Supporting Information

NIS-mediated oxidative arene C(sp^2)-H amidation toward 3,4-dihydro-2(^{1}H)-quinolinone and phenanthridone derivatives

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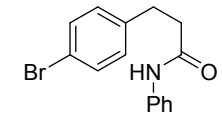
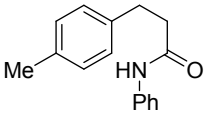
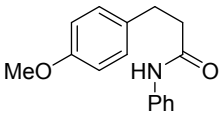
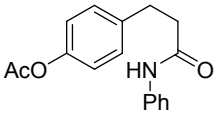
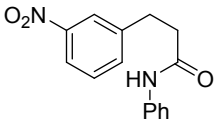
Unsuccessful substrates





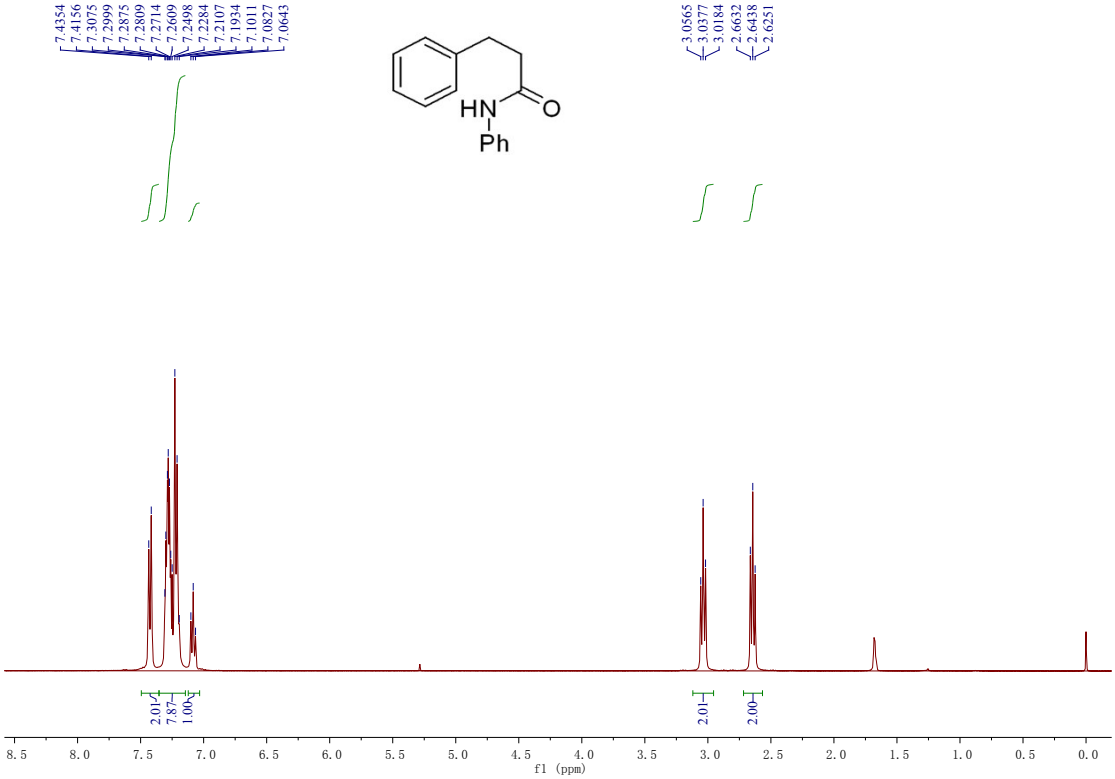




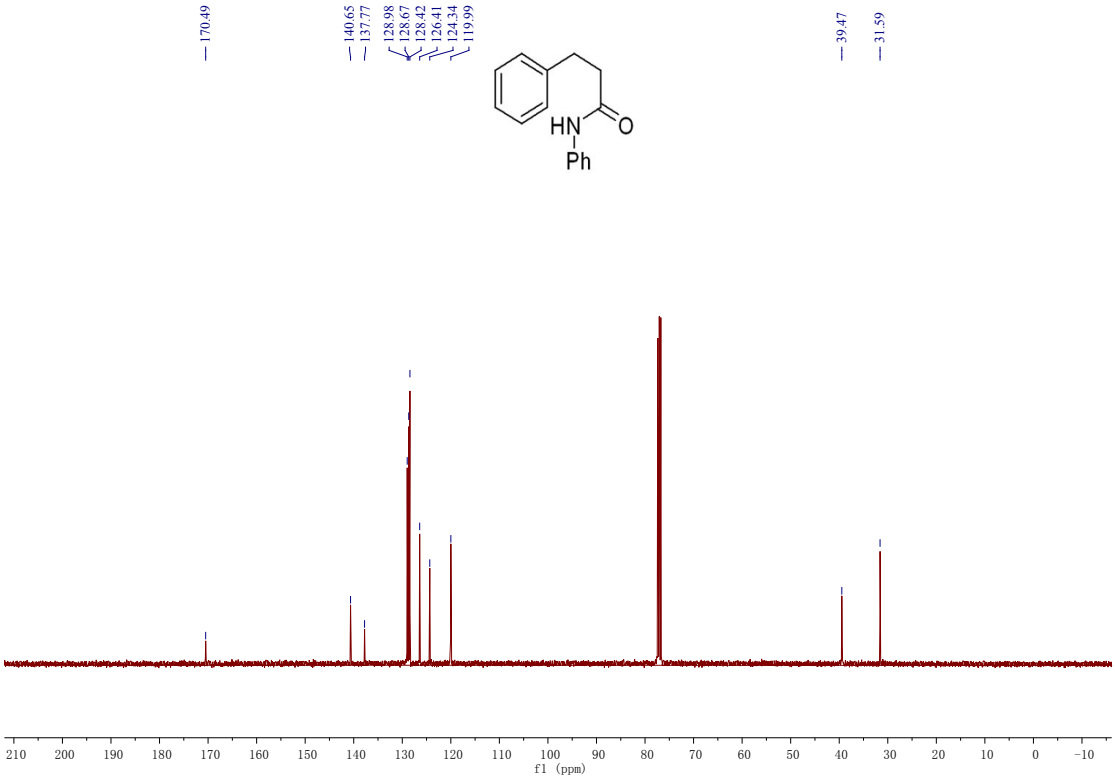


NMR Spectra

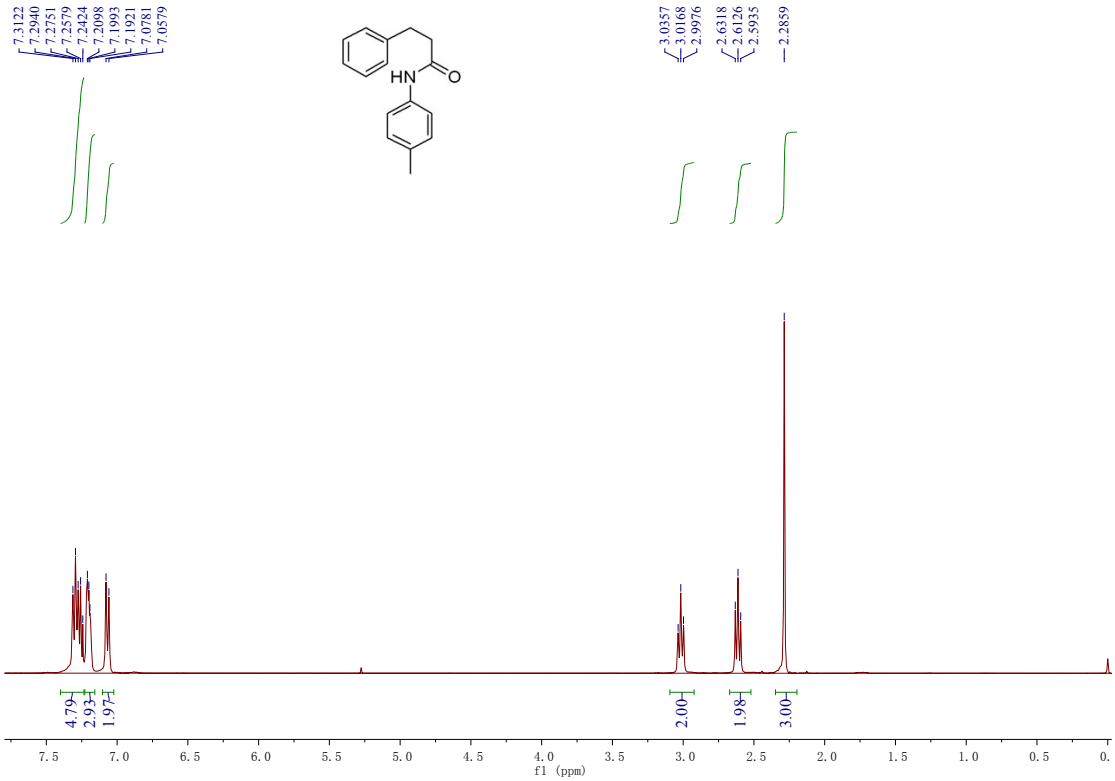
^{1}H NMR spectrum of compound **1a**



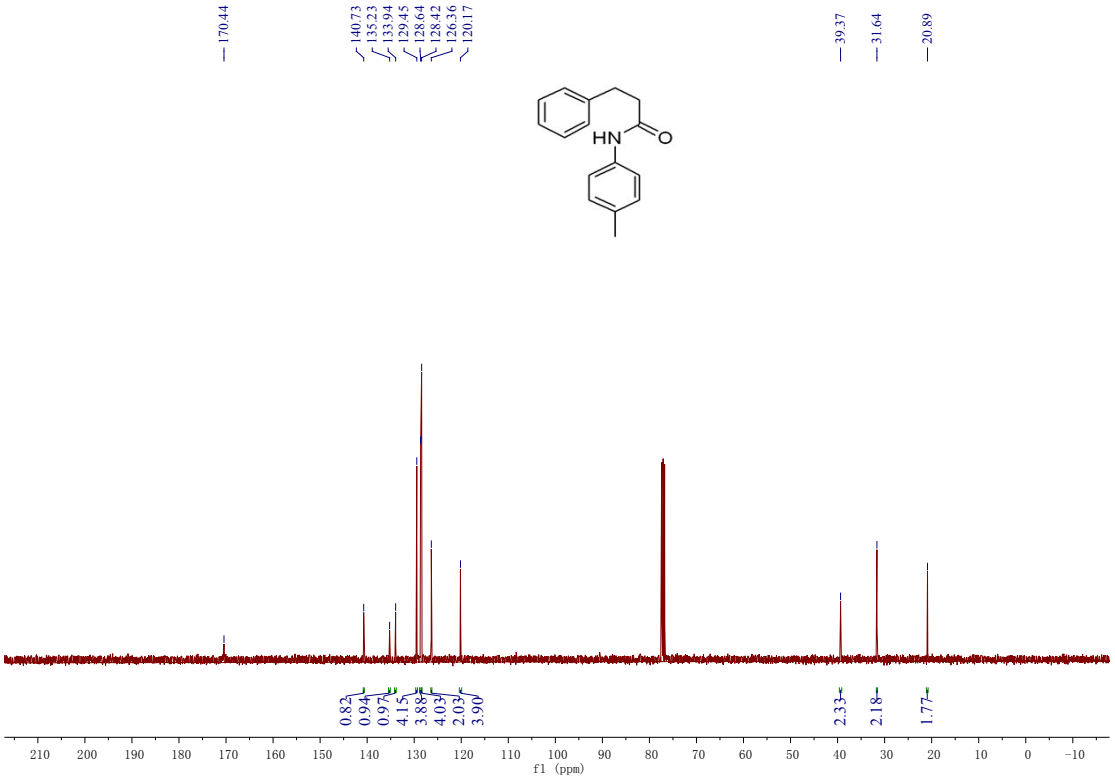
^{13}C NMR spectrum of compound **1a**



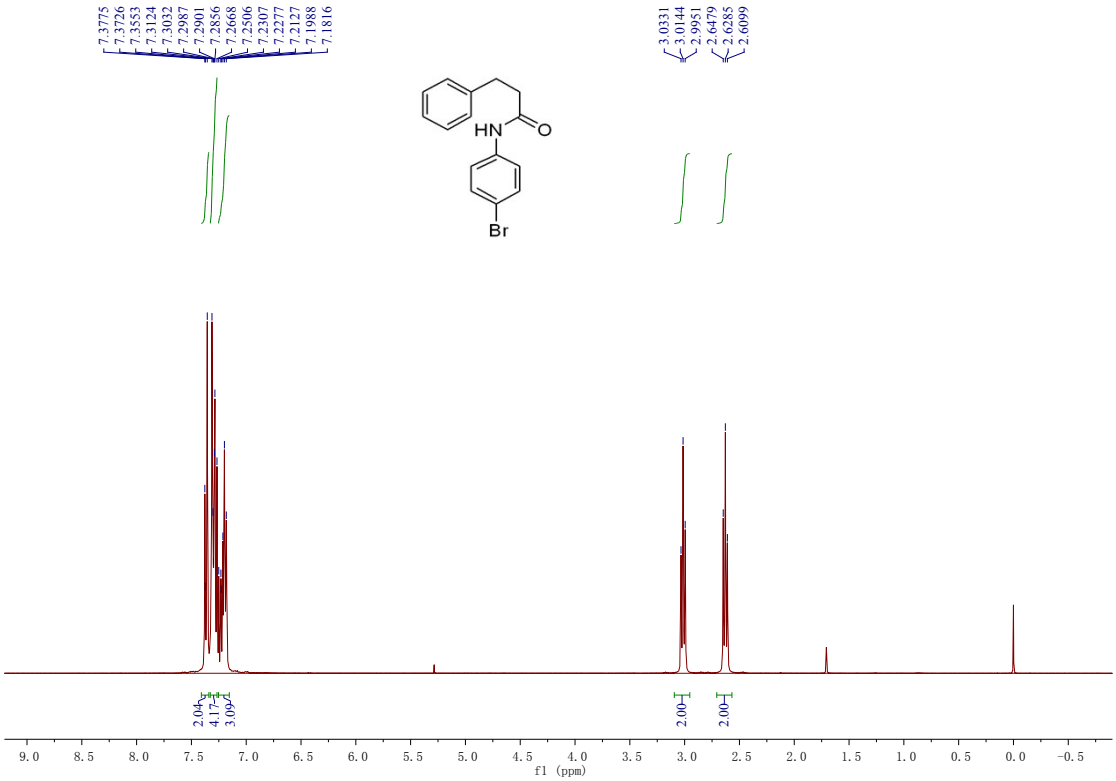
^{1}H NMR spectrum of compound **1b**



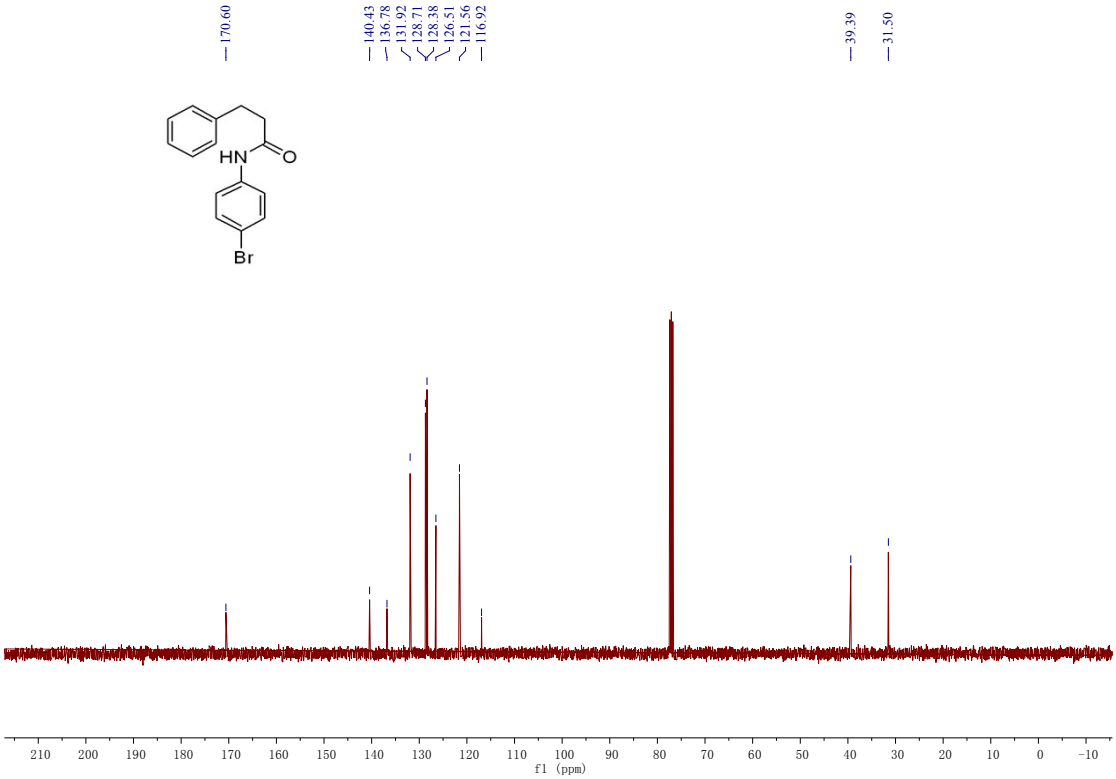
^{13}C NMR spectrum of compound **1b**



^{1}H NMR spectrum of compound **1c**



^{13}C NMR spectrum of compound **1c**



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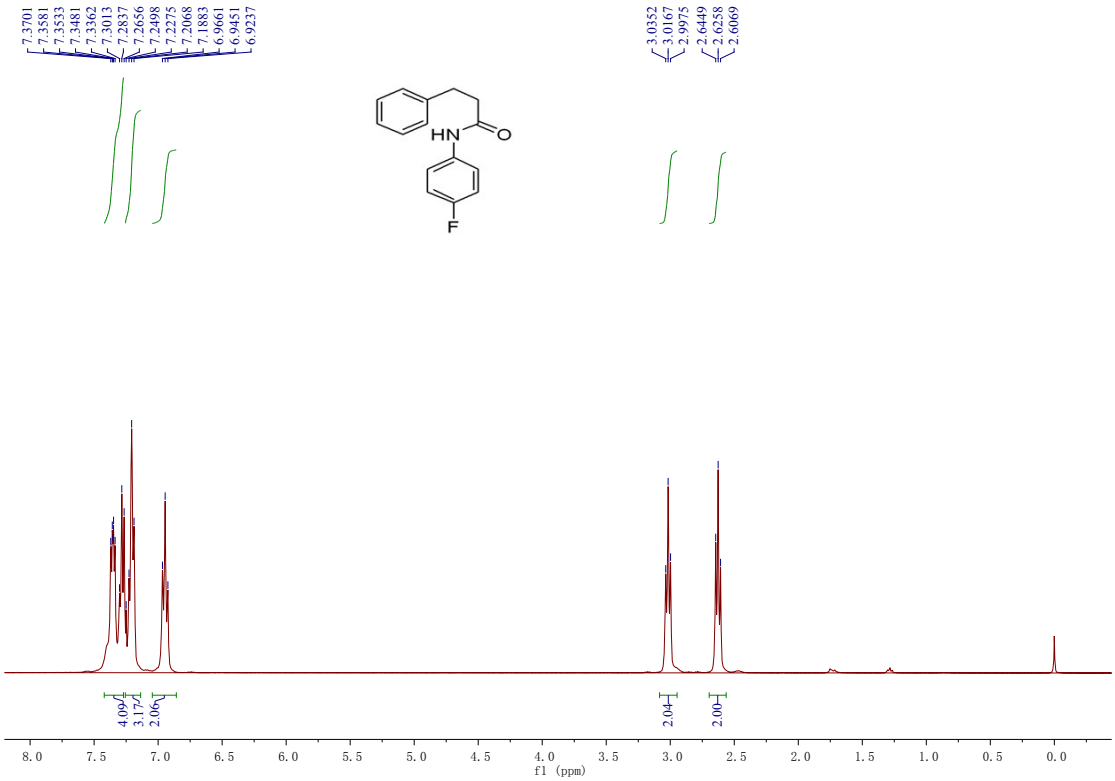

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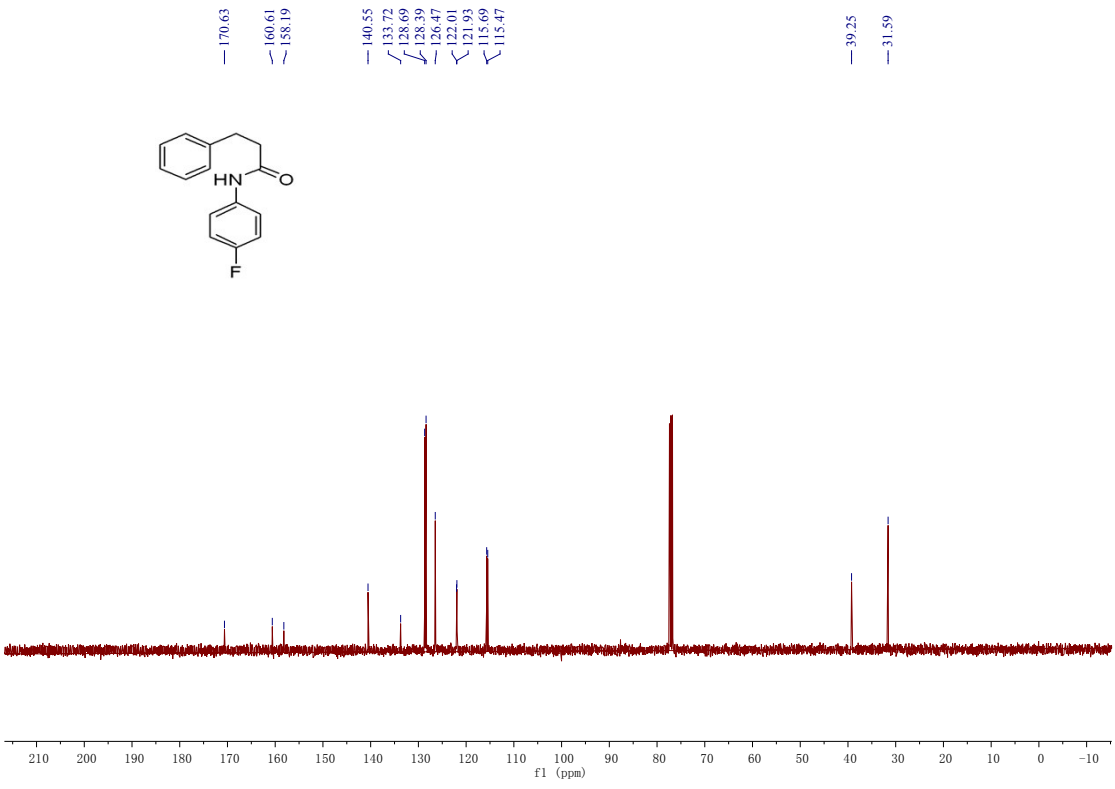
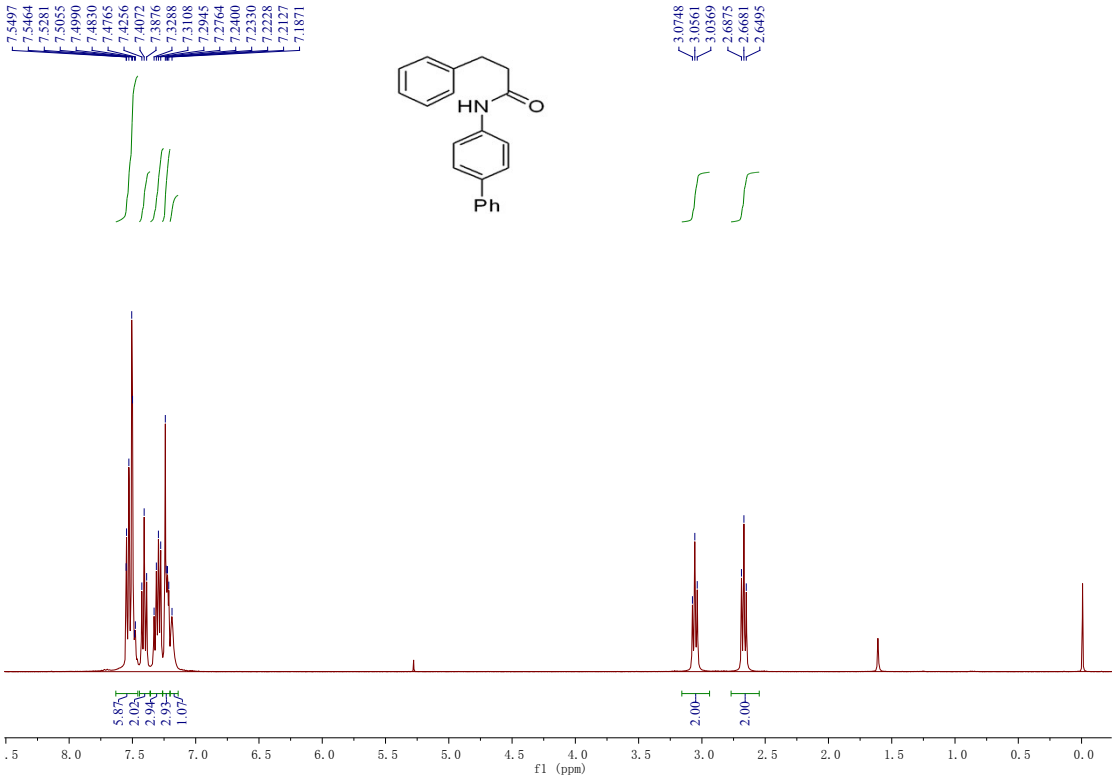
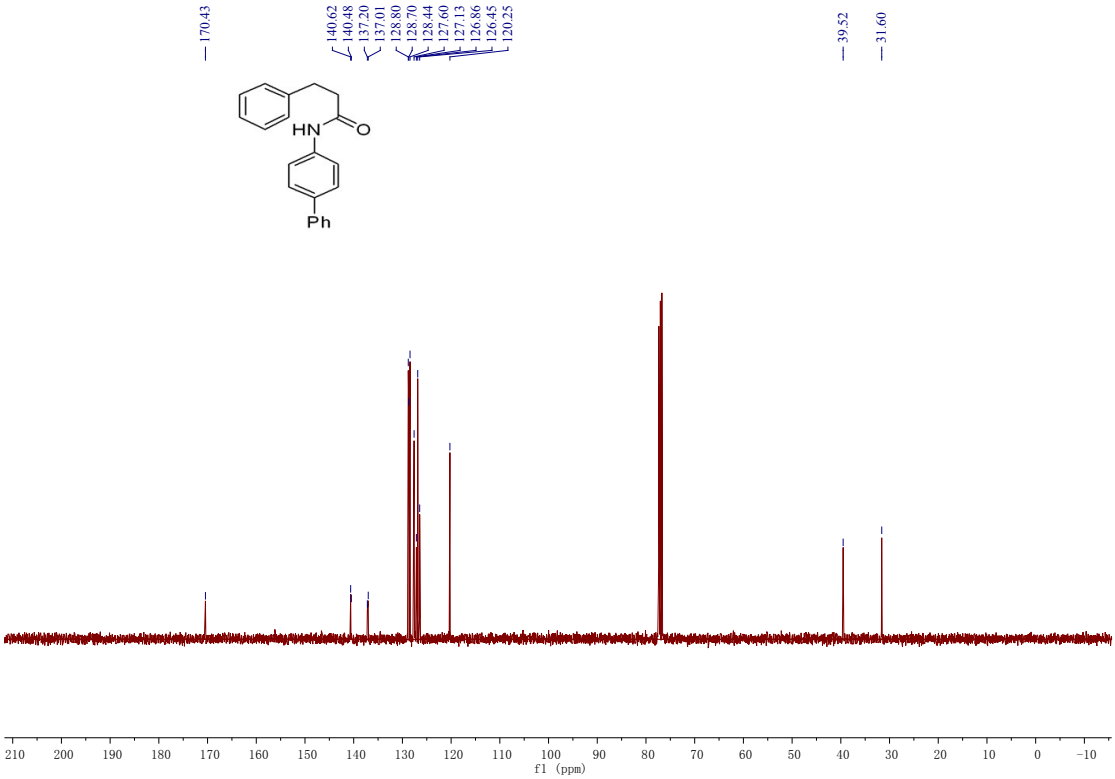


