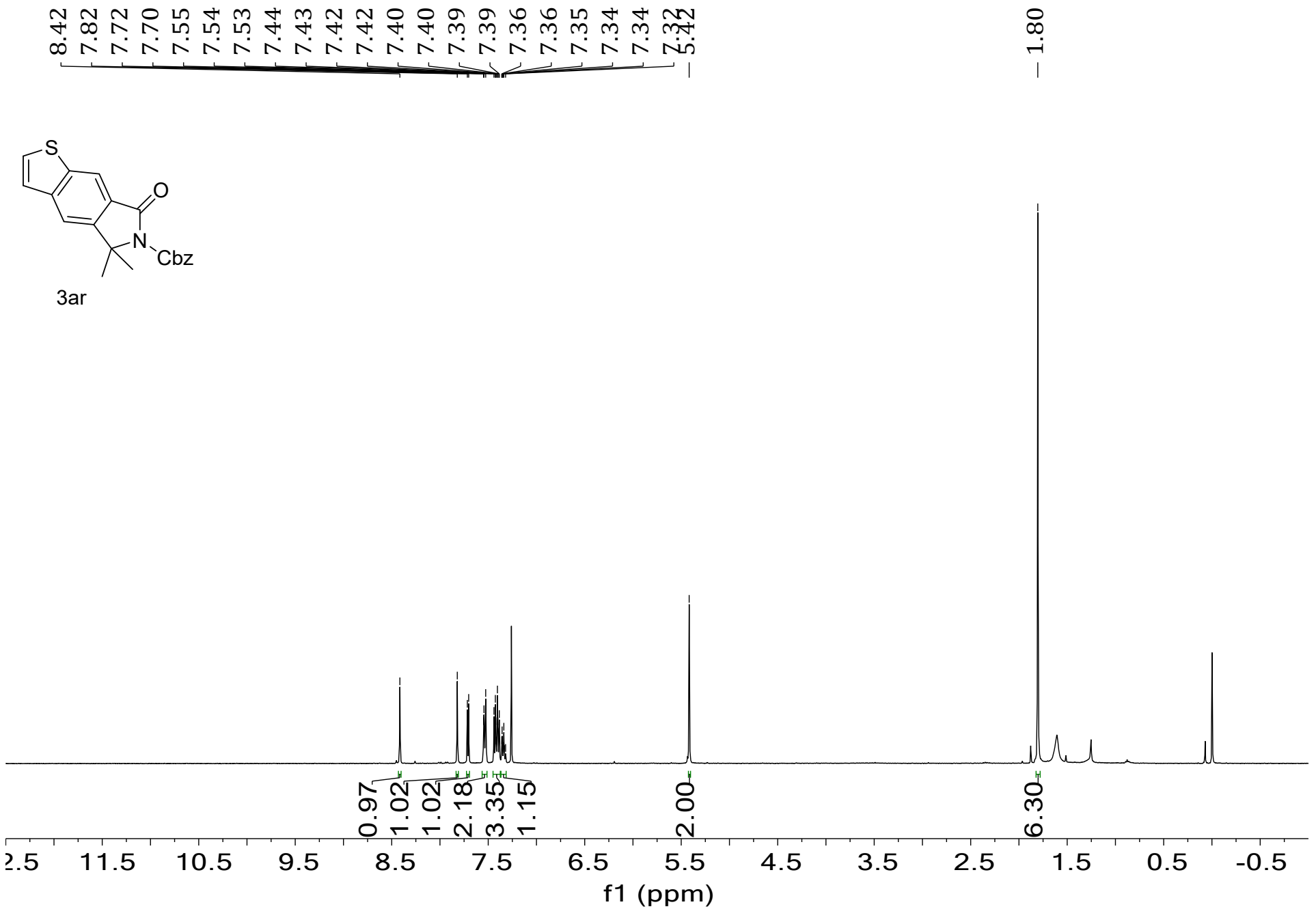
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ap**.



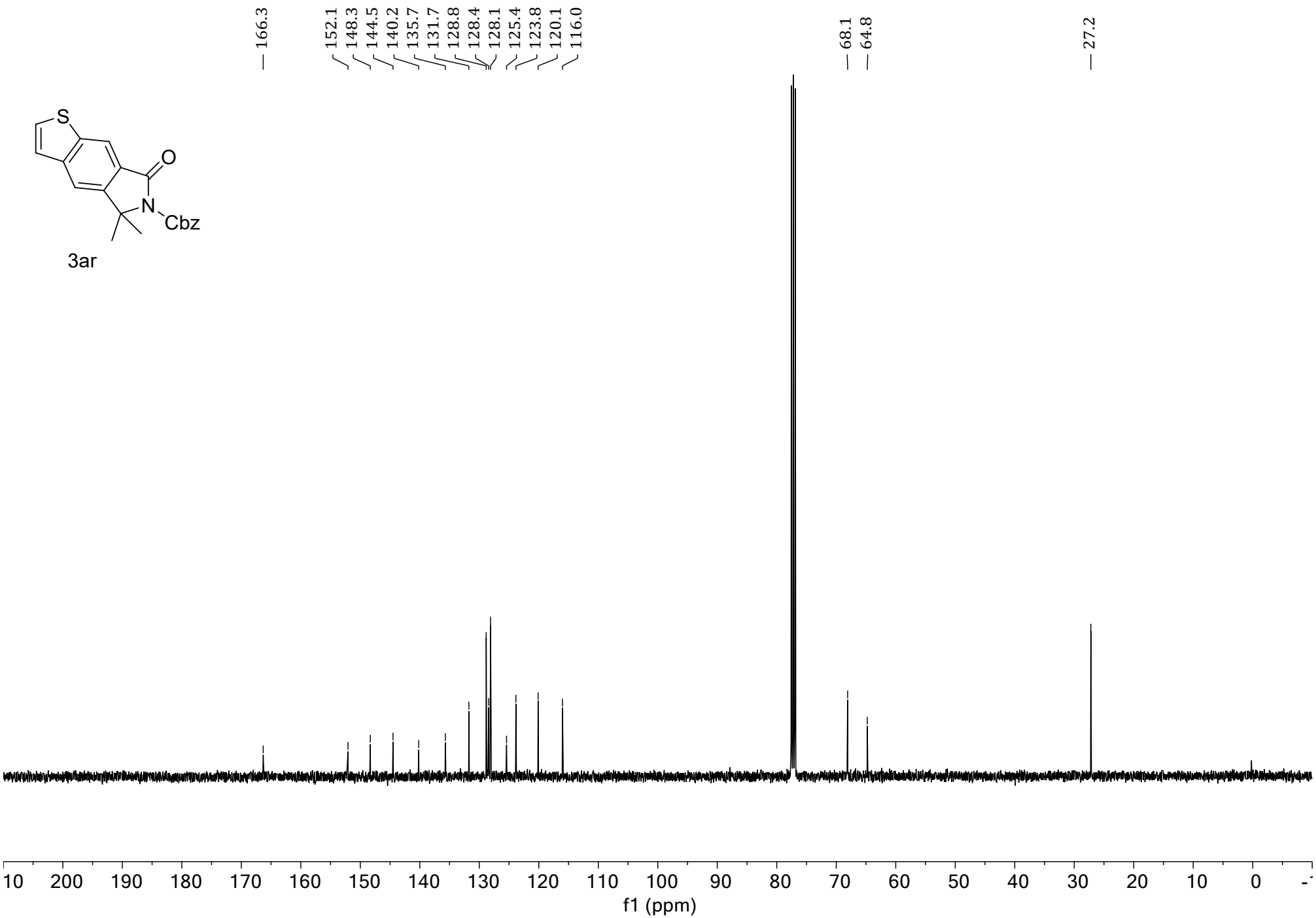
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3aq**.



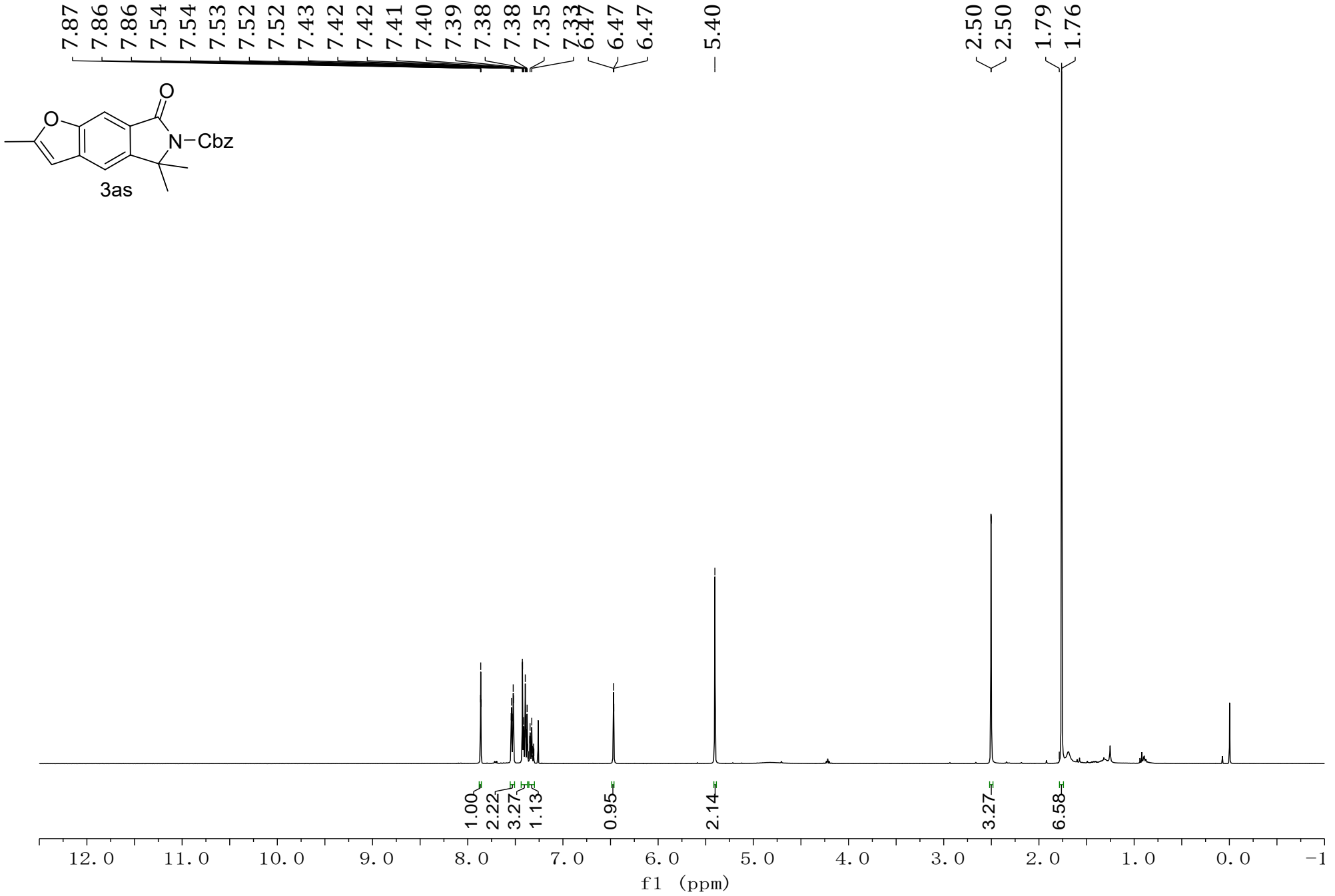
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3aq**.



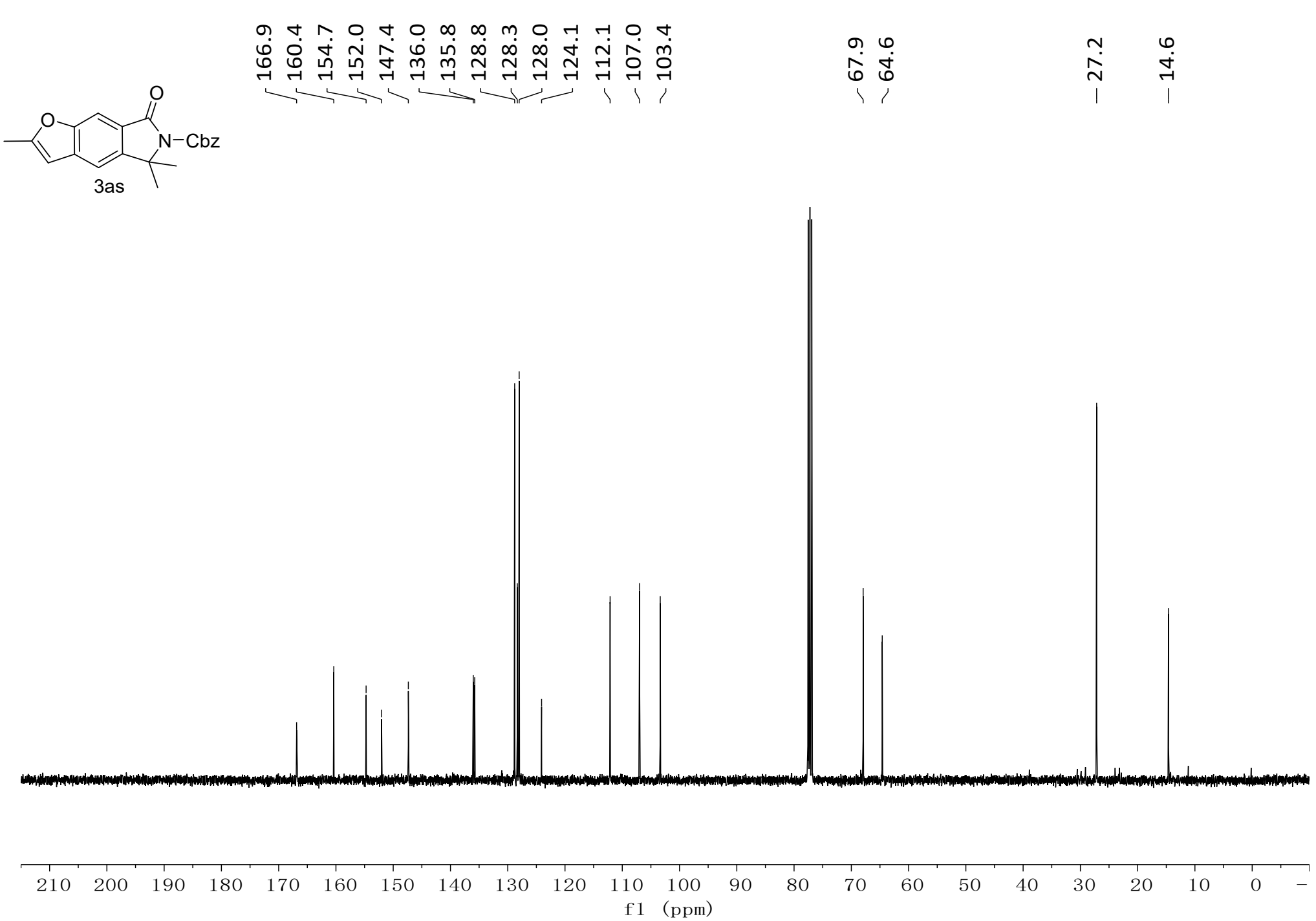
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ar**.



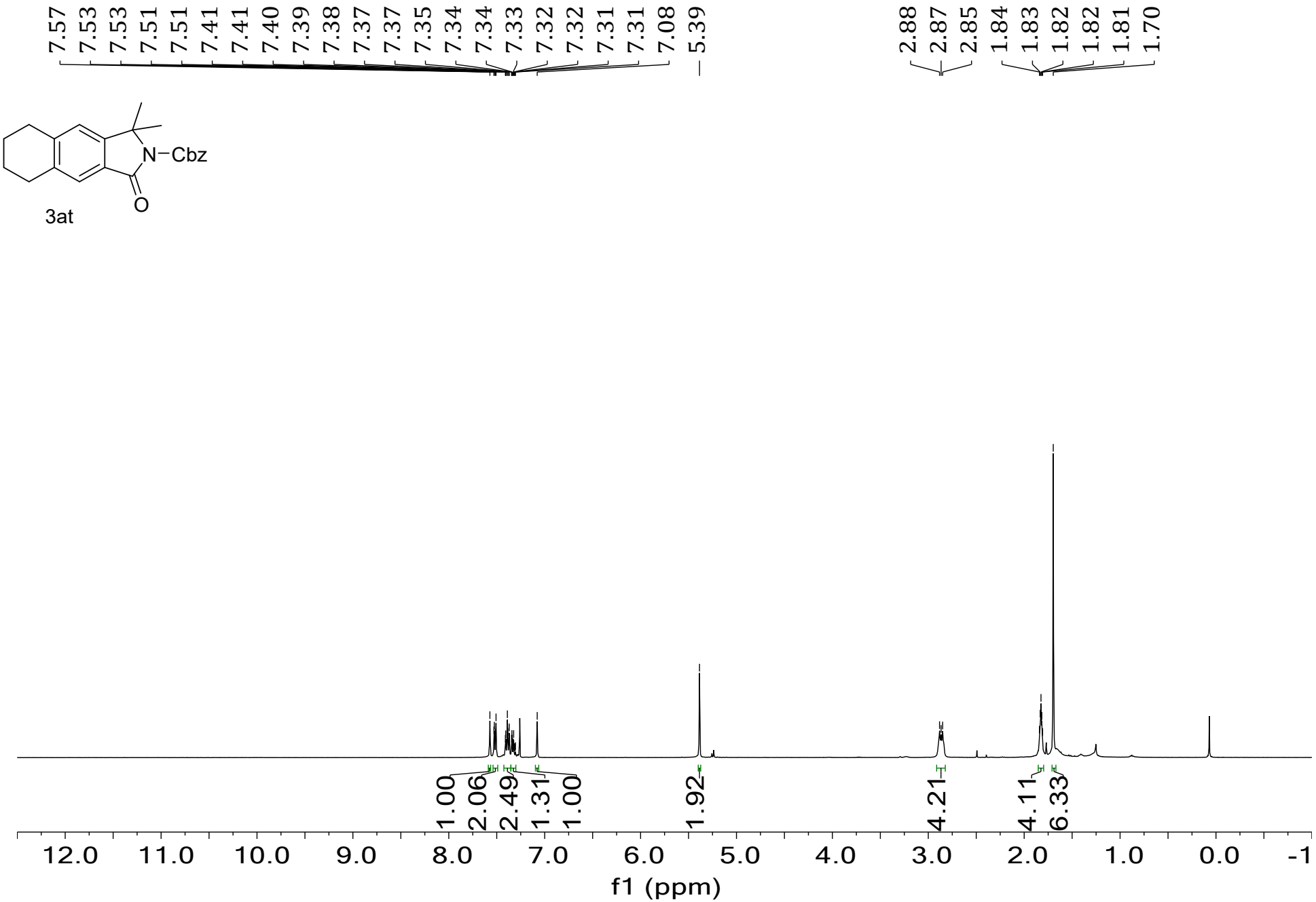
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ar**.



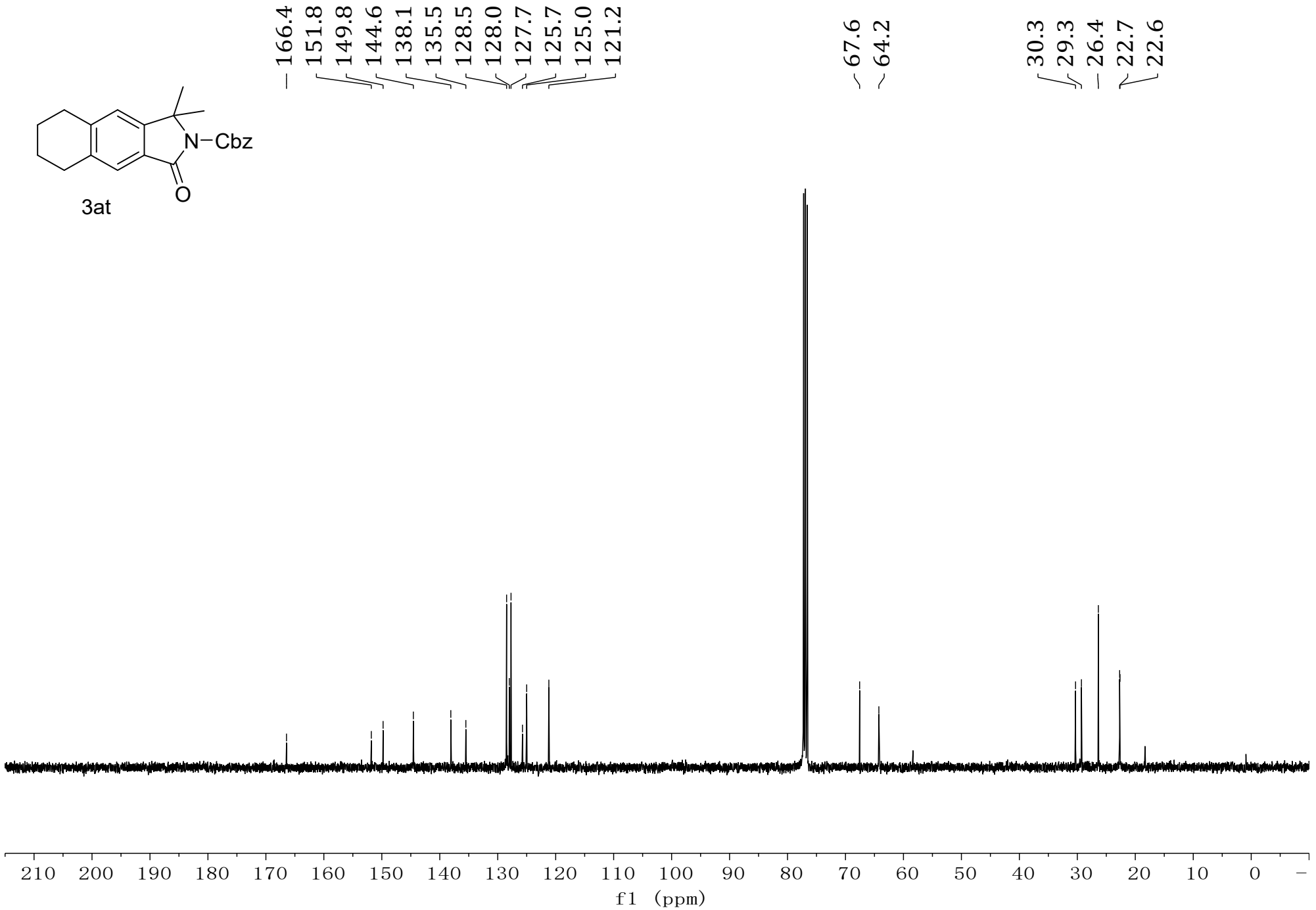
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3as**.



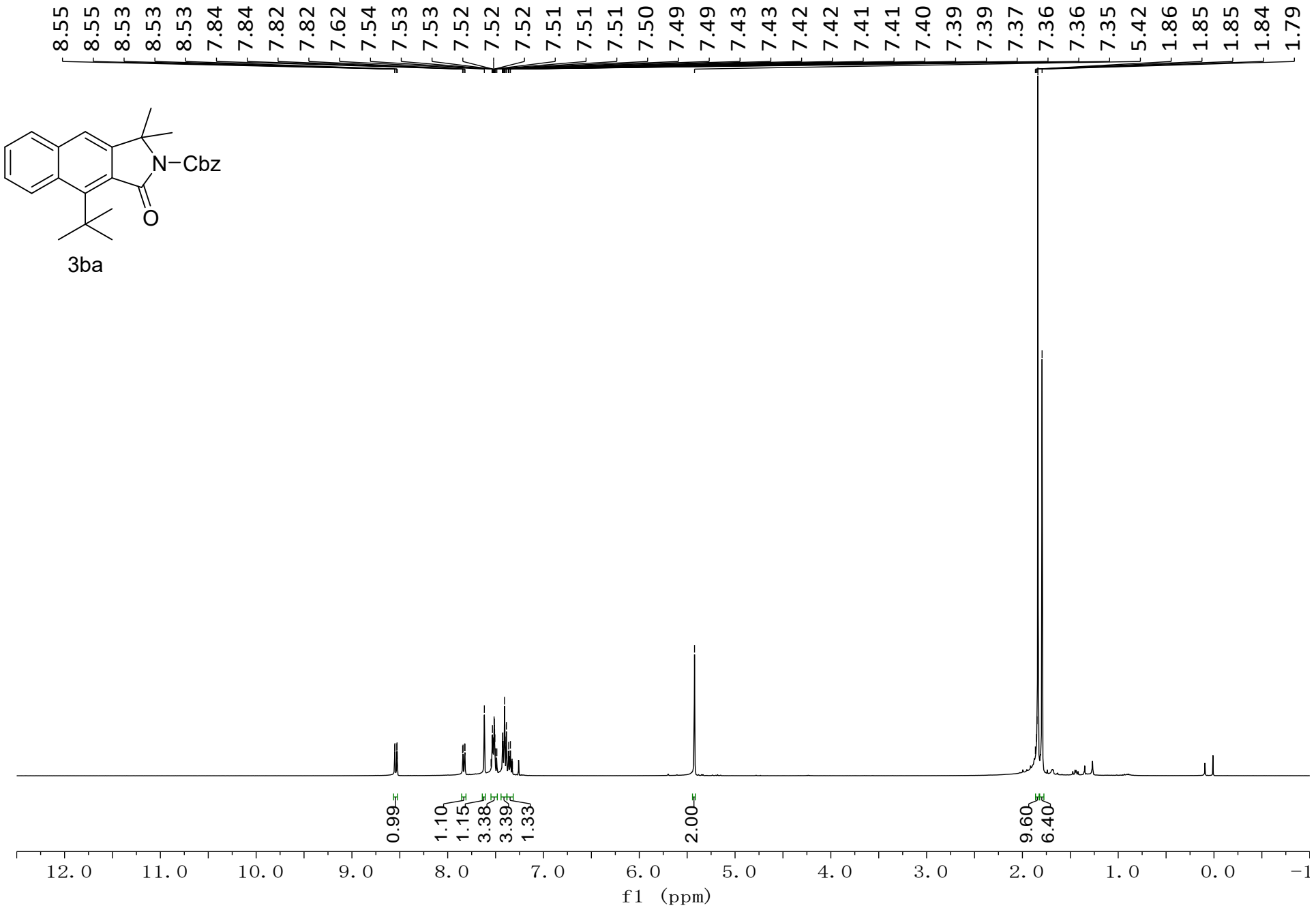
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3as**.