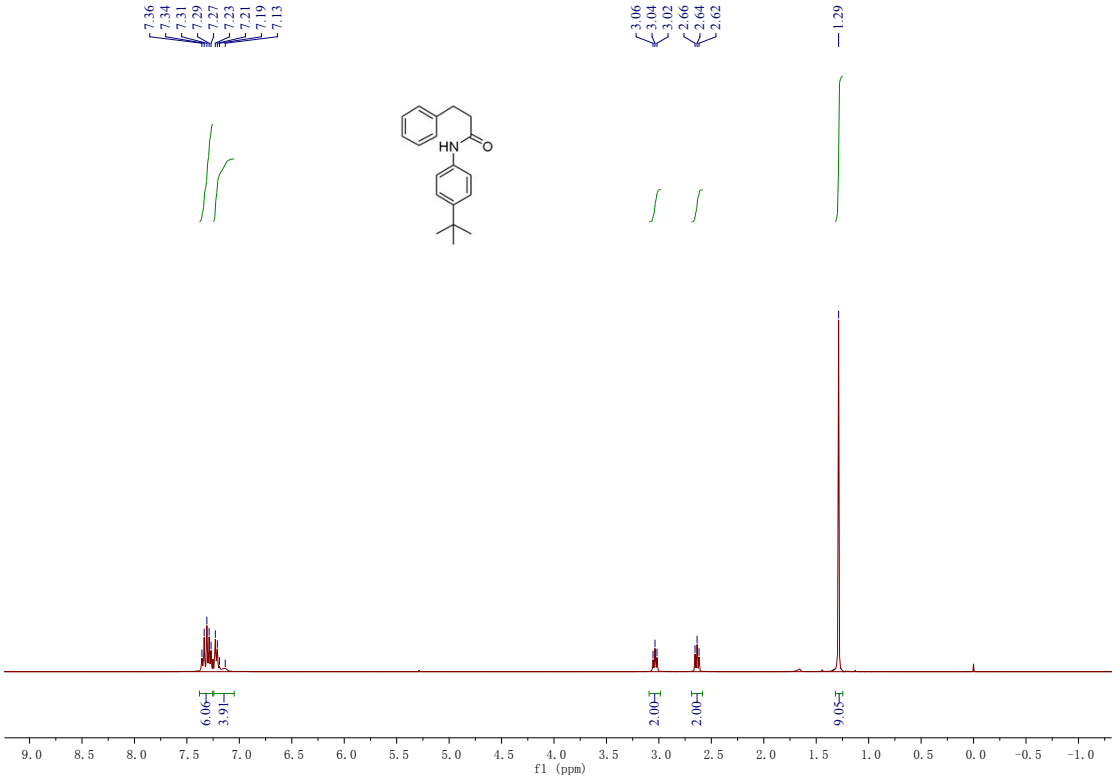
^{1}H NMR spectrum of compound **1e**



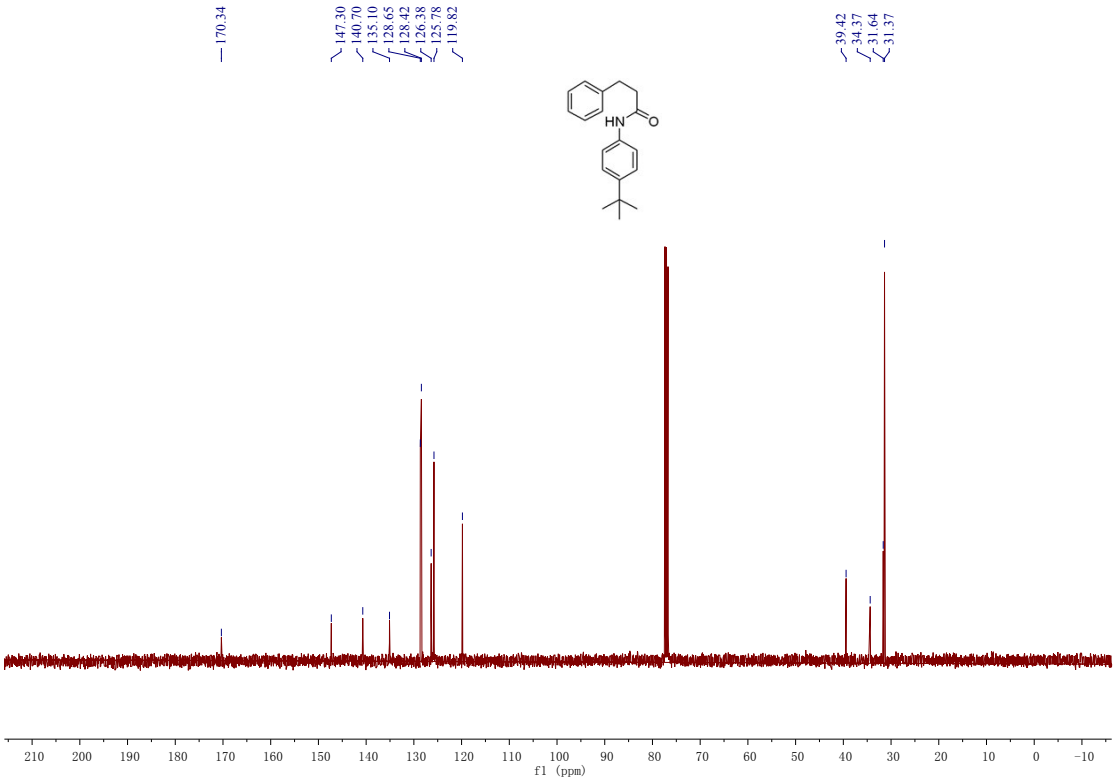
^{13}C NMR spectrum of compound **1e**



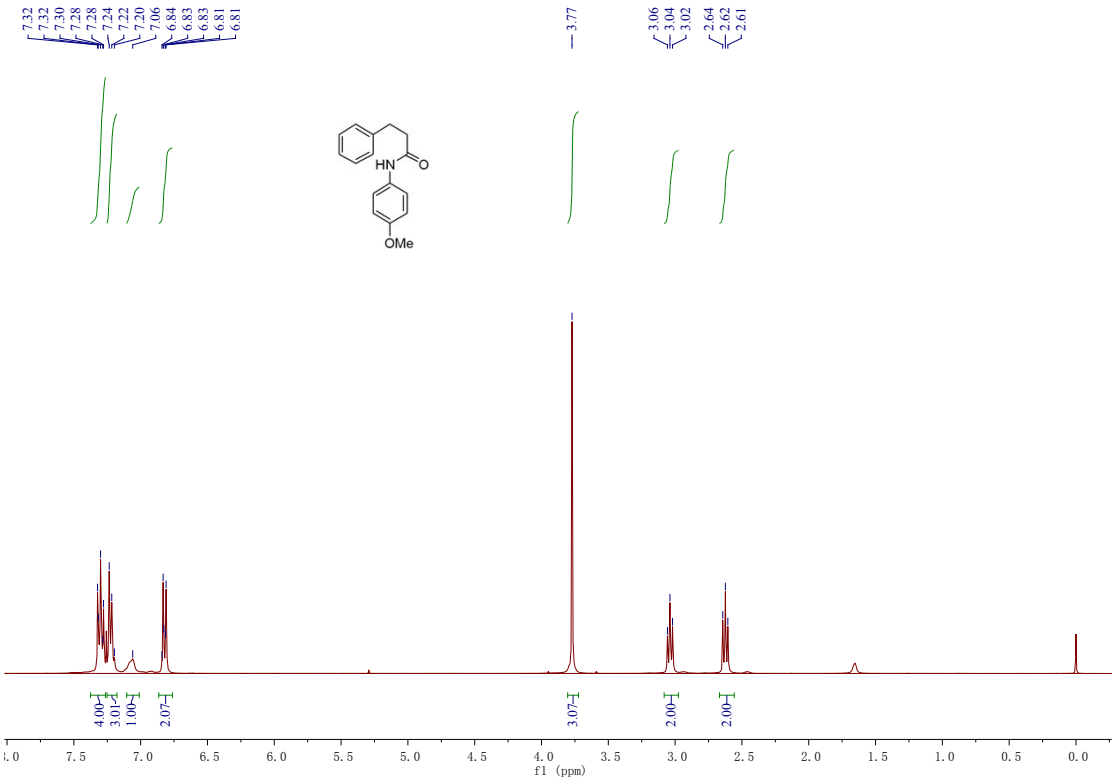
^{1}H NMR spectrum of compound **1f**



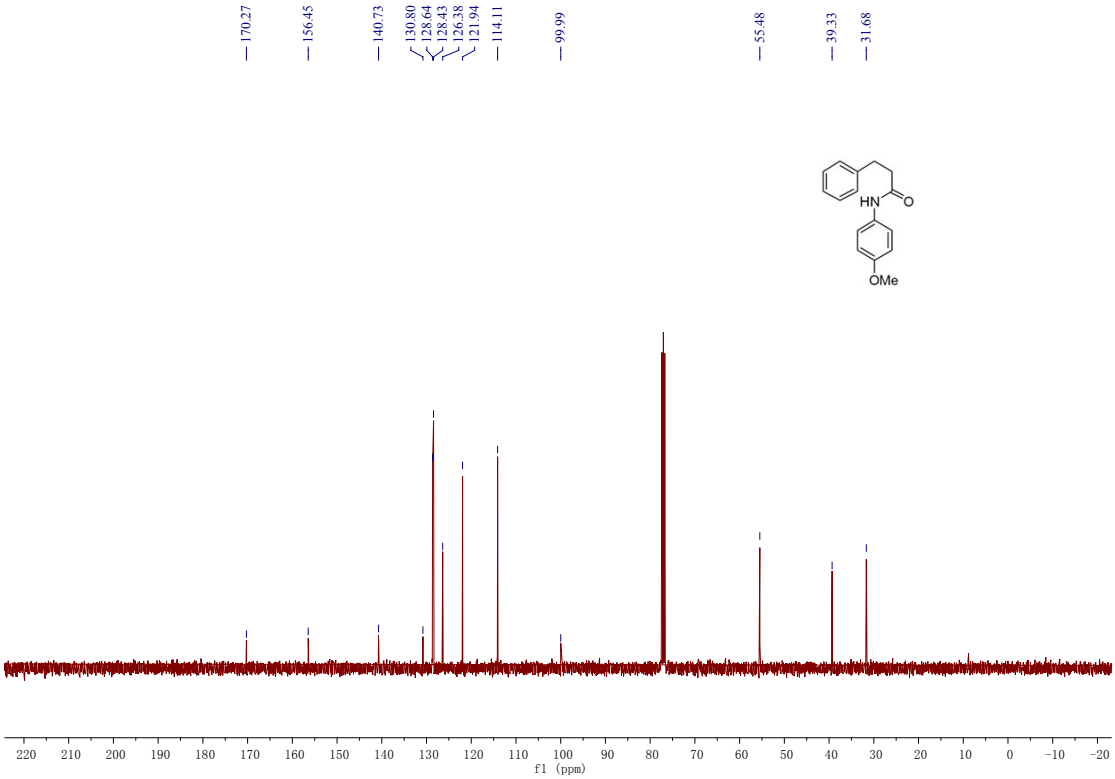
^{13}C NMR spectrum of compound **1f**



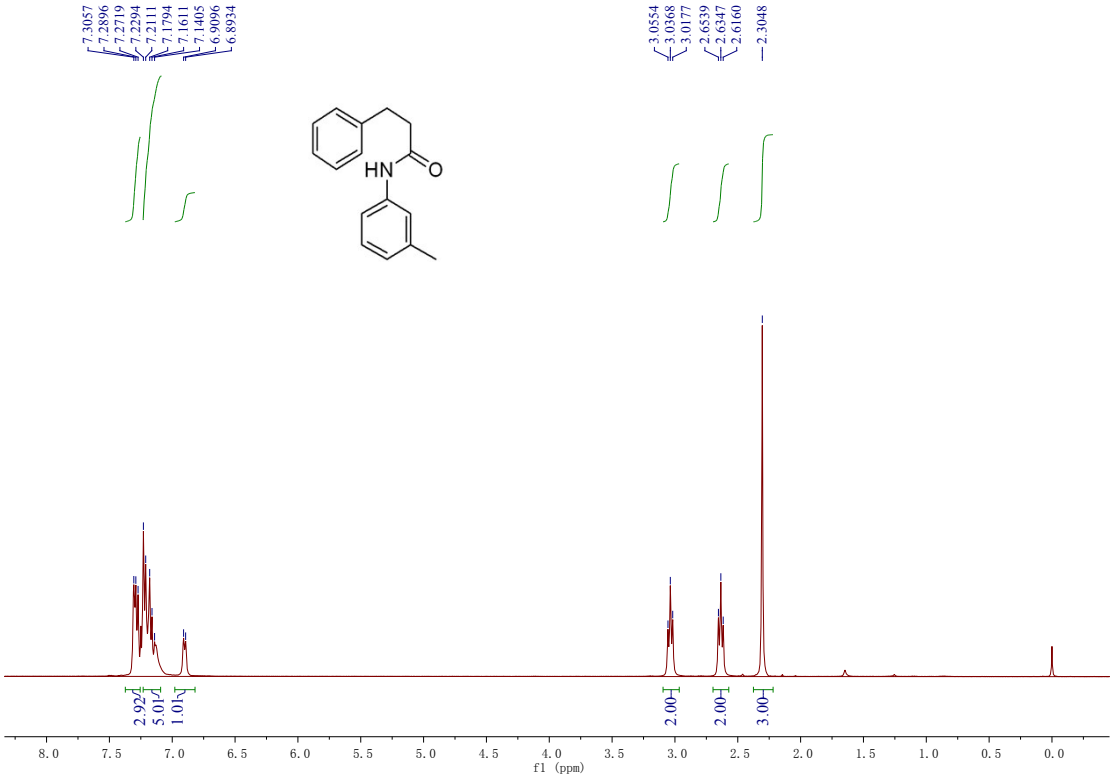
^{1}H NMR spectrum of compound **1g**



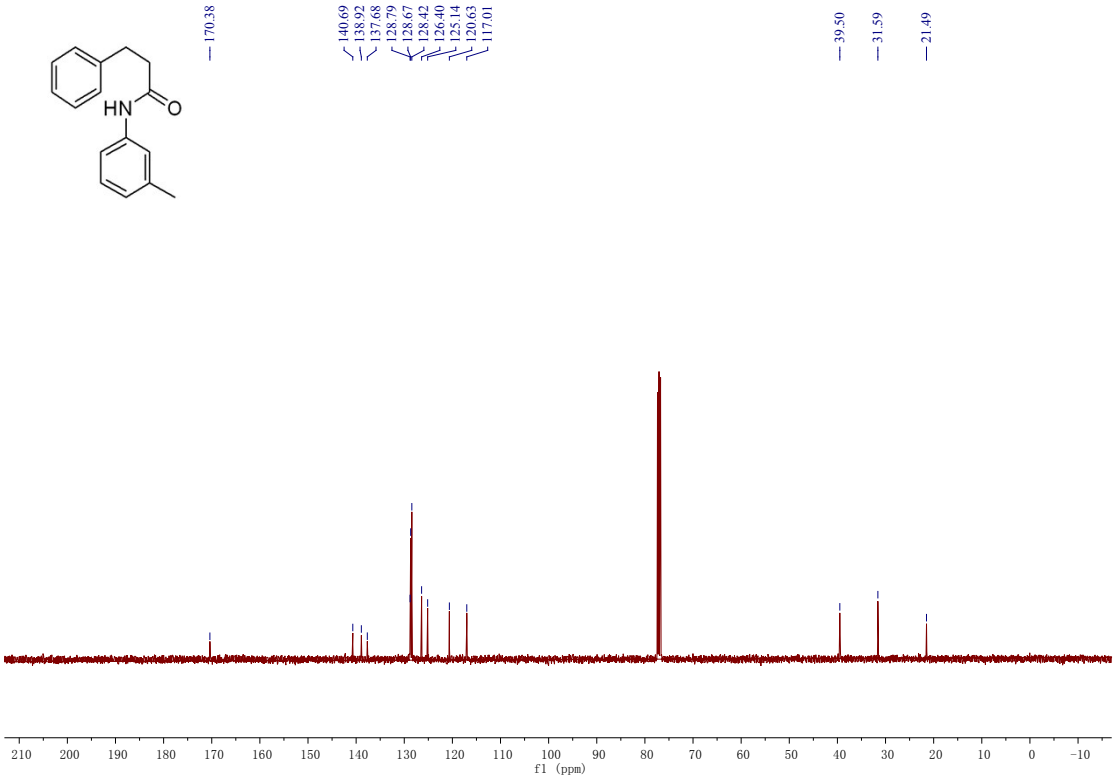
^{13}C NMR spectrum of compound **1g**



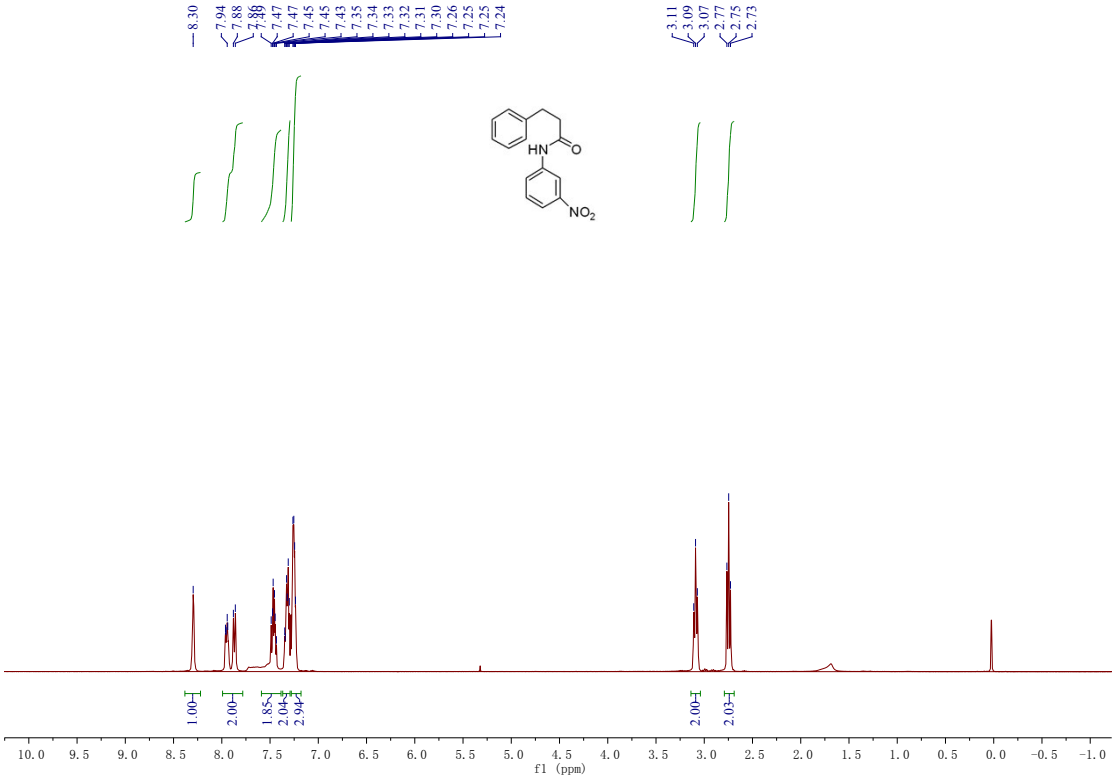
^{1}H NMR spectrum of compound **1h**



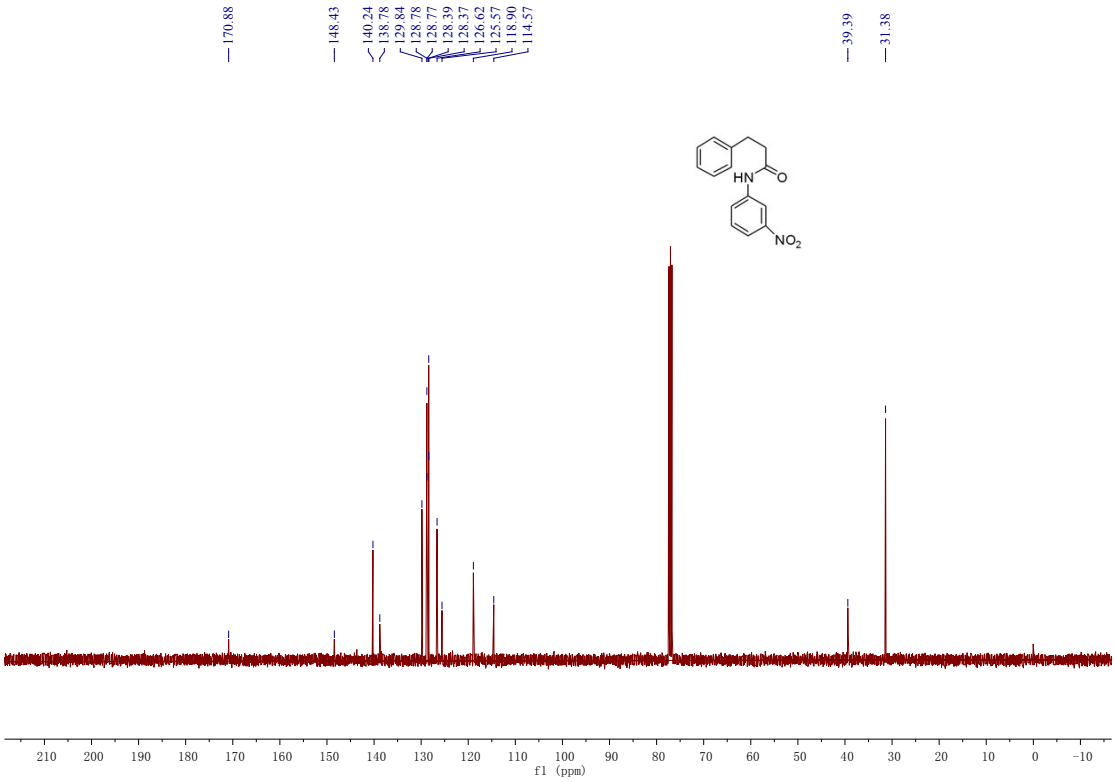
^{13}C NMR spectrum of compound **1h**



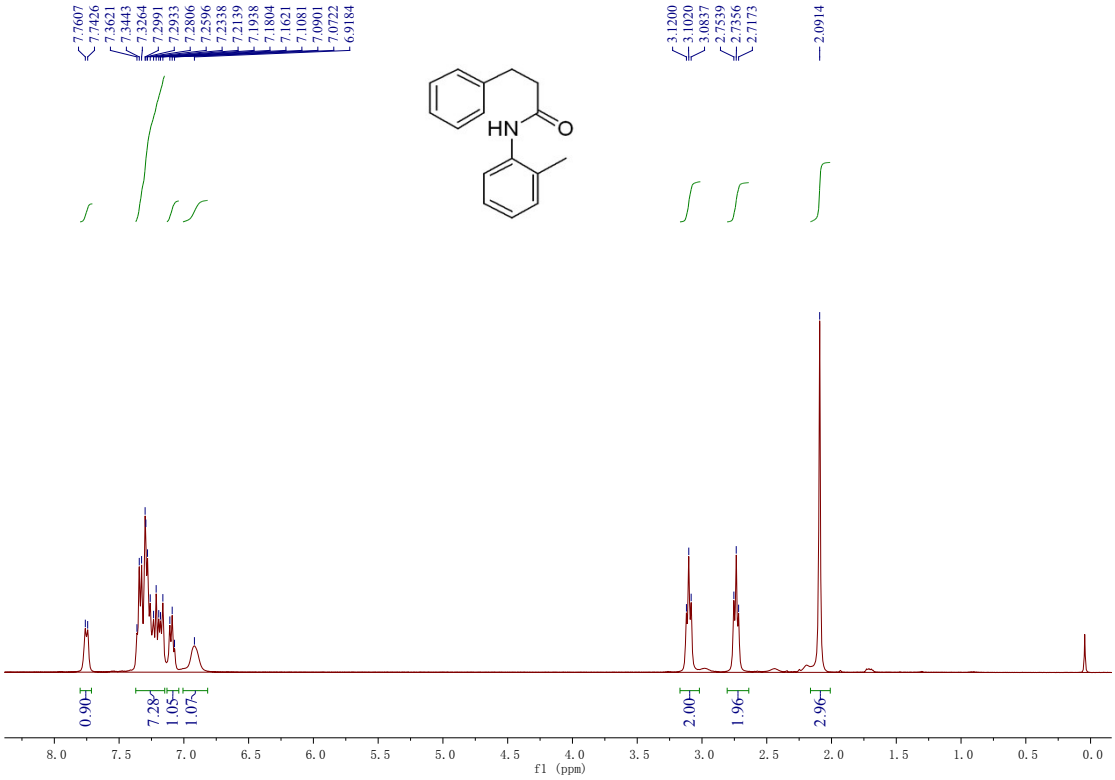
^{1}H NMR spectrum of compound **1i**



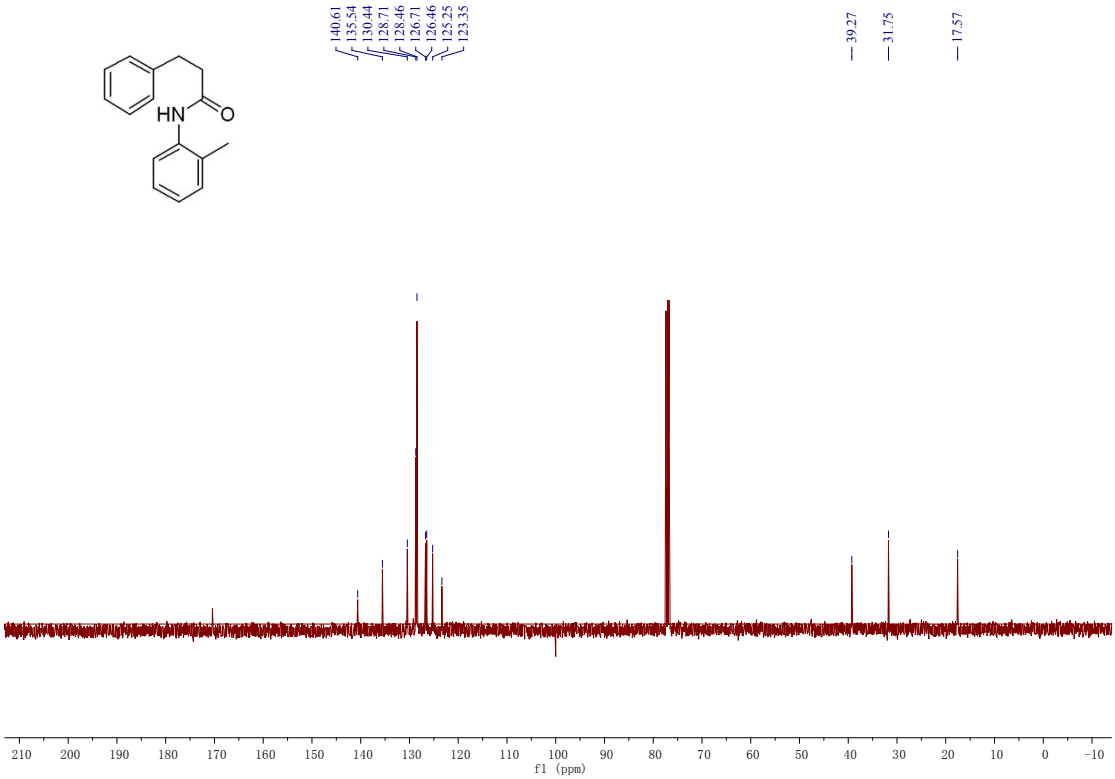
^{13}C NMR spectrum of compound **1i**



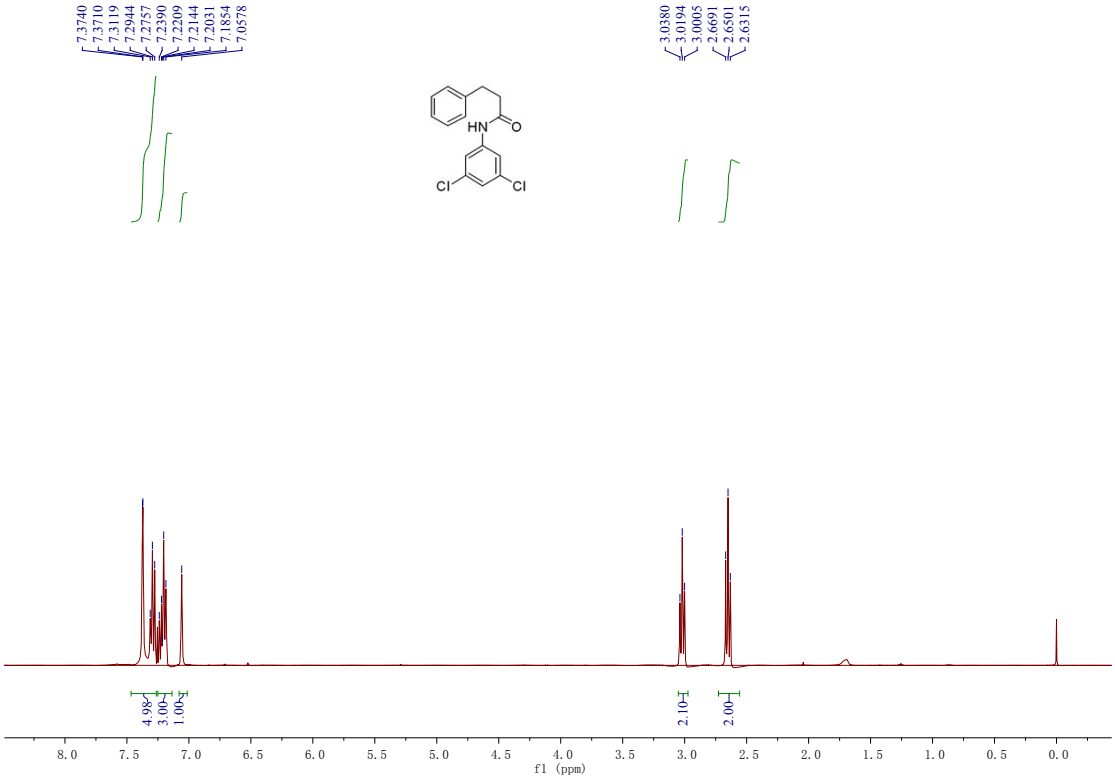
^{1}H NMR spectrum of compound **1j**



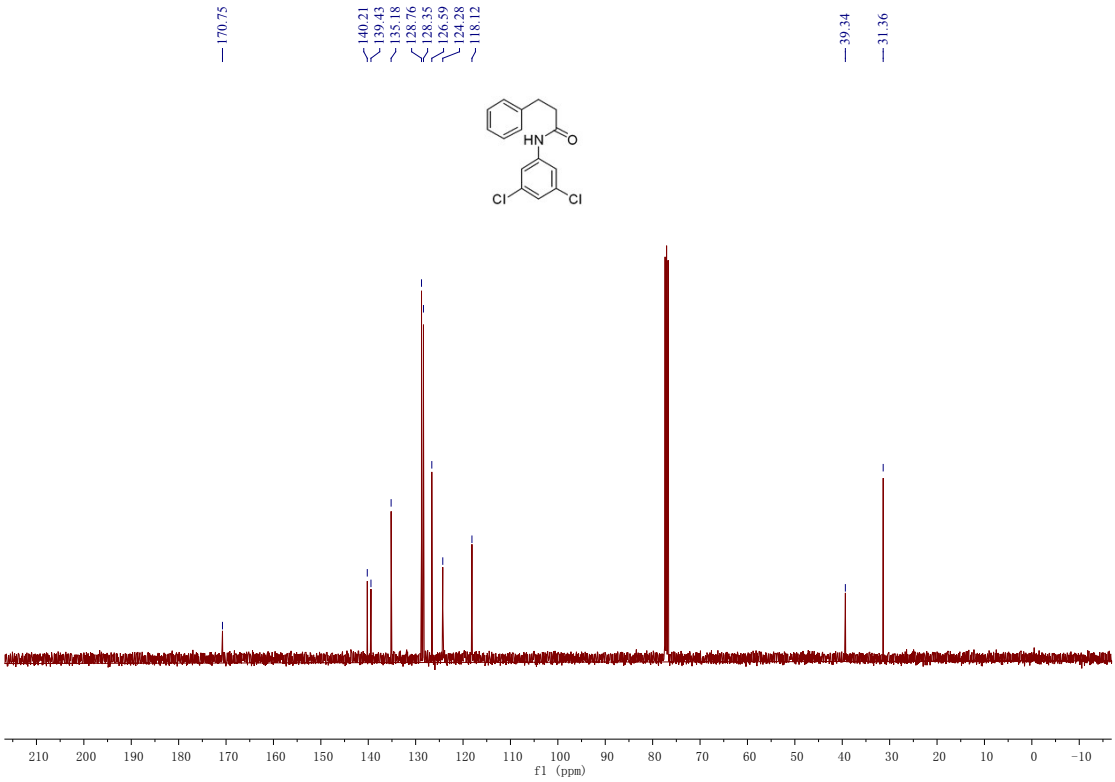
^{13}C NMR spectrum of compound **1j**



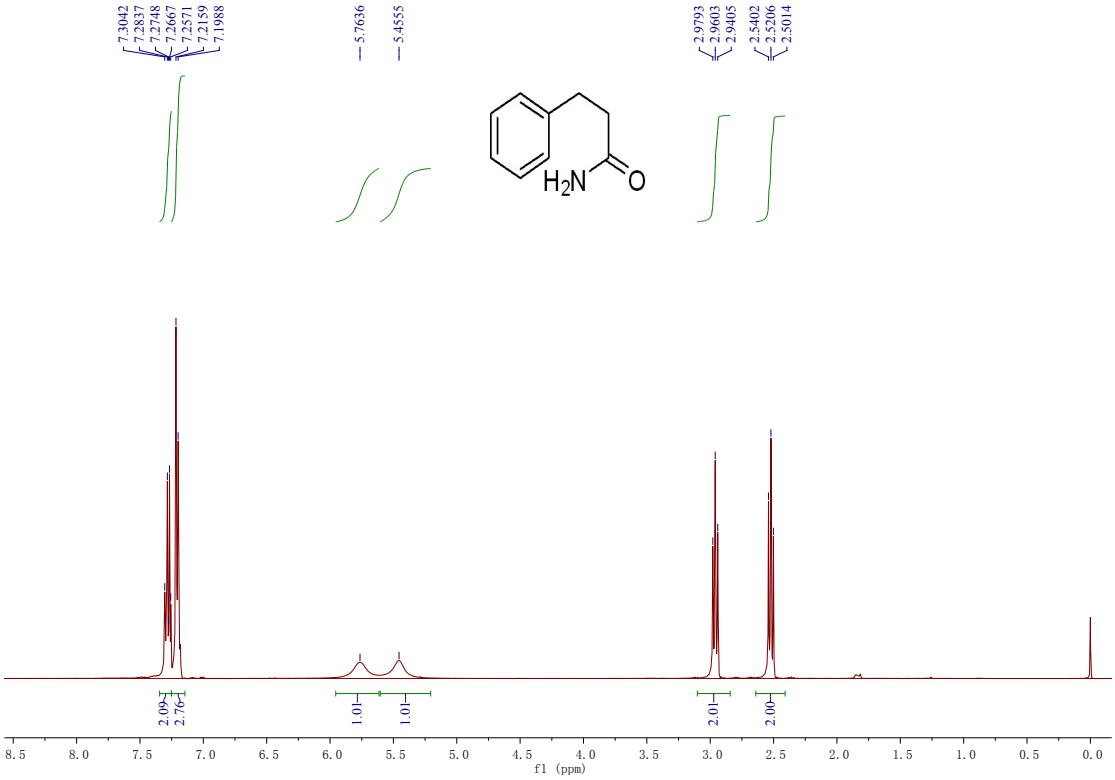
^{1}H NMR spectrum of compound **1k**



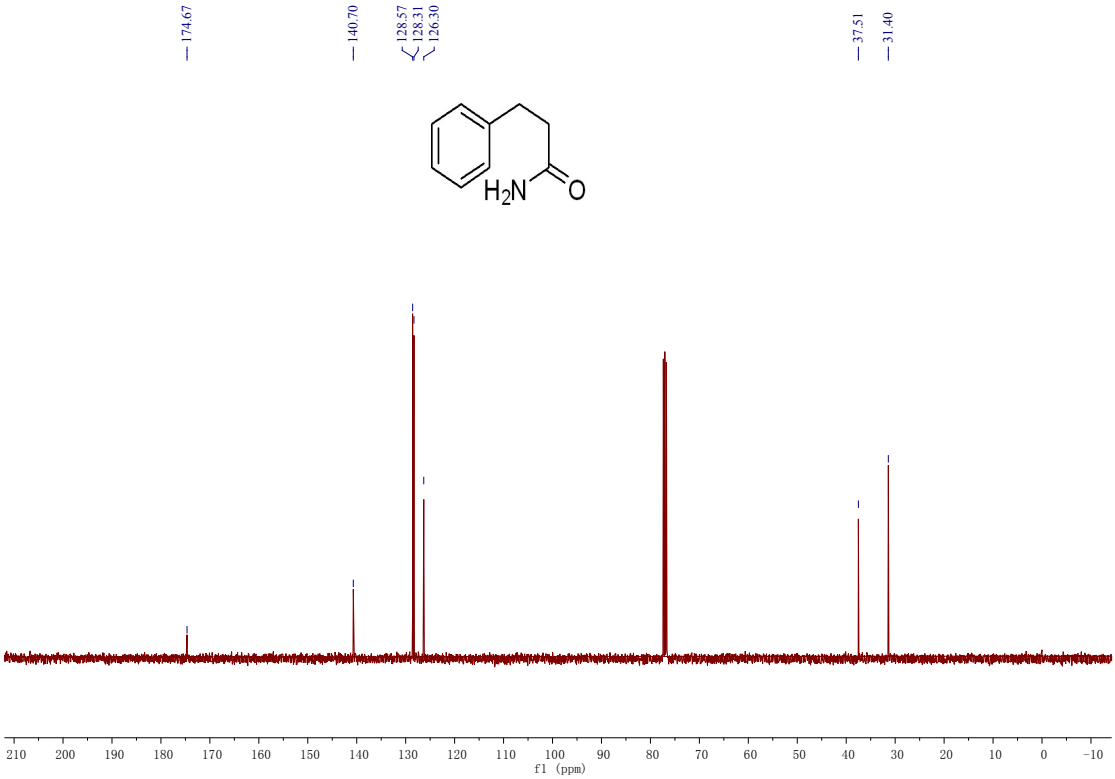
^{13}C NMR spectrum of compound **1k**



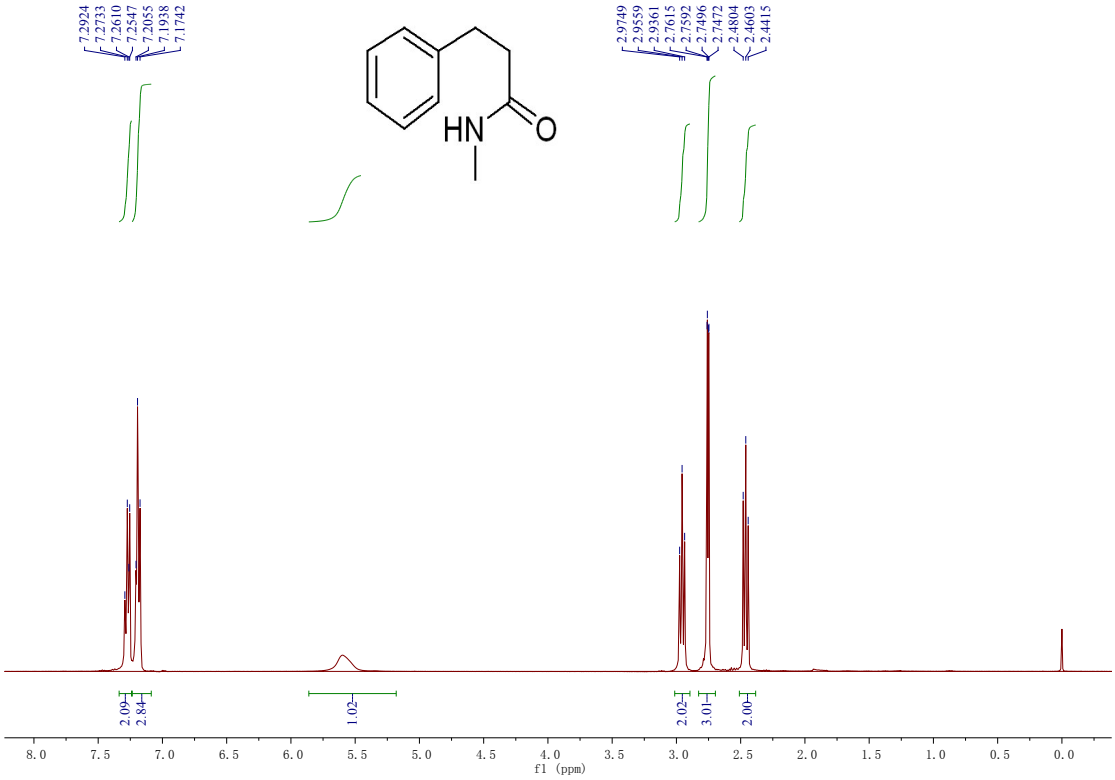
^{1}H NMR spectrum of compound **1l**



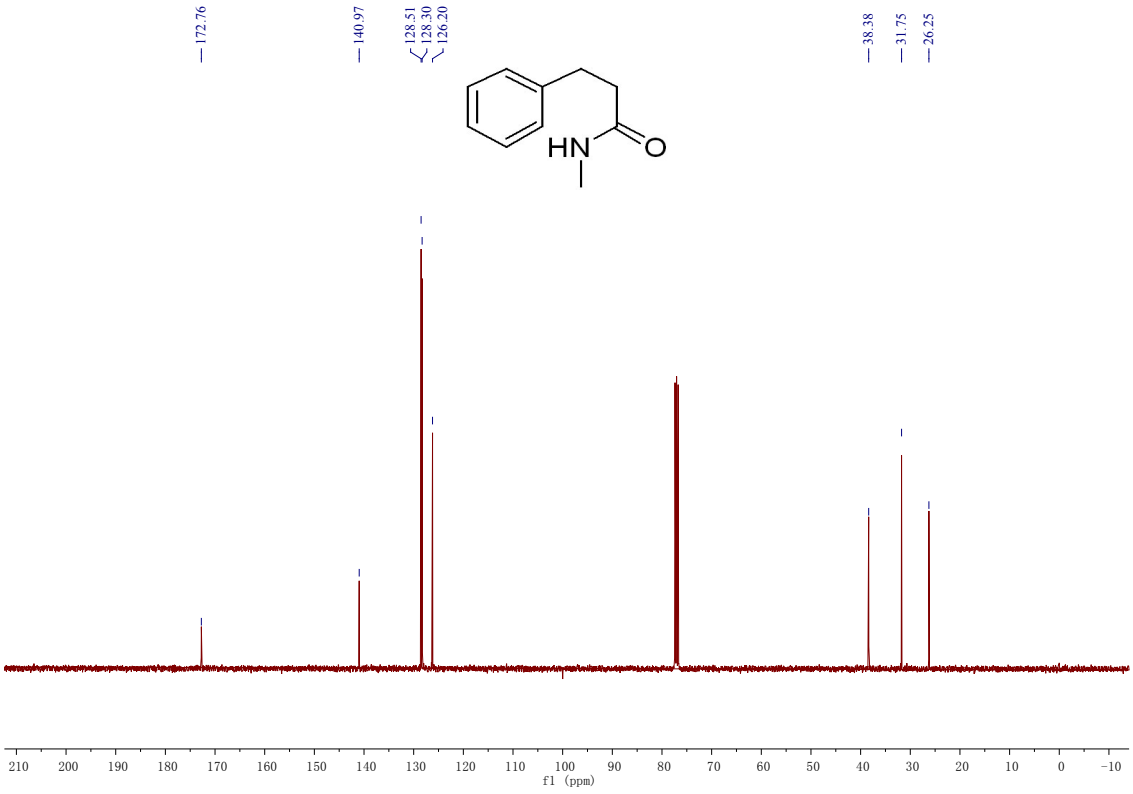