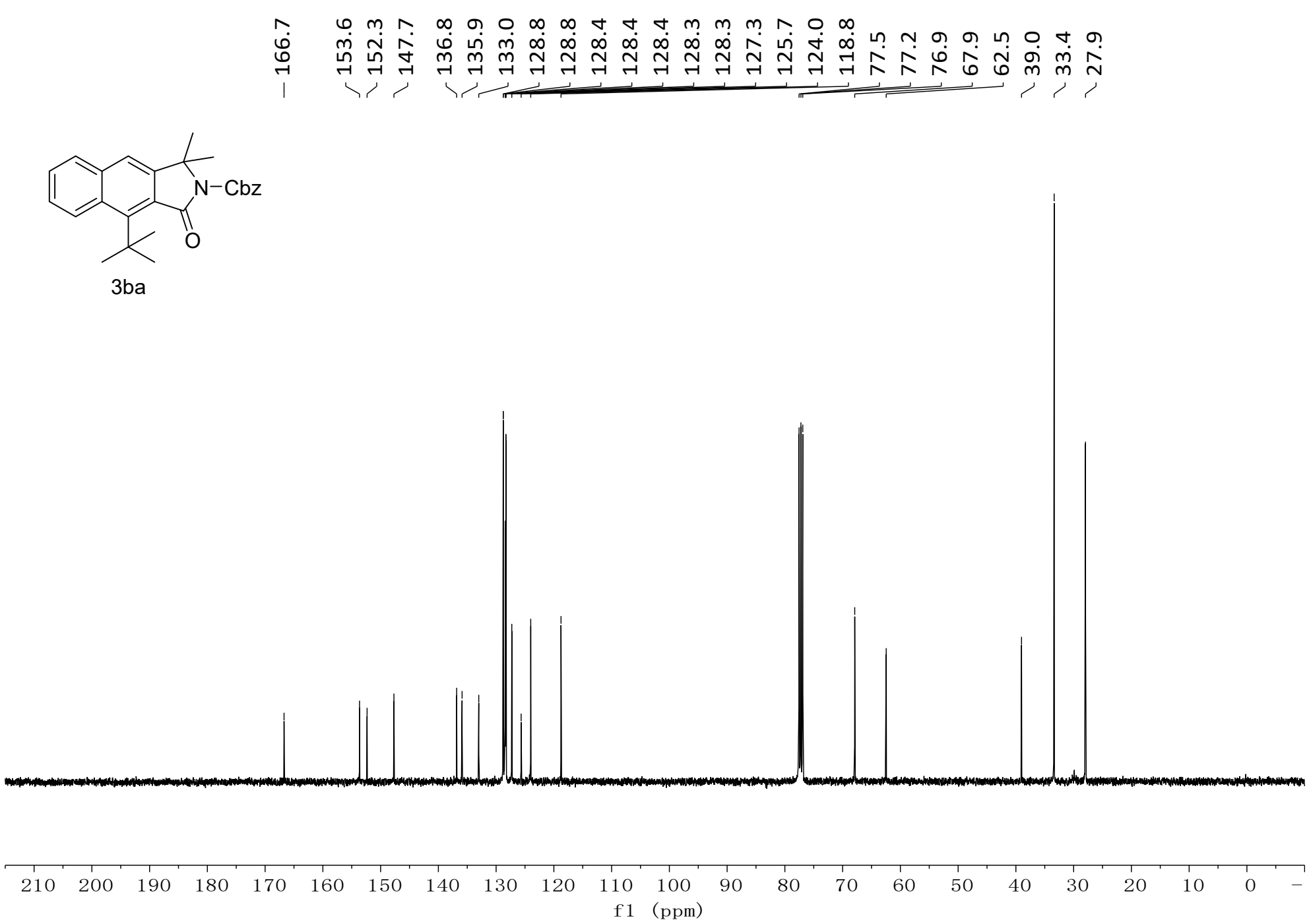
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3at**.



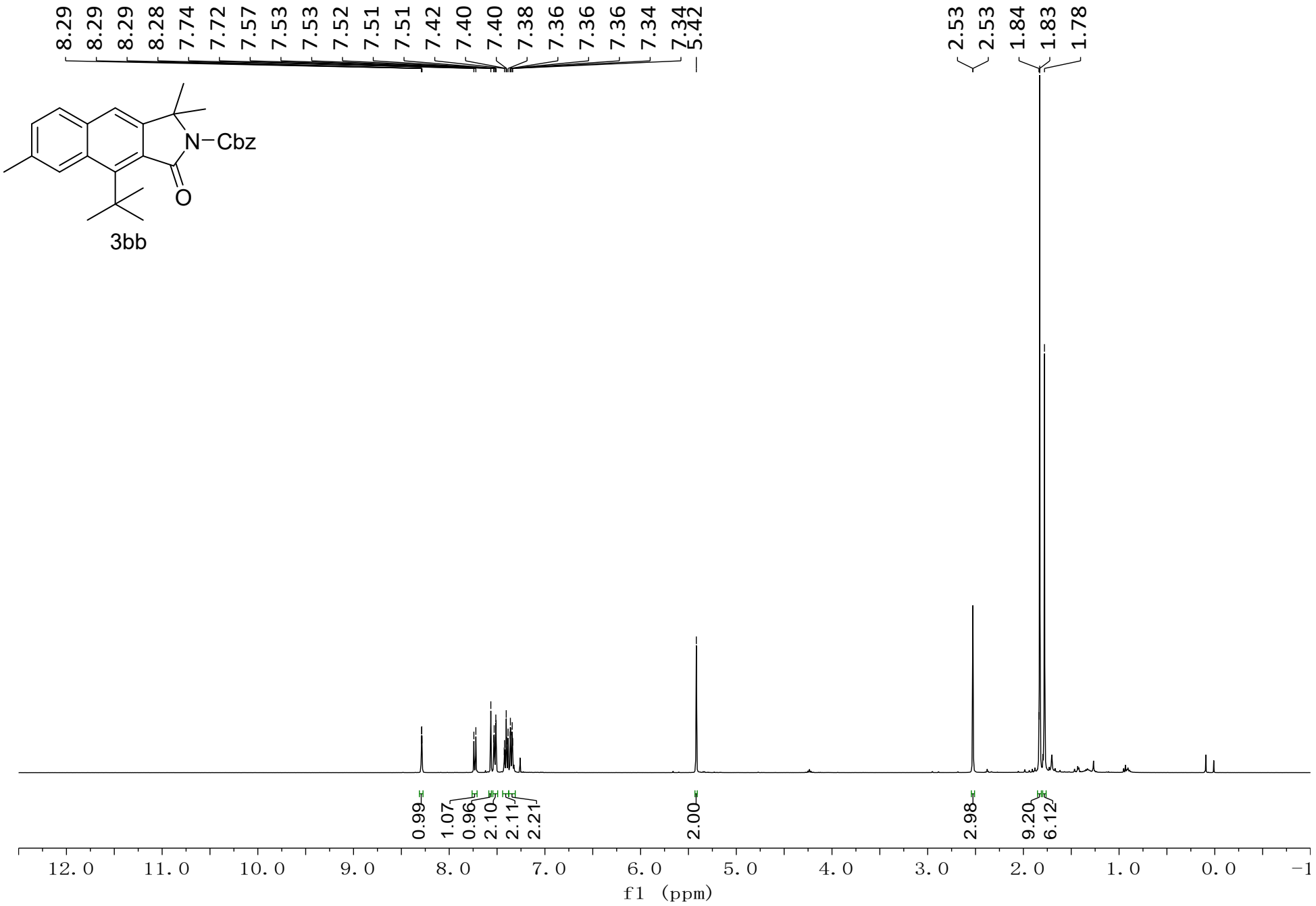
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3at**.



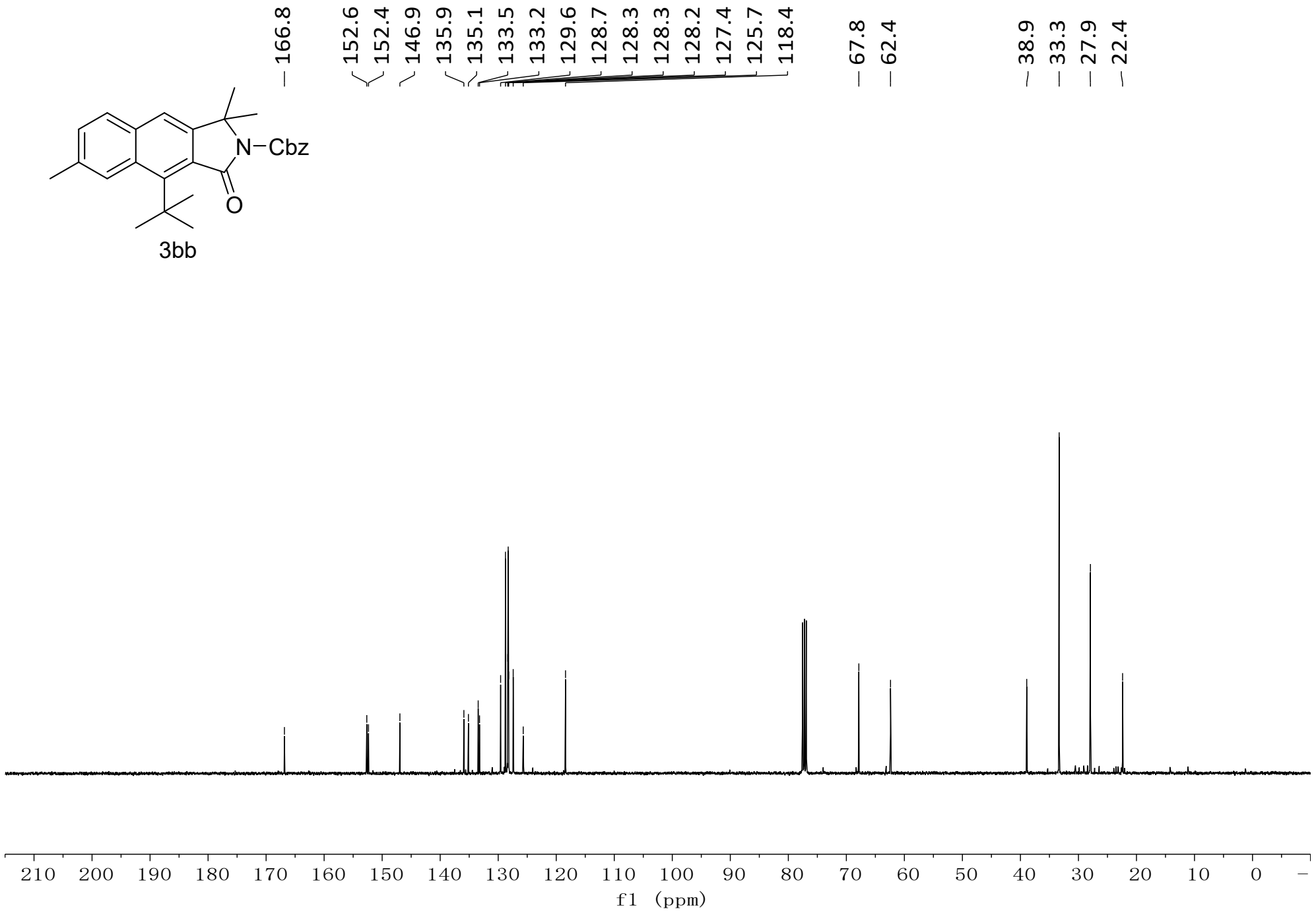
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3ba**.



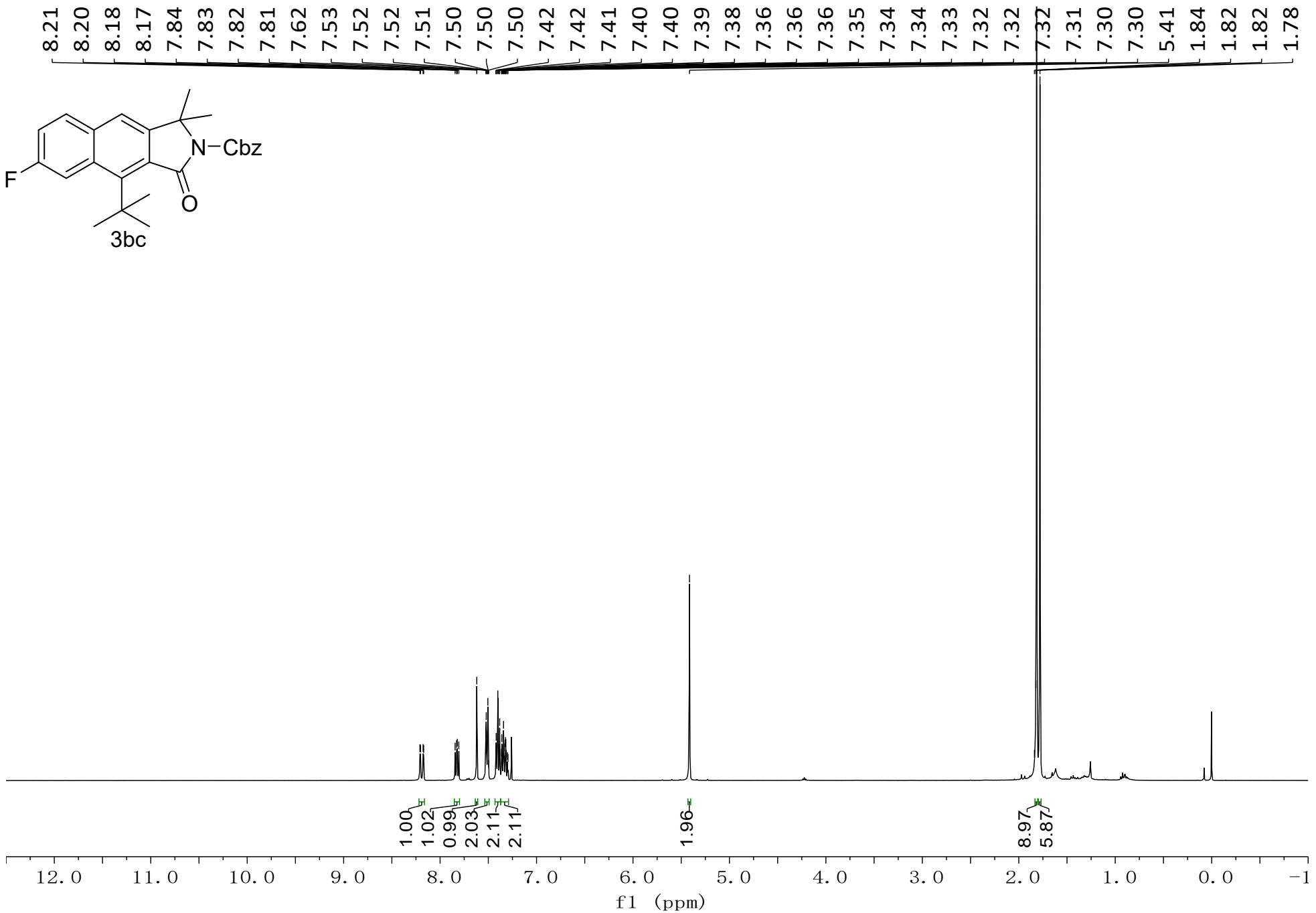
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3ba**.



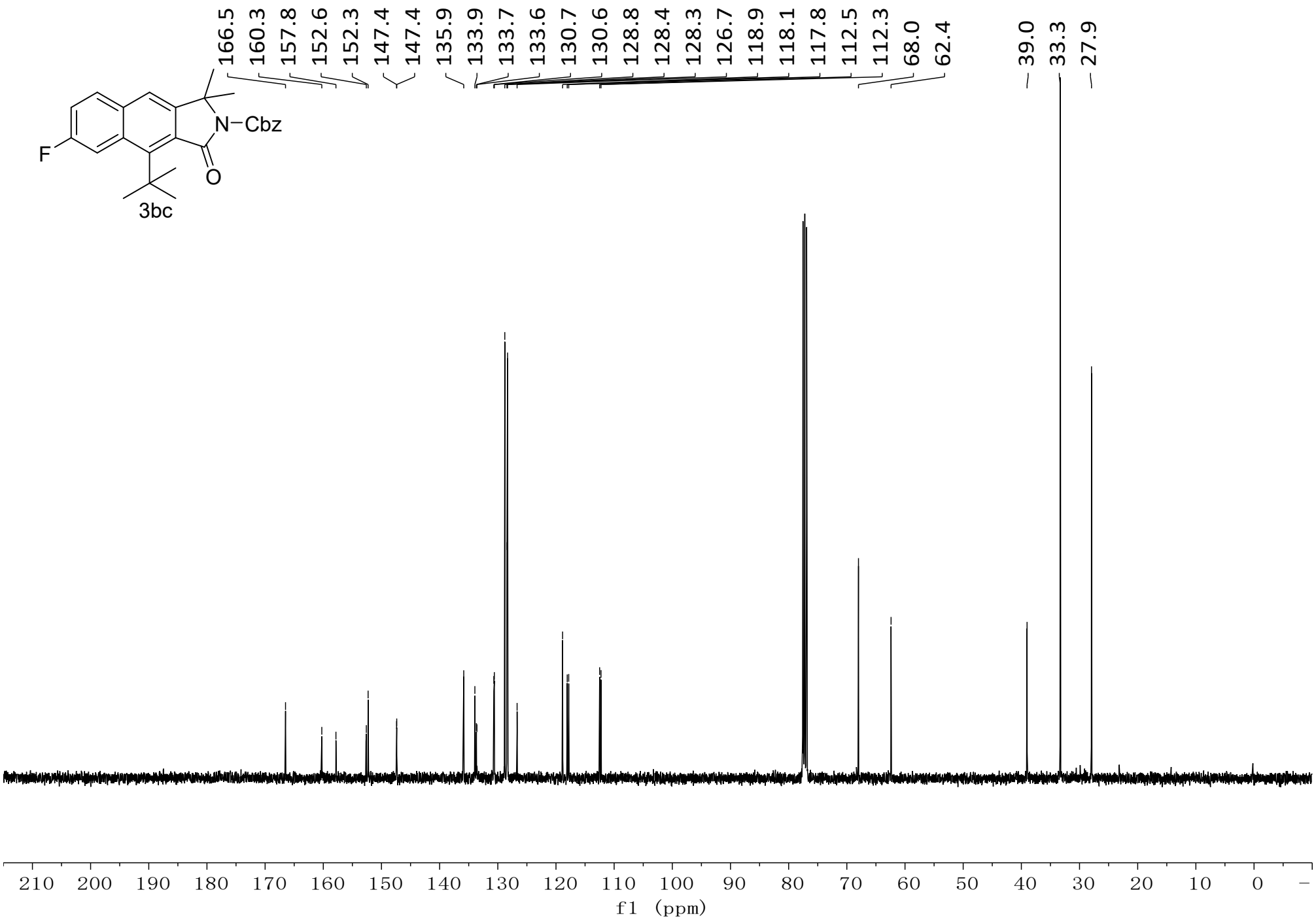
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bb**.



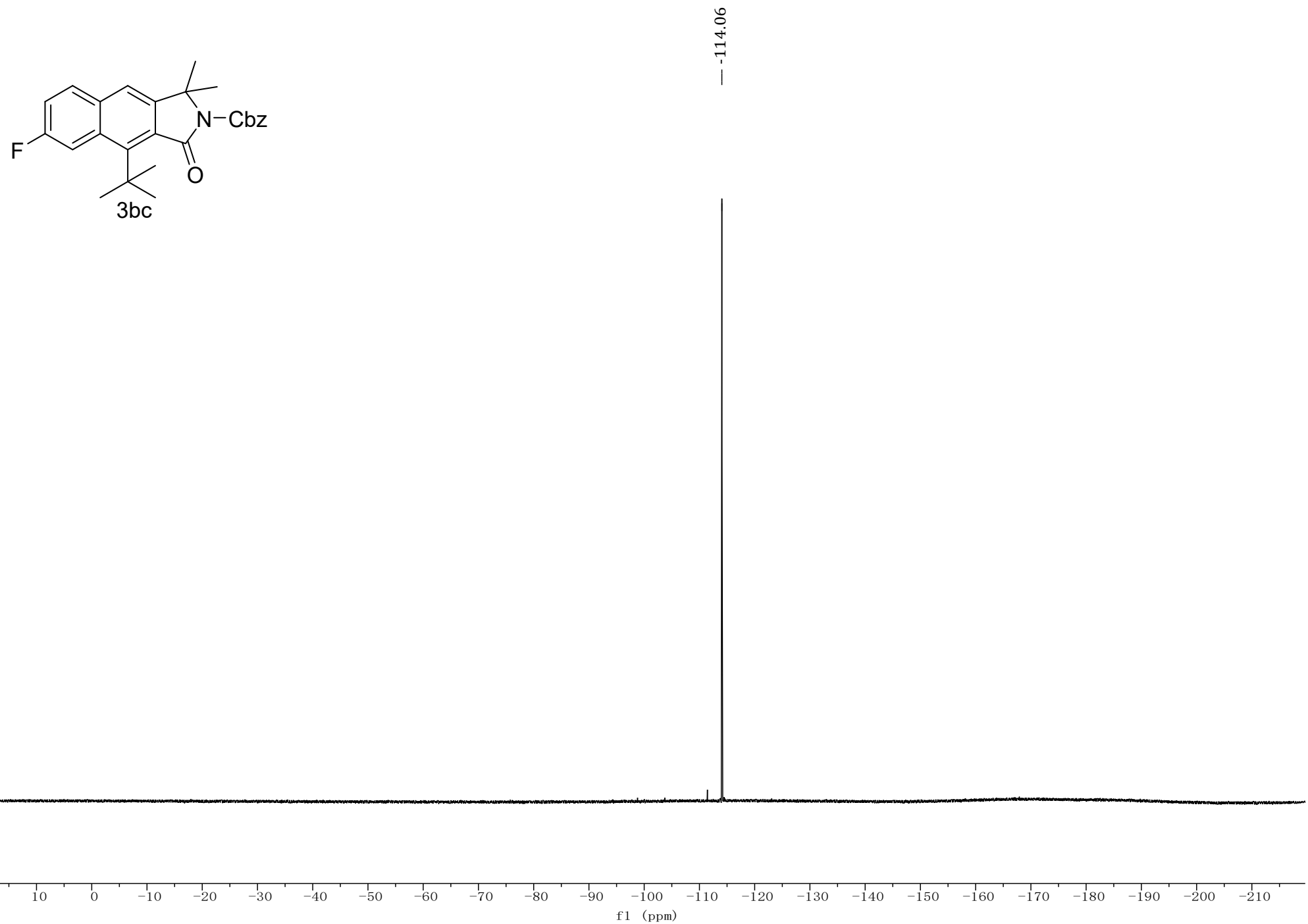
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bb**.



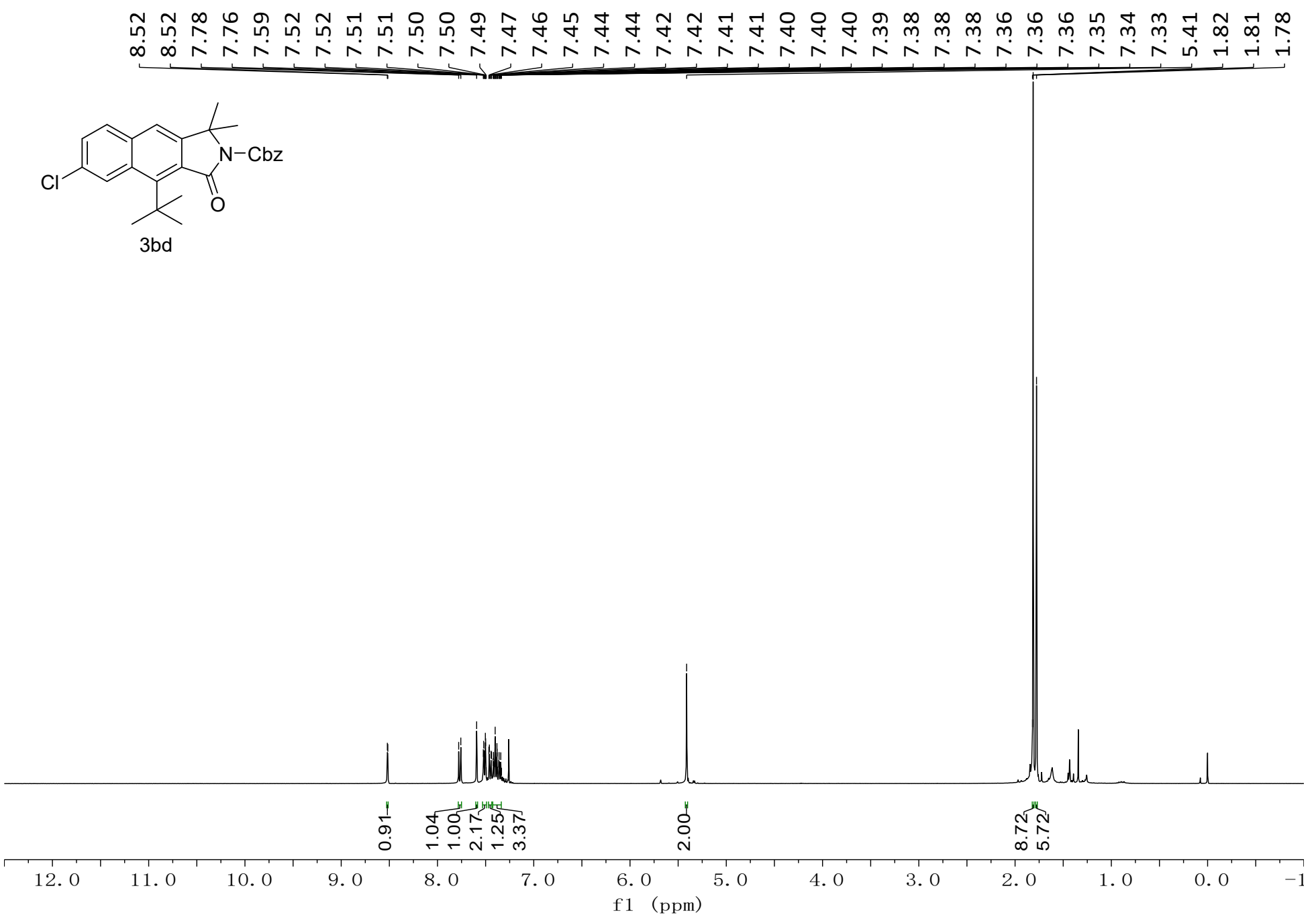
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bc**.



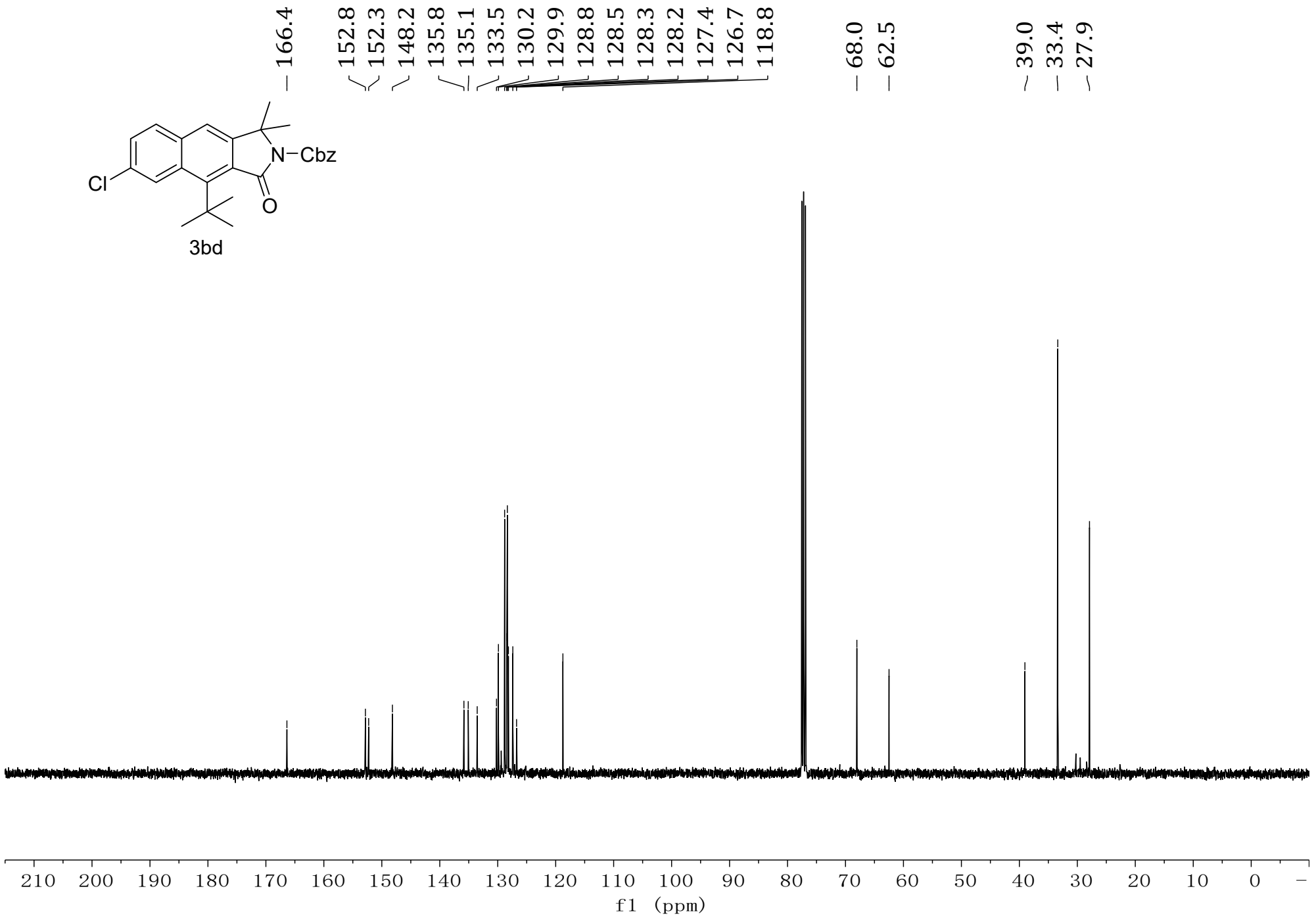
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bc**.