^{13}C NMR spectrum of compound **1l**



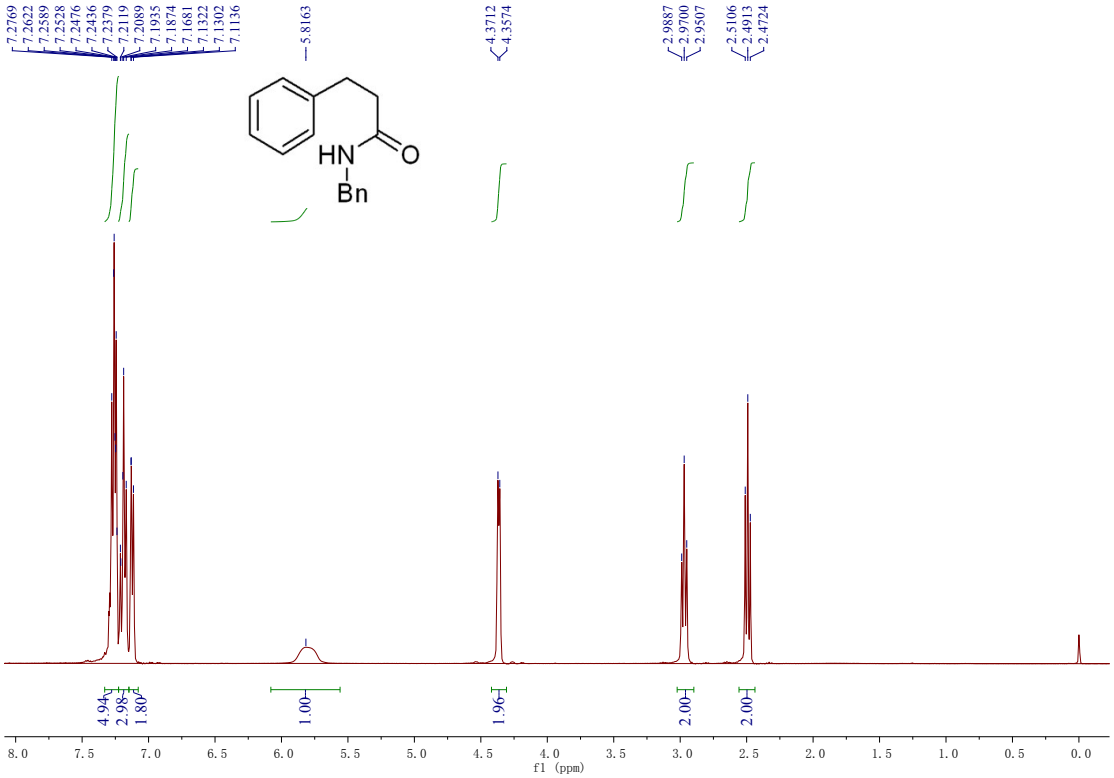
^{1}H NMR spectrum of compound **1m**



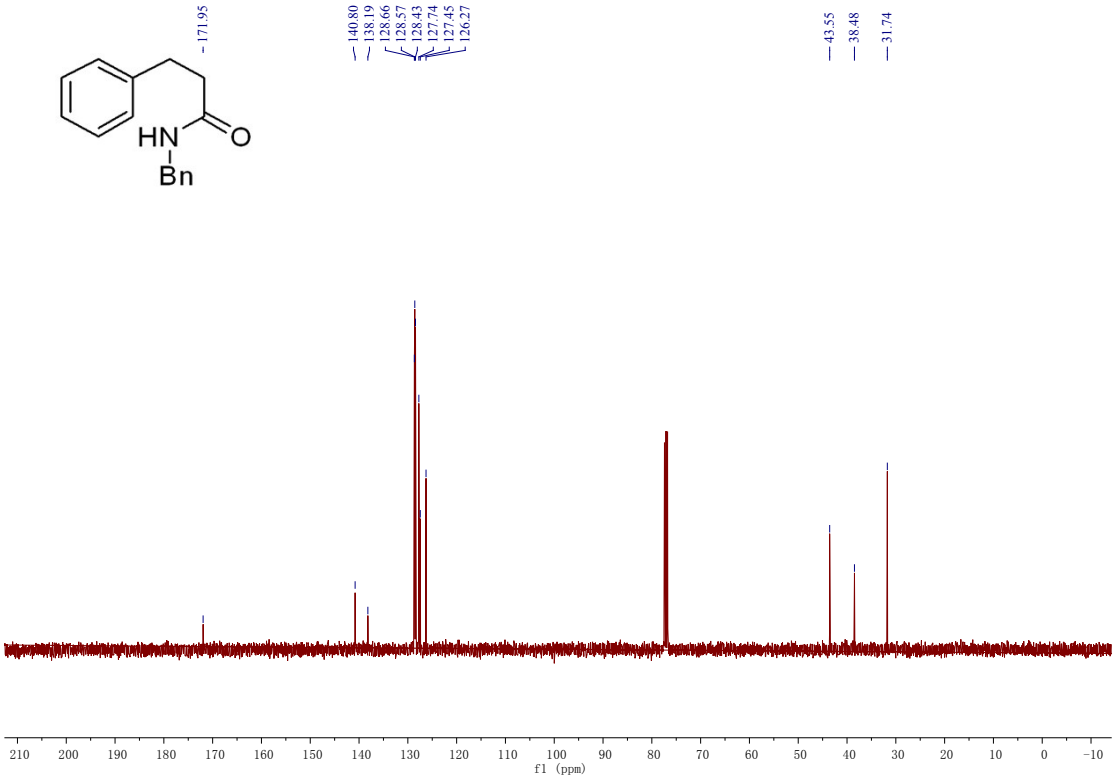
^{13}C NMR spectrum of compound **1m**



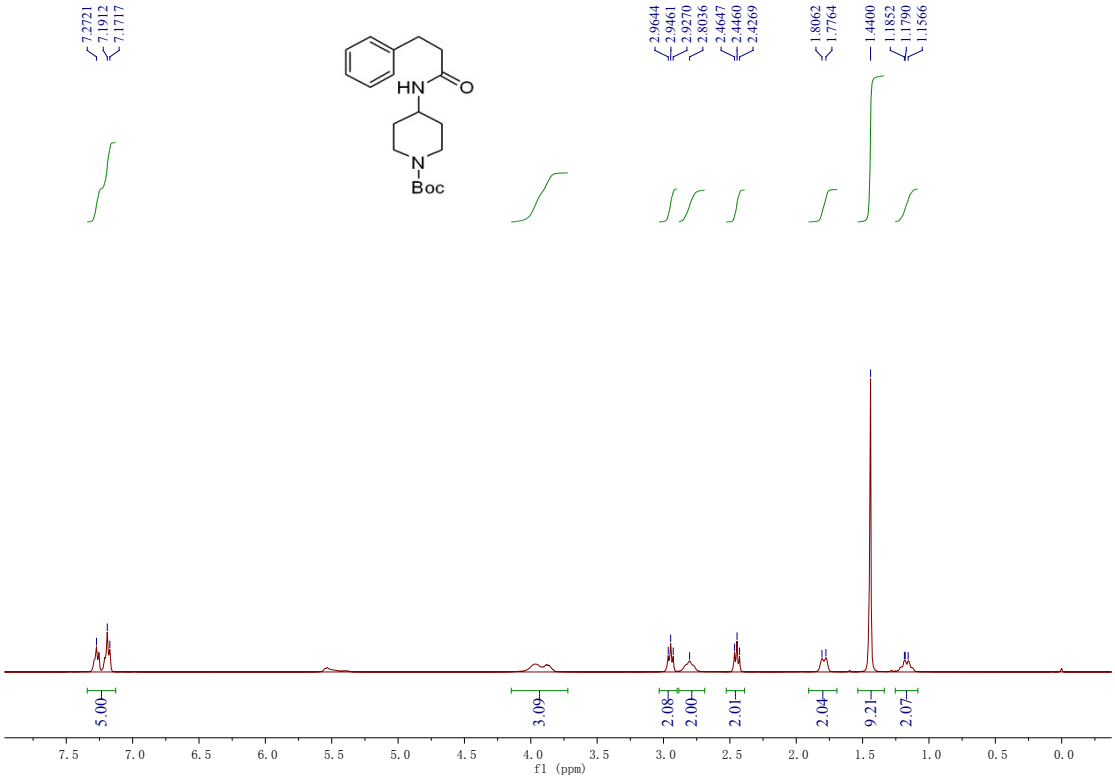
^{1}H NMR spectrum of compound **1n**



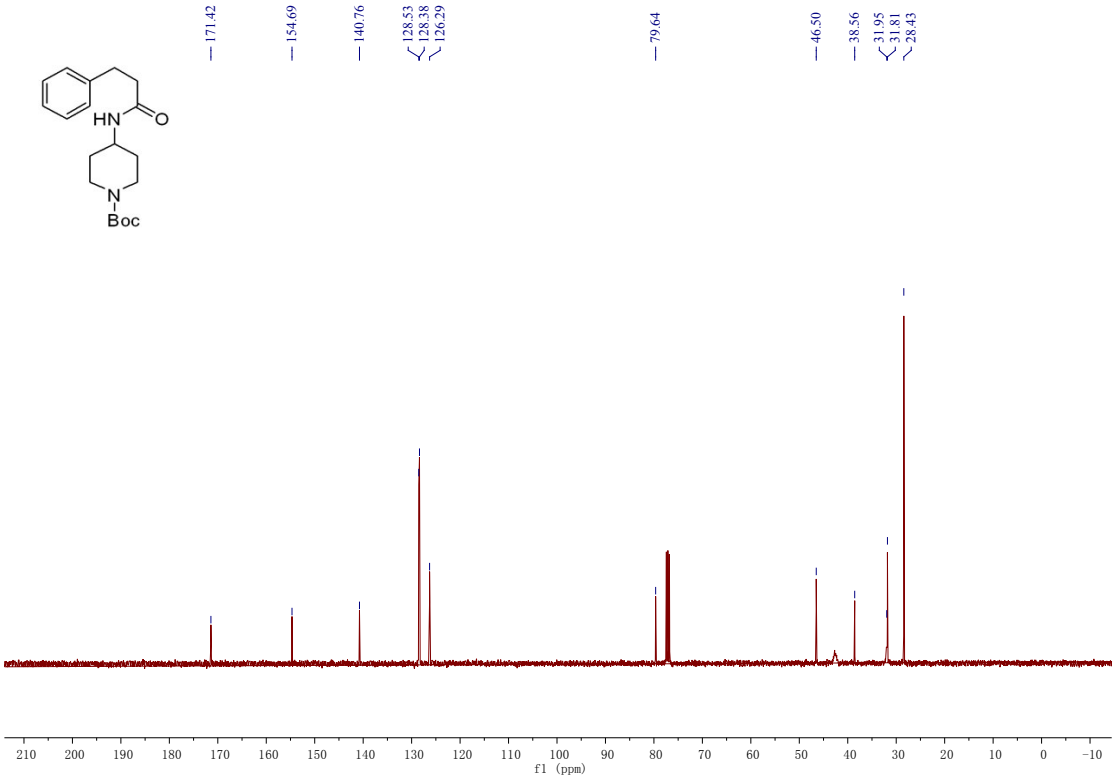
^{13}C NMR spectrum of compound **1n**



^{1}H NMR spectrum of compound **1o**



^{13}C NMR spectrum of compound **1o**



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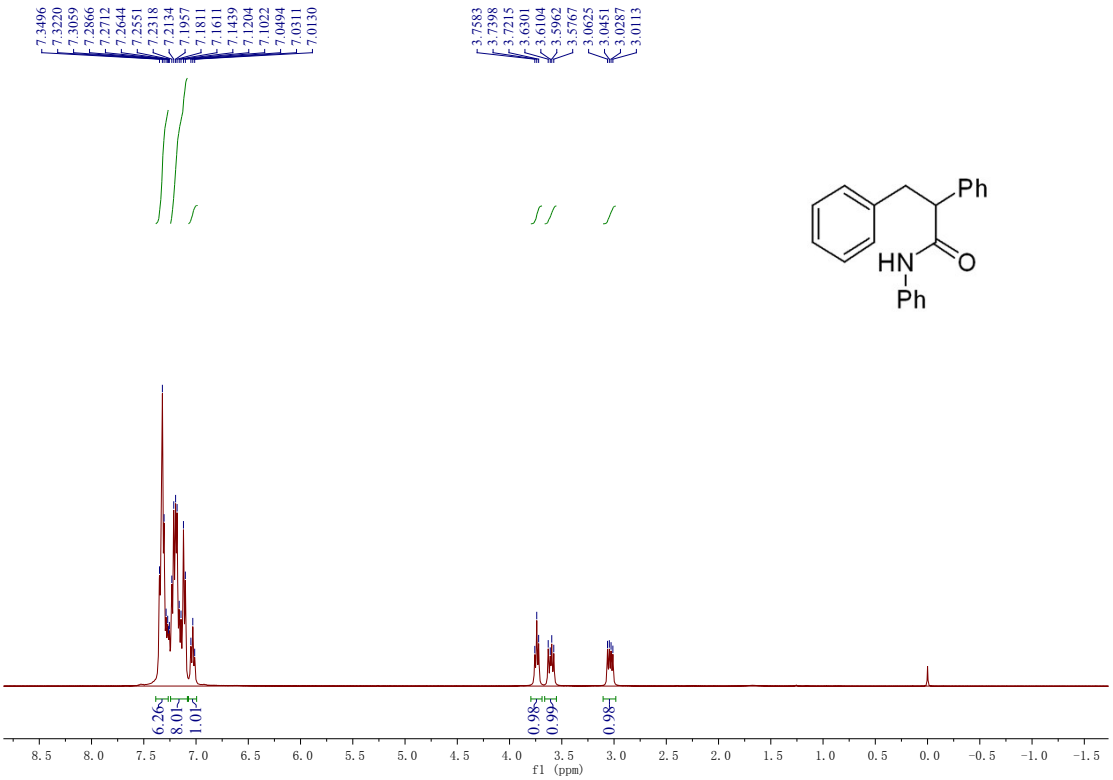
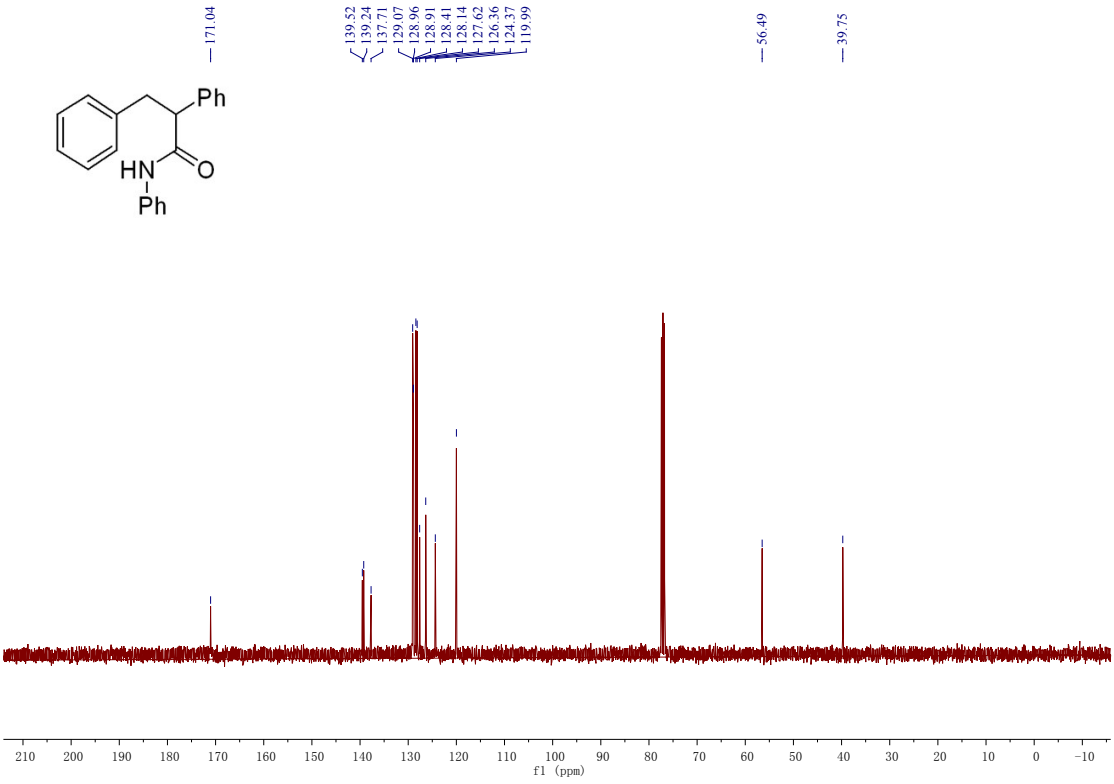
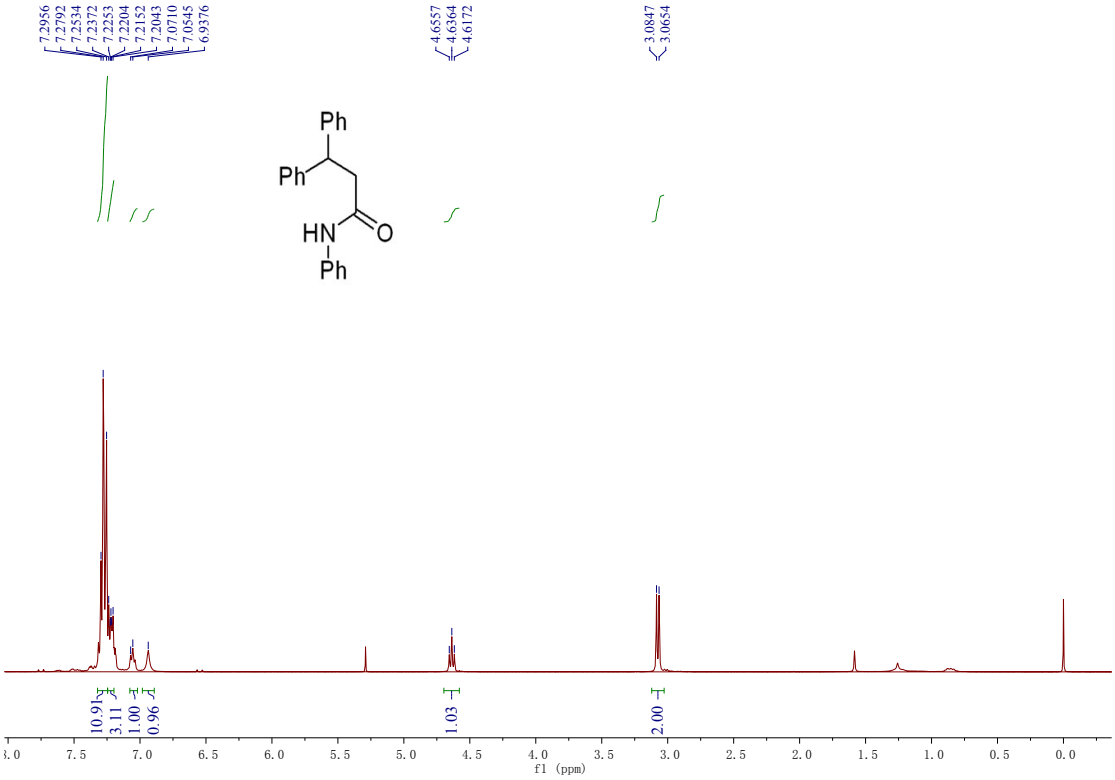