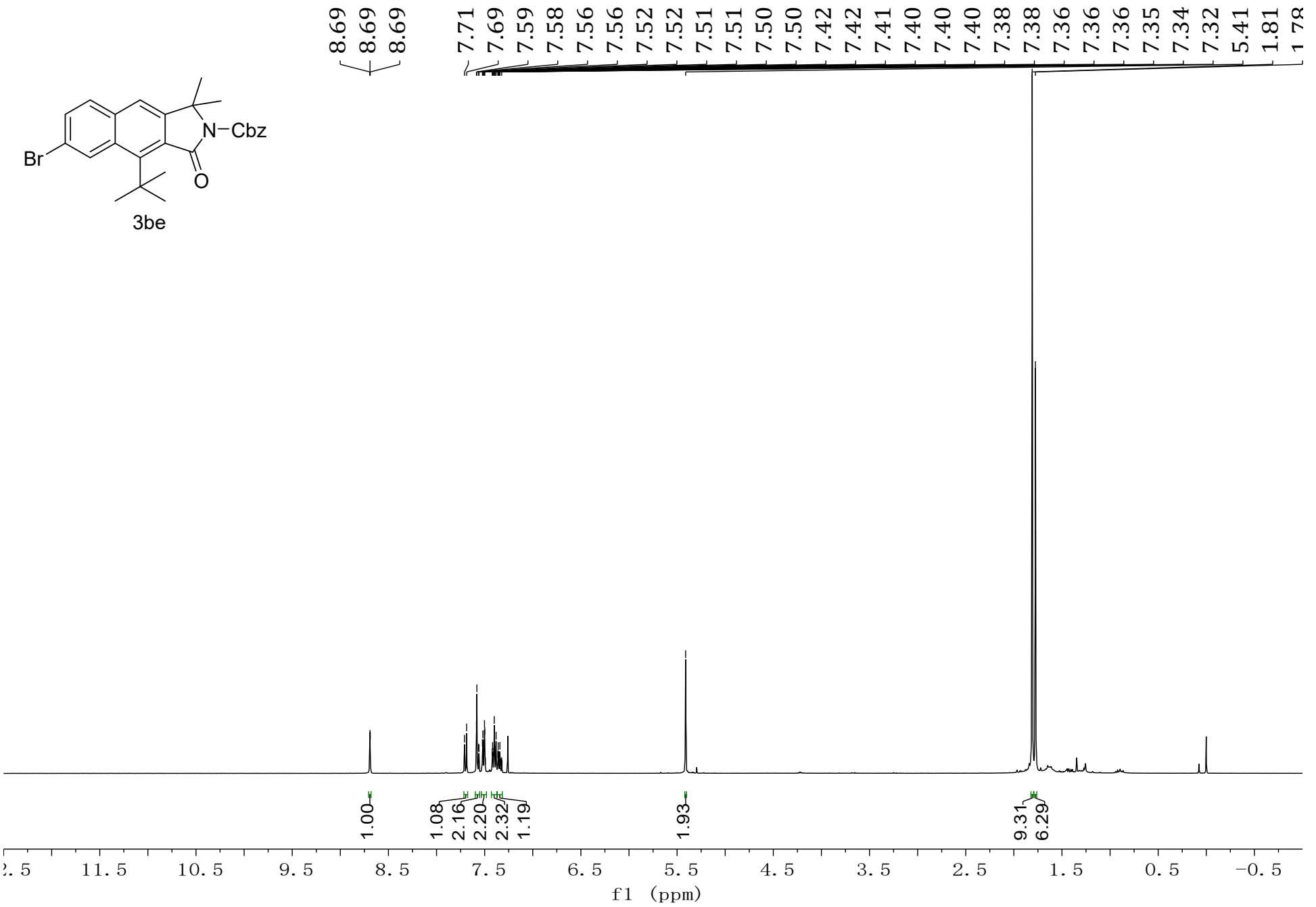
^{19}F NMR (400 MHz, $CDCl_3$) spectra of **3bc**.



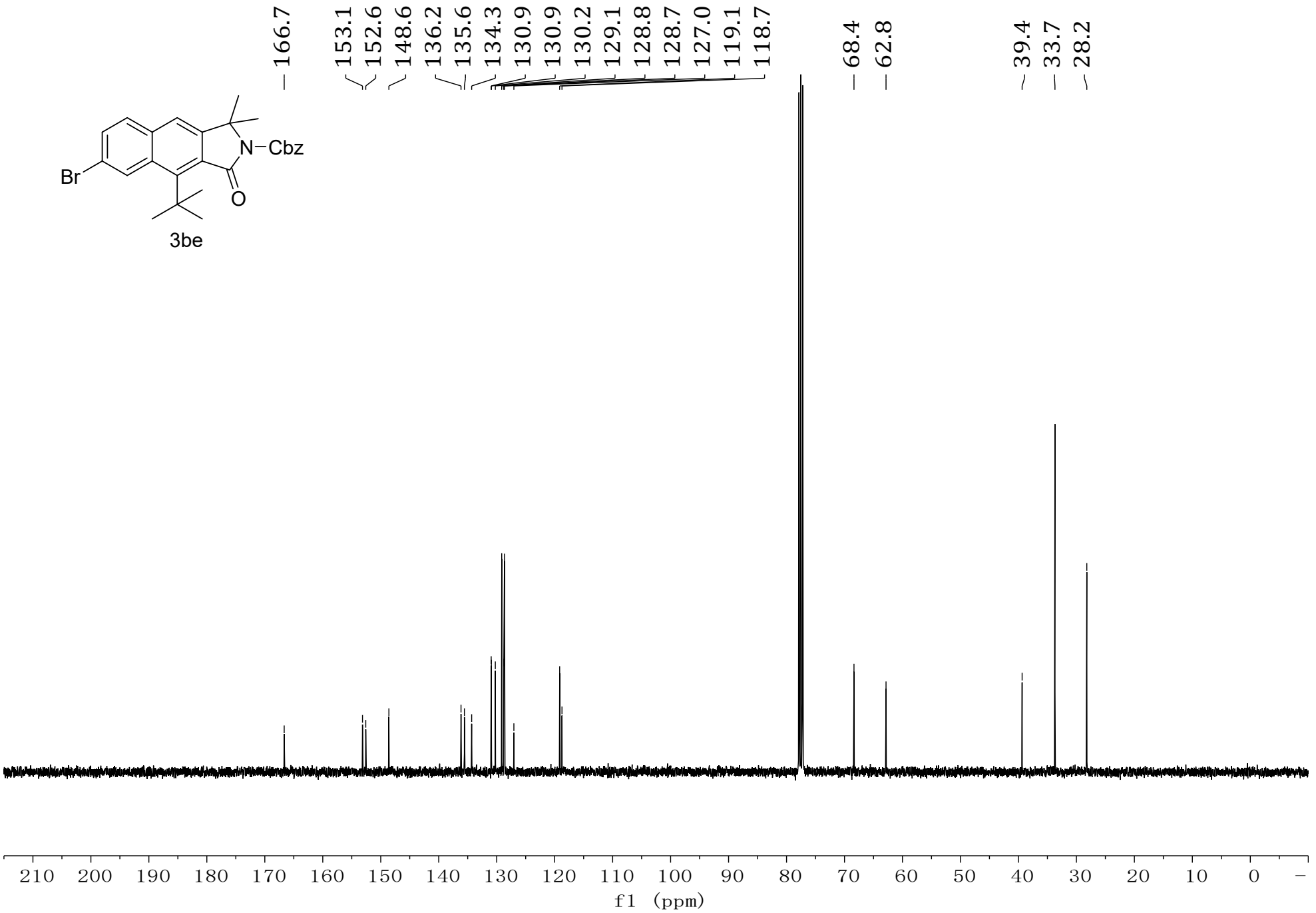
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bd**.



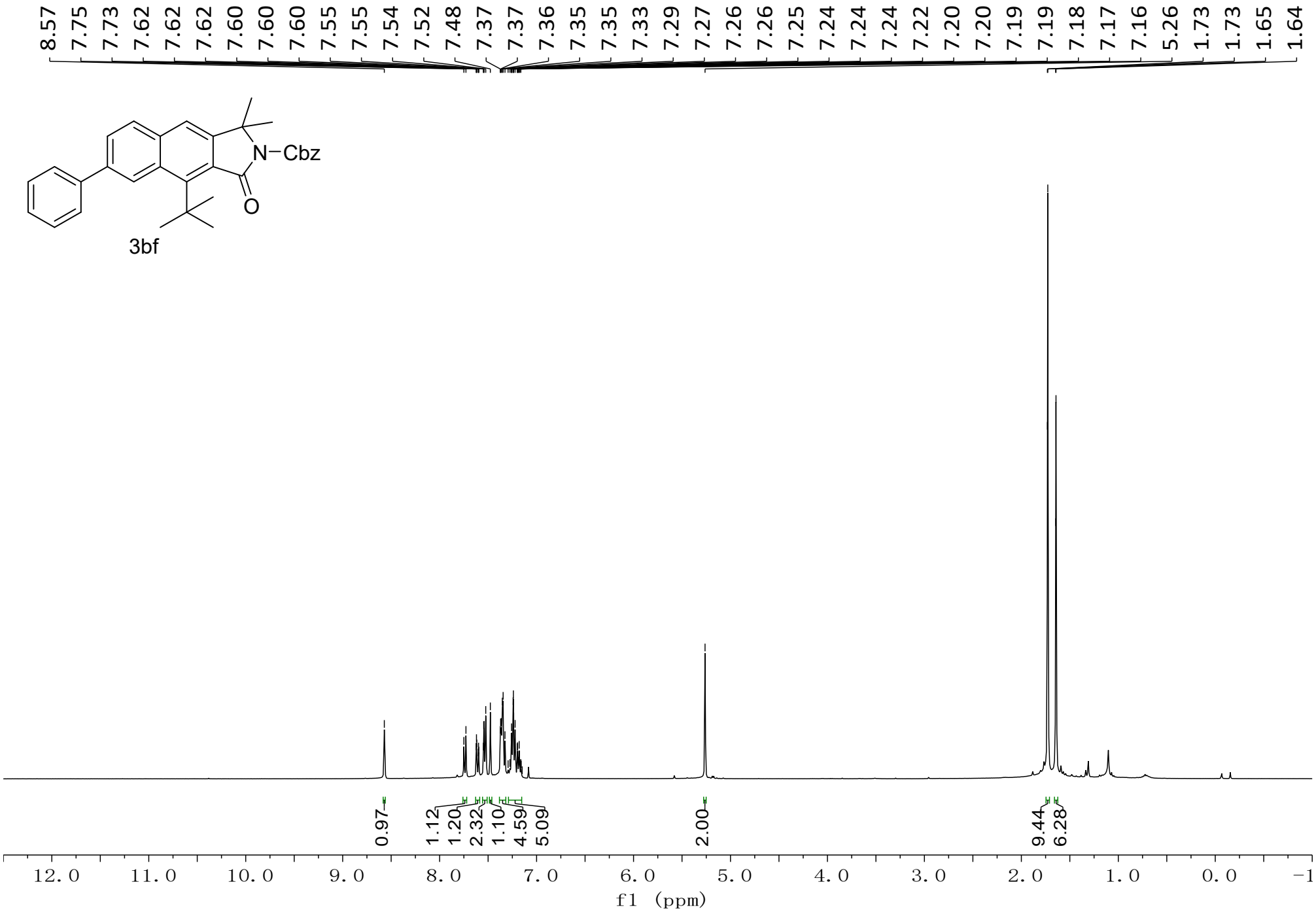
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bd**.



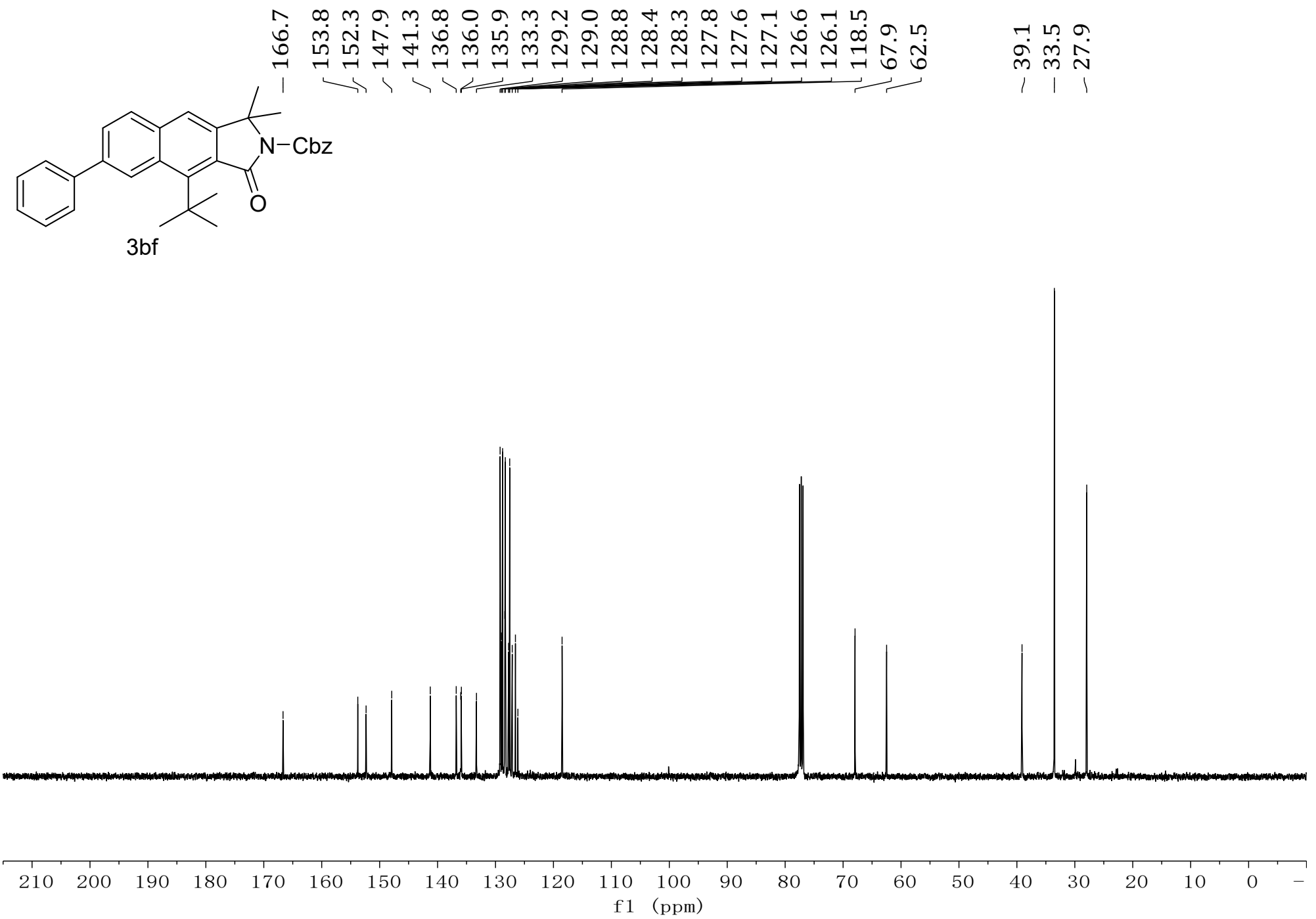
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3be**.



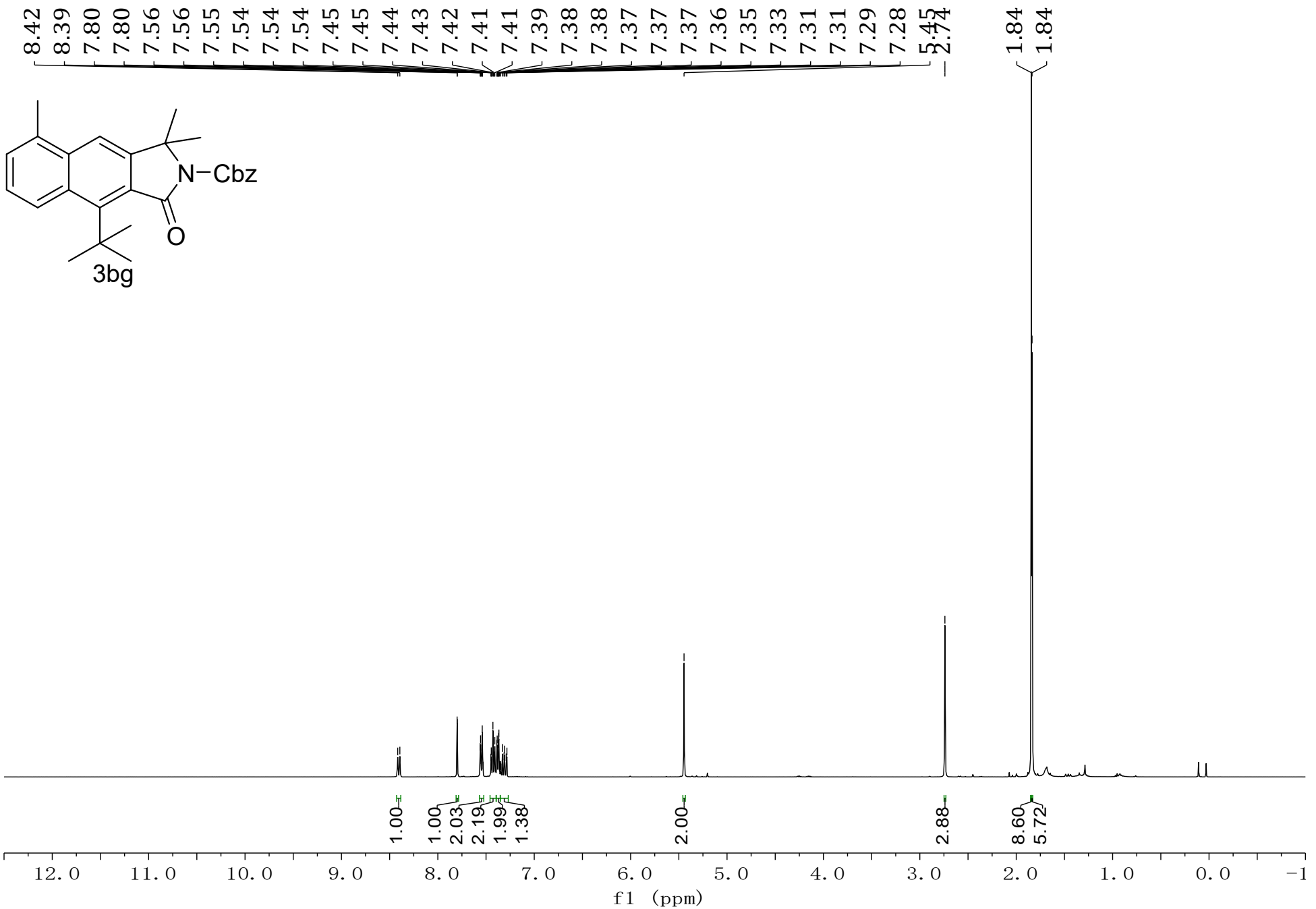
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3be**.



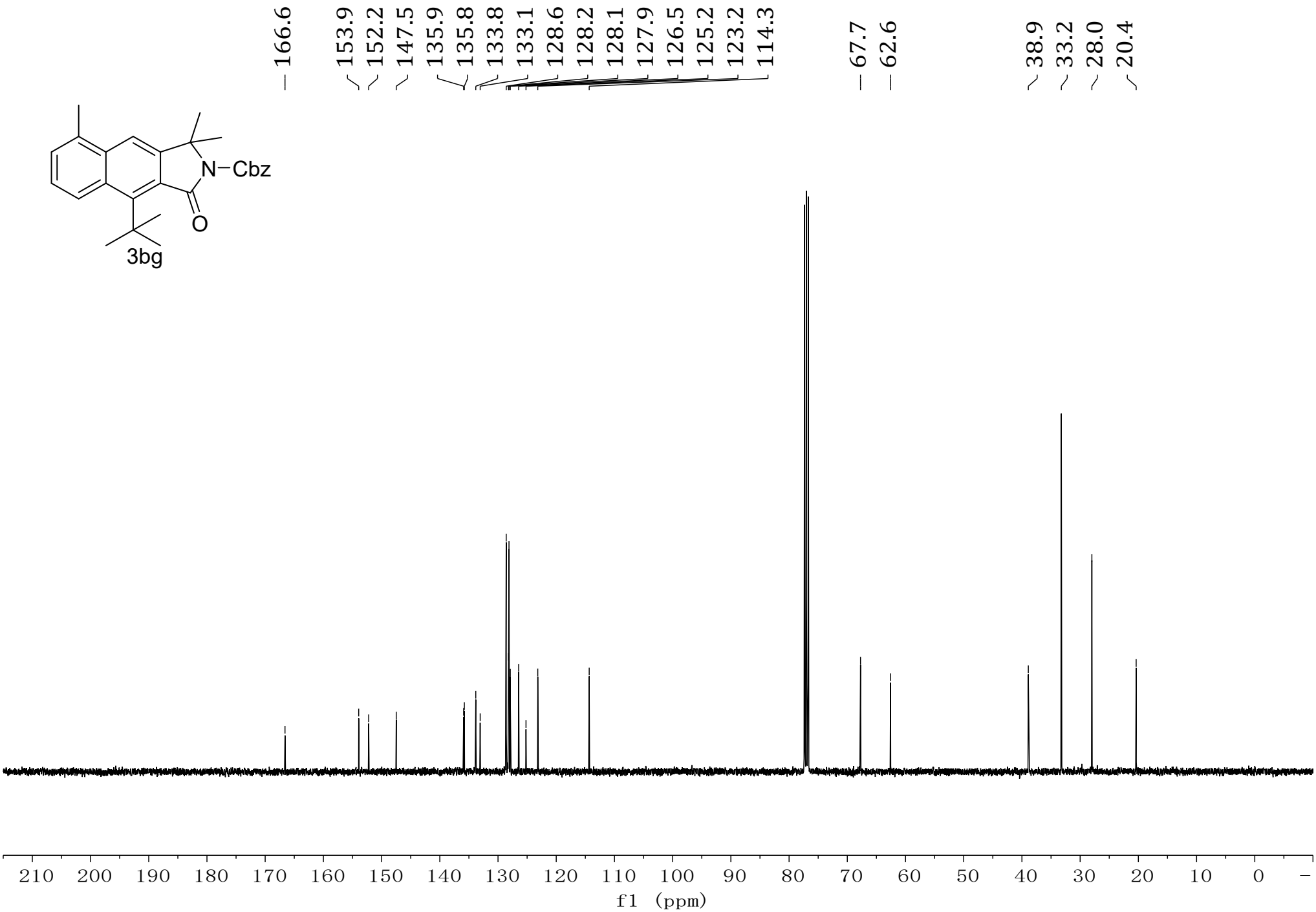
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bf**.



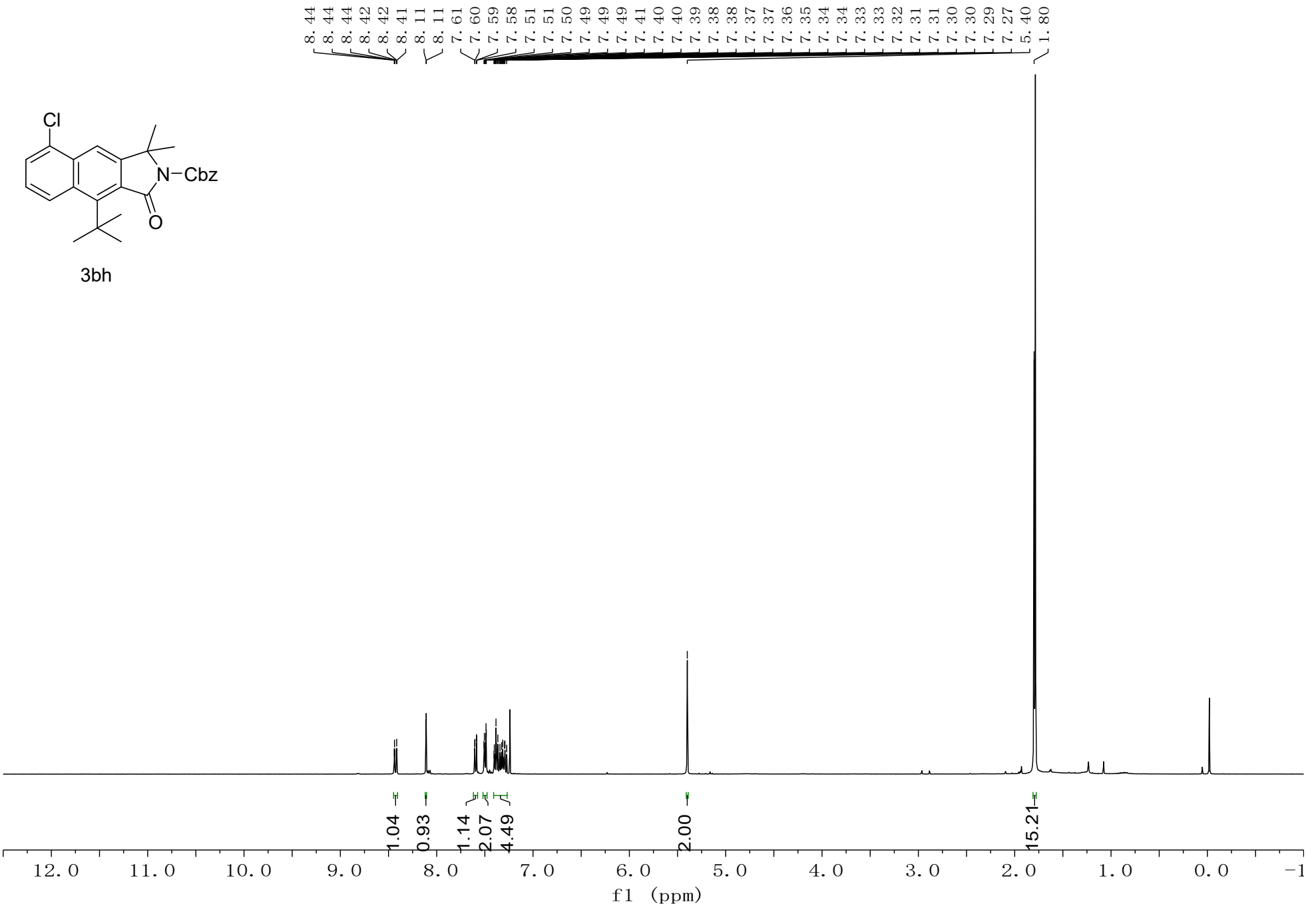
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bf**.