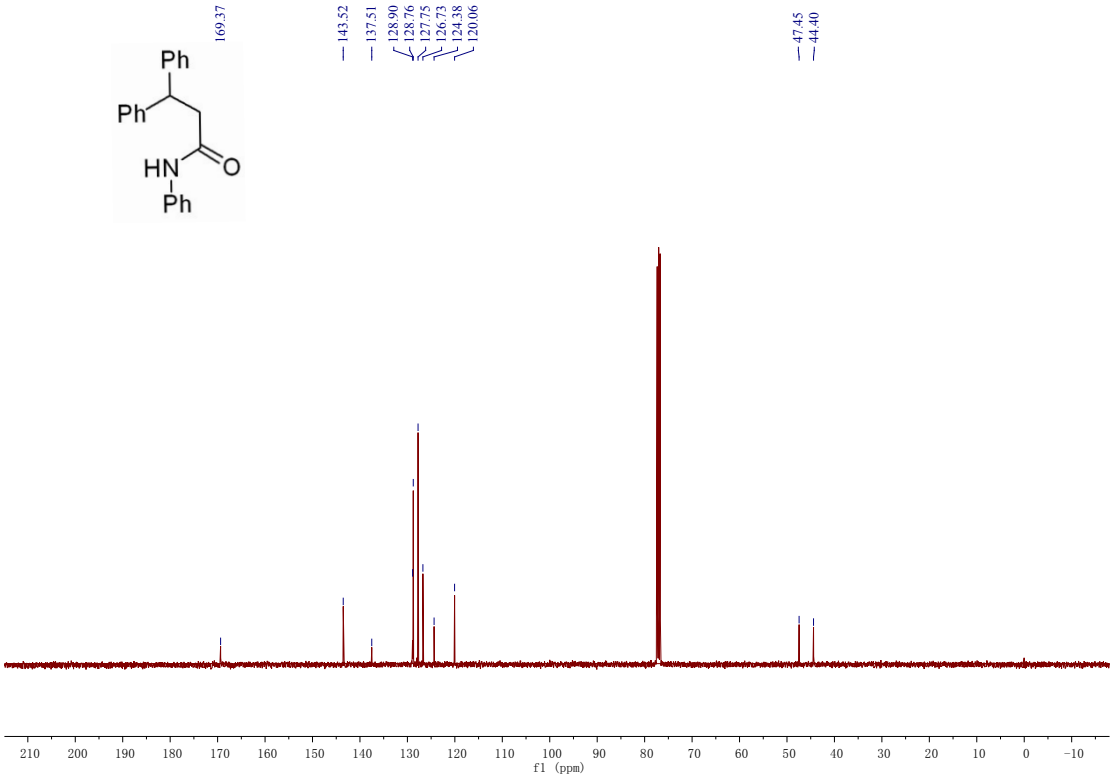
^{13}C NMR spectrum of compound **1p**



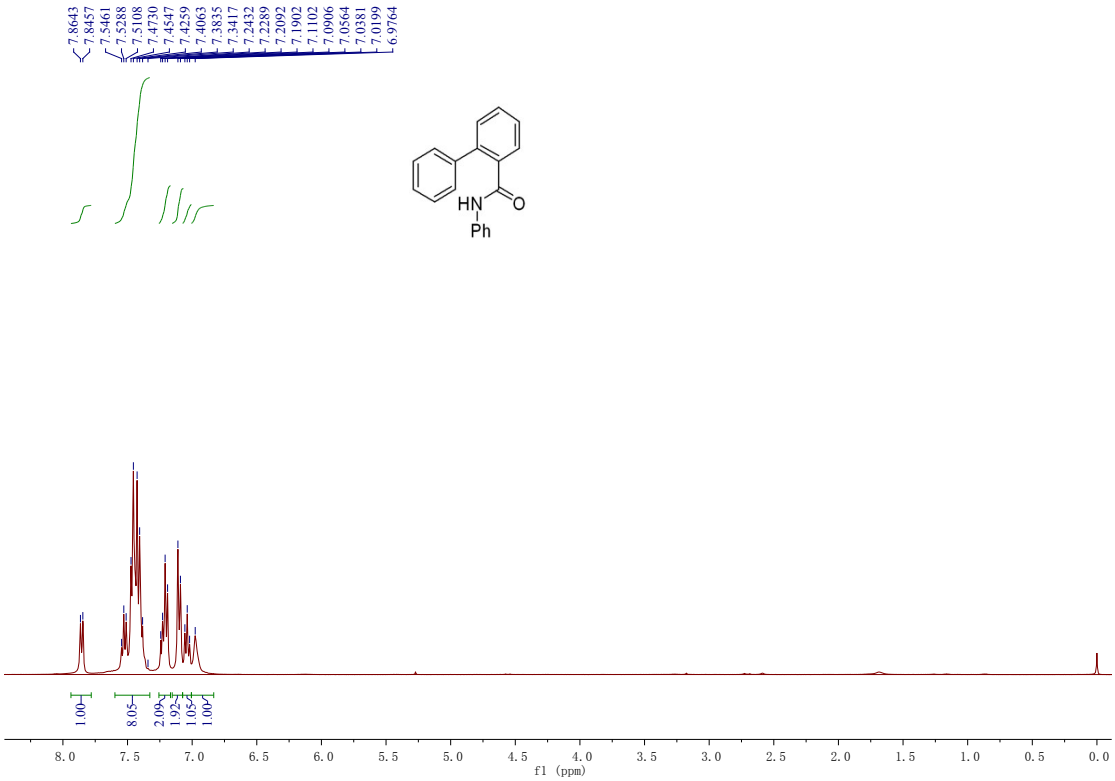
^{1}H NMR spectrum of compound **1q**



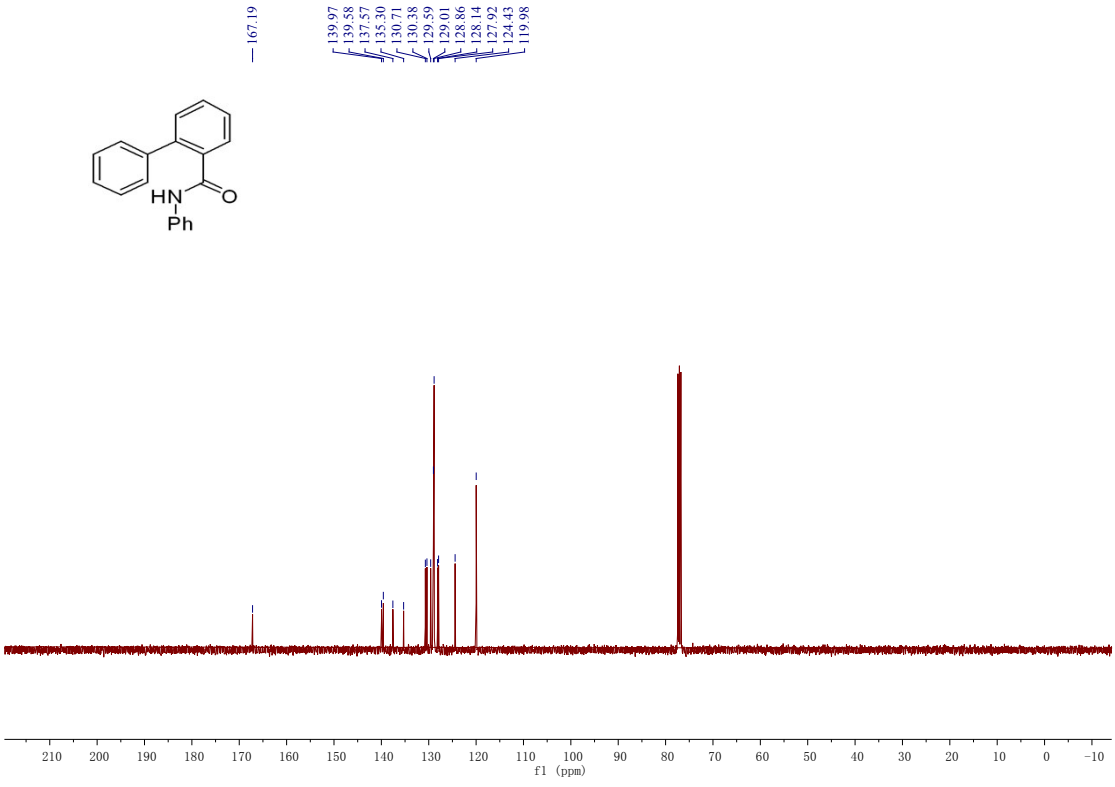
^{13}C NMR spectrum of compound **1q**



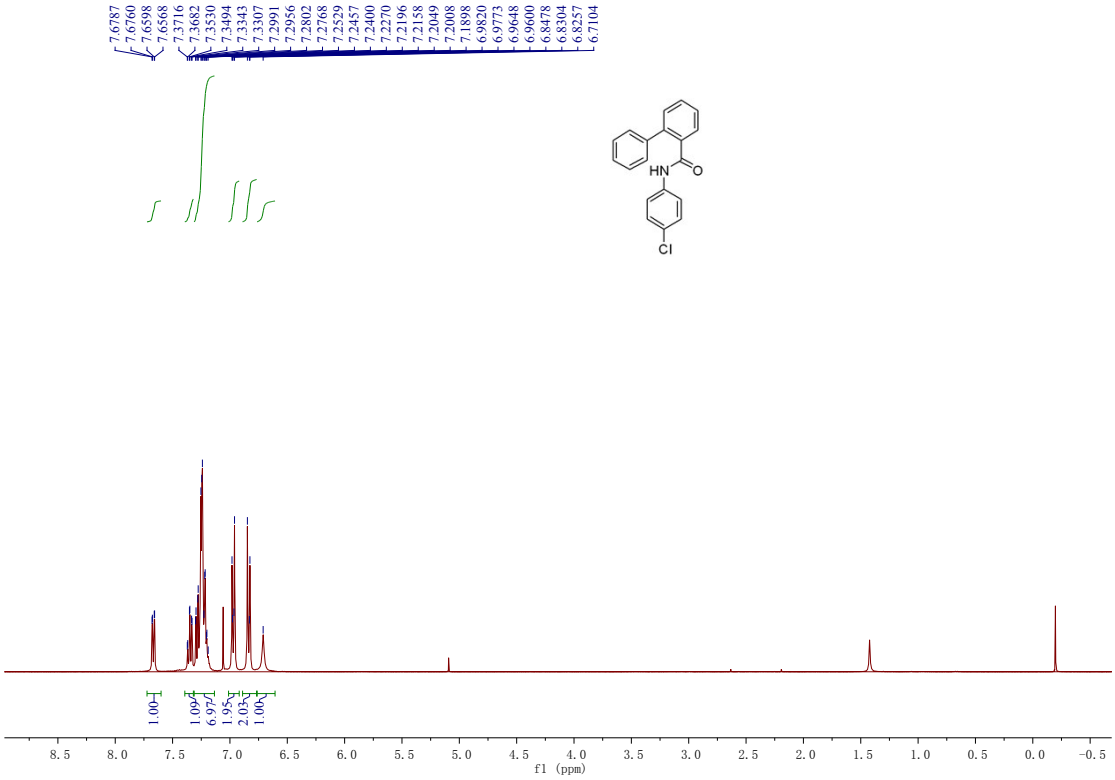
^{1}H NMR spectrum of compound **1r**



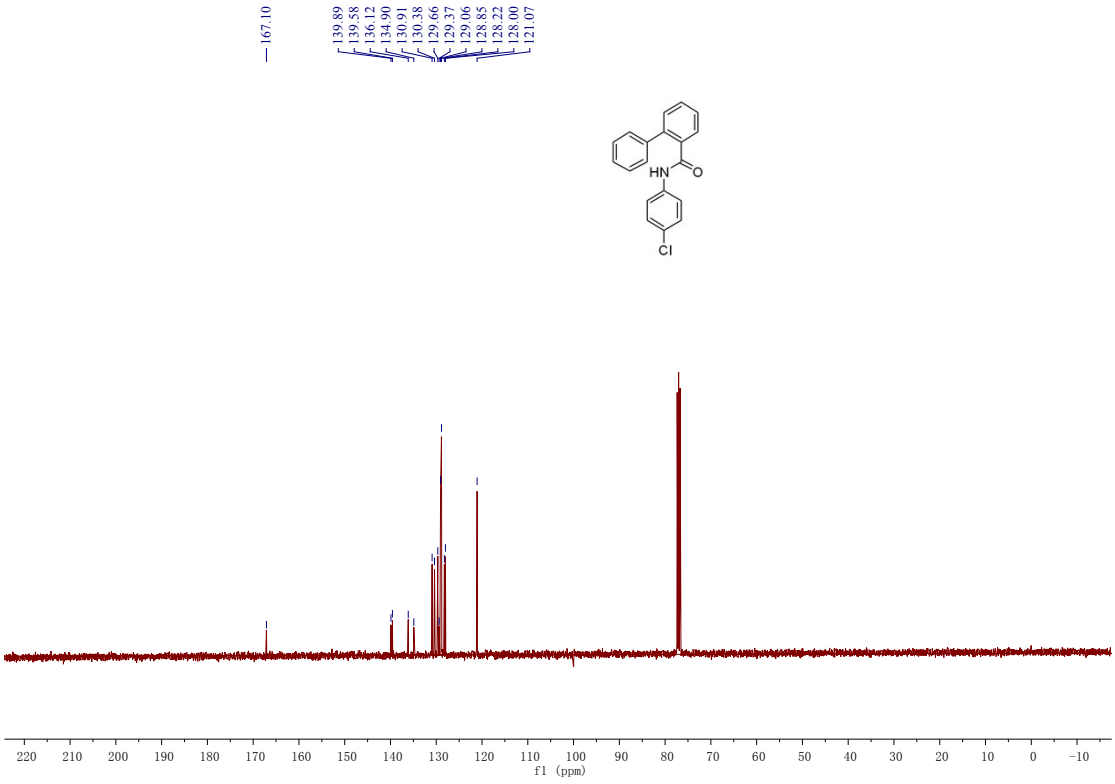
^{13}C NMR spectrum of compound **1r**



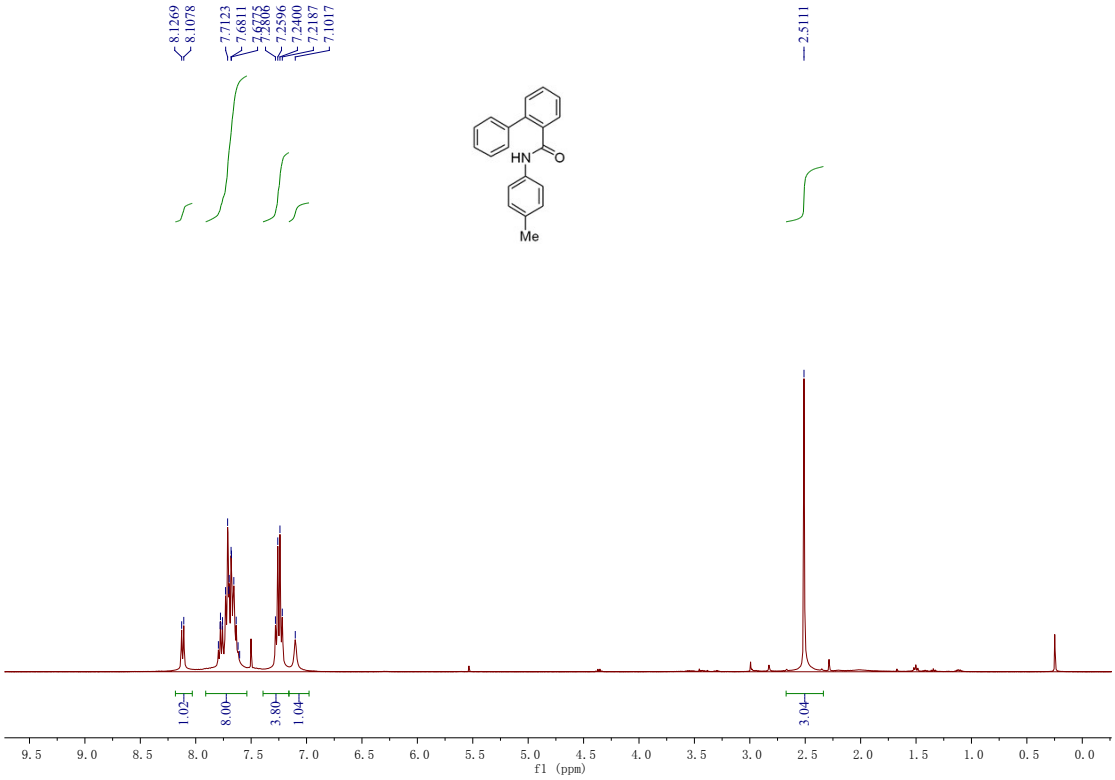
^{1}H NMR spectrum of compound **1s**



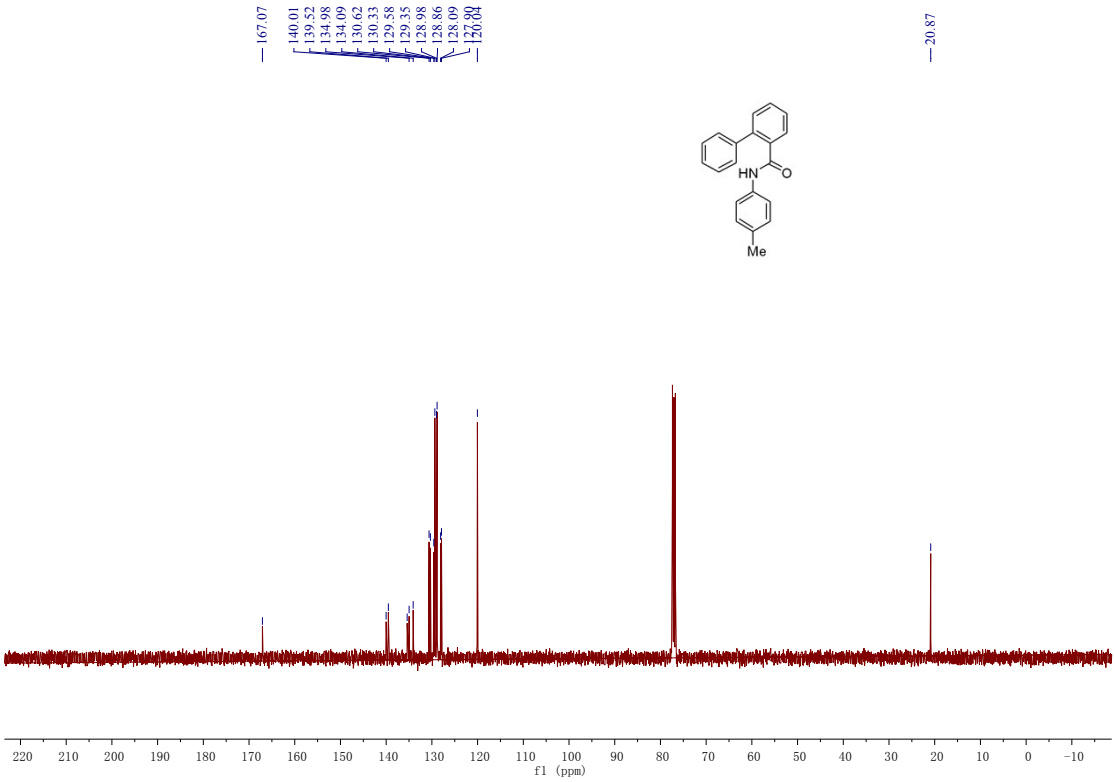
^{13}C NMR spectrum of compound **1s**



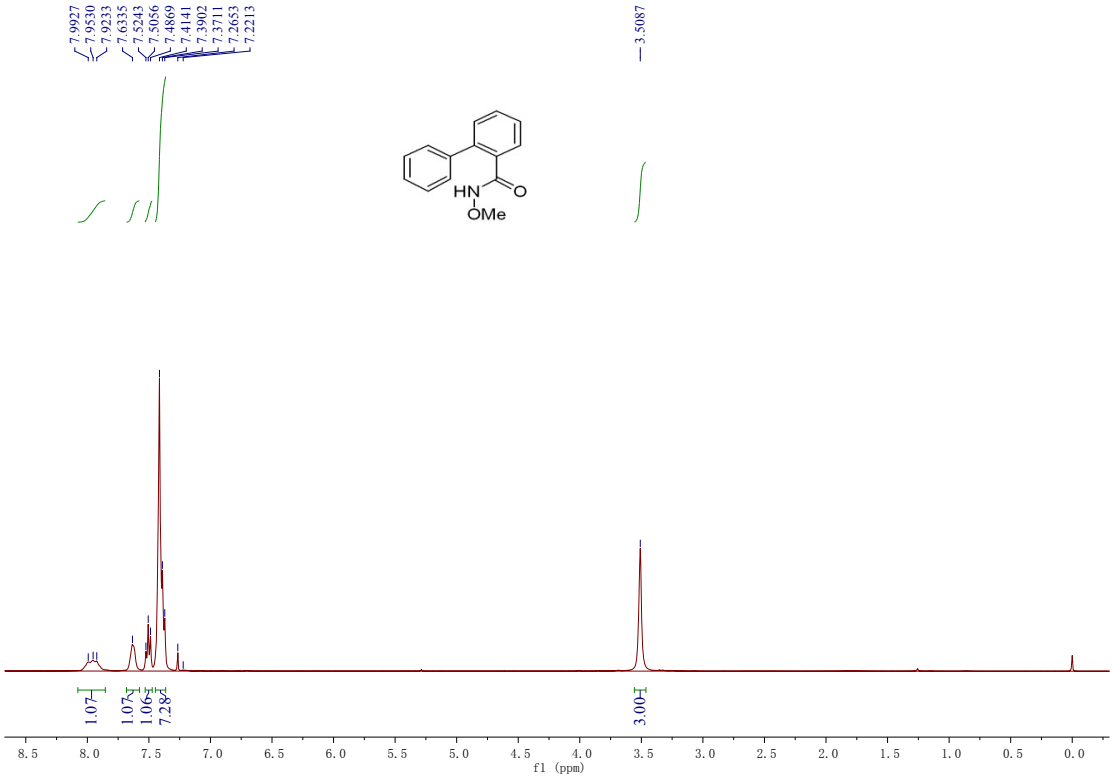
^{1}H NMR spectrum of compound **1t**



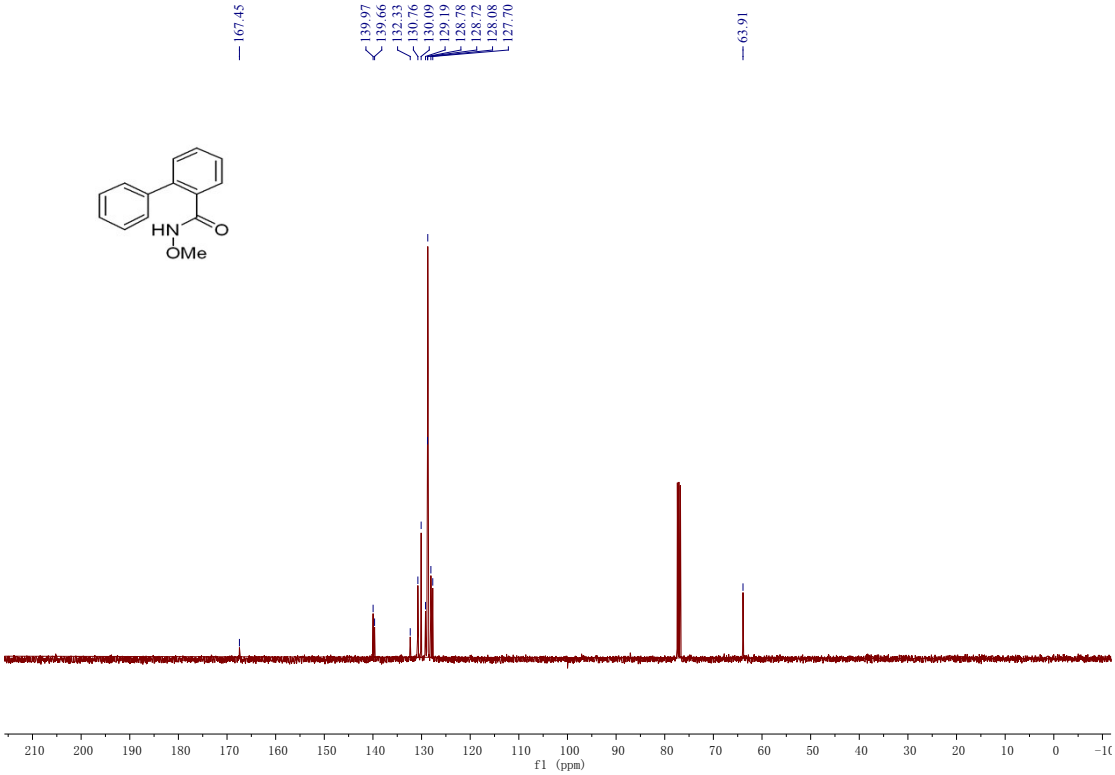
^{13}C NMR spectrum of compound **1t**



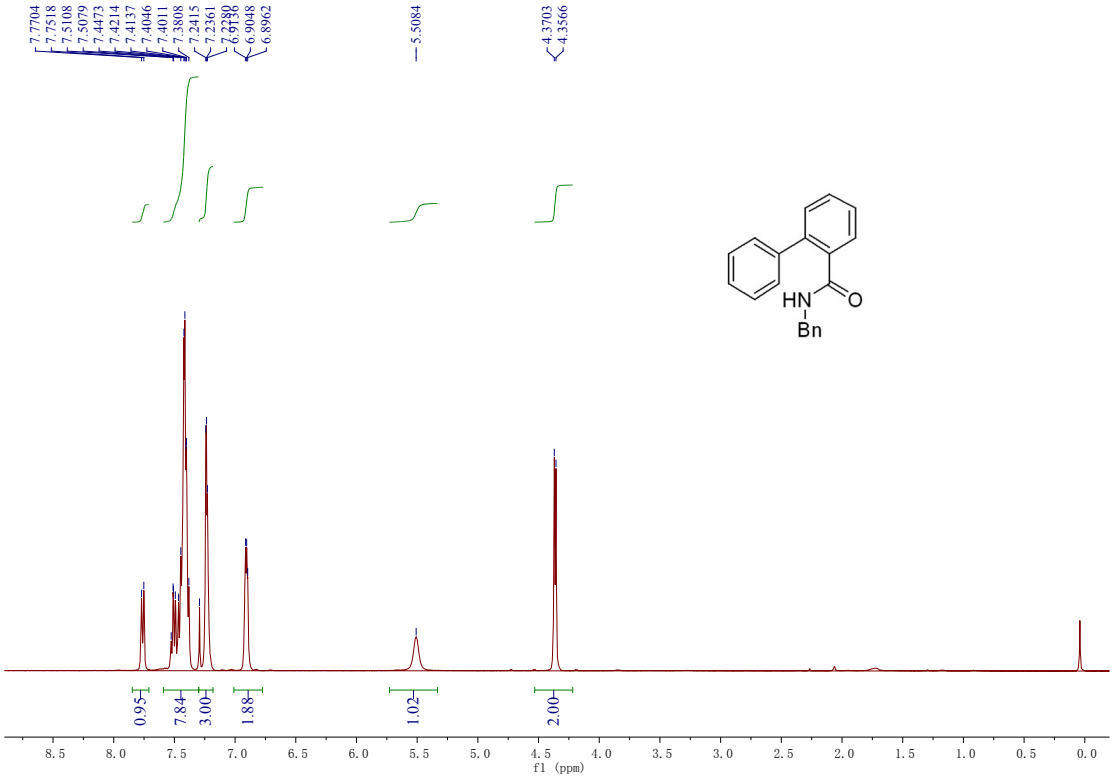