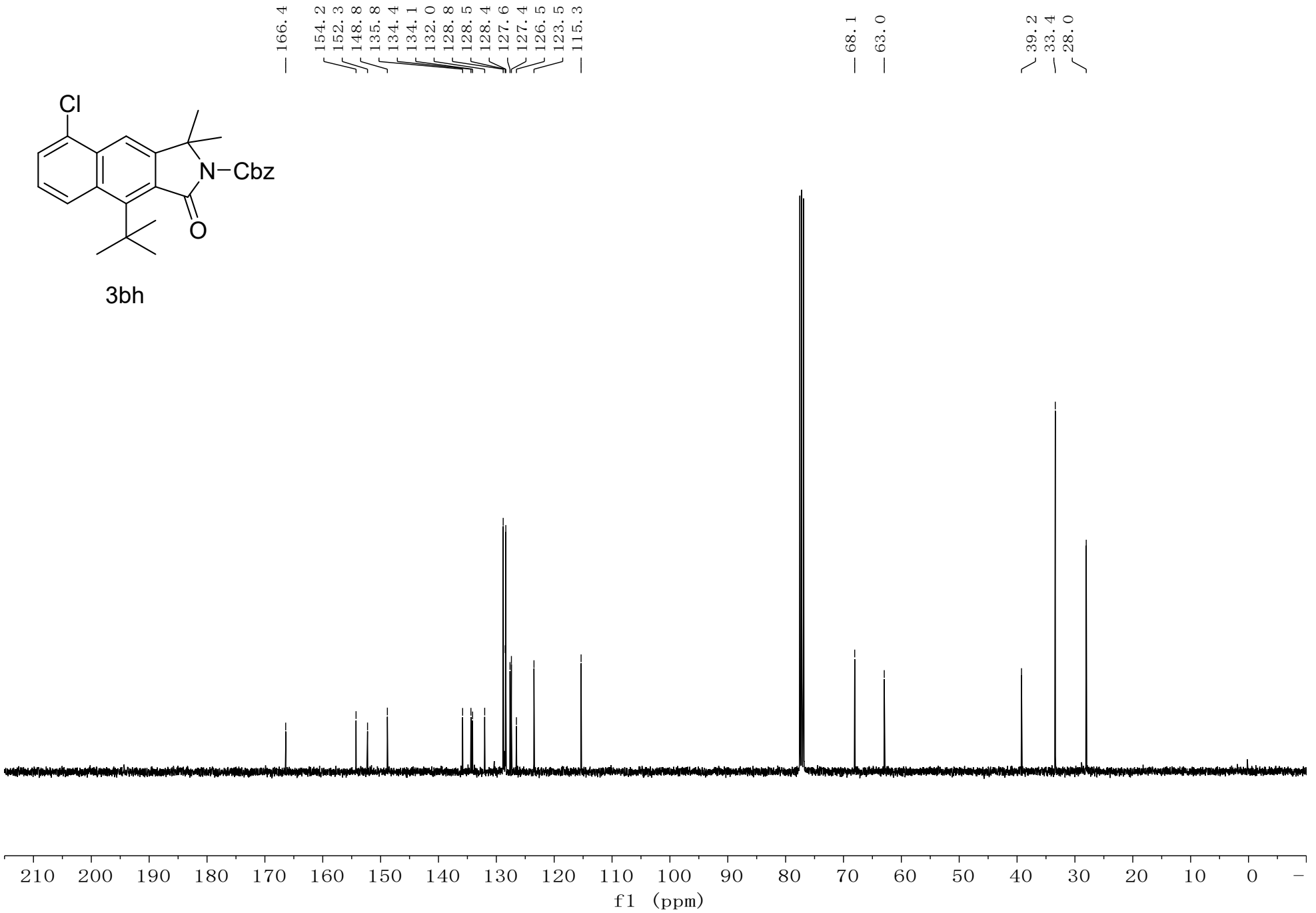
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bg**.



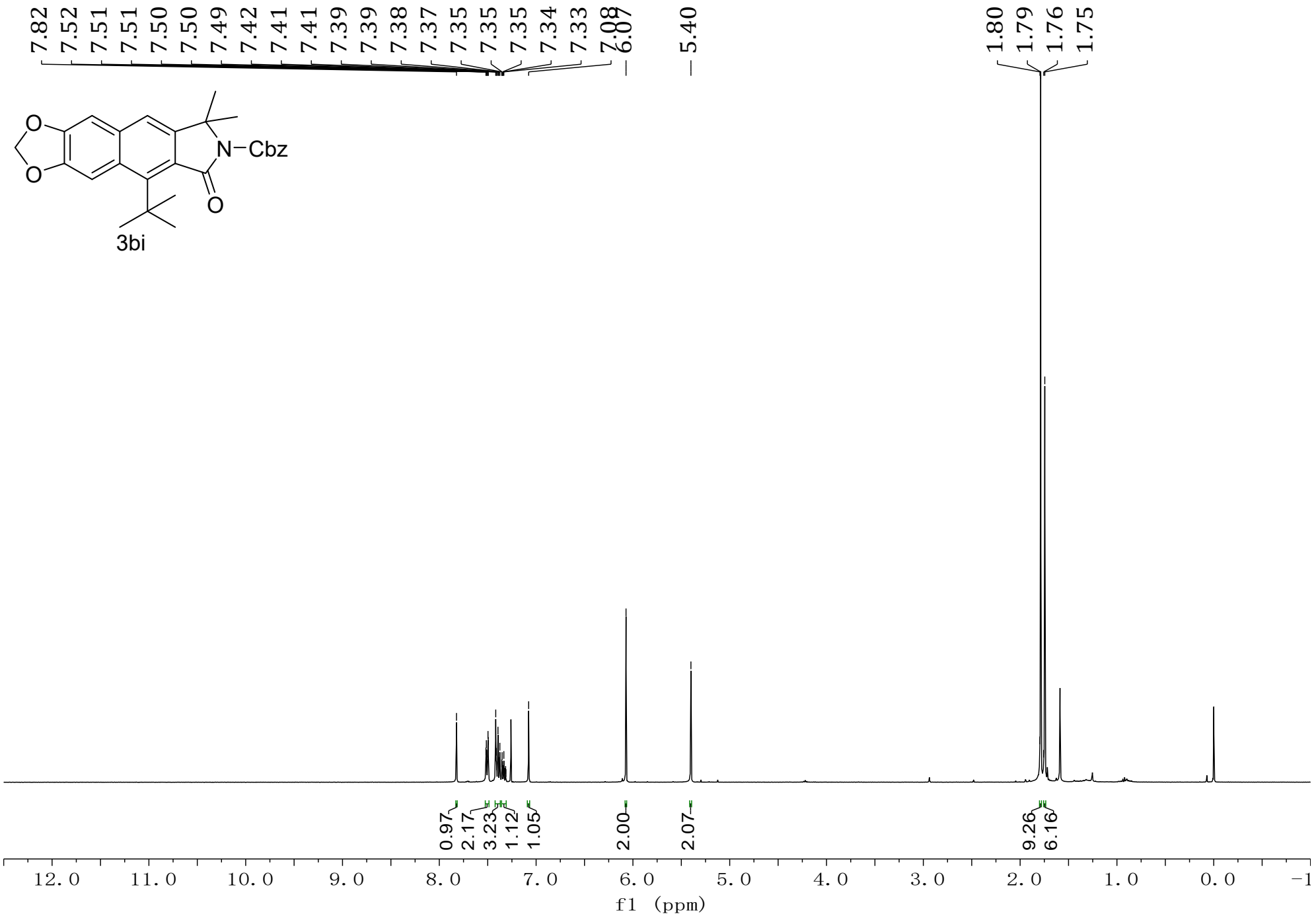
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bg**.



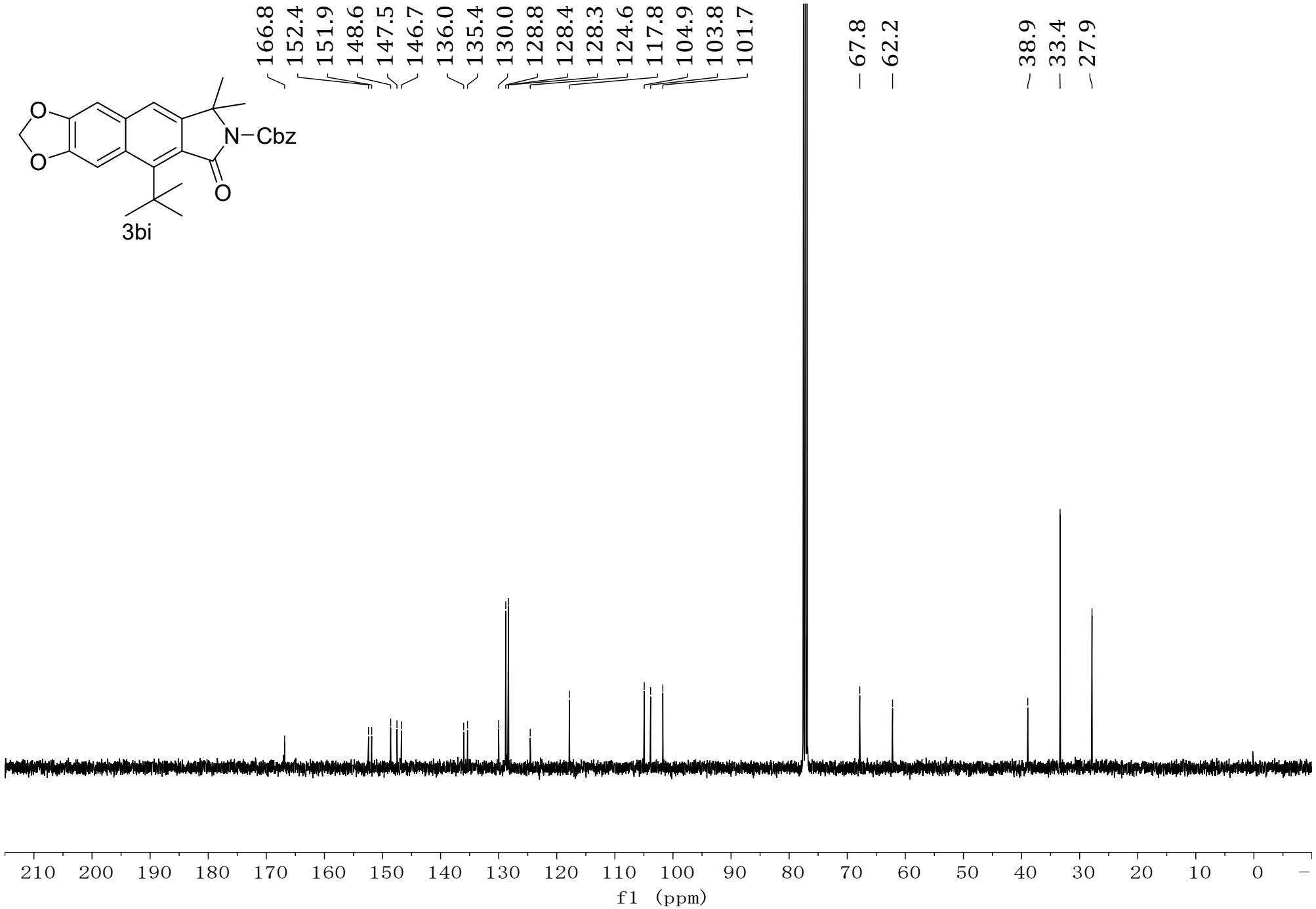
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bh**.



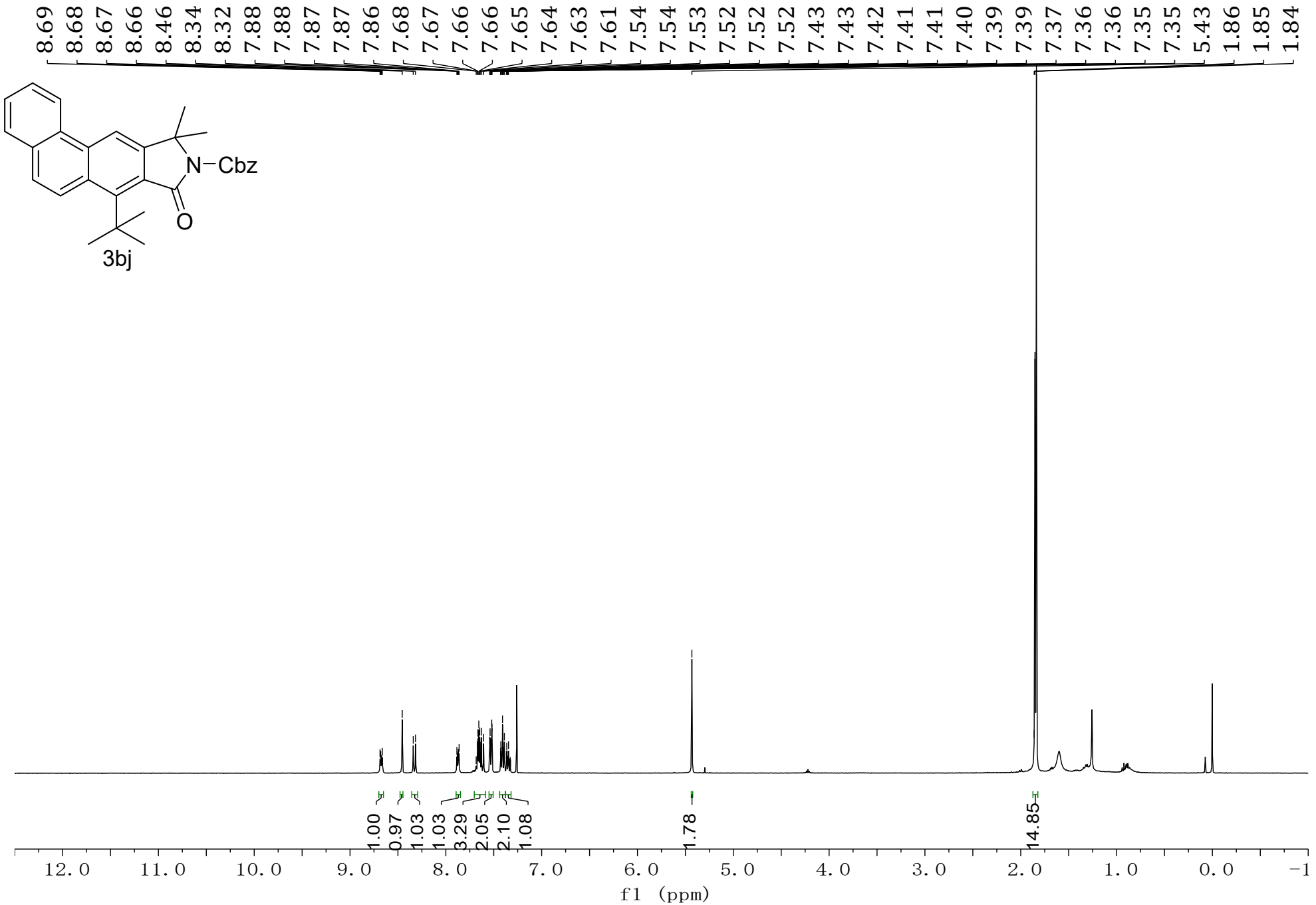
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bh**.



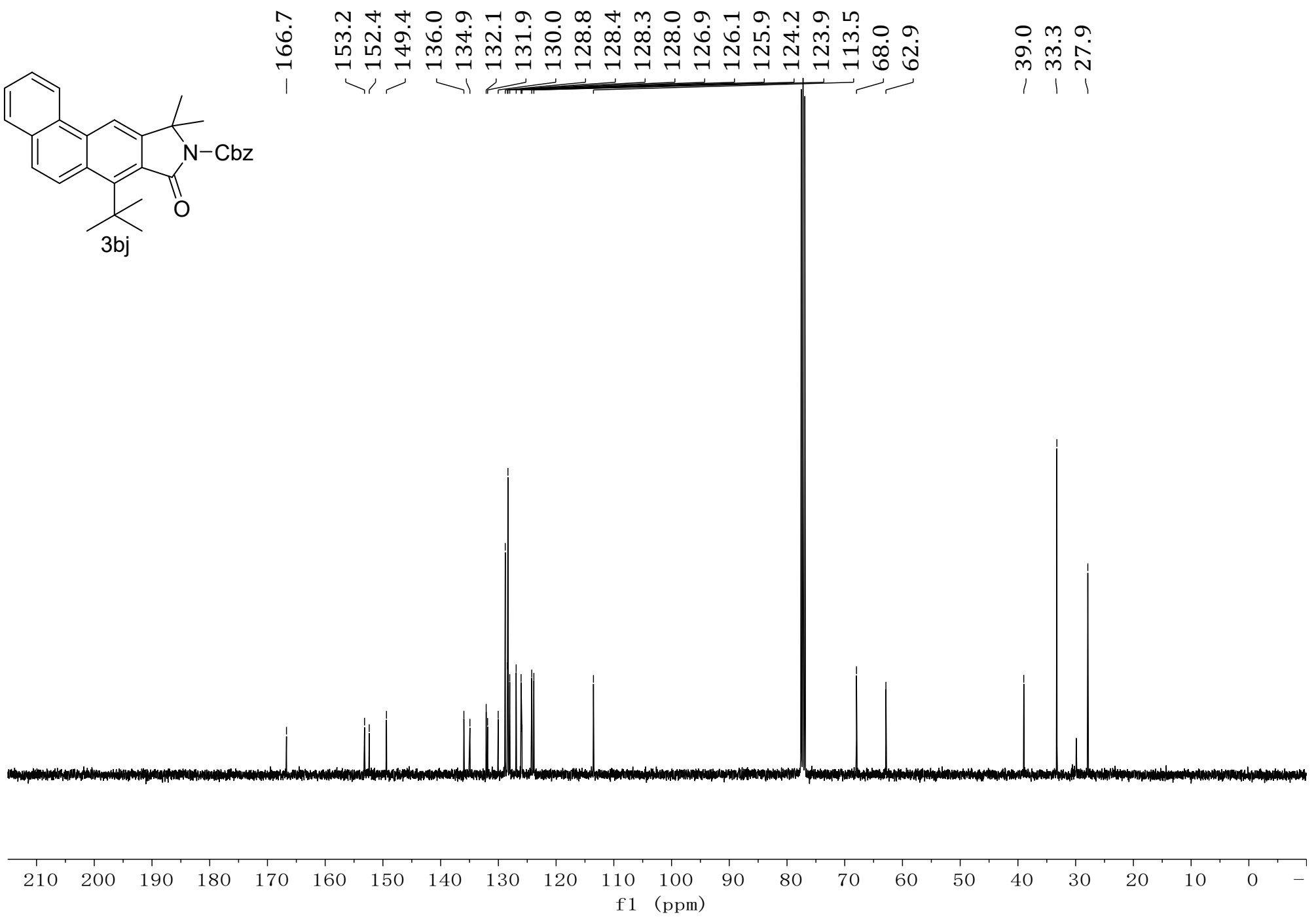
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bi**.



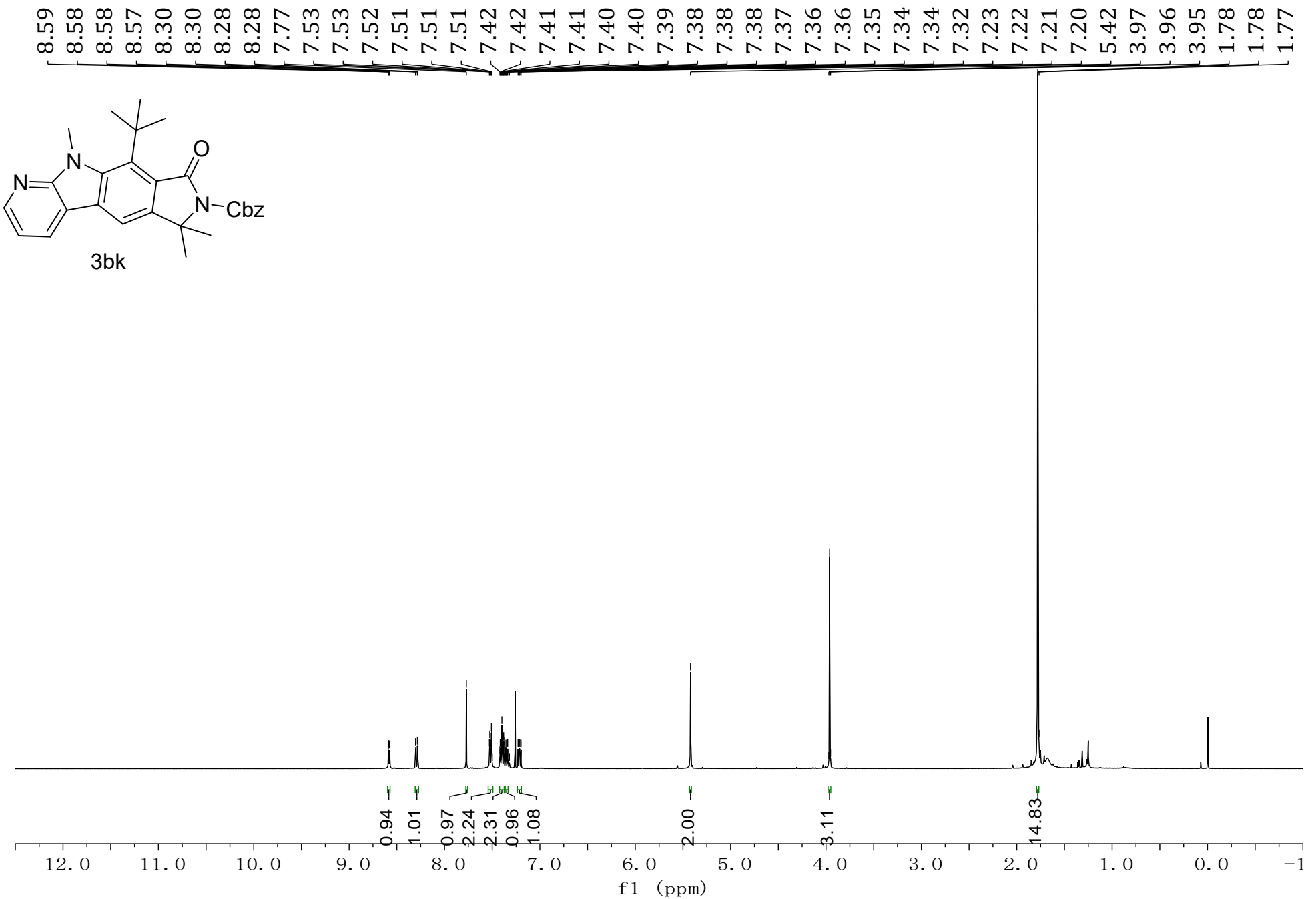
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bi**.



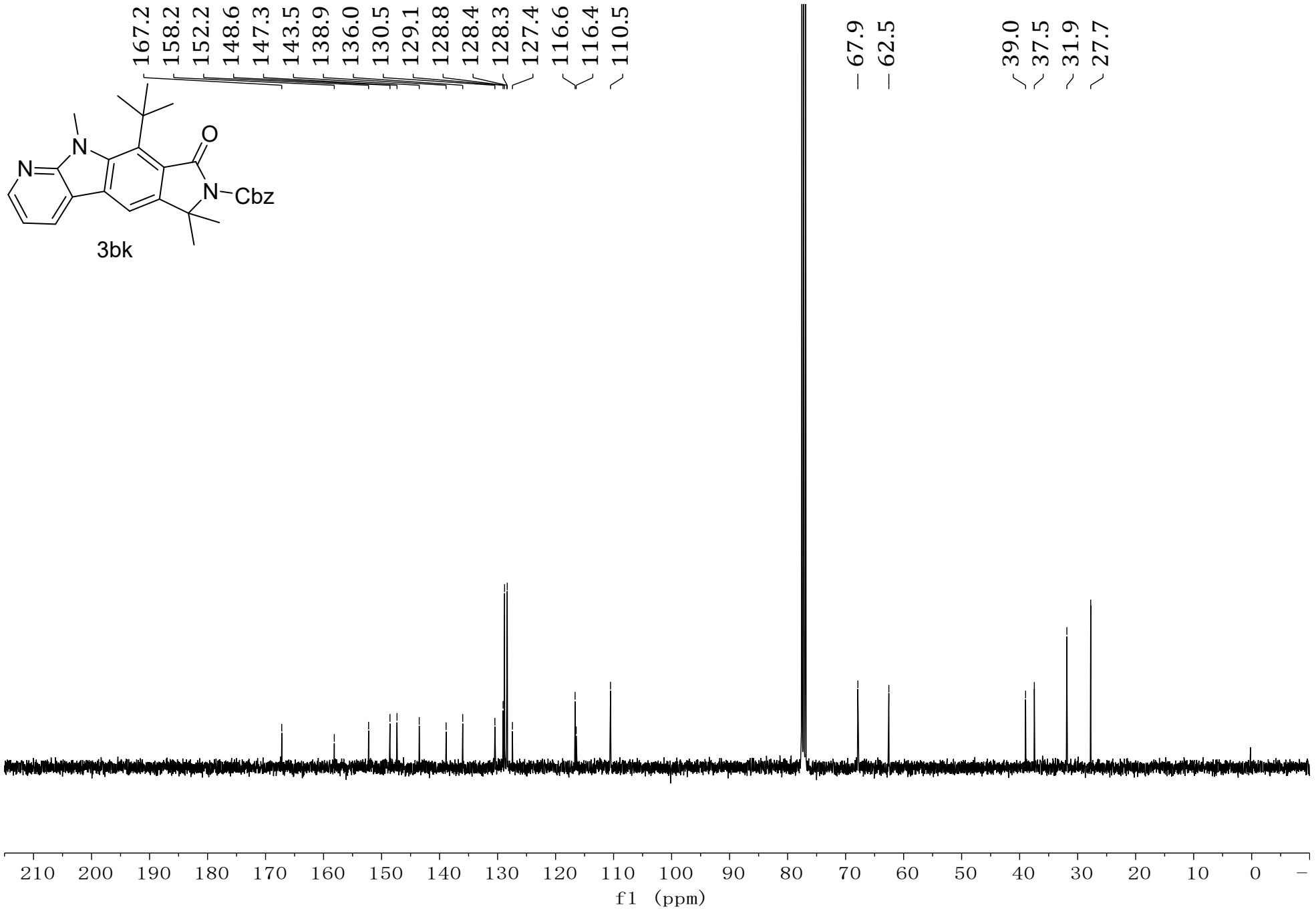
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bj**.



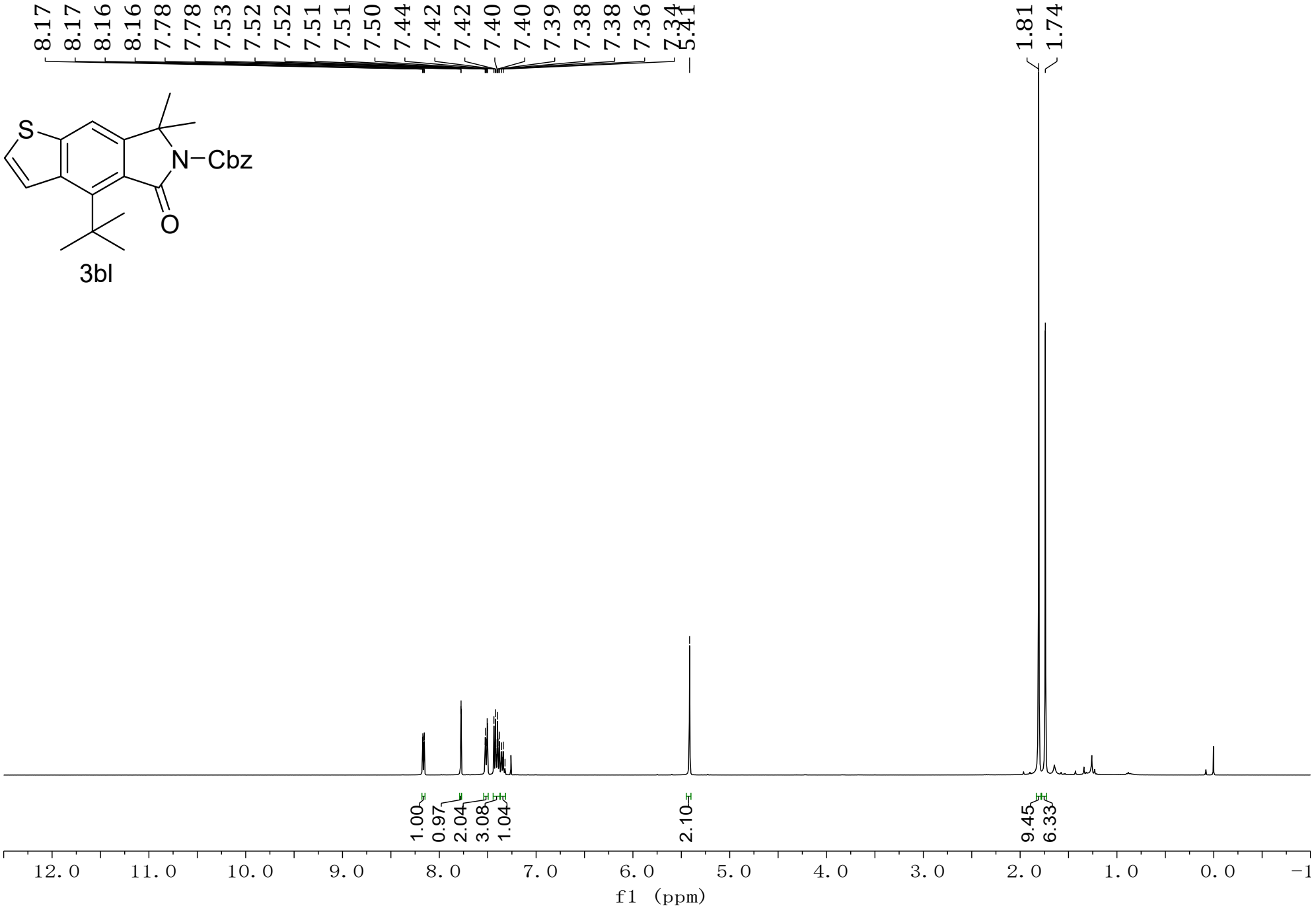
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bj**.