^{1}H NMR spectrum of compound **1u**



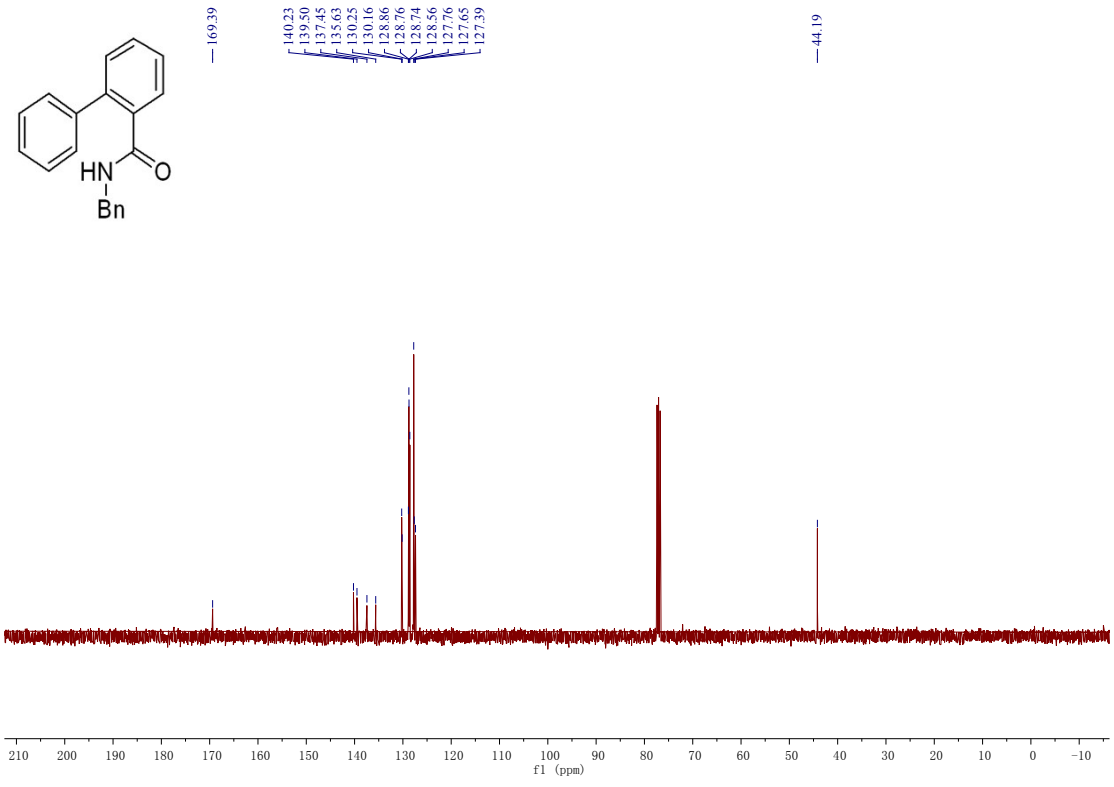
^{13}C NMR spectrum of compound **1u**



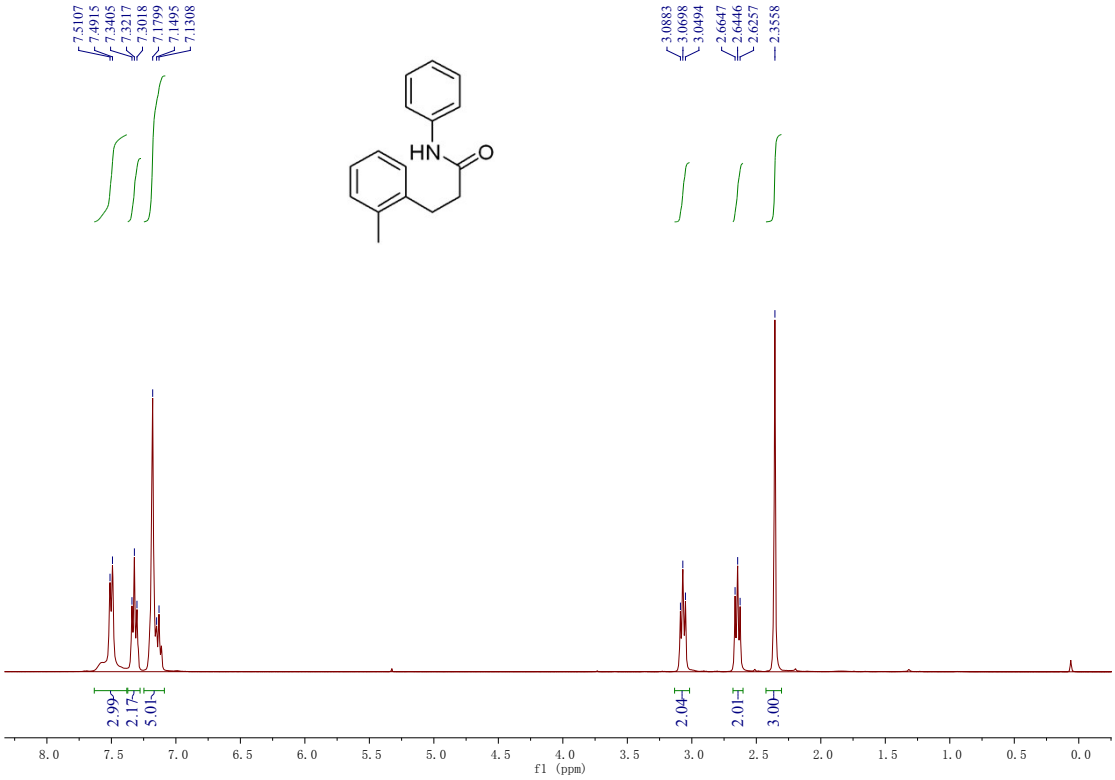
^{1}H NMR spectrum of compound **1v**



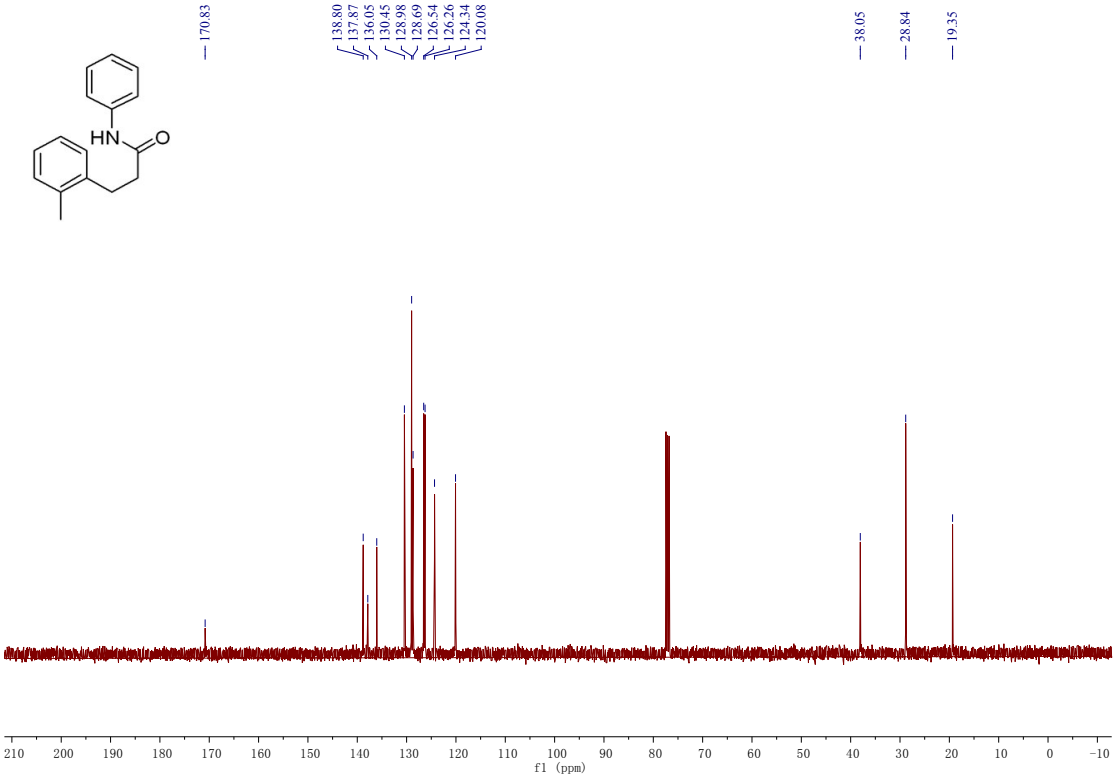
^{13}C NMR spectrum of compound **1v**



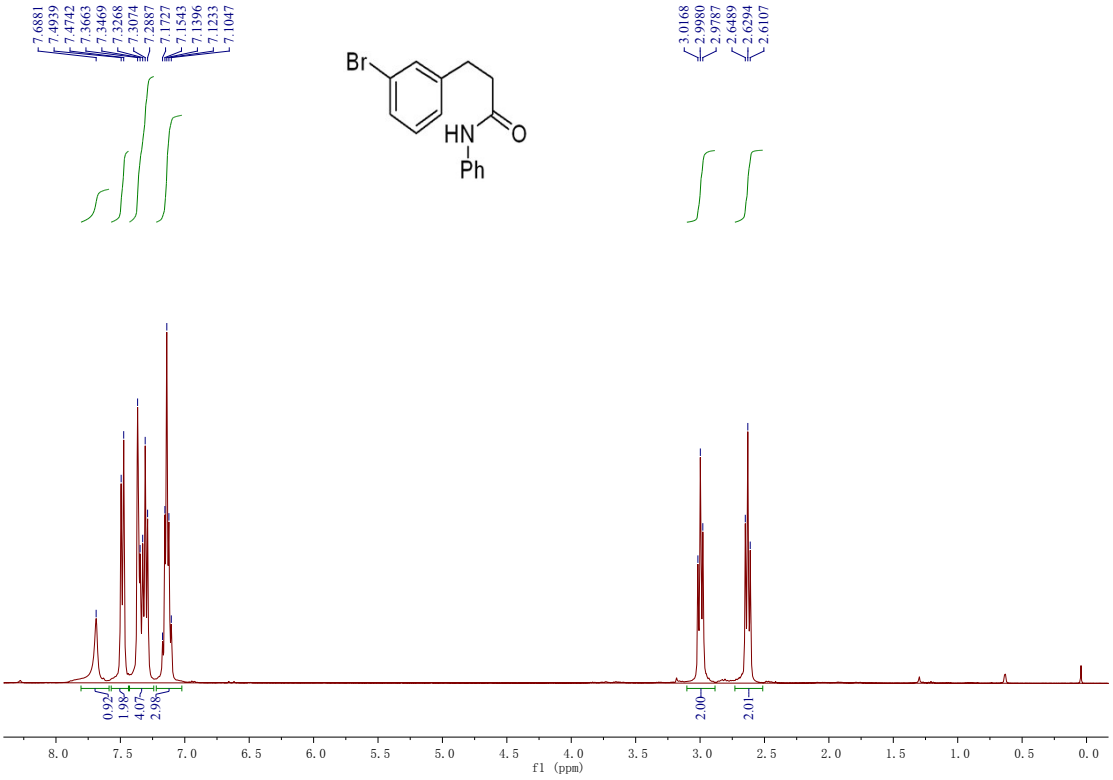
^{1}H NMR spectrum of compound **1w**



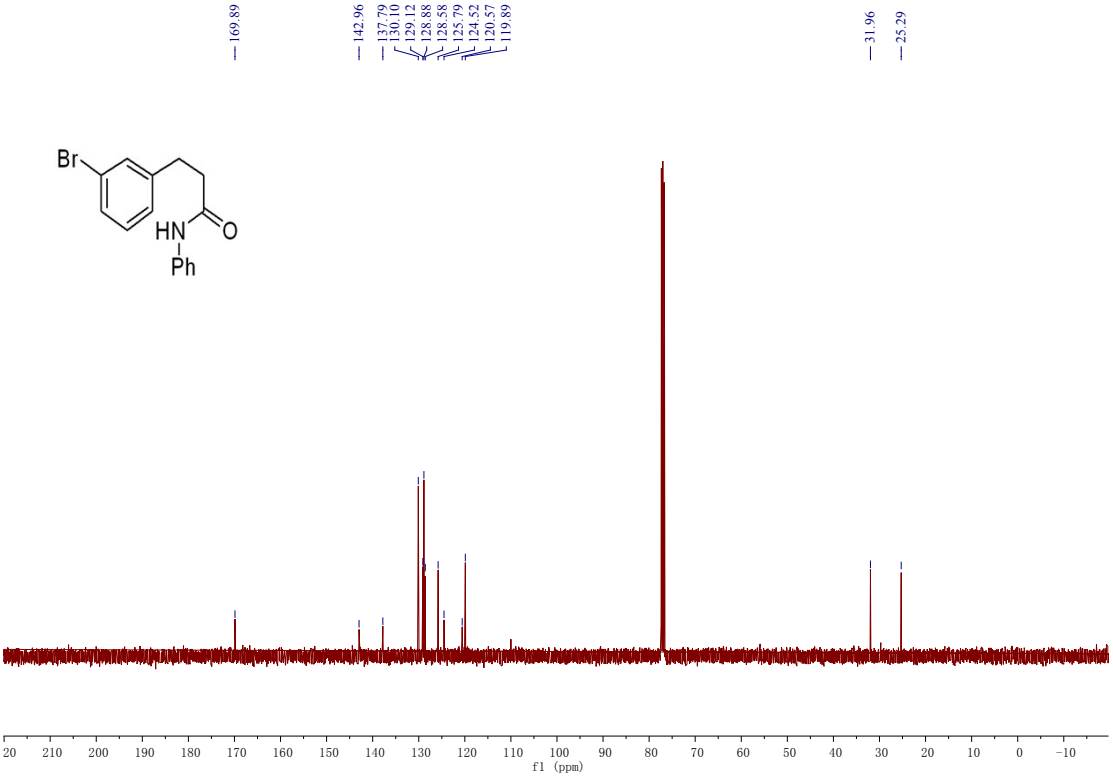
^{13}C NMR spectrum of compound **1w**



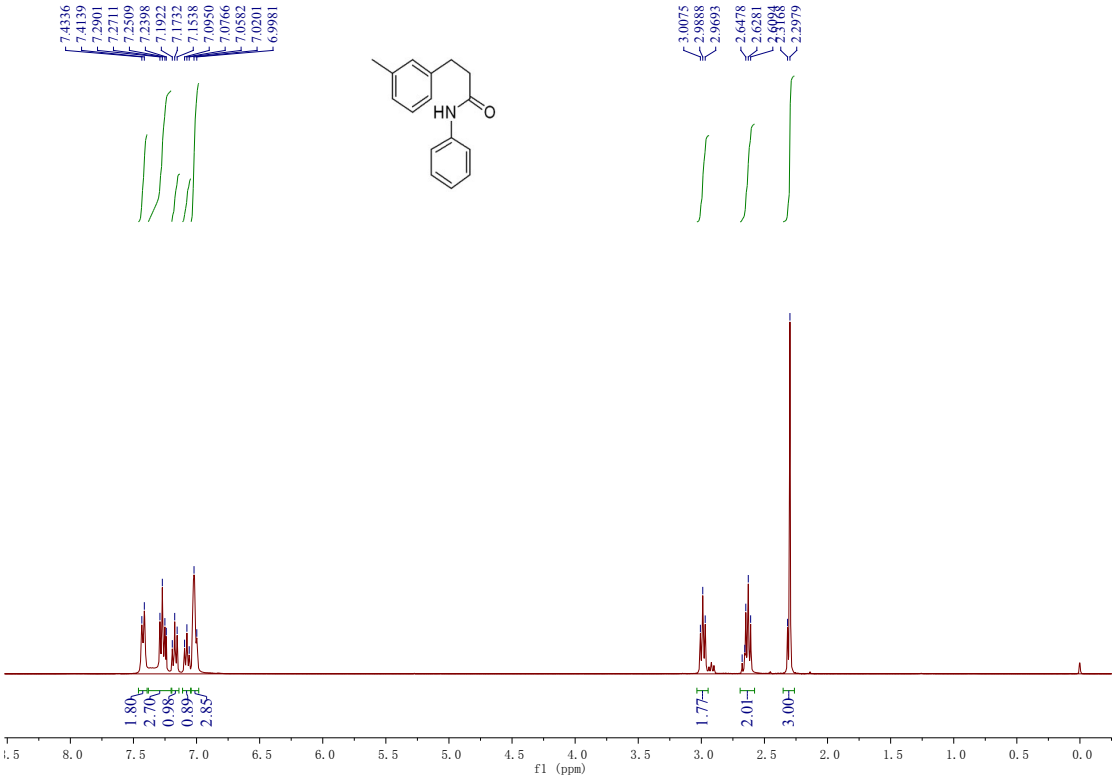
^{1}H NMR spectrum of compound **1x**



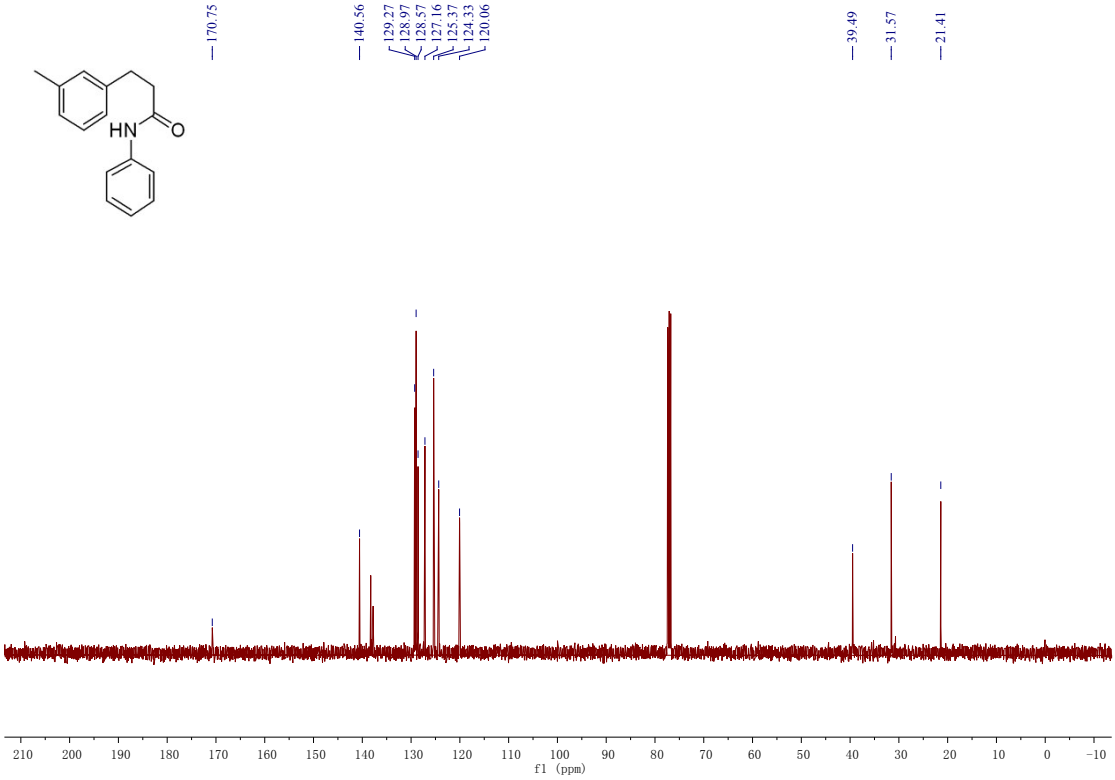
^{13}C NMR spectrum of compound **1x**



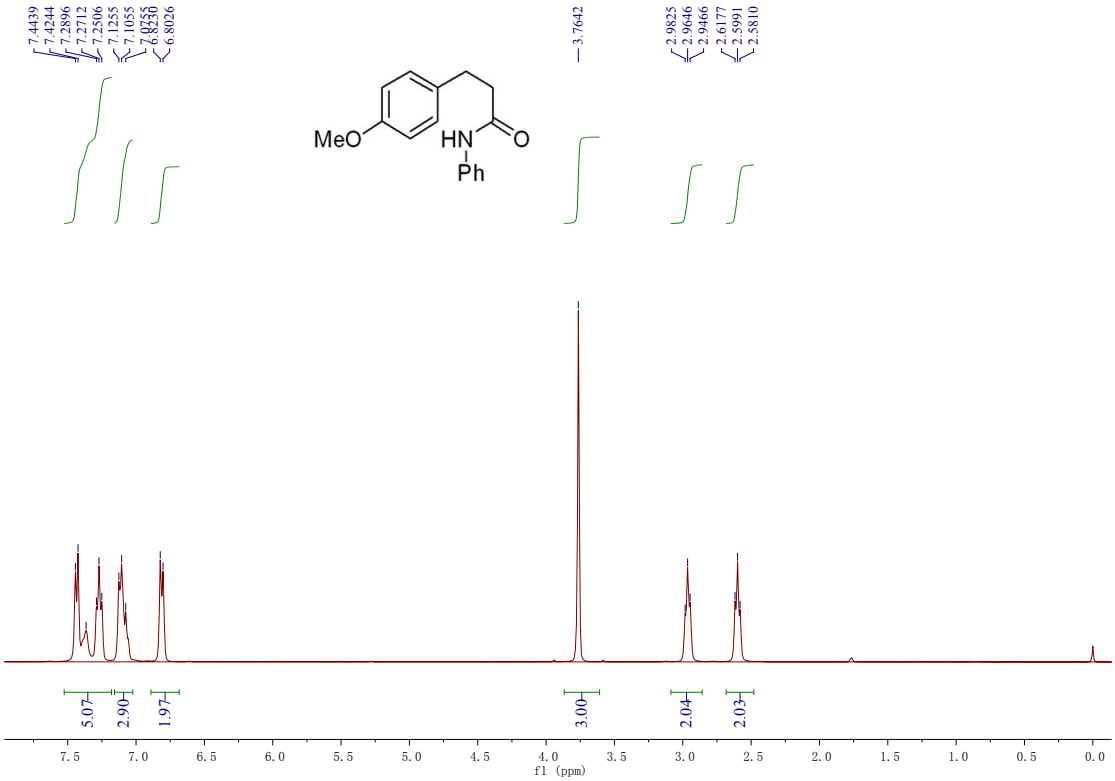
^{1}H NMR spectrum of compound **1y**



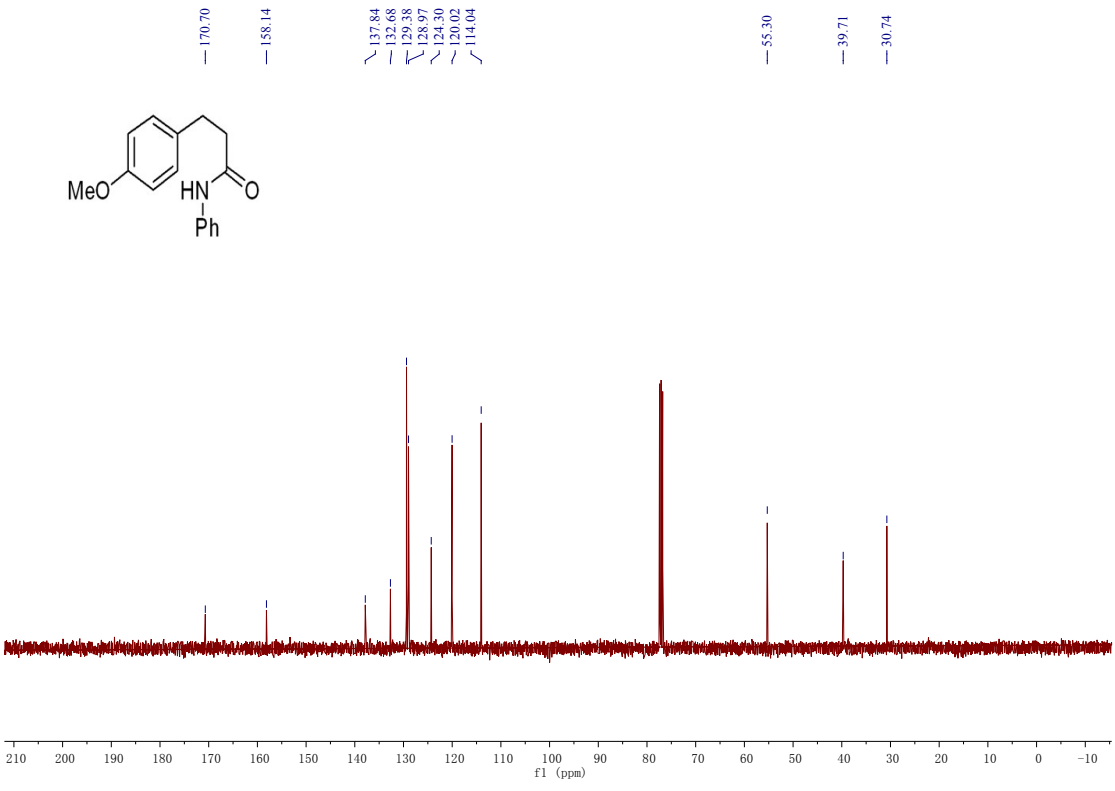
^{13}C NMR spectrum of compound **1y**