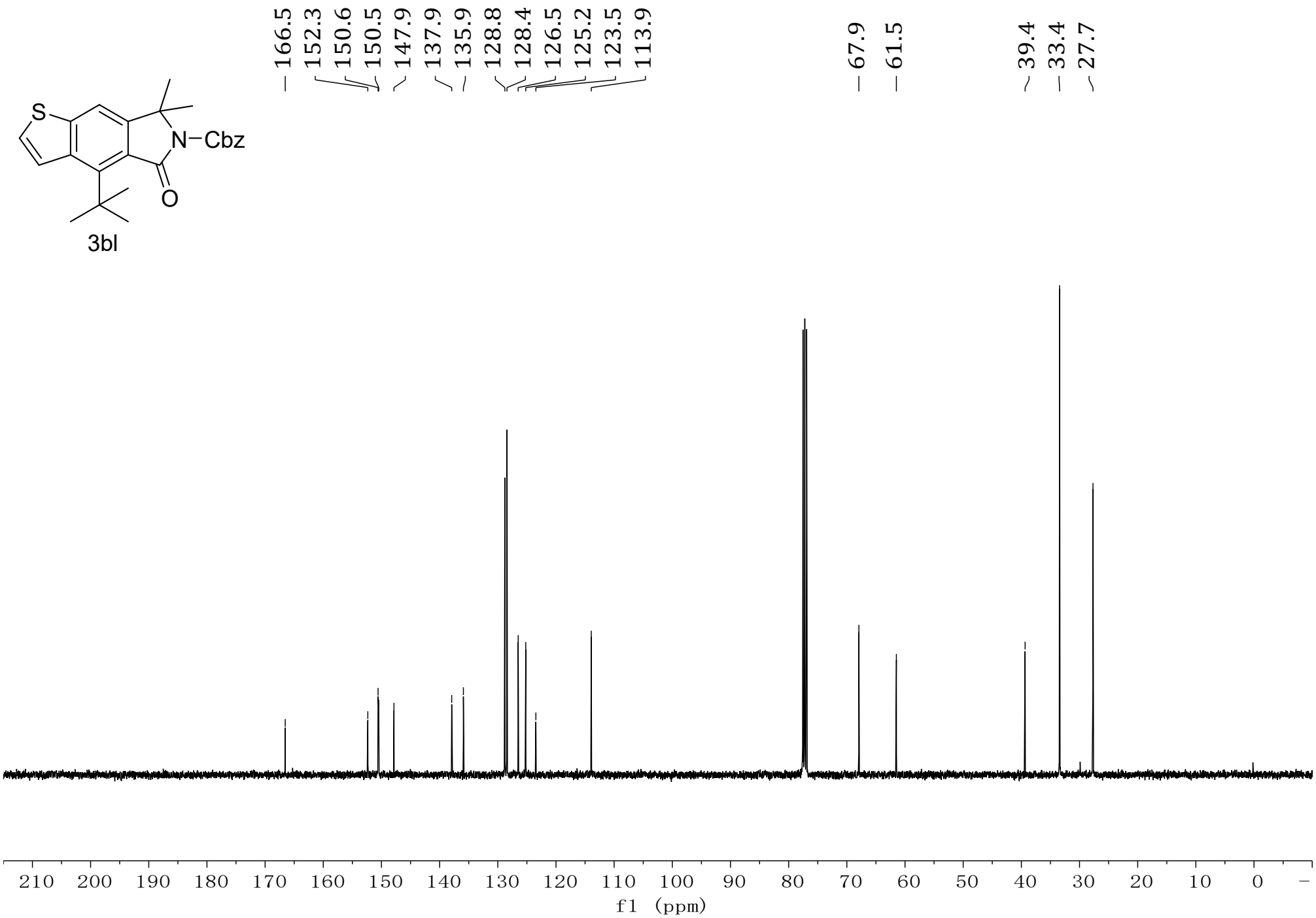
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bk**.



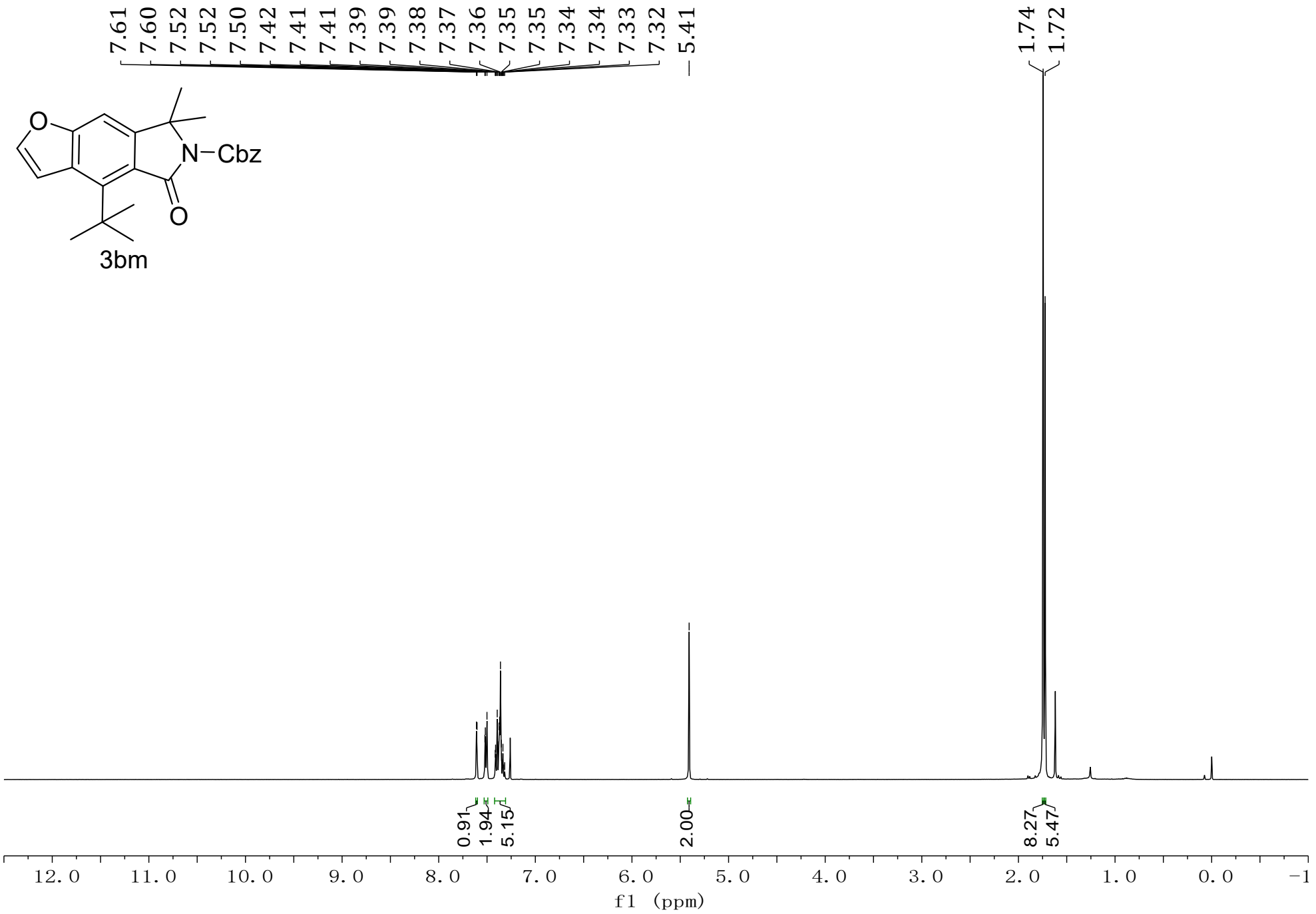
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bk**.



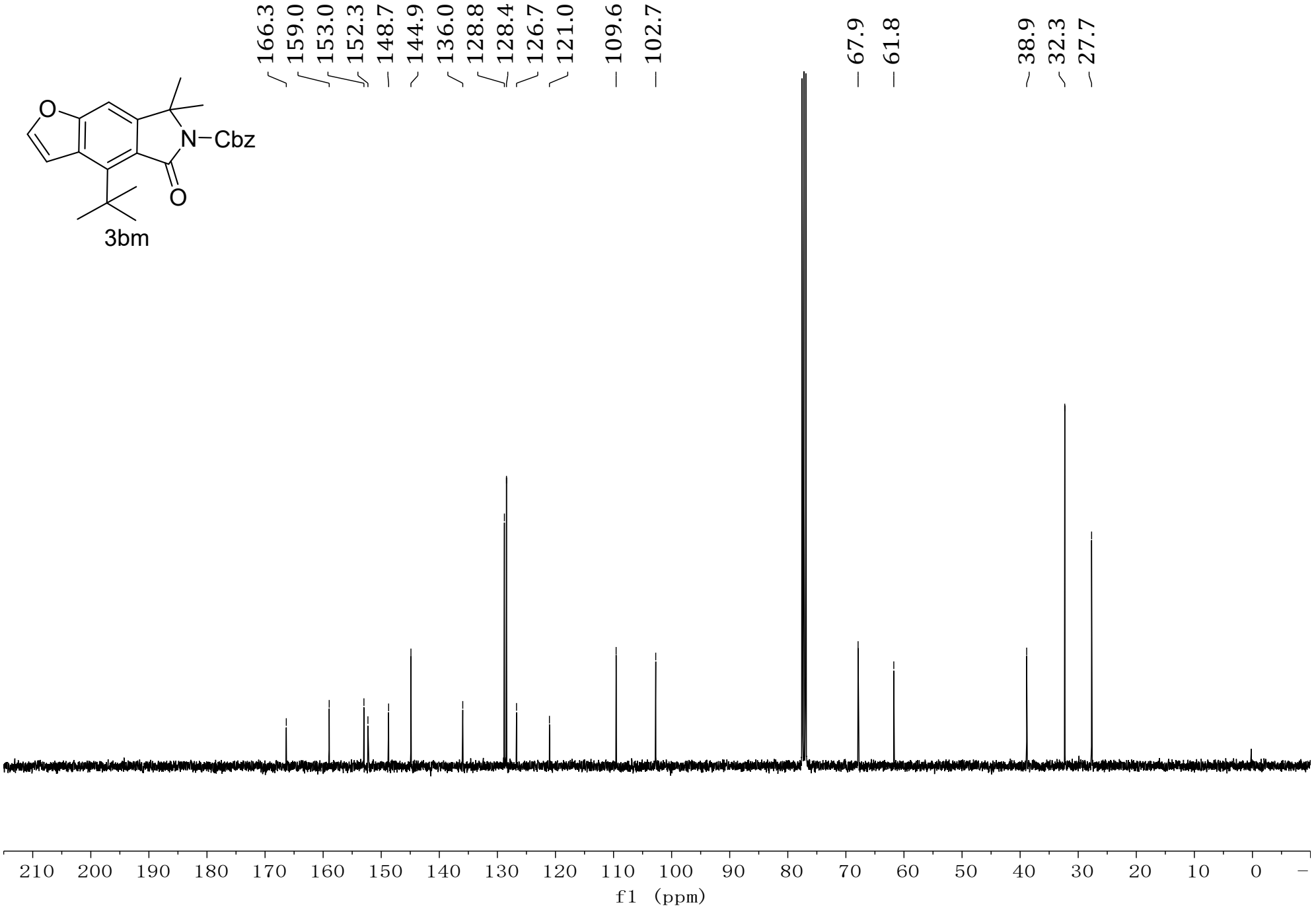
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bl**.



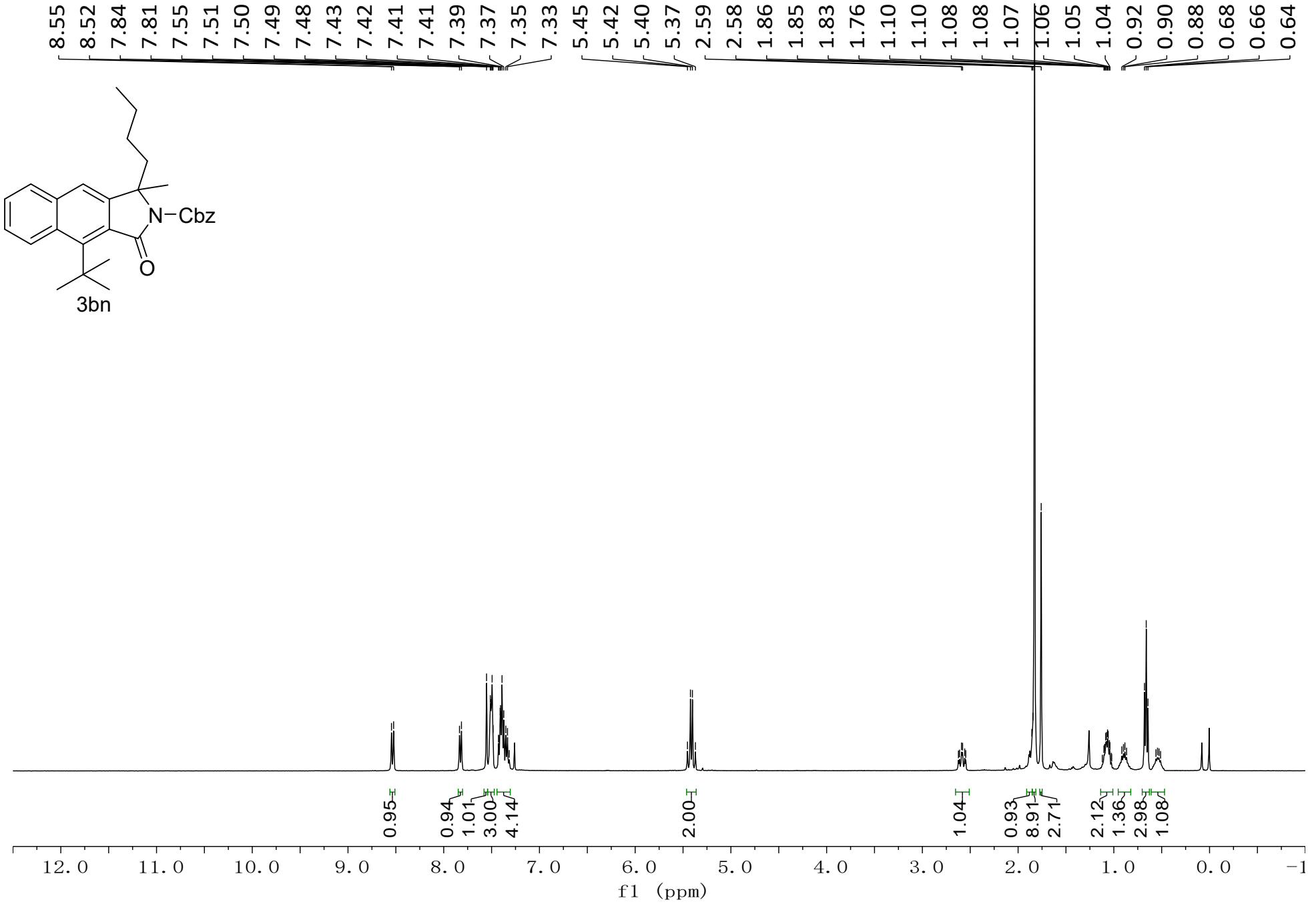
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bl**.



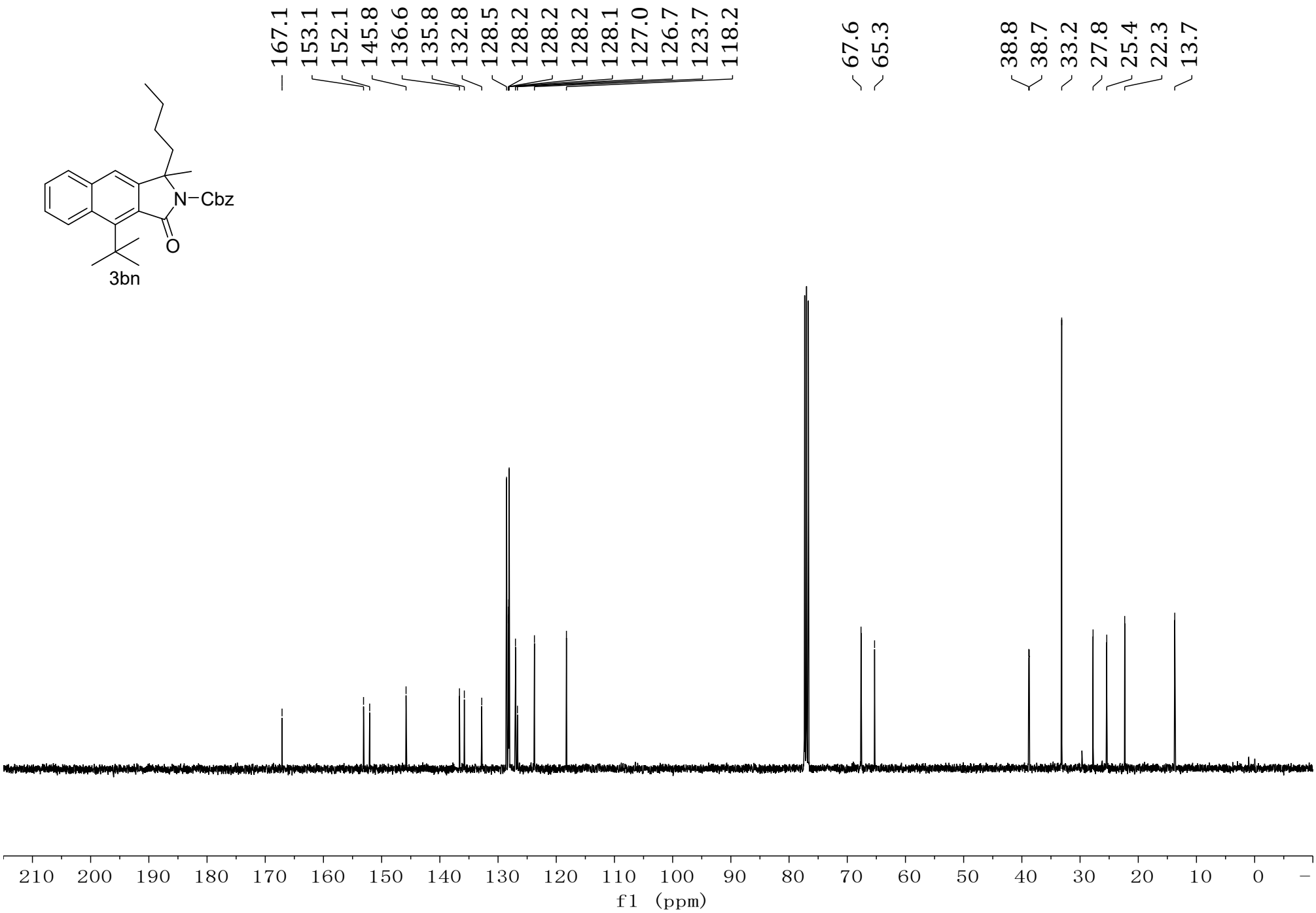
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bm**.



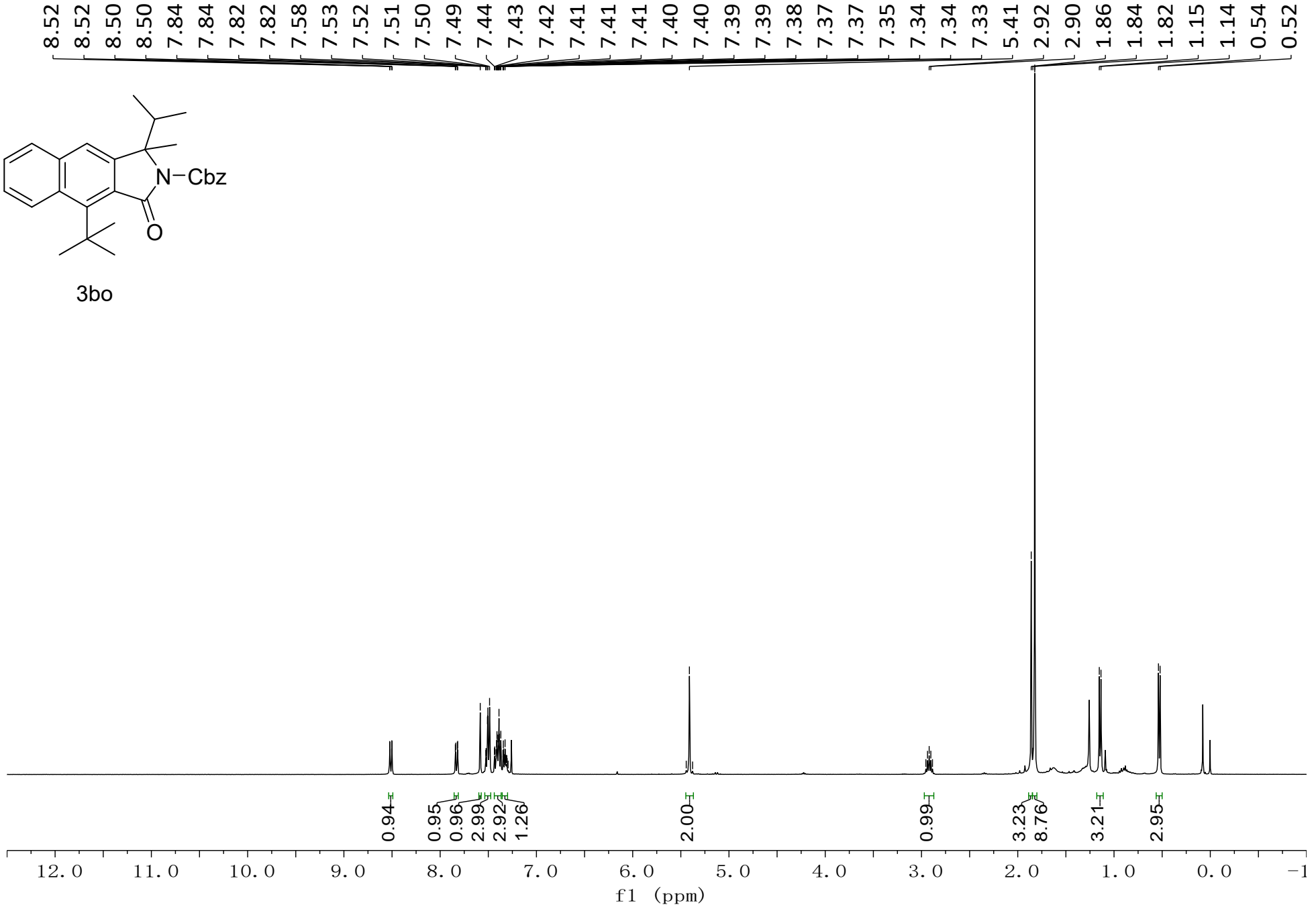
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bm**.



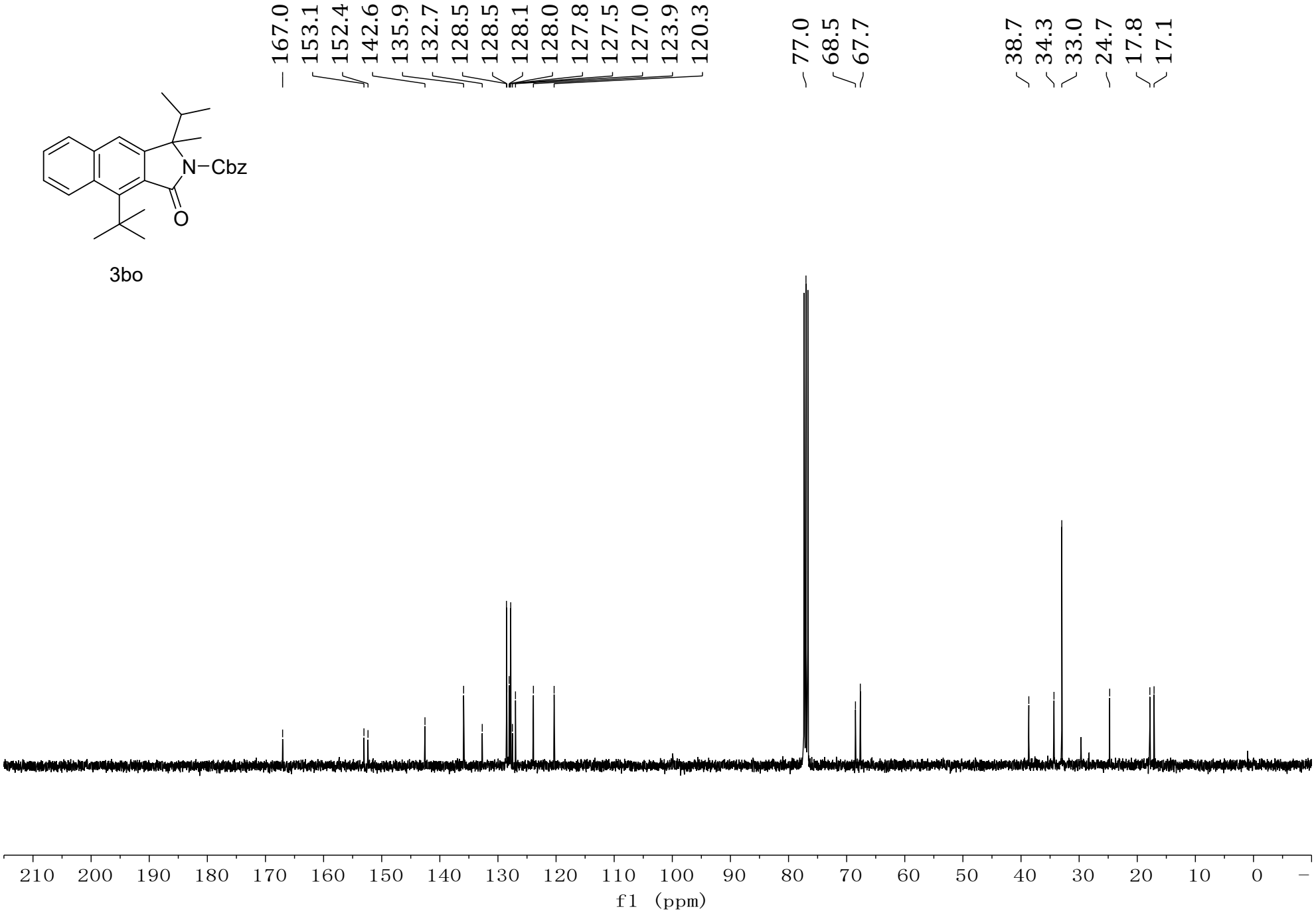
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bn**.



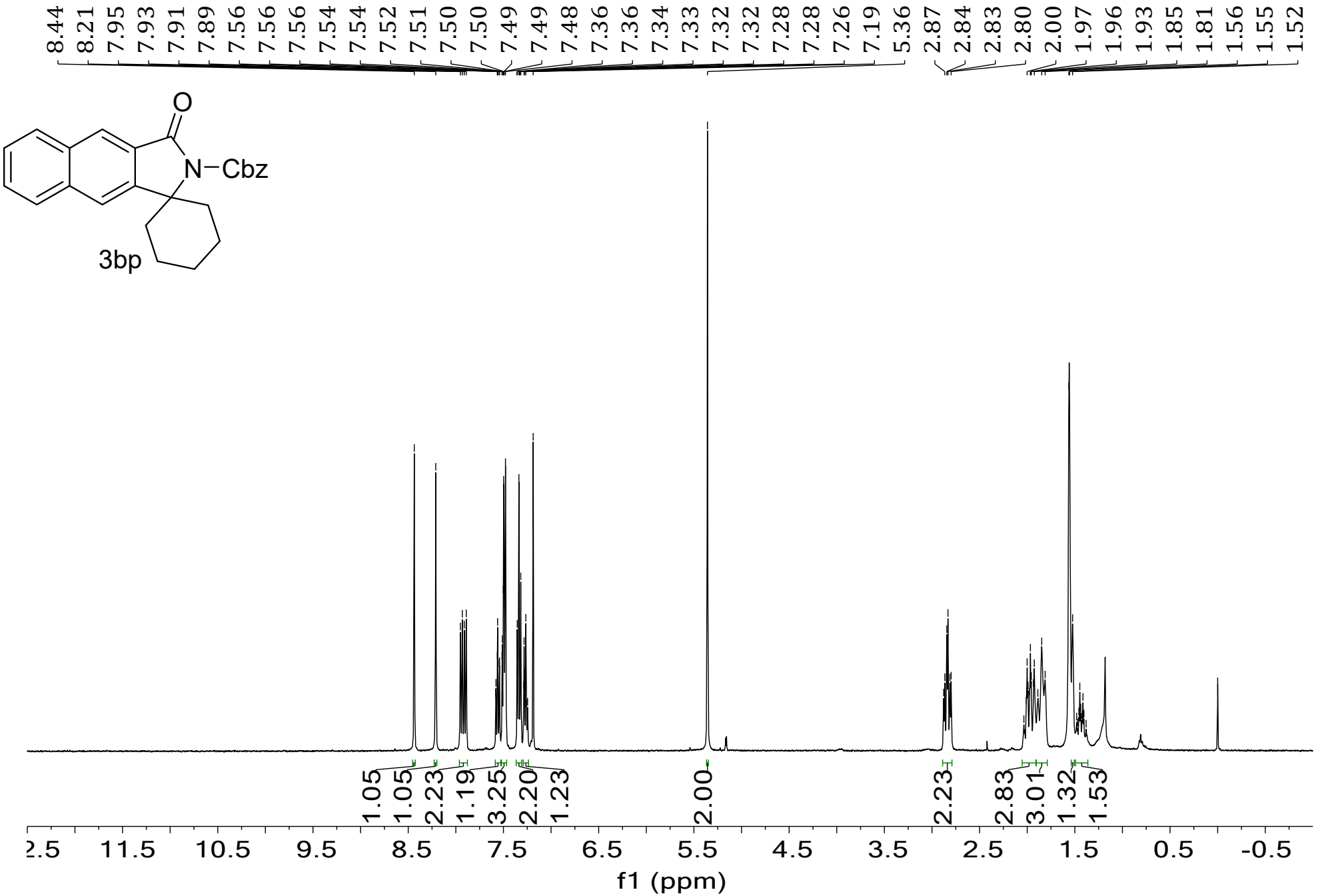
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bn**.



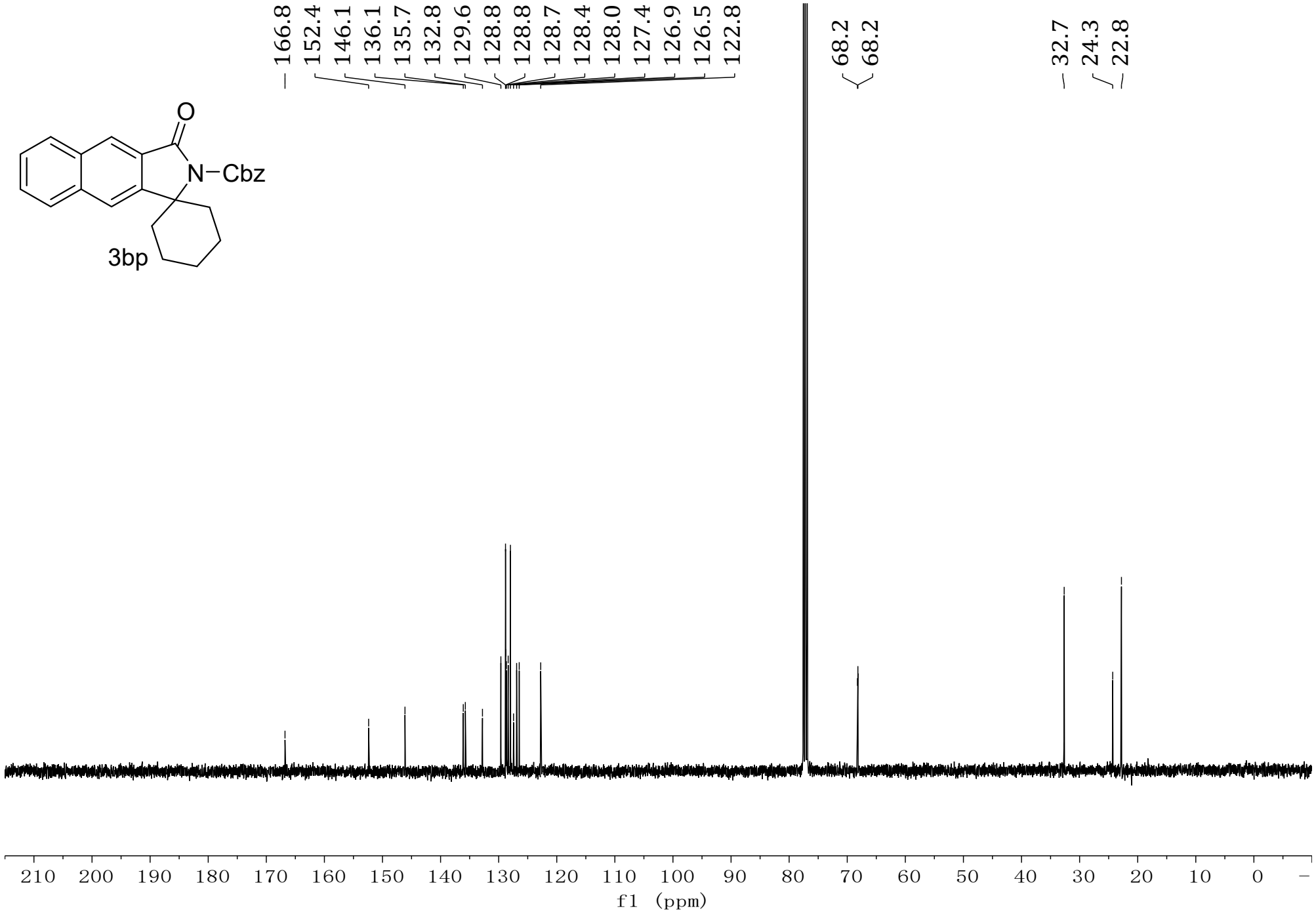
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bo**.



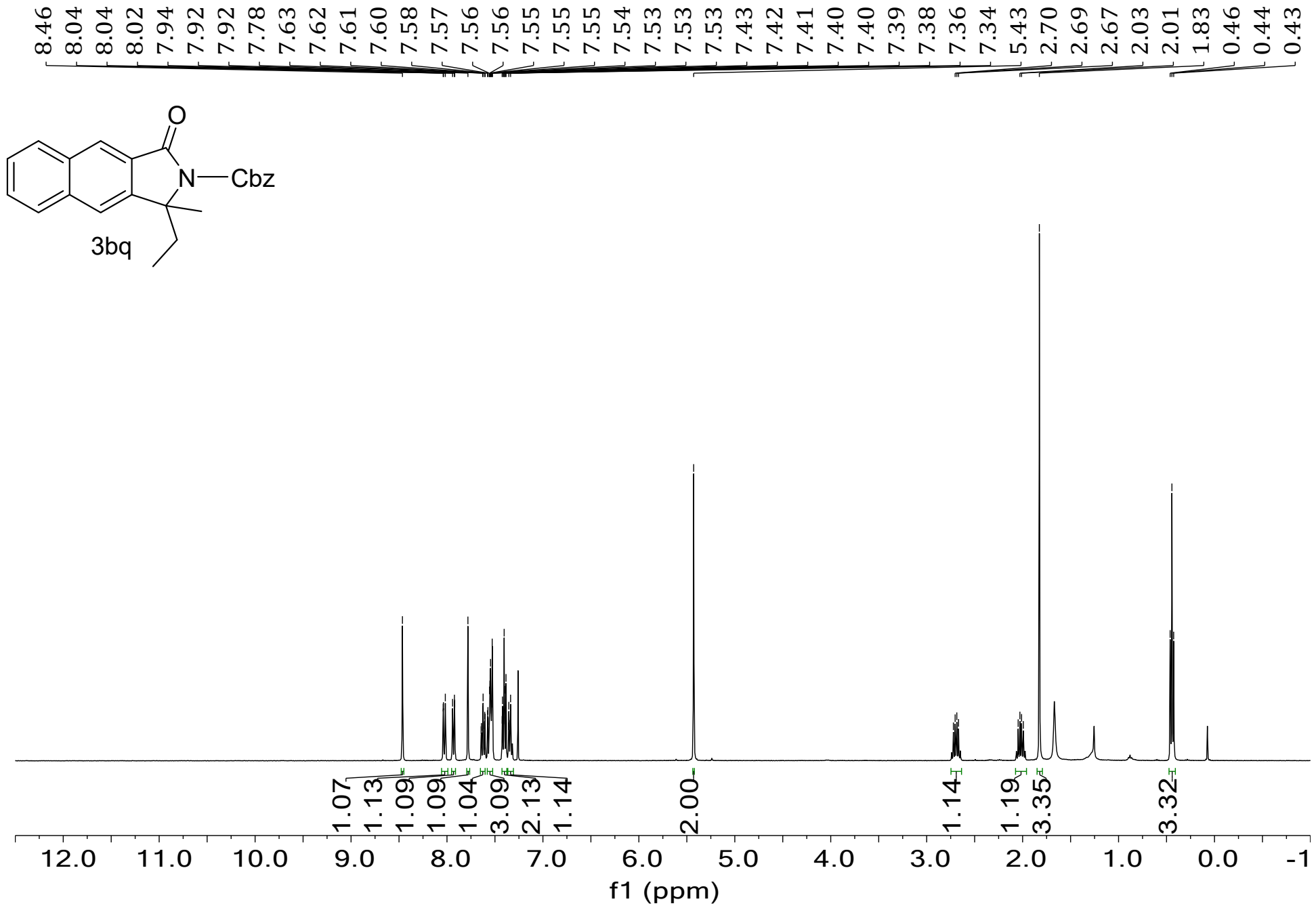
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bo**.



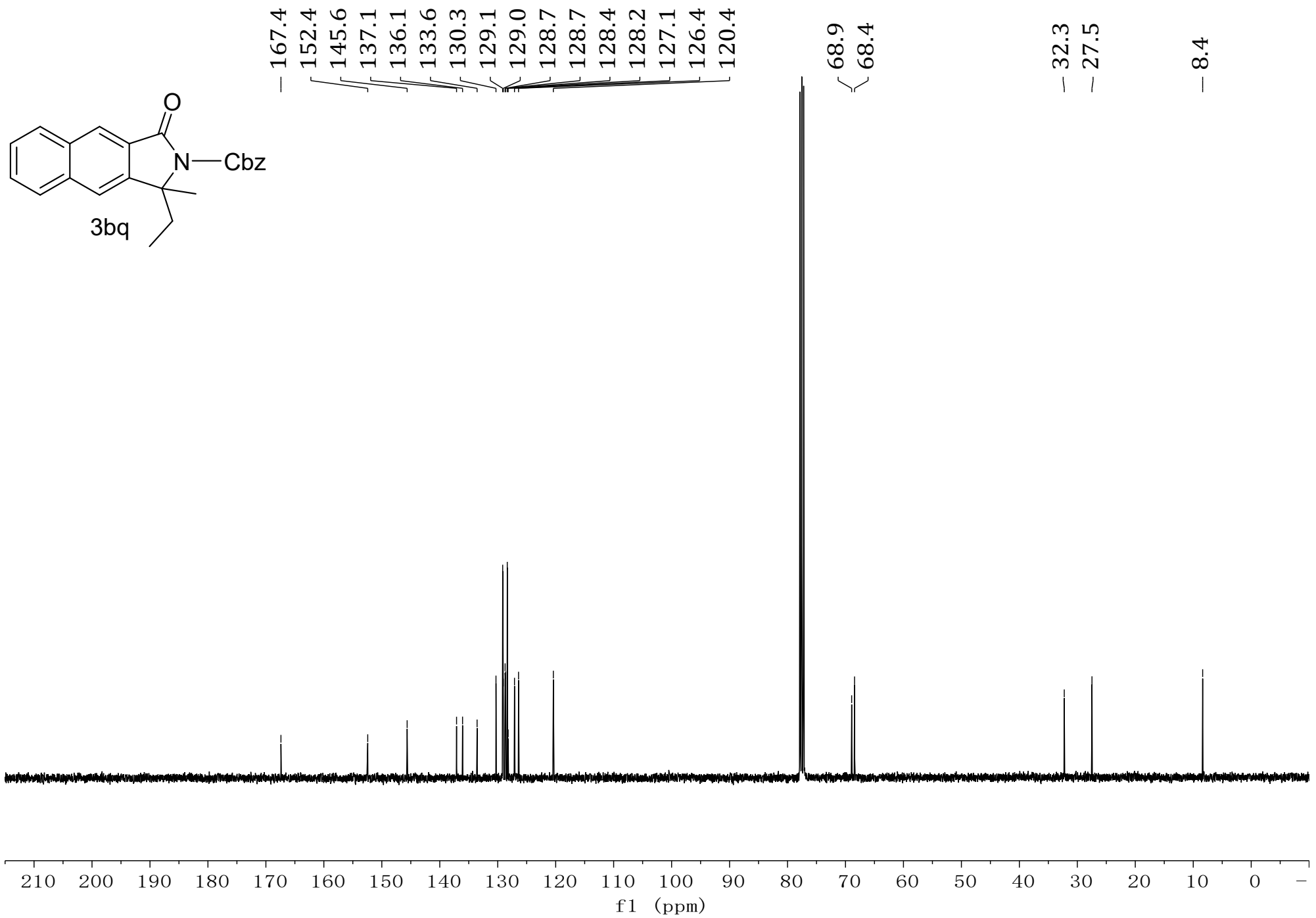
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bp**.



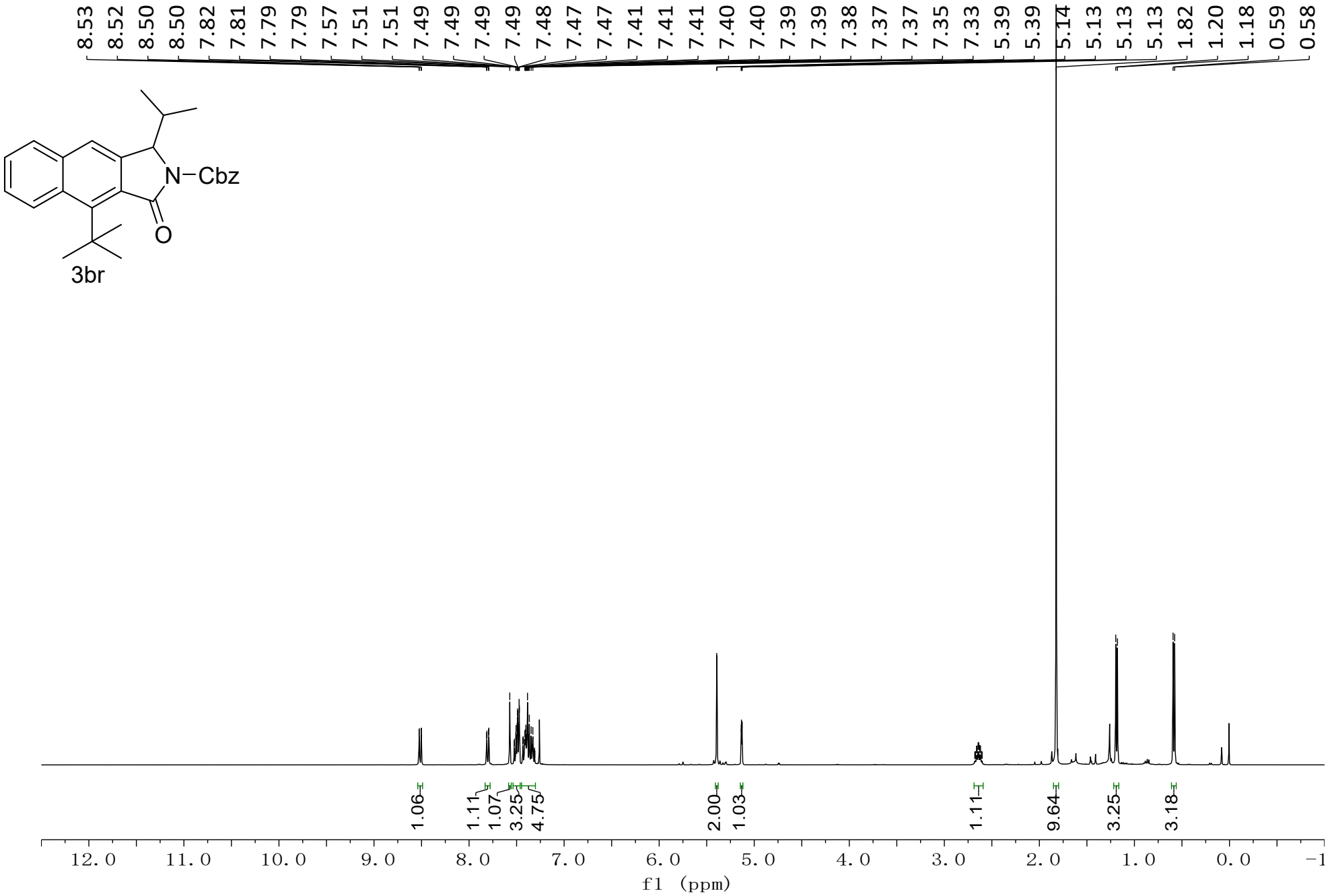
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bp**.



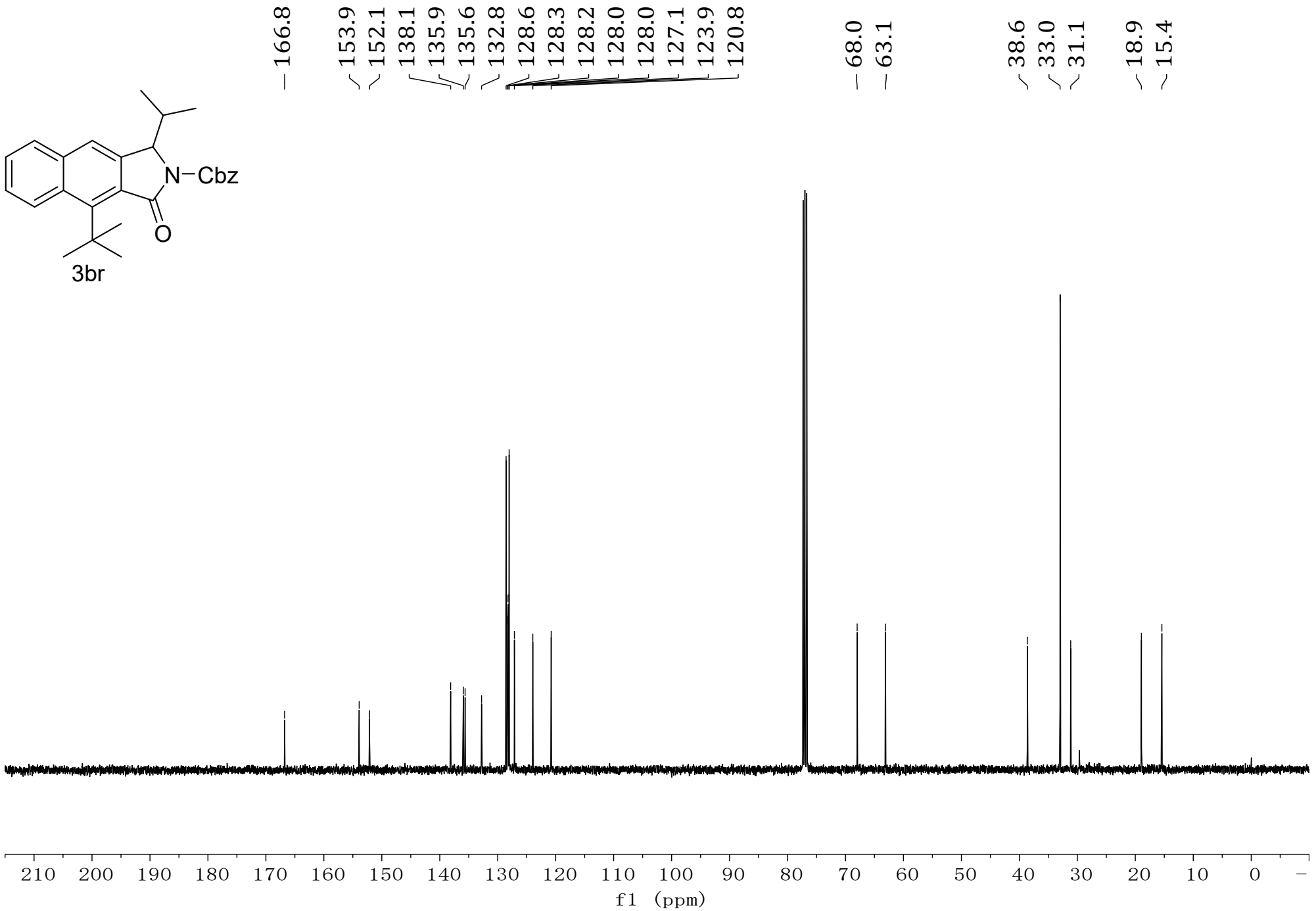
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bq**



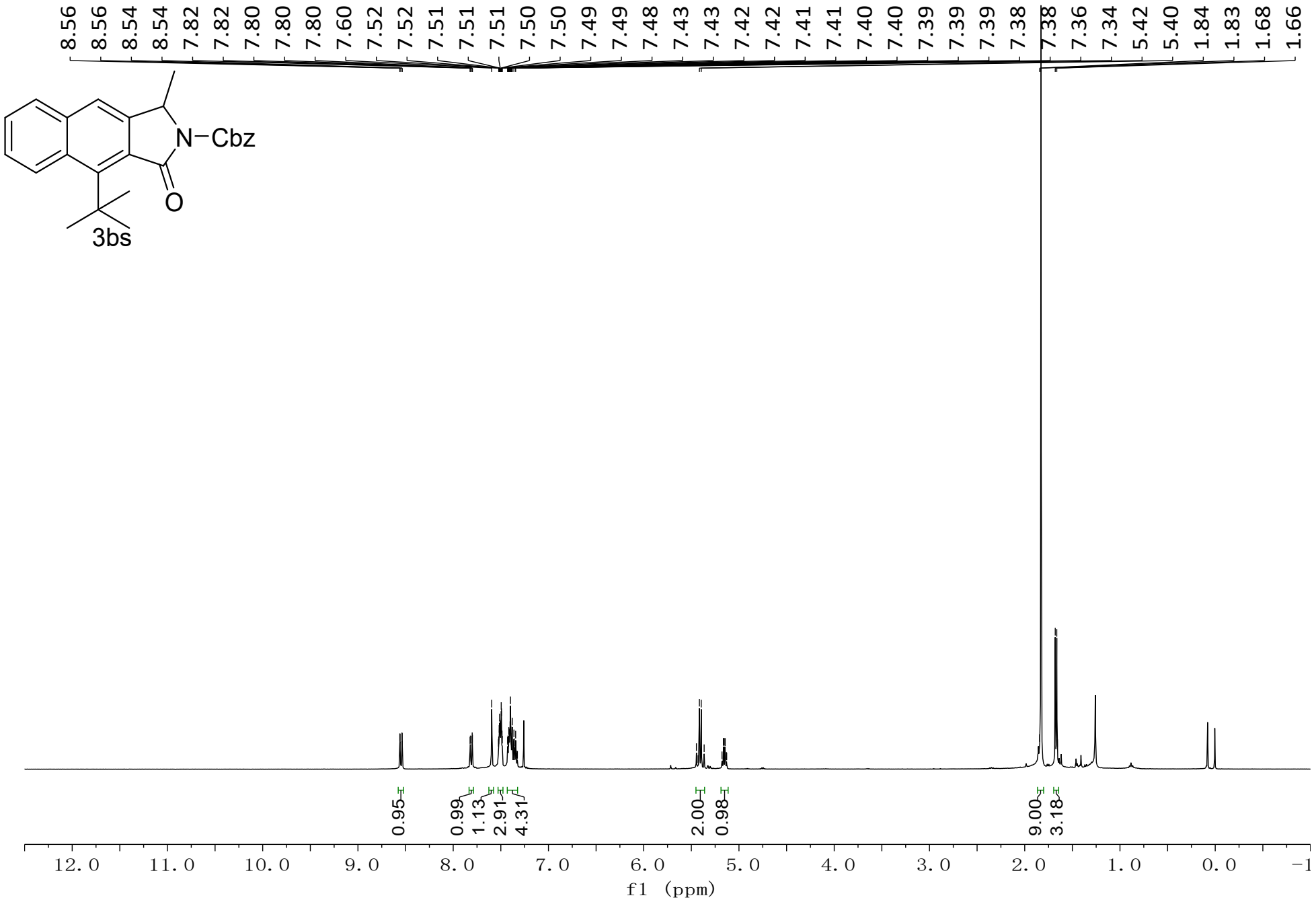
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bq**.



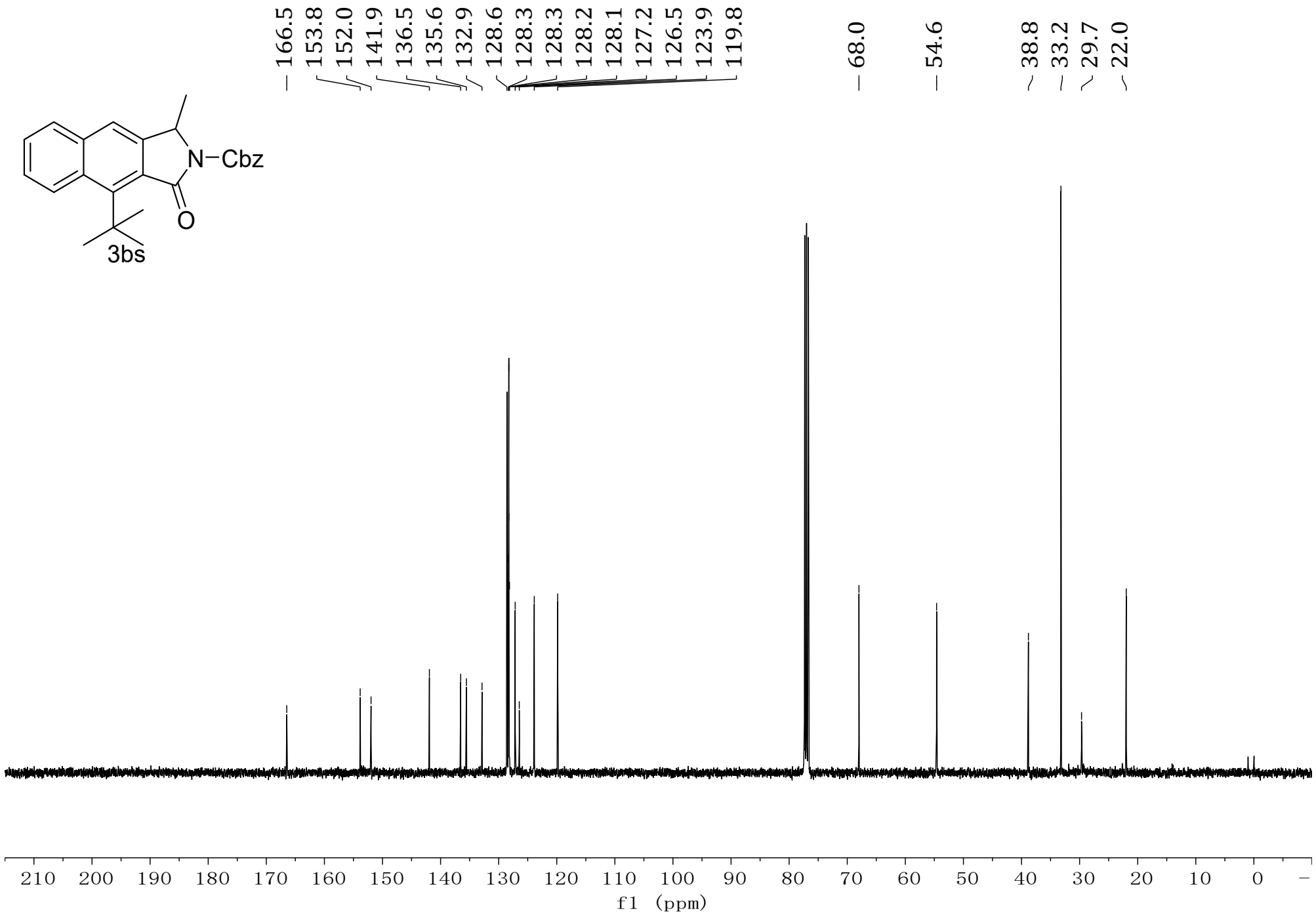
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3br**.