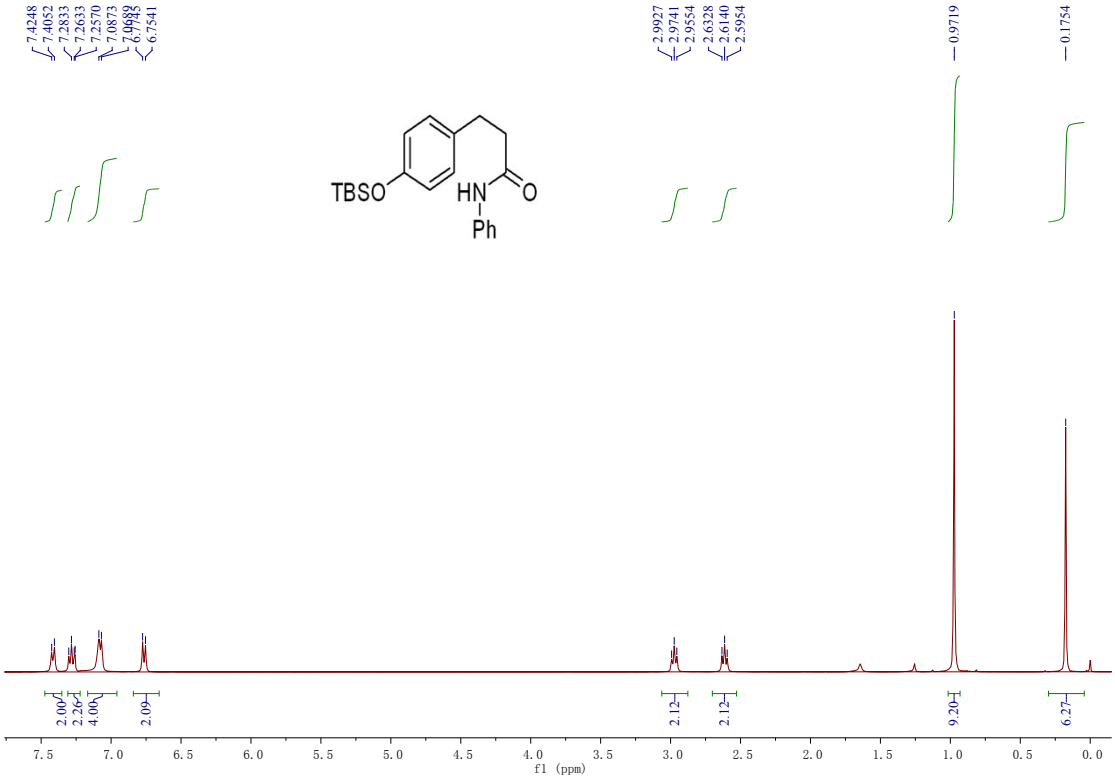
^{1}H NMR spectrum of compound **1z**



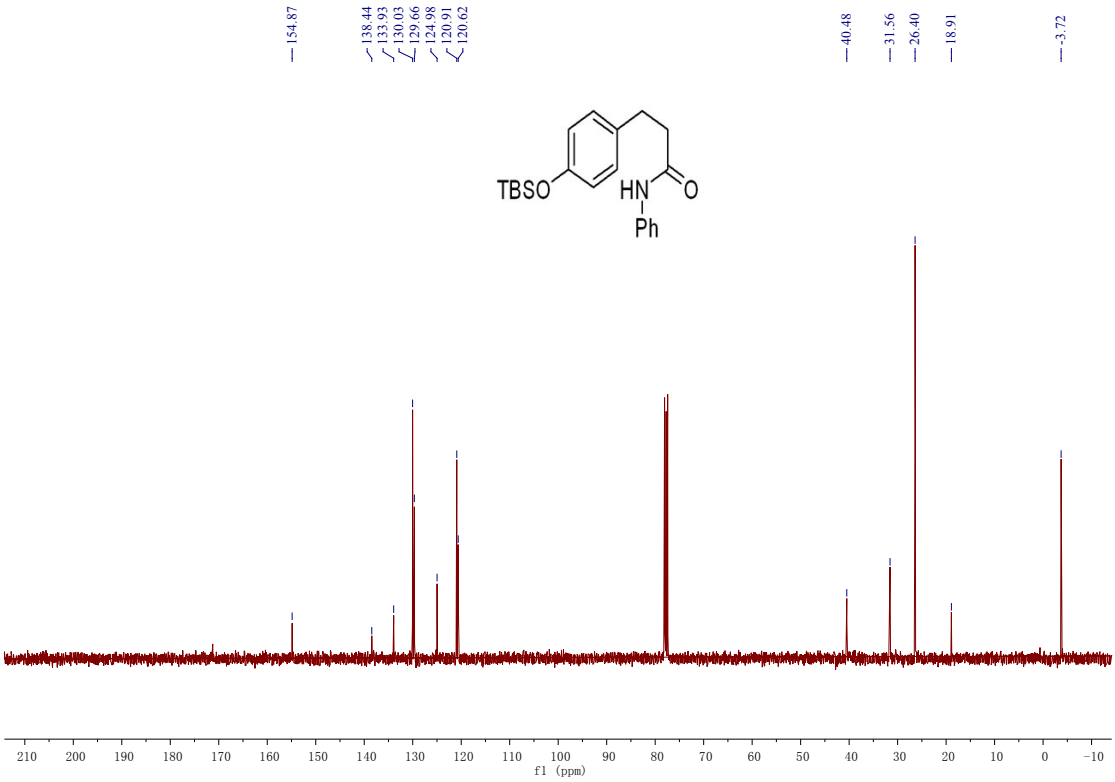
^{13}C NMR spectrum of compound **1z**



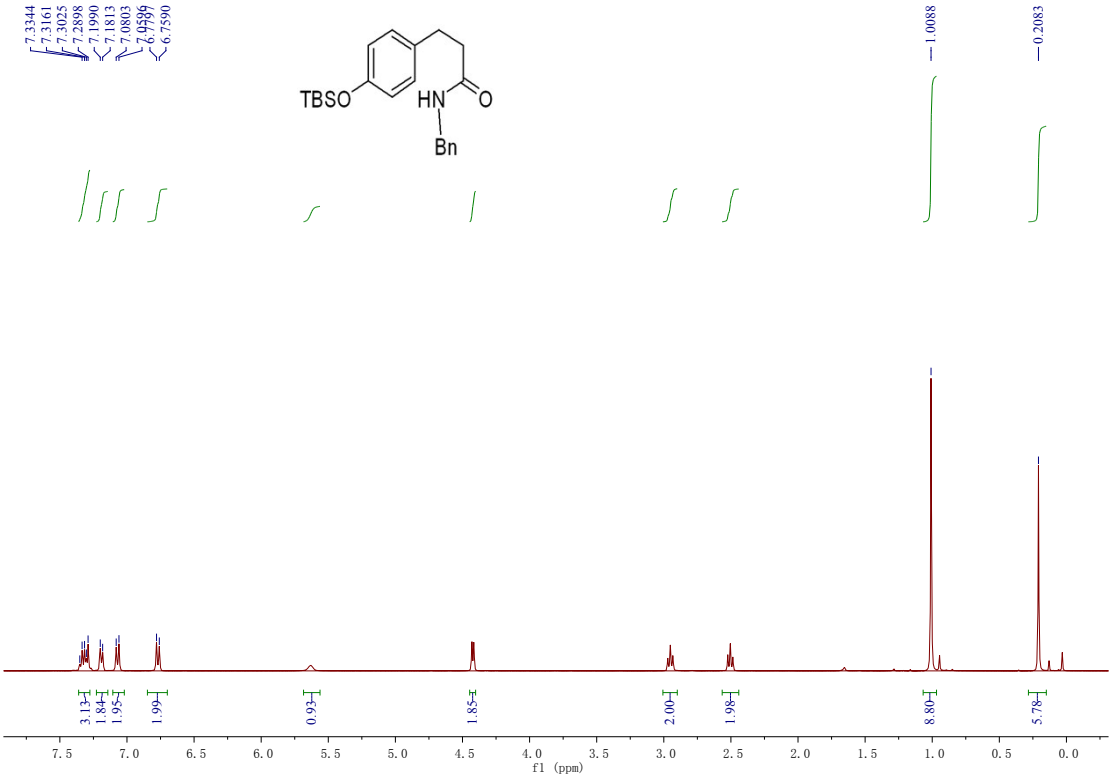
^{1}H NMR spectrum of compound **1aa**



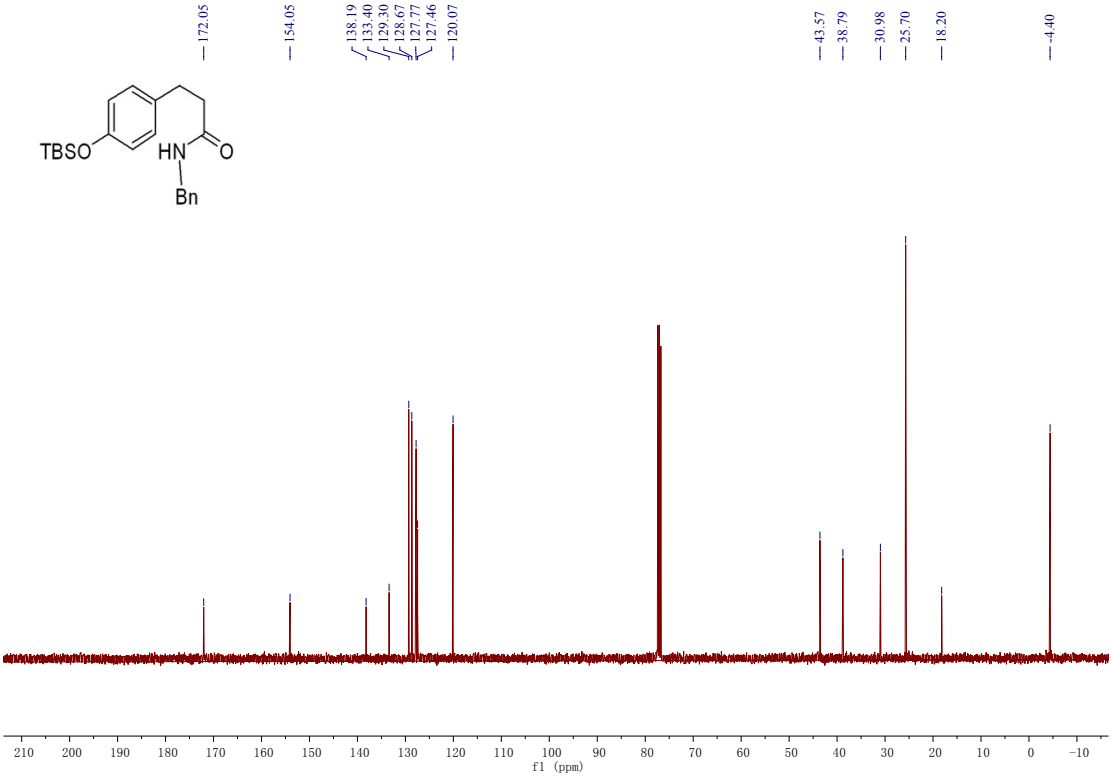
^{13}C NMR spectrum of compound **1aa**



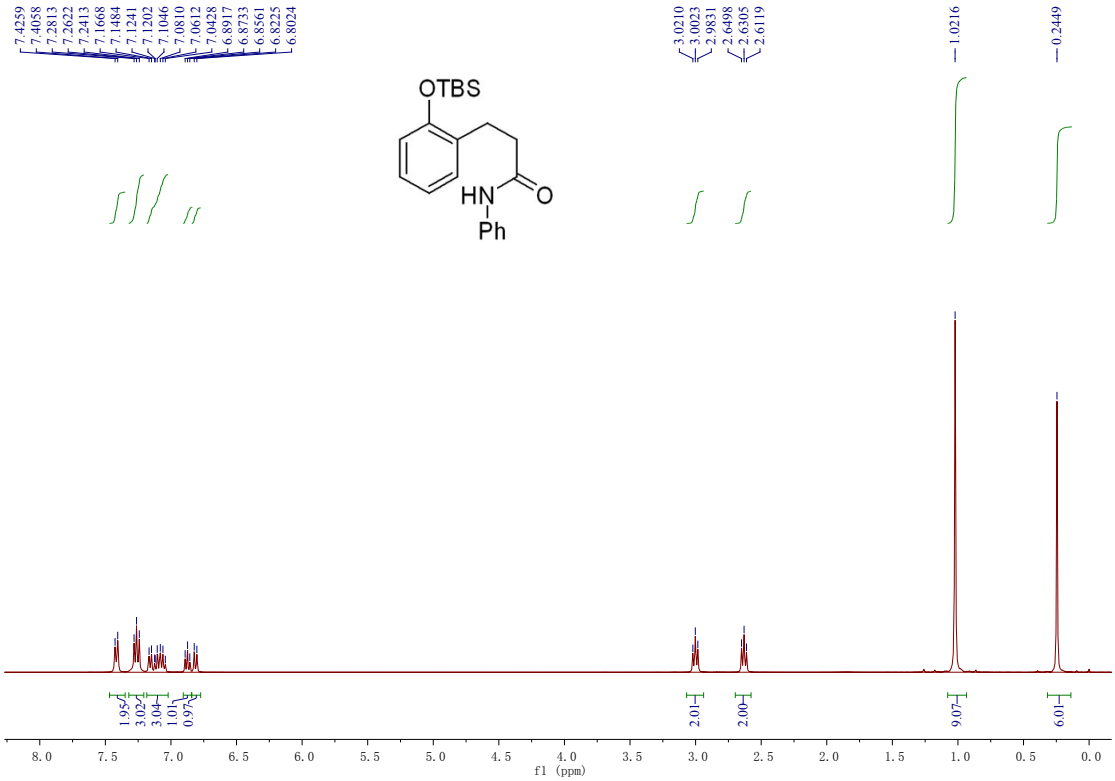
^{1}H NMR spectrum of compound **1ab**



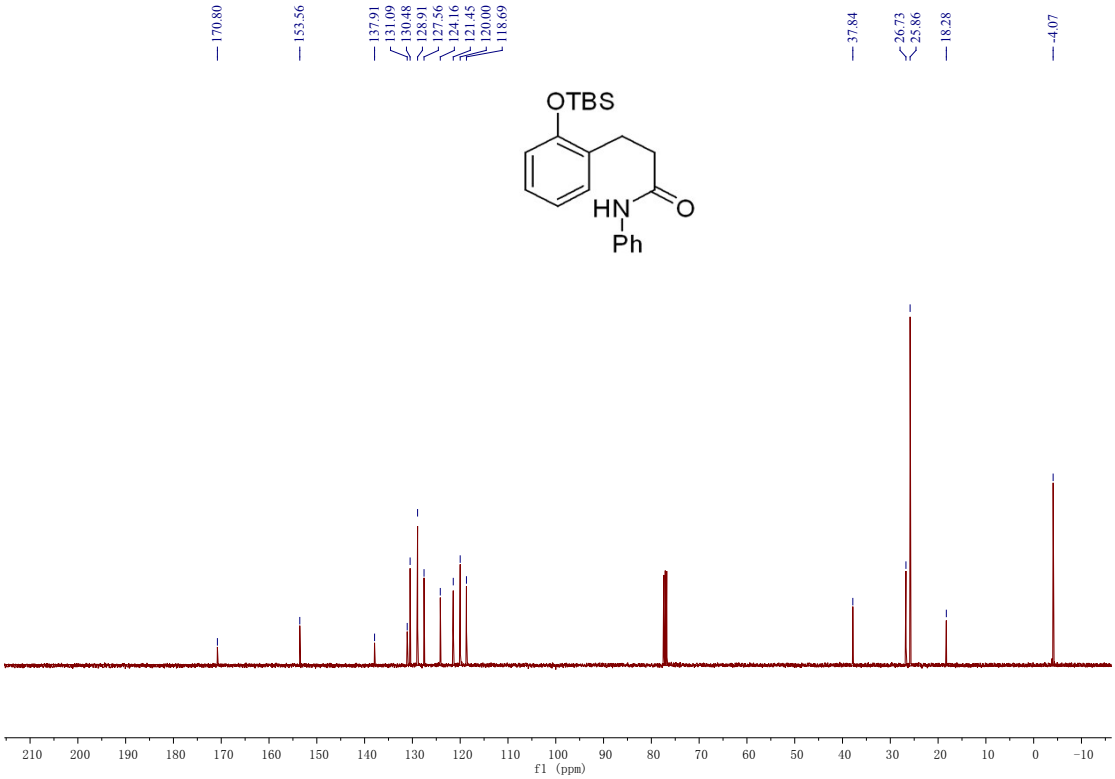
^{13}C NMR spectrum of compound **1ab**



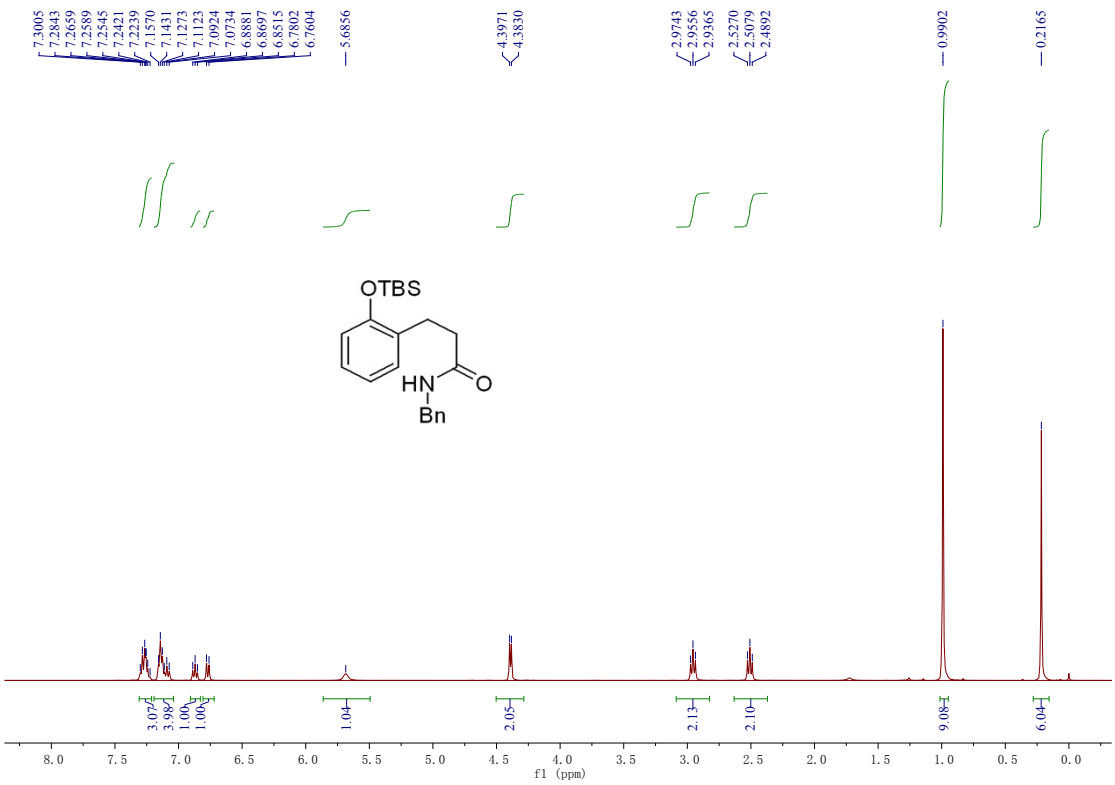
^{1}H NMR spectrum of compound **1ac**



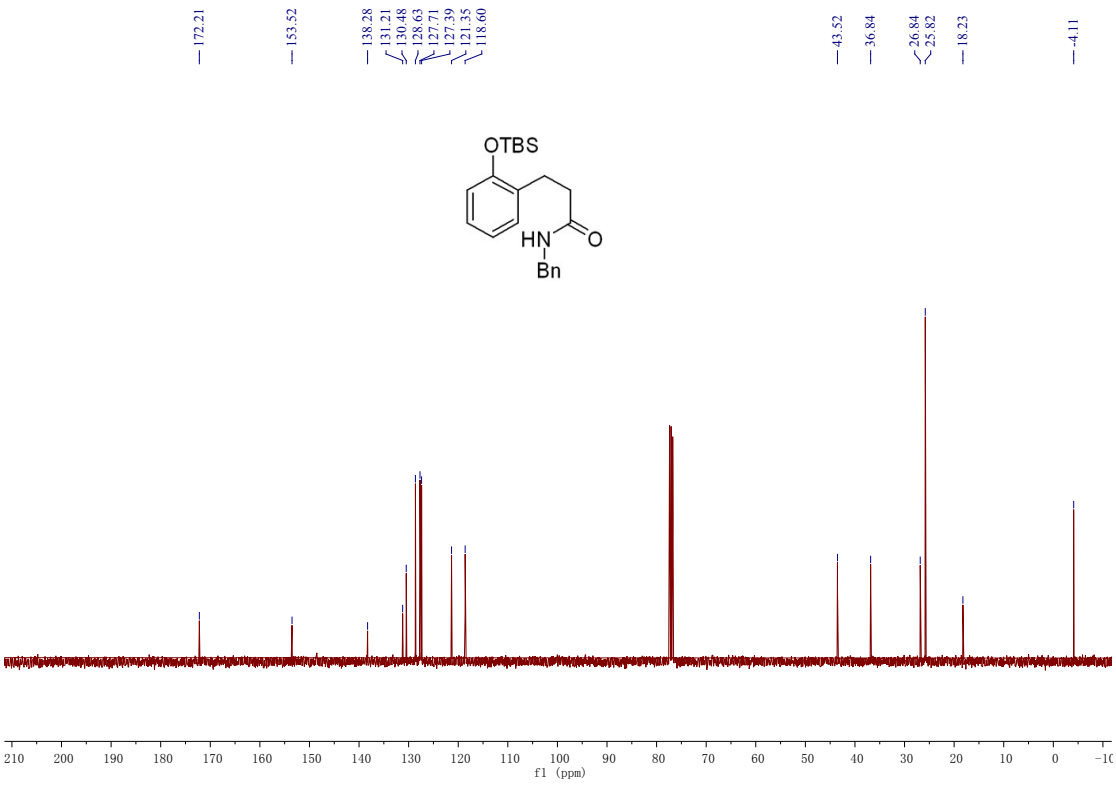
^{13}C NMR spectrum of compound **1ac**



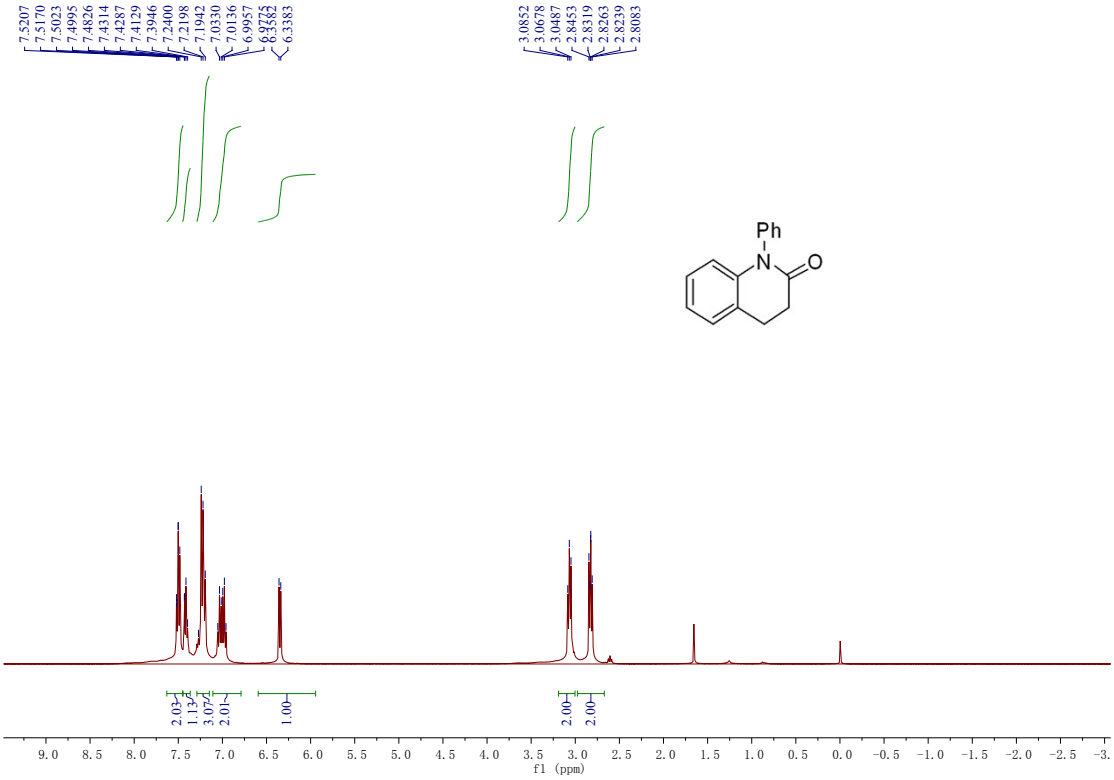
^{1}H NMR spectrum of compound **1ad**



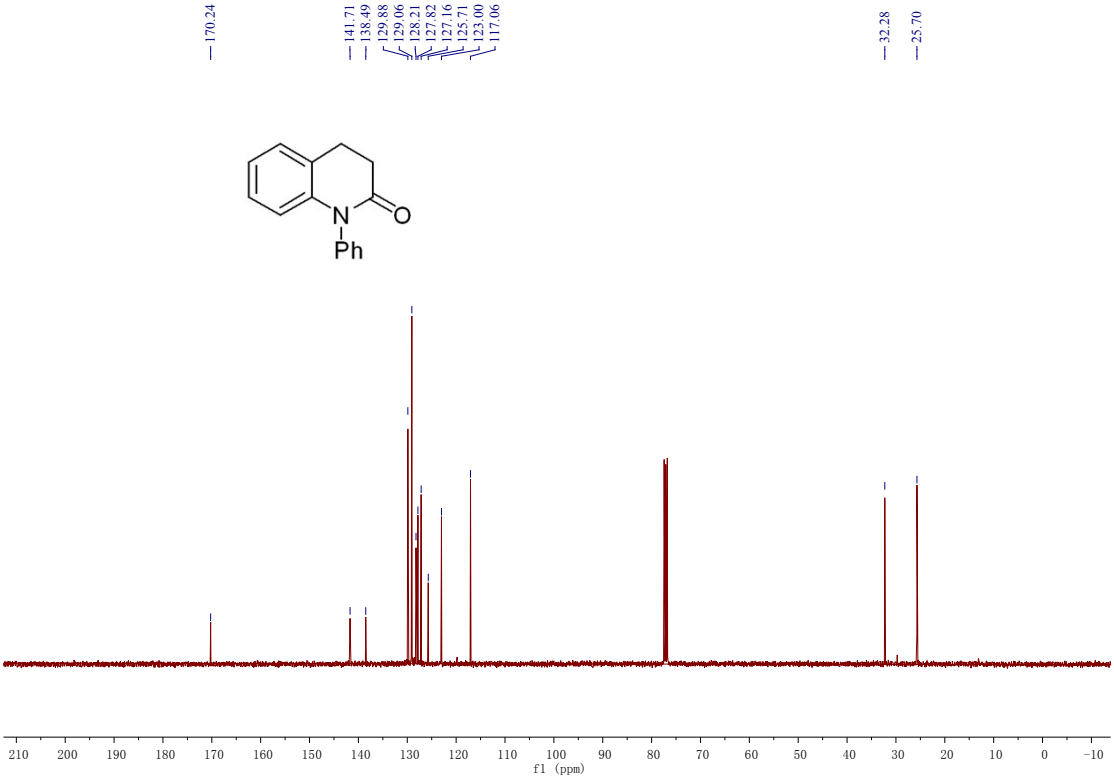