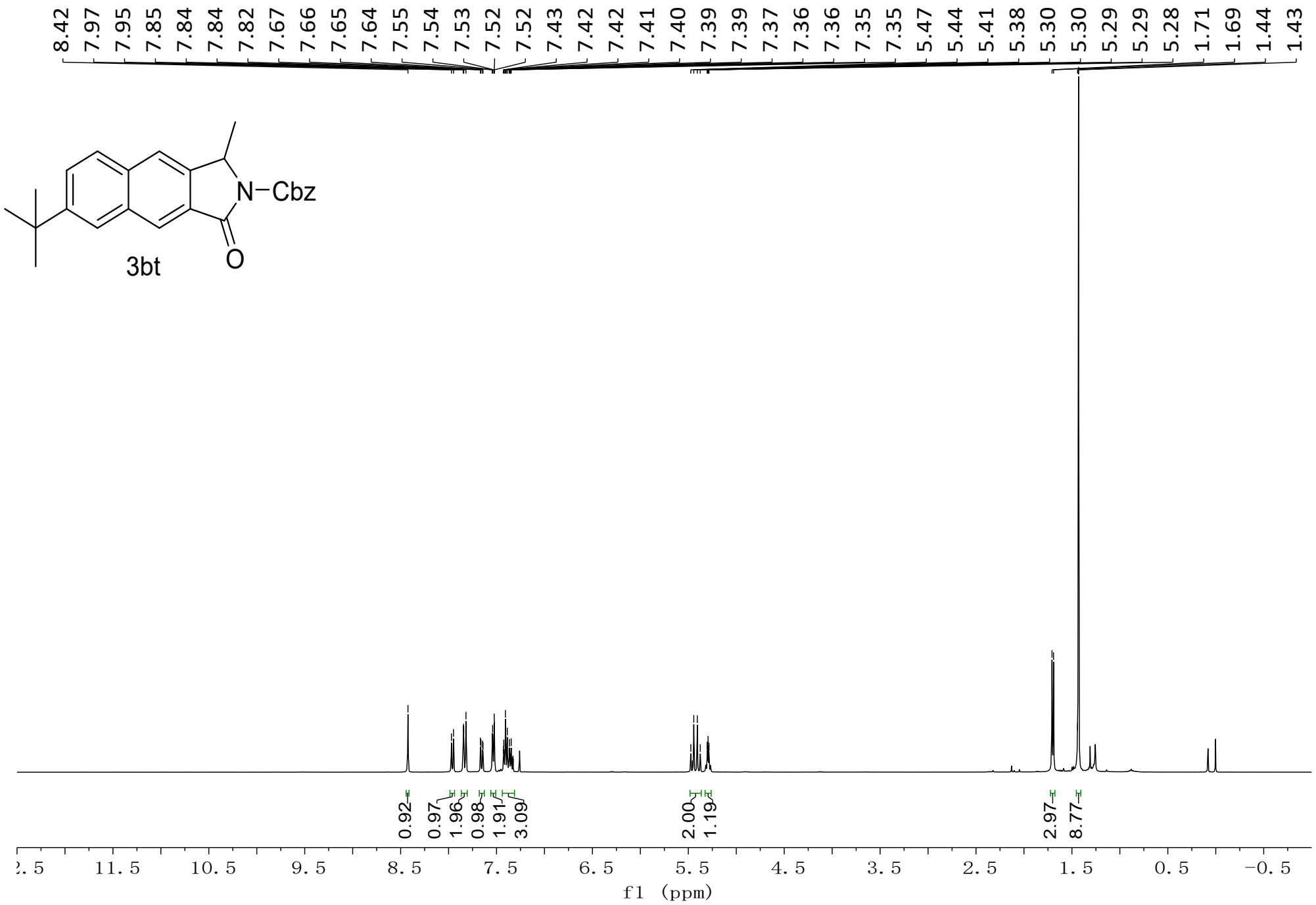
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3br**.



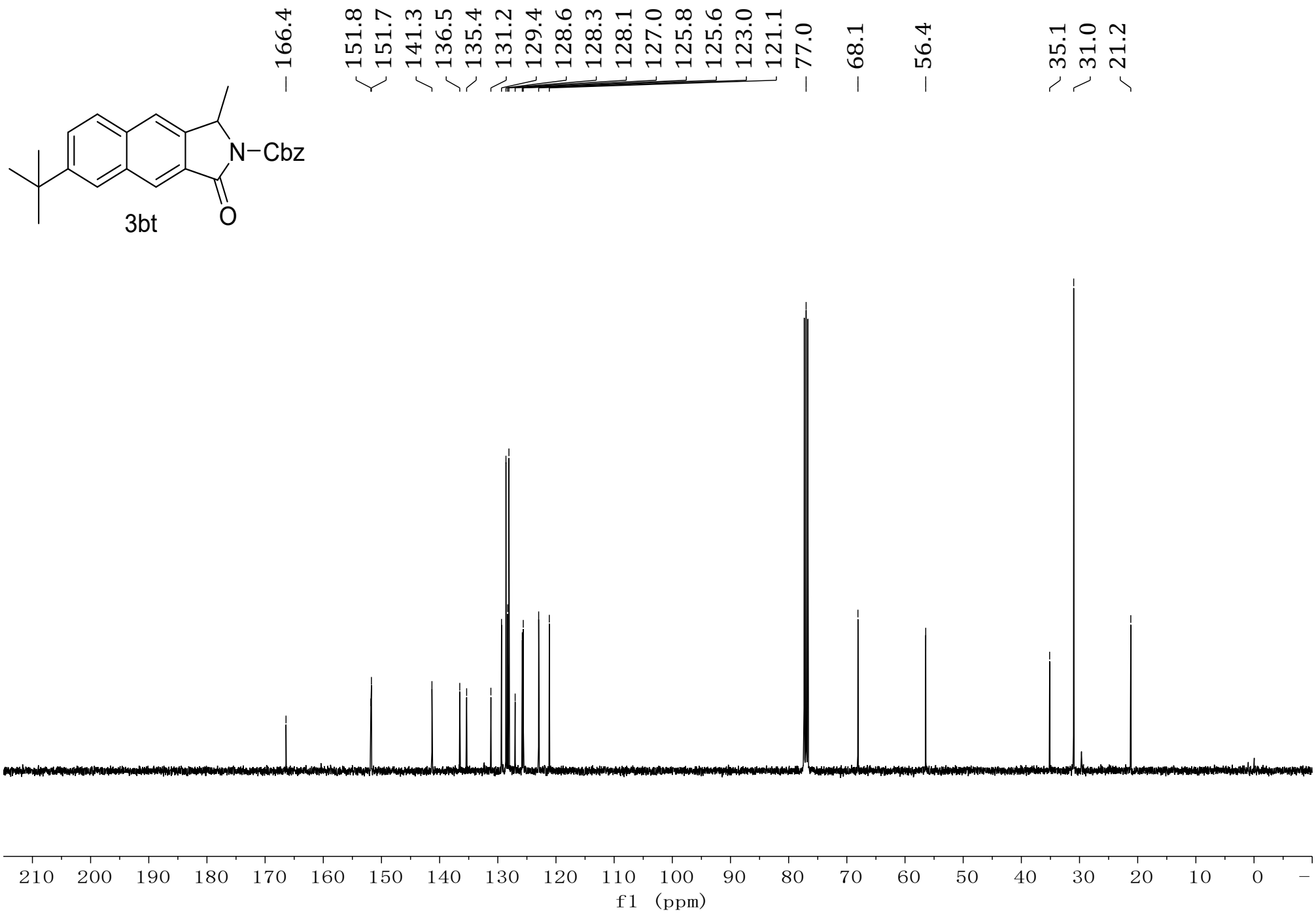
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bs**.



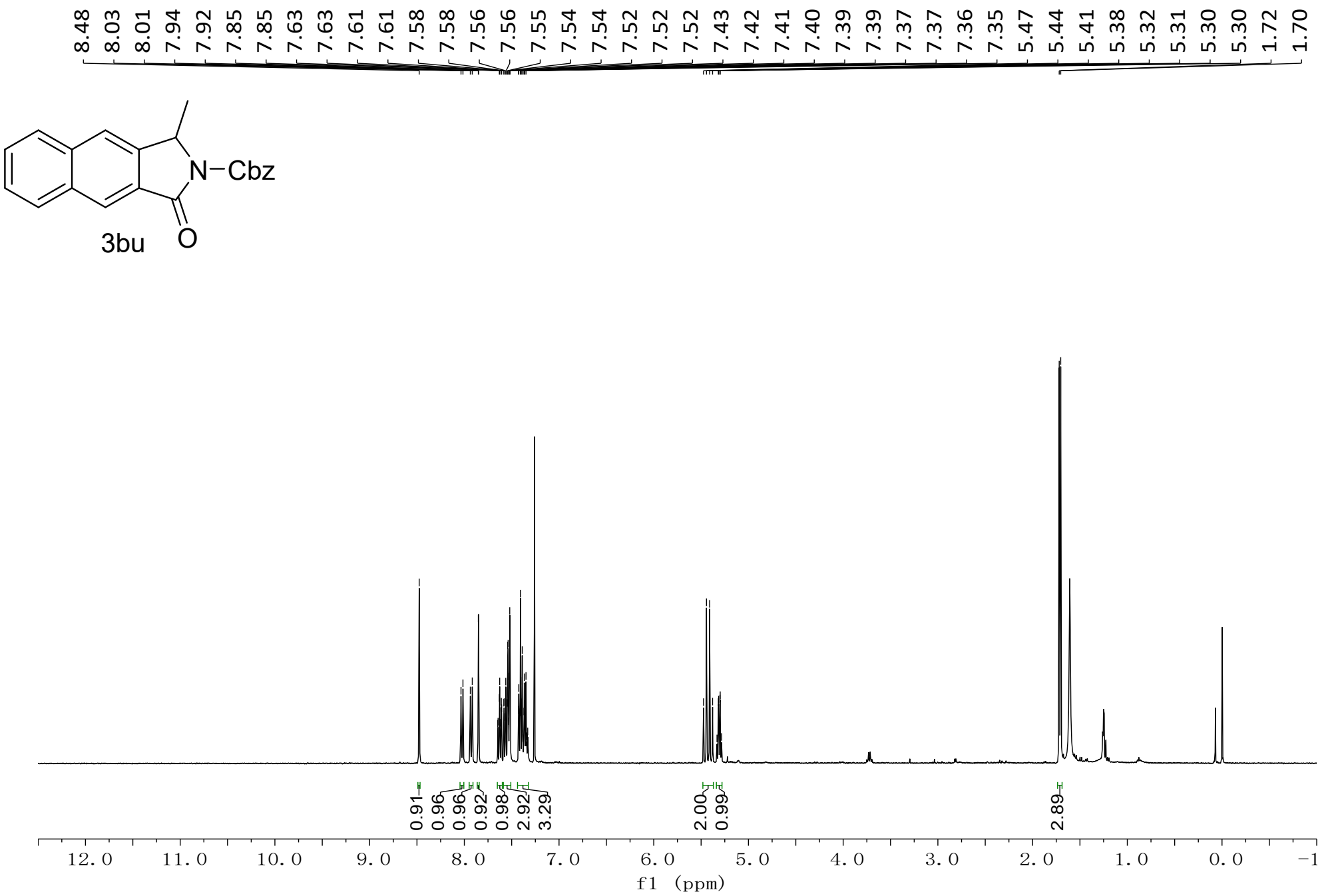
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bs**.



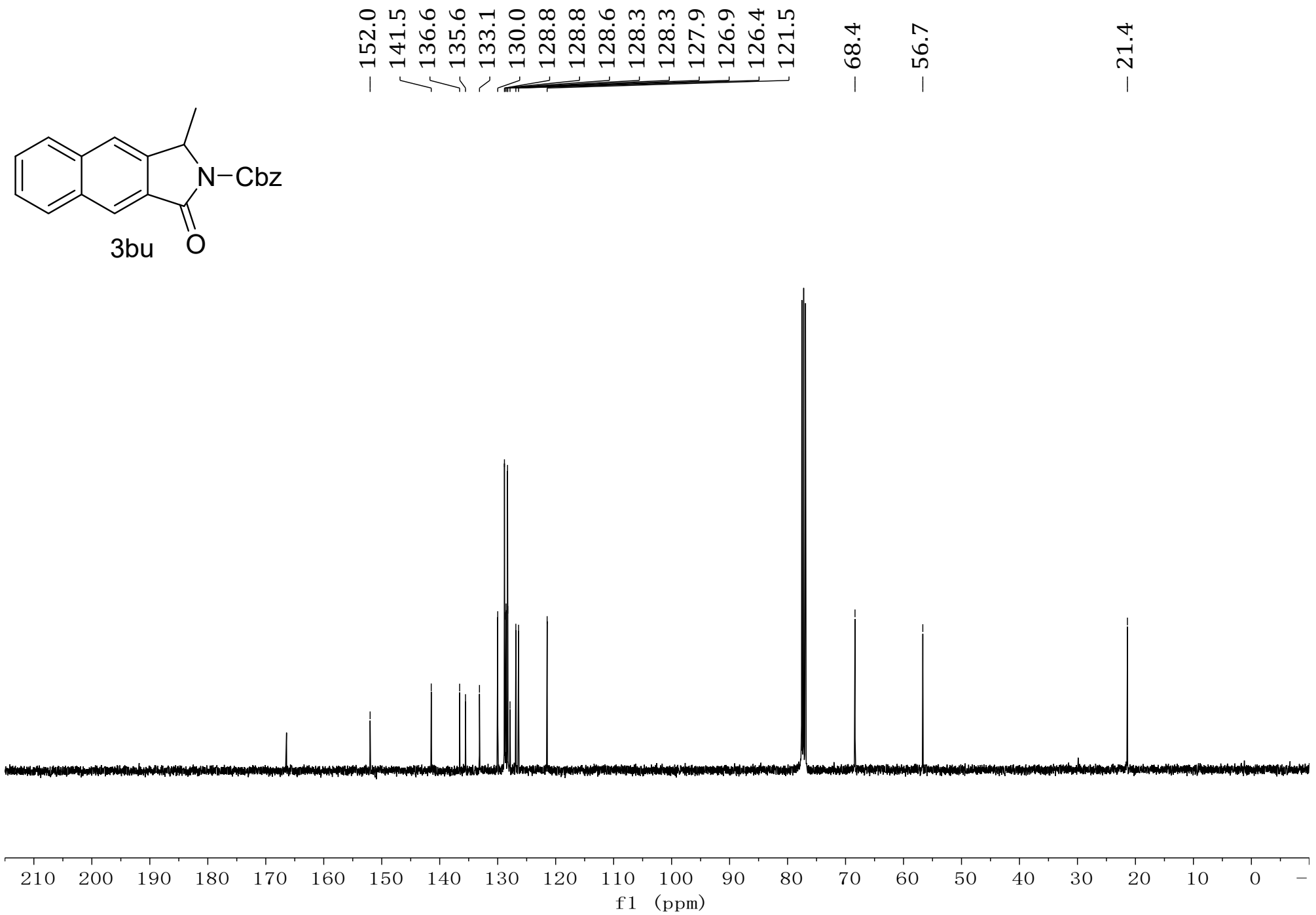
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bt**.



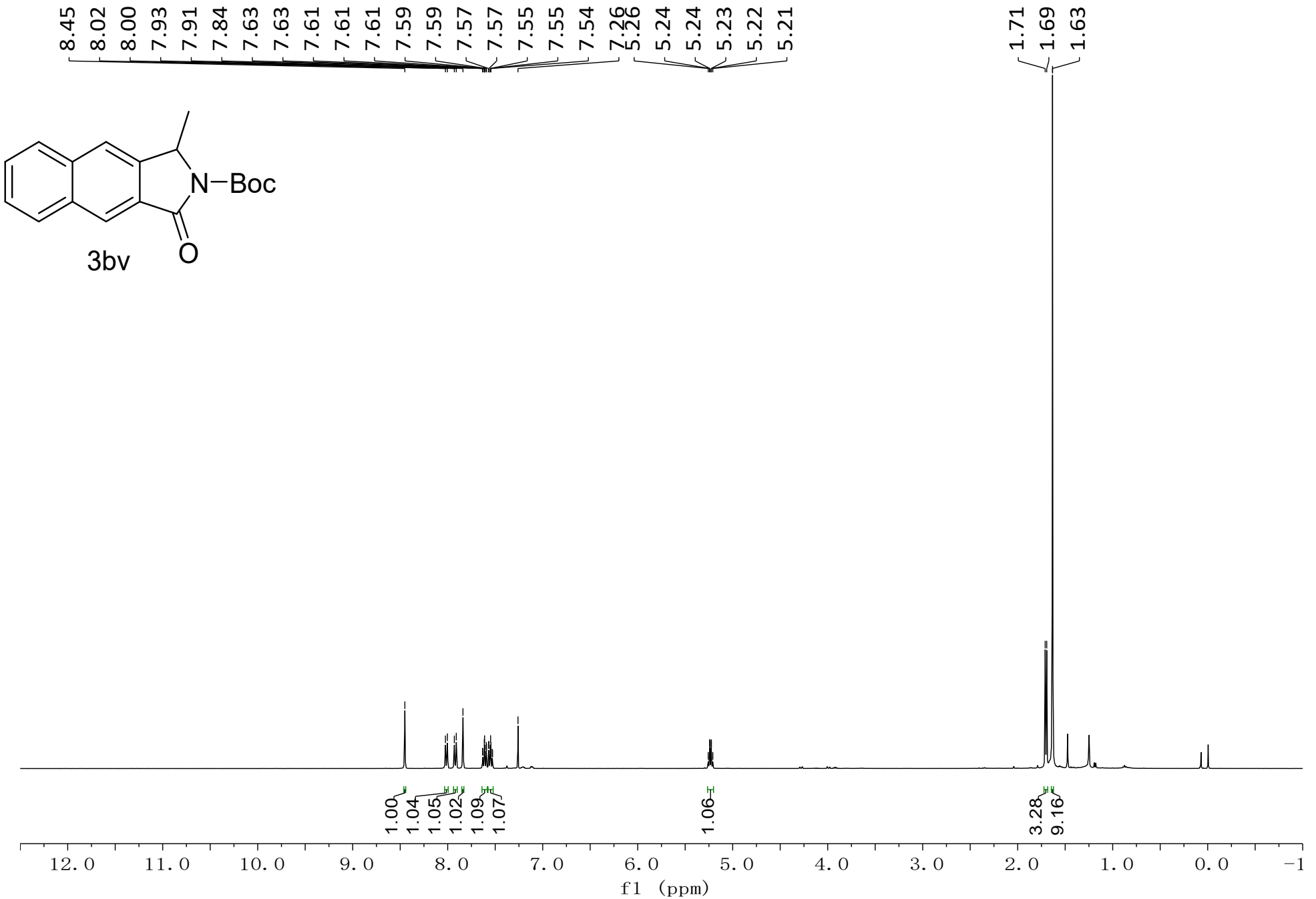
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bt**.



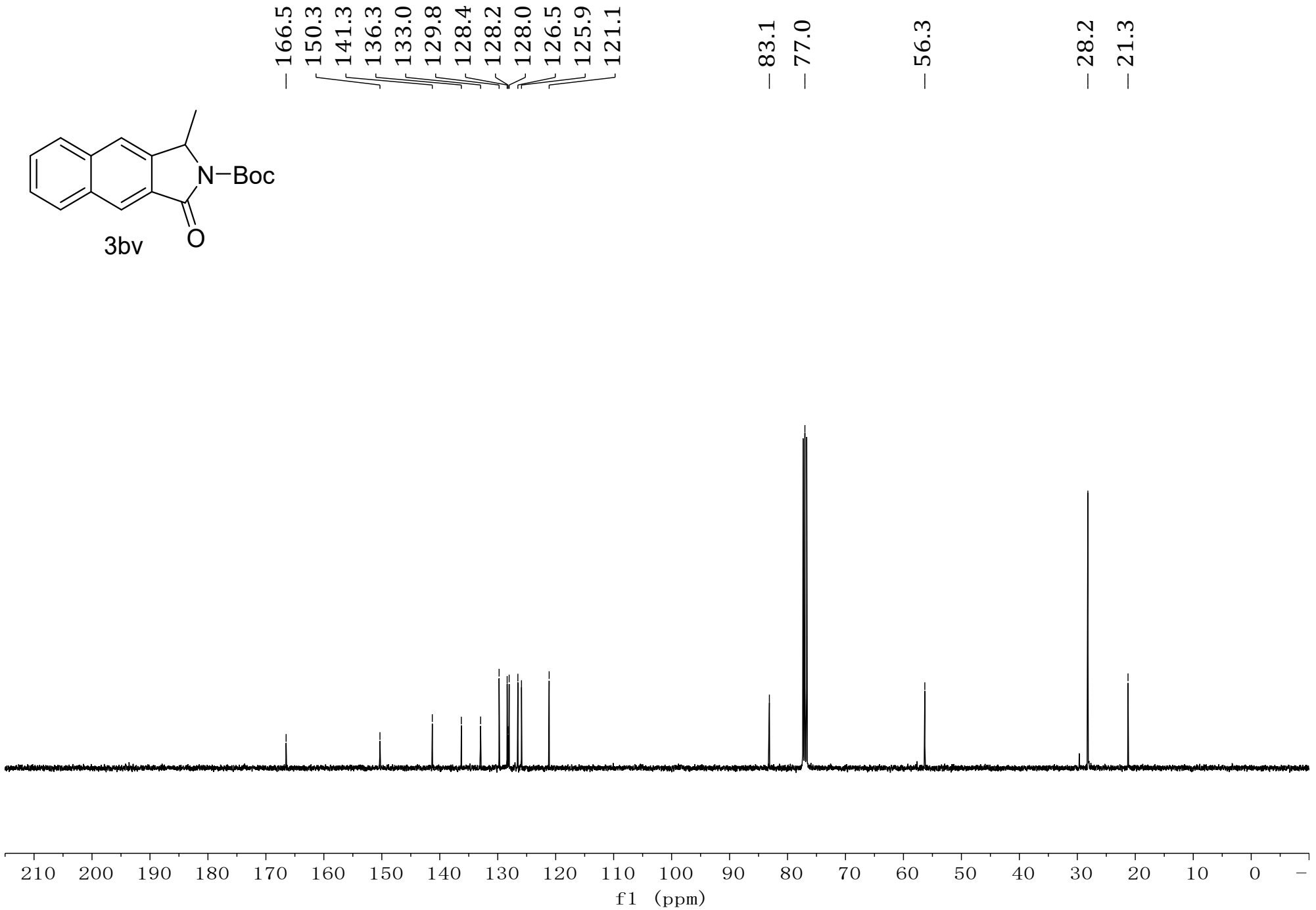
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bu**.



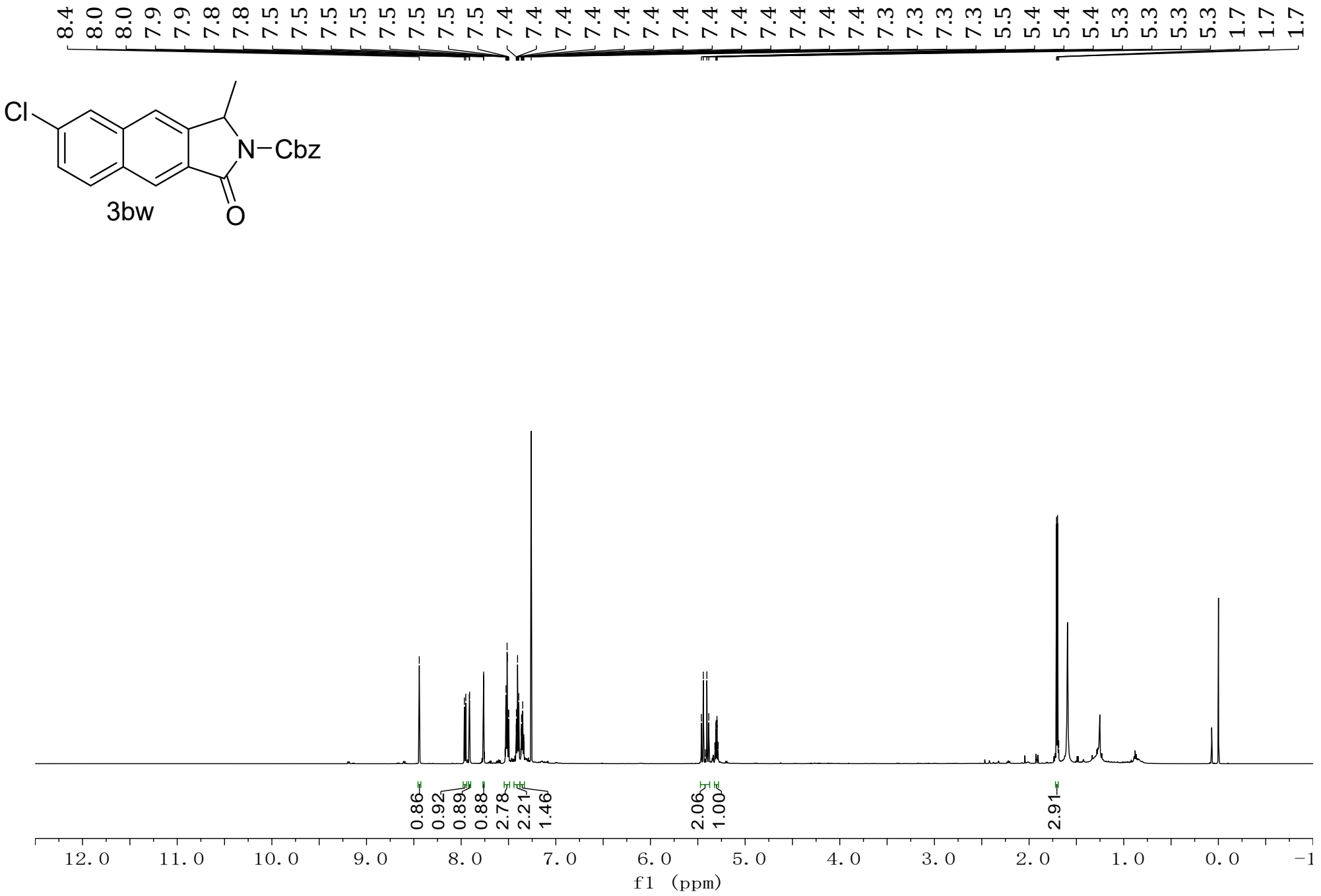
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bu**.



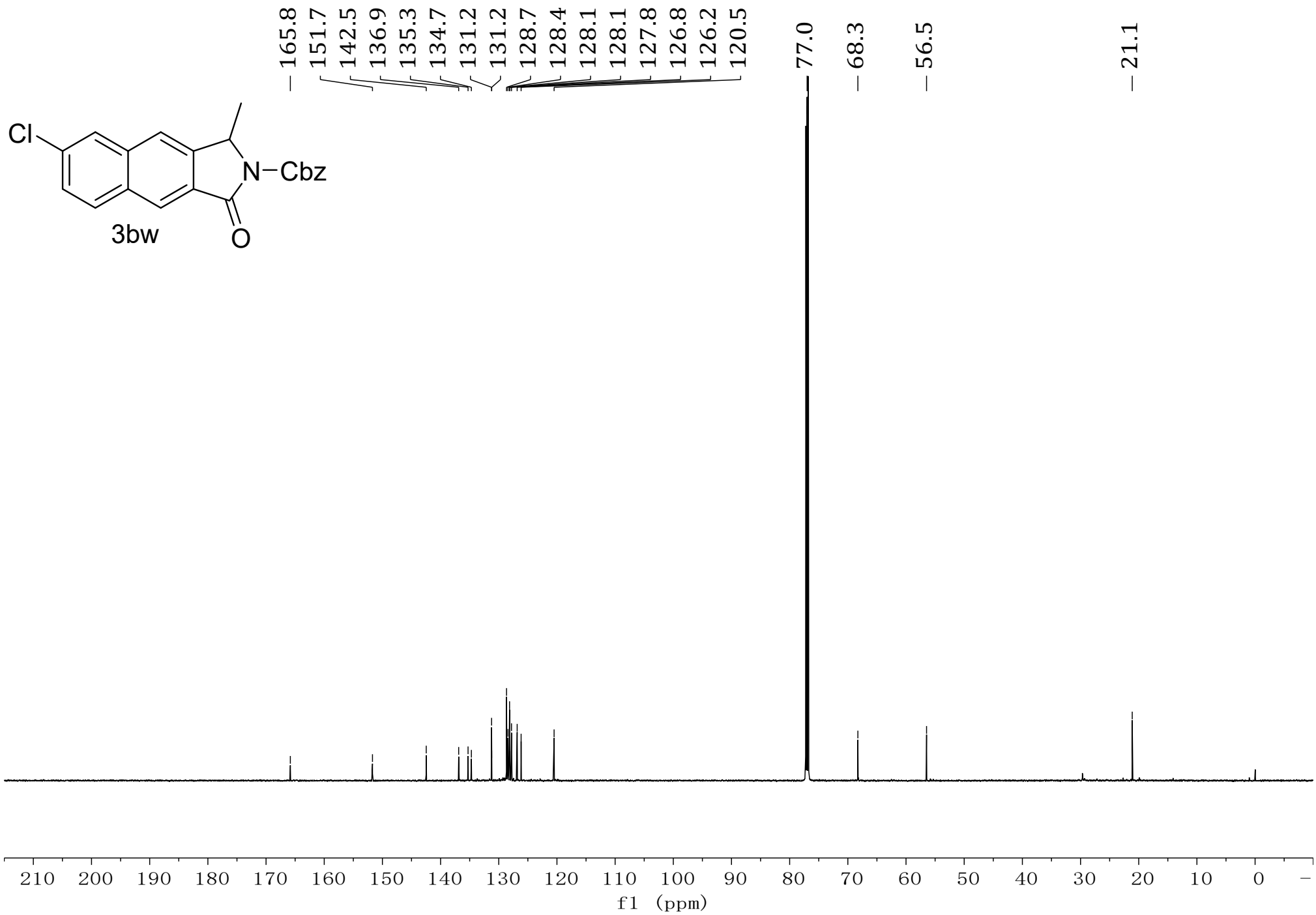
^{1}H NMR (400 MHz, $CDCl_3$) spectra of **3bv**.



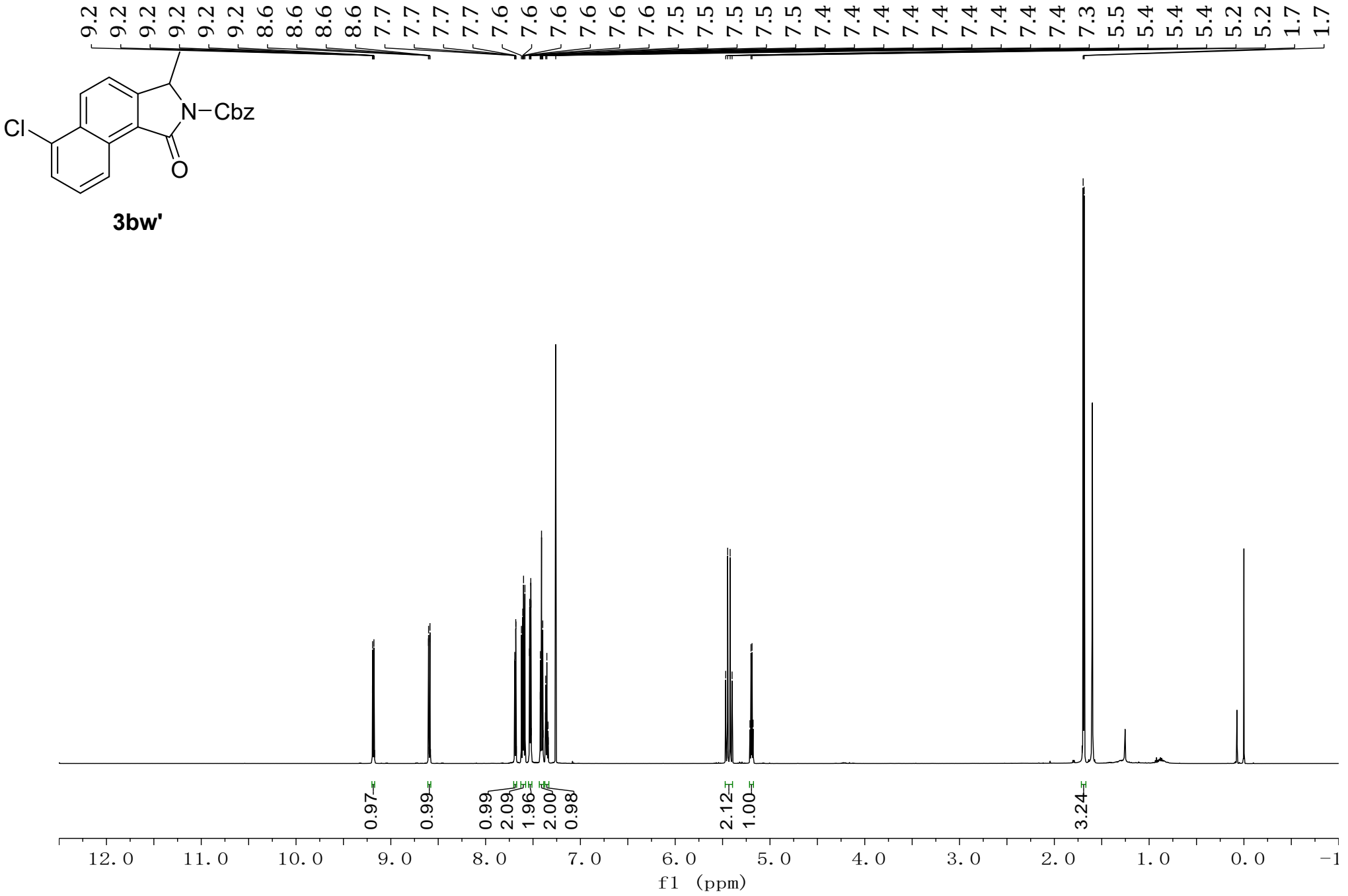
^{13}C NMR (100 MHz, $CDCl_3$) spectra of **3bv**.



^{1}H NMR (600 MHz, $CDCl_3$) spectra of **3bw**.

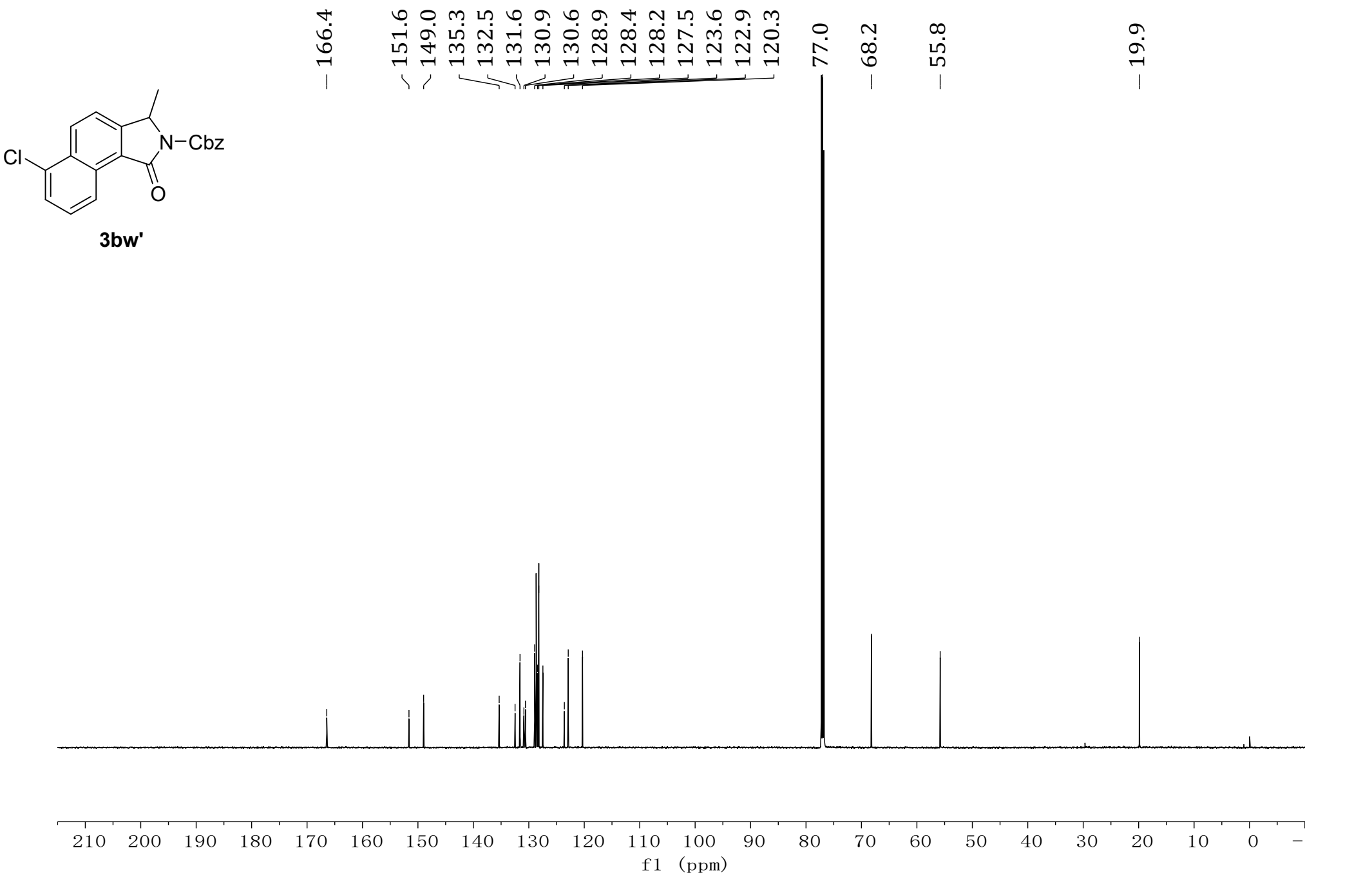


^{13}C NMR (150 MHz, $CDCl_3$) spectra of **3bw**.



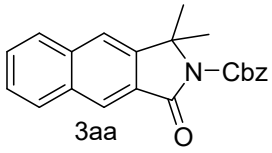
3bw'

^{1}H NMR (600 MHz, $CDCl_3$) spectra of **3bw'**.



^{13}C NMR (150 MHz, $CDCl_3$) spectra of **3bw'**.

X-ray Crystal Structure and Details of Compound 3aa



3aa

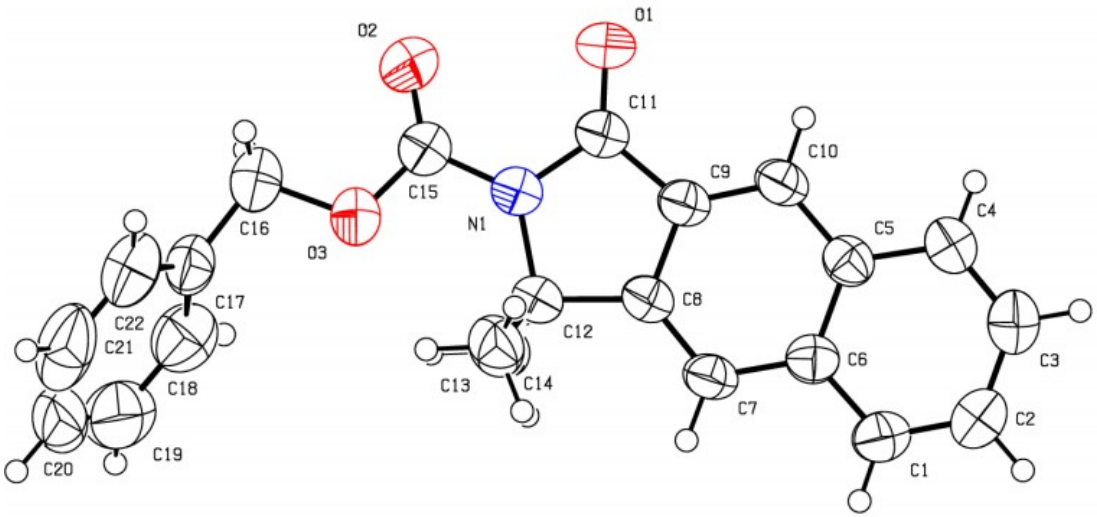


Table 1. Crystal data and structure refinement for 3a.

Identification code	1_a
Empirical formula	C22 H19 N O3
Formula weight	345.38
Temperature	293(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 9.7838(2) Å α= 90°.
	b = 9.39690(10) Å β= 95.2820(10)°.
	c = 19.7446(3) Å γ = 90°.
Volume	1807.56(5) $Å^3$
Z	4
Density (calculated)	1.269 Mg/m^3
Absorption coefficient	0.681 mm^{-1}
F(000)	728
Crystal size	0.220 x 0.200 x 0.180 mm^3
Theta range for data collection	4.498 to 73.837°.
Index ranges	-12<=h<=12, -11<=k<=11, -24<=l<=24
Reflections collected	42473
Independent reflections	3632 [R(int) = 0.0347]
Completeness to theta = 67.679°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3632 / 1 / 225
Goodness-of-fit on F^2	1.075
Final R indices [I>2sigma(I)]	R1 = 0.0732, wR2 = 0.2078
R indices (all data)	R1 = 0.0757, wR2 = 0.2115
Extinction coefficient	n/a
Largest diff. peak and hole	0.355 and -0.409 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for 1_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4067(2)	9579(2)	2008(1)	59(1)
C(2)	3477(2)	10886(2)	1937(1)	64(1)
C(3)	3351(2)	11756(2)	2507(1)	66(1)
C(4)	3755(2)	11275(2)	3142(1)	59(1)
C(5)	4343(2)	9899(2)	3242(1)	50(1)
C(6)	4549(2)	9048(2)	2660(1)	49(1)
C(7)	5194(2)	7703(2)	2744(1)	53(1)
C(8)	5590(2)	7222(2)	3385(1)	50(1)
C(9)	5330(2)	8038(2)	3954(1)	52(1)
C(10)	4735(2)	9353(2)	3897(1)	54(1)
C(11)	5837(2)	7277(2)	4577(1)	63(1)
C(12)	6322(2)	5860(2)	3598(1)	54(1)
C(13)	5452(3)	4571(2)	3373(1)	70(1)
C(14)	7734(2)	5826(3)	3323(1)	74(1)
C(15)	7016(2)	5032(3)	4824(1)	72(1)
C(16)	8267(4)	2904(3)	4943(2)	104(1)
C(17)	8881(2)	1858(2)	4497(1)	67(1)
C(18)	8051(2)	995(2)	4060(1)	85(1)
C(19)	8640(3)	-24(2)	3667(1)	123(1)
C(20)	10058(3)	-179(2)	3710(1)	139(2)
C(21)	10888(2)	684(3)	4147(1)	120(2)
C(22)	10299(2)	1703(2)	4540(1)	85(1)
N(1)	6440(2)	6022(2)	4360(1)	60(1)
O(1)	5760(2)	7642(2)	5159(1)	94(1)
O(2)	6969(3)	5081(3)	5422(1)	122(1)

O(3)	7630(2)	4000(2)	4501(1)	83(1)

Table 3. Bond lengths [Å] and angles [°] for 1_a.

C(1)-C(2)	1.359(3)
C(1)-C(6)	1.420(3)
C(1)-H(1)	0.9300
C(2)-C(3)	1.405(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.357(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.422(3)
C(4)-H(4)	0.9300
C(5)-C(10)	1.410(3)
C(5)-C(6)	1.429(2)
C(6)-C(7)	1.416(3)
C(7)-C(8)	1.366(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.402(2)
C(8)-C(12)	1.508(2)
C(9)-C(10)	1.367(3)
C(9)-C(11)	1.468(3)
C(10)-H(10)	0.9300
C(11)-O(1)	1.209(2)
C(11)-N(1)	1.403(2)
C(12)-N(1)	1.507(2)
C(12)-C(13)	1.523(3)
C(12)-C(14)	1.530(3)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600

C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-O(2)	1.186(3)
C(15)-O(3)	1.333(3)
C(15)-N(1)	1.388(3)
C(16)-O(3)	1.452(3)
C(16)-C(17)	1.483(3)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.3900
C(17)-C(22)	1.3900
C(18)-C(19)	1.3900
C(18)-H(18)	0.9300
C(19)-C(20)	1.3900
C(19)-H(19)	0.9300
C(20)-C(21)	1.3900
C(20)-H(20)	0.9300
C(21)-C(22)	1.3900
C(21)-H(21)	0.9300
C(22)-H(22)	0.9300

C(2)-C(1)-C(6)	120.91(18)
C(2)-C(1)-H(1)	119.5
C(6)-C(1)-H(1)	119.5
C(1)-C(2)-C(3)	120.68(19)
C(1)-C(2)-H(2)	119.7
C(3)-C(2)-H(2)	119.7
C(4)-C(3)-C(2)	120.45(19)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8

C(3)-C(4)-C(5)	120.73(19)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(10)-C(5)-C(4)	122.02(16)
C(10)-C(5)-C(6)	119.15(16)
C(4)-C(5)-C(6)	118.82(17)
C(7)-C(6)-C(1)	121.80(16)
C(7)-C(6)-C(5)	119.95(16)
C(1)-C(6)-C(5)	118.23(17)
C(8)-C(7)-C(6)	119.28(15)
C(8)-C(7)-H(7)	120.4
C(6)-C(7)-H(7)	120.4
C(7)-C(8)-C(9)	120.34(17)
C(7)-C(8)-C(12)	128.73(15)
C(9)-C(8)-C(12)	110.94(15)
C(10)-C(9)-C(8)	122.32(17)
C(10)-C(9)-C(11)	128.21(16)
C(8)-C(9)-C(11)	109.43(16)
C(9)-C(10)-C(5)	118.86(16)
C(9)-C(10)-H(10)	120.6
C(5)-C(10)-H(10)	120.6
O(1)-C(11)-N(1)	126.4(2)
O(1)-C(11)-C(9)	127.75(19)
N(1)-C(11)-C(9)	105.85(15)
N(1)-C(12)-C(8)	100.55(13)
N(1)-C(12)-C(13)	111.12(16)
C(8)-C(12)-C(13)	110.86(16)
N(1)-C(12)-C(14)	111.57(17)
C(8)-C(12)-C(14)	109.92(16)
C(13)-C(12)-C(14)	112.24(17)

C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(2)-C(15)-O(3)	124.3(2)
O(2)-C(15)-N(1)	125.5(2)
O(3)-C(15)-N(1)	110.22(18)
O(3)-C(16)-C(17)	106.8(2)
O(3)-C(16)-H(16A)	110.4
C(17)-C(16)-H(16A)	110.4
O(3)-C(16)-H(16B)	110.4
C(17)-C(16)-H(16B)	110.4
H(16A)-C(16)-H(16B)	108.6
C(18)-C(17)-C(22)	120.0
C(18)-C(17)-C(16)	120.6(2)
C(22)-C(17)-C(16)	119.3(2)
C(17)-C(18)-C(19)	120.0
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(20)-C(19)-C(18)	120.0
C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0

C(21)-C(20)-C(19)	120.0
C(21)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
C(20)-C(21)-C(22)	120.0
C(20)-C(21)-H(21)	120.0
C(22)-C(21)-H(21)	120.0
C(21)-C(22)-C(17)	120.0
C(21)-C(22)-H(22)	120.0
C(17)-C(22)-H(22)	120.0
C(15)-N(1)-C(11)	121.24(17)
C(15)-N(1)-C(12)	125.50(16)
C(11)-N(1)-C(12)	113.18(15)
C(15)-O(3)-C(16)	114.63(18)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	66(1)	62(1)	49(1)	-1(1)	3(1)	-7(1)
C(2)	62(1)	69(1)	62(1)	12(1)	0(1)	-2(1)
C(3)	60(1)	60(1)	78(1)	8(1)	6(1)	7(1)
C(4)	59(1)	54(1)	65(1)	-4(1)	9(1)	6(1)
C(5)	46(1)	49(1)	54(1)	-6(1)	5(1)	-1(1)
C(6)	49(1)	50(1)	49(1)	-3(1)	4(1)	-6(1)
C(7)	63(1)	51(1)	46(1)	-10(1)	8(1)	-2(1)
C(8)	54(1)	47(1)	48(1)	-8(1)	7(1)	0(1)
C(9)	57(1)	54(1)	46(1)	-9(1)	4(1)	3(1)
C(10)	60(1)	54(1)	49(1)	-13(1)	6(1)	5(1)
C(11)	76(1)	62(1)	49(1)	-10(1)	1(1)	14(1)
C(12)	65(1)	52(1)	47(1)	-6(1)	8(1)	8(1)
C(13)	94(2)	51(1)	63(1)	-6(1)	4(1)	1(1)
C(14)	76(1)	72(1)	76(1)	4(1)	23(1)	19(1)
C(15)	88(2)	72(1)	55(1)	1(1)	3(1)	24(1)
C(16)	144(3)	94(2)	74(2)	15(1)	7(2)	58(2)
C(17)	78(1)	59(1)	65(1)	16(1)	9(1)	15(1)
C(18)	86(2)	84(2)	85(2)	13(1)	2(1)	-11(1)
C(19)	220(3)	62(2)	85(2)	7(1)	0(2)	-11(2)
C(20)	245(4)	104(3)	77(2)	35(2)	64(3)	93(3)
C(21)	97(2)	153(3)	119(3)	69(2)	51(2)	60(2)
C(22)	79(2)	80(2)	92(2)	28(1)	-3(1)	-3(1)
N(1)	72(1)	59(1)	48(1)	-5(1)	4(1)	14(1)
O(1)	147(2)	89(1)	45(1)	-14(1)	-1(1)	43(1)
O(2)	189(2)	123(2)	53(1)	7(1)	8(1)	81(2)

O(3)	113(1)	74(1)	63(1)	7(1)	9(1)	40(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1_a.

x	y	z	U(eq)
H(1)	4158	9025	1625	71
H(2)	3152	11208	1507	77
H(3)	2989	12667	2449	79
H(4)	3646	11852	3516	71
H(7)	5346	7152	2367	63
H(10)	4591	9880	4283	65
H(13A)	4624	4576	3599	104
H(13B)	5959	3716	3489	104
H(13C)	5225	4606	2890	104
H(14A)	7627	5927	2837	110
H(14B)	8175	4936	3440	110
H(14C)	8285	6593	3519	110
H(16A)	7587	2446	5196	125
H(16B)	8970	3314	5262	125
H(18)	7102	1099	4031	102
H(19)	8084	-601	3375	148
H(20)	10451	-860	3447	167
H(21)	11837	581	4176	144
H(22)	10854	2280	4833	101

Table 6. Torsion angles [°] for 1_a.

C(6)-C(1)-C(2)-C(3)	1.2(3)
C(1)-C(2)-C(3)-C(4)	-3.4(3)
C(2)-C(3)-C(4)-C(5)	1.6(3)
C(3)-C(4)-C(5)-C(10)	-178.10(18)
C(3)-C(4)-C(5)-C(6)	2.3(3)
C(2)-C(1)-C(6)-C(7)	-178.63(17)
C(2)-C(1)-C(6)-C(5)	2.6(3)
C(10)-C(5)-C(6)-C(7)	-2.7(2)
C(4)-C(5)-C(6)-C(7)	176.92(15)
C(10)-C(5)-C(6)-C(1)	176.05(16)
C(4)-C(5)-C(6)-C(1)	-4.3(2)
C(1)-C(6)-C(7)-C(8)	-177.52(16)
C(5)-C(6)-C(7)-C(8)	1.2(3)
C(6)-C(7)-C(8)-C(9)	1.5(3)
C(6)-C(7)-C(8)-C(12)	-178.07(17)
C(7)-C(8)-C(9)-C(10)	-2.9(3)
C(12)-C(8)-C(9)-C(10)	176.81(16)
C(7)-C(8)-C(9)-C(11)	179.16(17)
C(12)-C(8)-C(9)-C(11)	-1.2(2)
C(8)-C(9)-C(10)-C(5)	1.3(3)
C(11)-C(9)-C(10)-C(5)	178.85(19)
C(4)-C(5)-C(10)-C(9)	-178.14(16)
C(6)-C(5)-C(10)-C(9)	1.5(3)
C(10)-C(9)-C(11)-O(1)	4.0(4)
C(8)-C(9)-C(11)-O(1)	-178.1(2)
C(10)-C(9)-C(11)-N(1)	-175.83(19)
C(8)-C(9)-C(11)-N(1)	2.0(2)
C(7)-C(8)-C(12)-N(1)	179.55(18)

C(9)-C(8)-C(12)-N(1)	-0.1(2)
C(7)-C(8)-C(12)-C(13)	-62.9(2)
C(9)-C(8)-C(12)-C(13)	117.51(18)
C(7)-C(8)-C(12)-C(14)	61.8(3)
C(9)-C(8)-C(12)-C(14)	-117.82(18)
O(3)-C(16)-C(17)-C(18)	-68.7(3)
O(3)-C(16)-C(17)-C(22)	114.1(2)
C(22)-C(17)-C(18)-C(19)	0.0
C(16)-C(17)-C(18)-C(19)	-177.18(18)
C(17)-C(18)-C(19)-C(20)	0.0
C(18)-C(19)-C(20)-C(21)	0.0
C(19)-C(20)-C(21)-C(22)	0.0
C(20)-C(21)-C(22)-C(17)	0.0
C(18)-C(17)-C(22)-C(21)	0.0
C(16)-C(17)-C(22)-C(21)	177.21(18)
O(2)-C(15)-N(1)-C(11)	6.0(4)
O(3)-C(15)-N(1)-C(11)	-174.4(2)
O(2)-C(15)-N(1)-C(12)	-170.8(3)
O(3)-C(15)-N(1)-C(12)	8.8(3)
O(1)-C(11)-N(1)-C(15)	0.9(4)
C(9)-C(11)-N(1)-C(15)	-179.25(19)
O(1)-C(11)-N(1)-C(12)	178.0(2)
C(9)-C(11)-N(1)-C(12)	-2.1(2)
C(8)-C(12)-N(1)-C(15)	178.4(2)
C(13)-C(12)-N(1)-C(15)	61.0(3)
C(14)-C(12)-N(1)-C(15)	-65.1(3)
C(8)-C(12)-N(1)-C(11)	1.4(2)
C(13)-C(12)-N(1)-C(11)	-116.0(2)
C(14)-C(12)-N(1)-C(11)	117.9(2)
O(2)-C(15)-O(3)-C(16)	-0.3(4)

N(1)-C(15)-O(3)-C(16)	-179.9(3)
C(17)-C(16)-O(3)-C(15)	179.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 1_a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)