^{13}C NMR spectrum of compound **1ad**



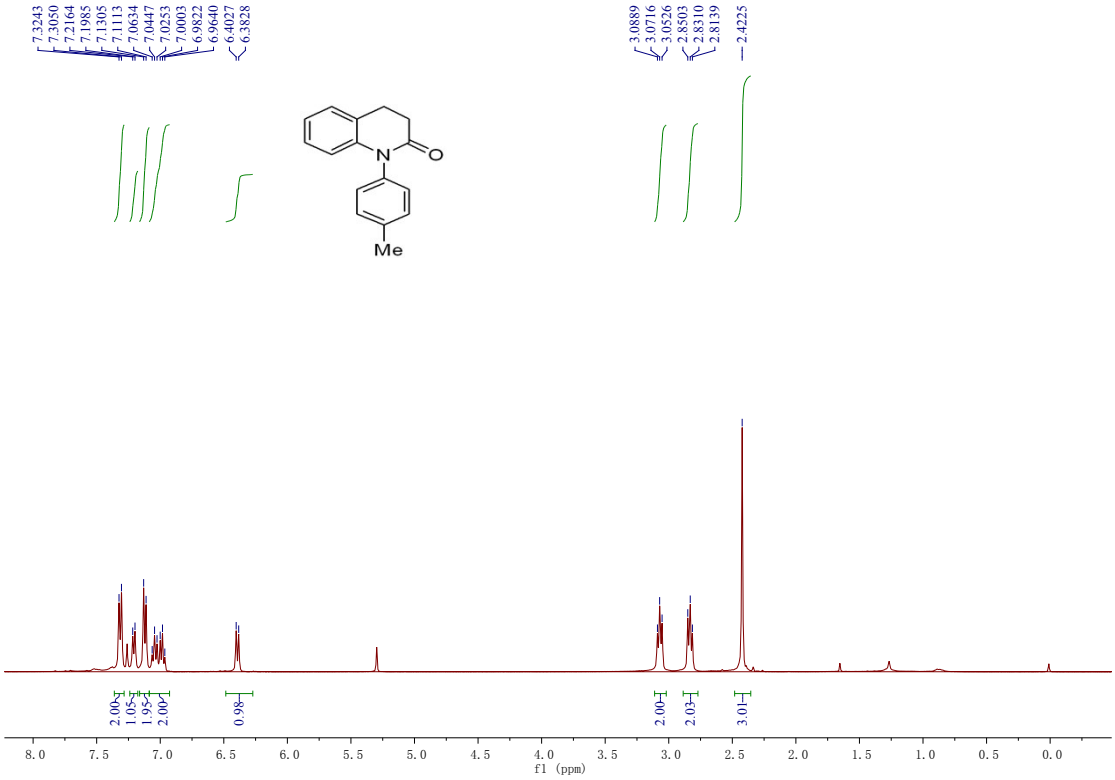
^{1}H NMR spectrum of compound **2a**



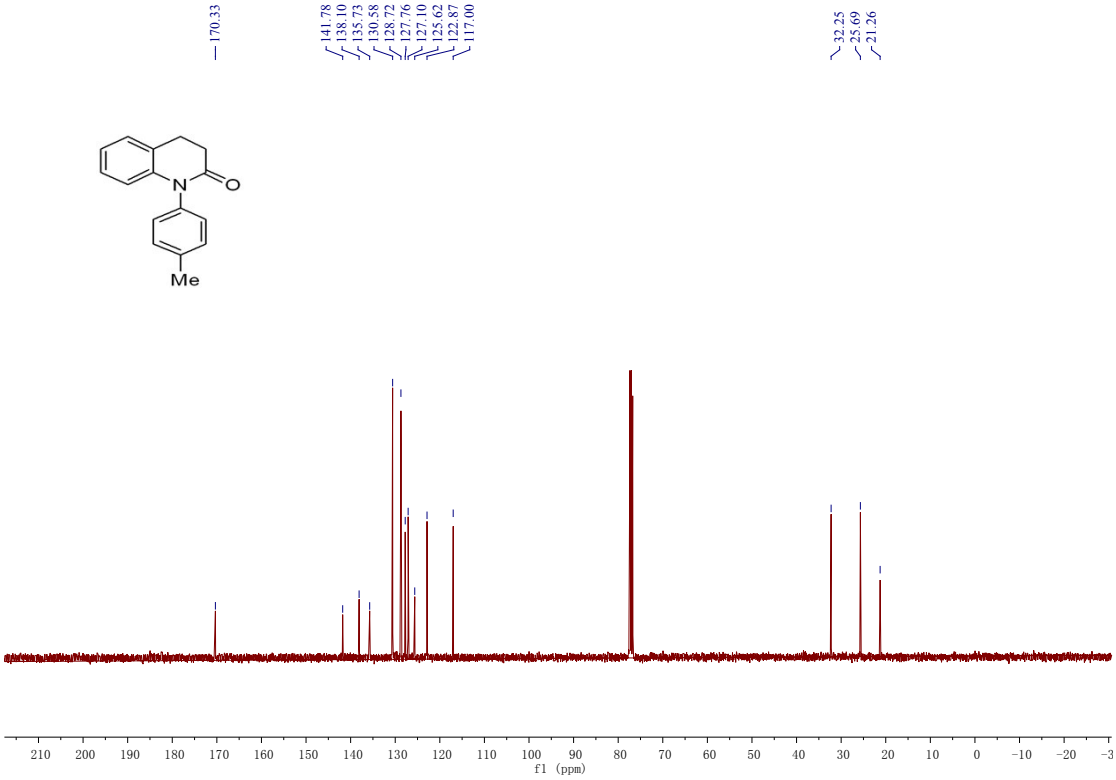
^{13}C NMR spectrum of compound **2a**



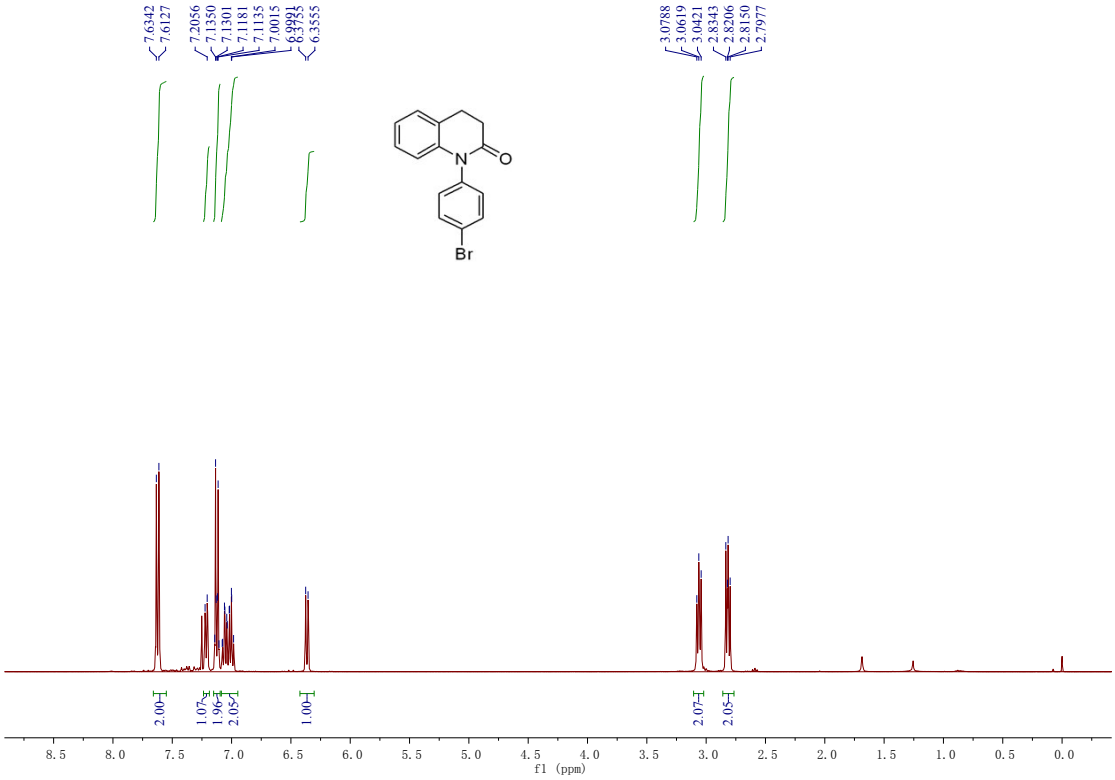
^{1}H NMR spectrum of compound **2b**



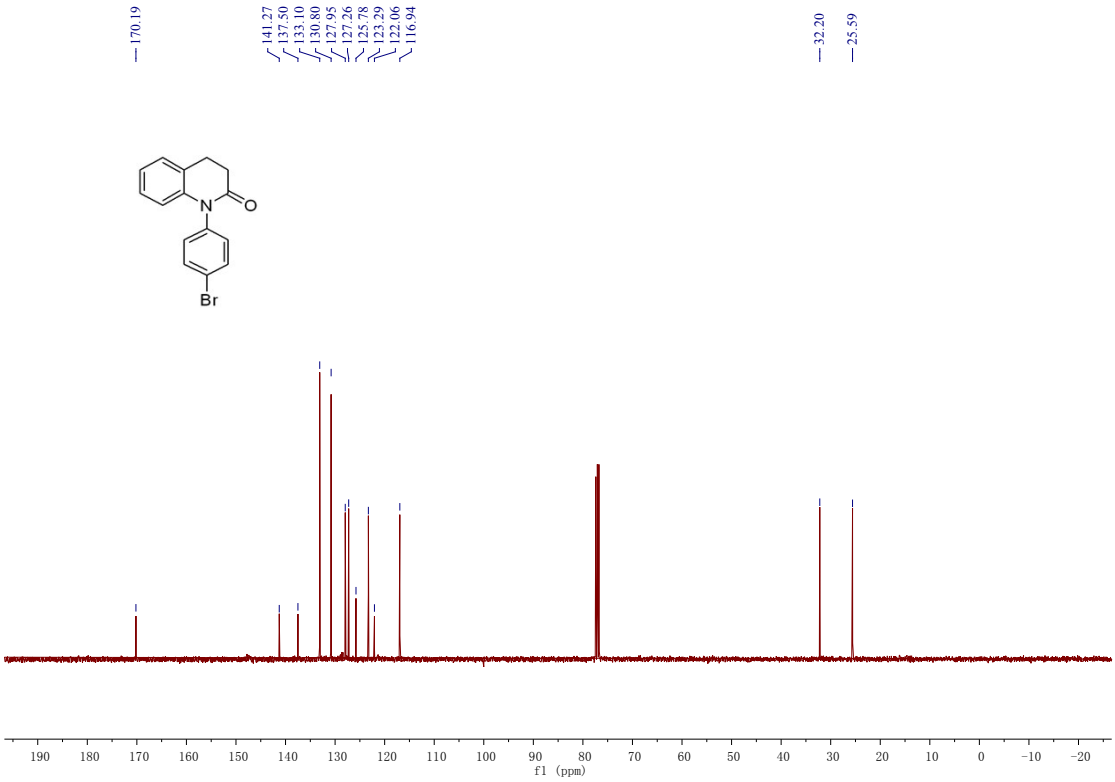
^{13}C NMR spectrum of compound **2b**



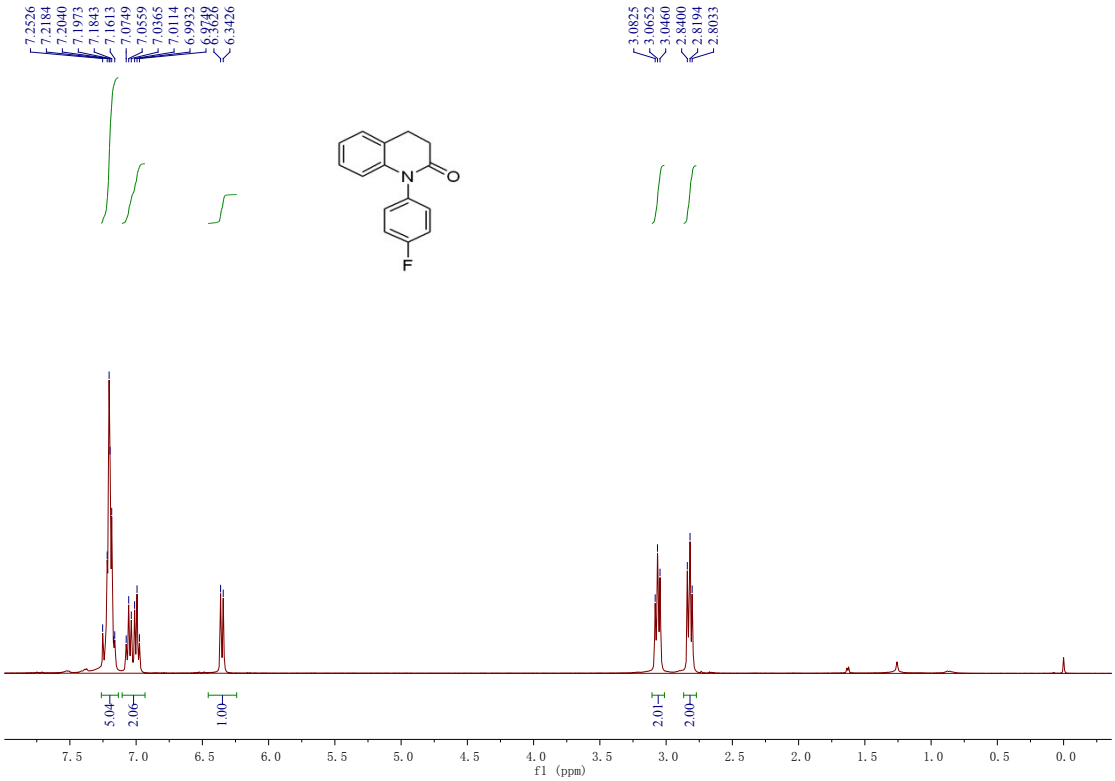
^{1}H NMR spectrum of compound **2c**



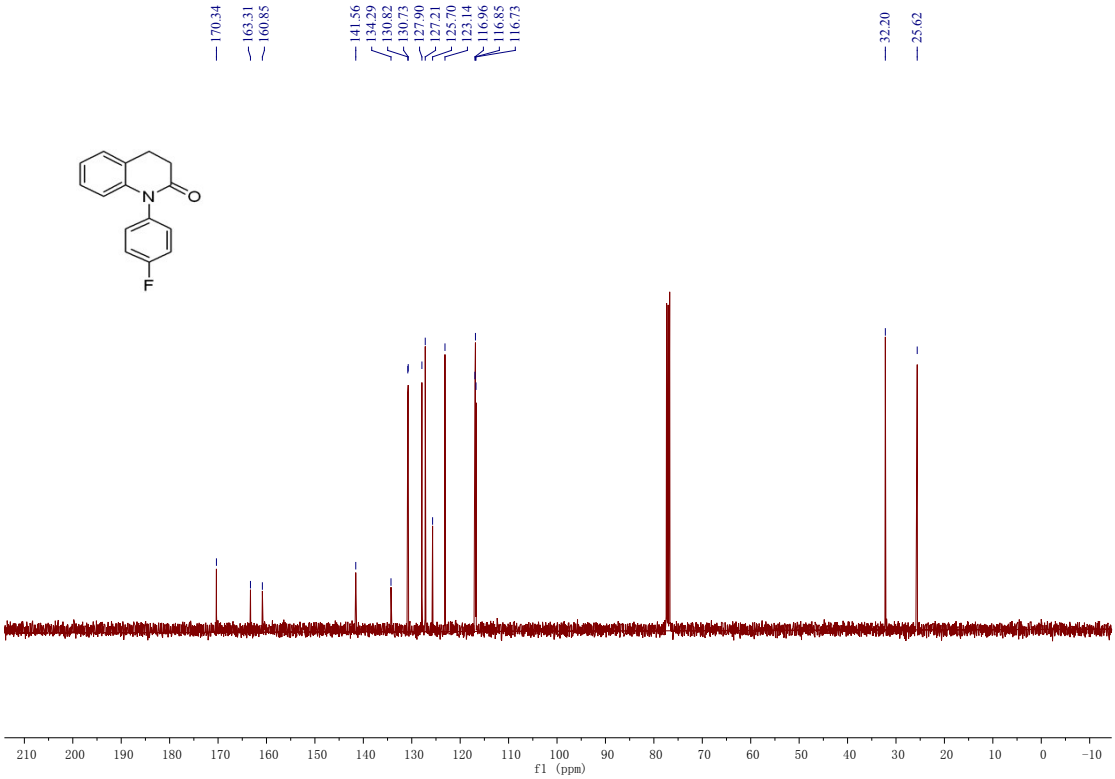
^{13}C NMR spectrum of compound **2c**



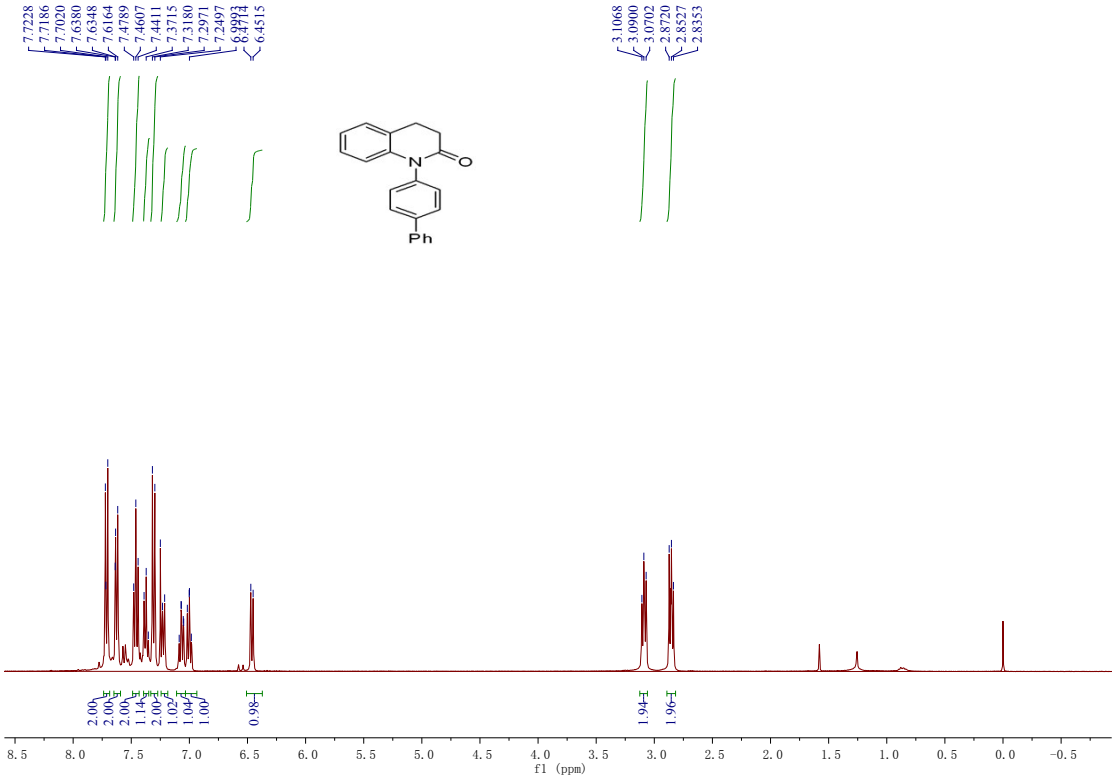
^{1}H NMR spectrum of compound **2d**



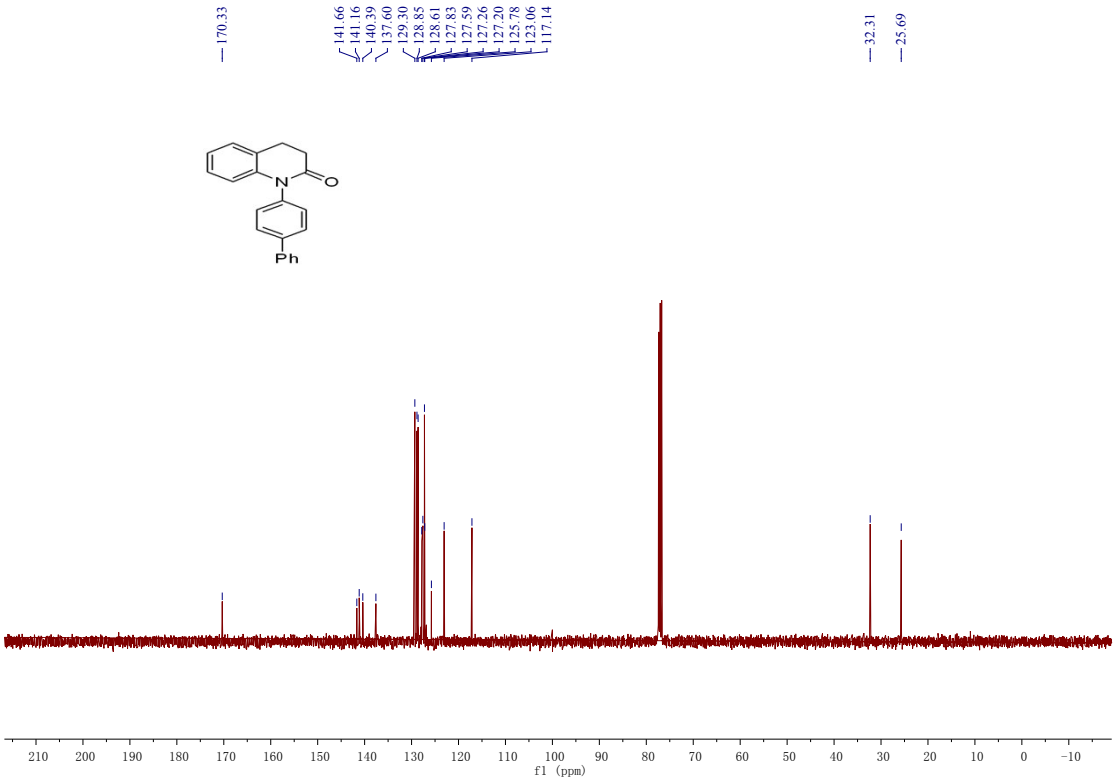
^{13}C NMR spectrum of compound **2d**



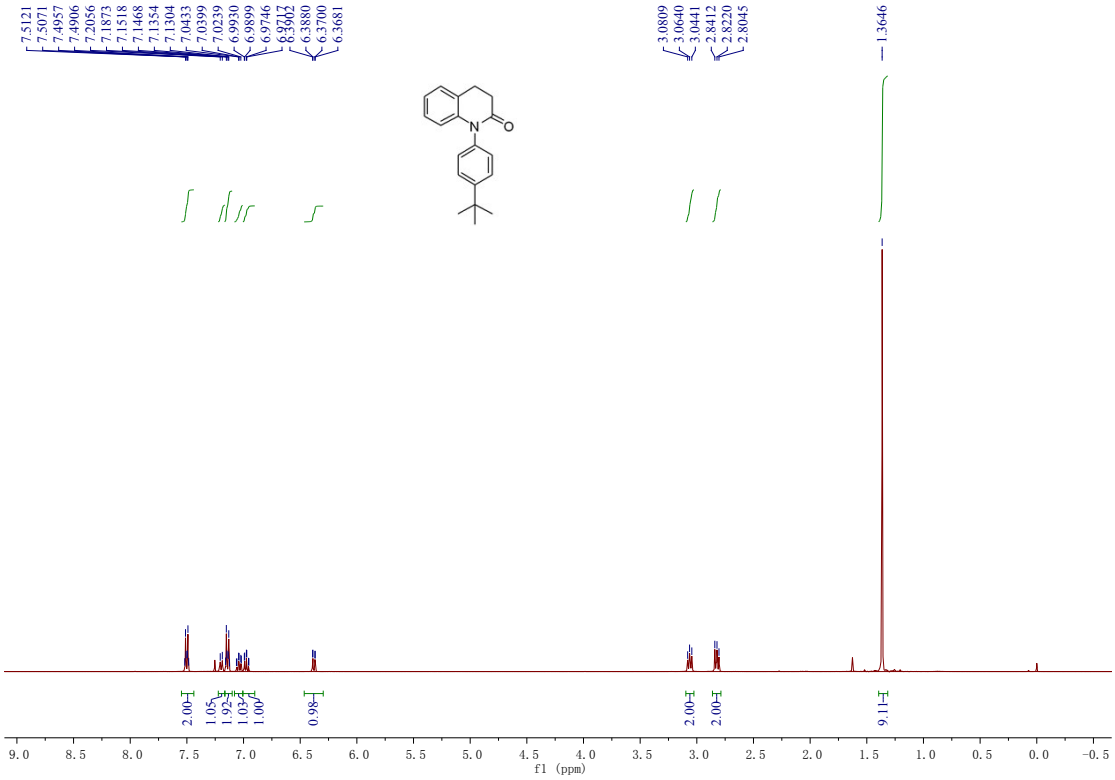
^{1}H NMR spectrum of compound **2e**



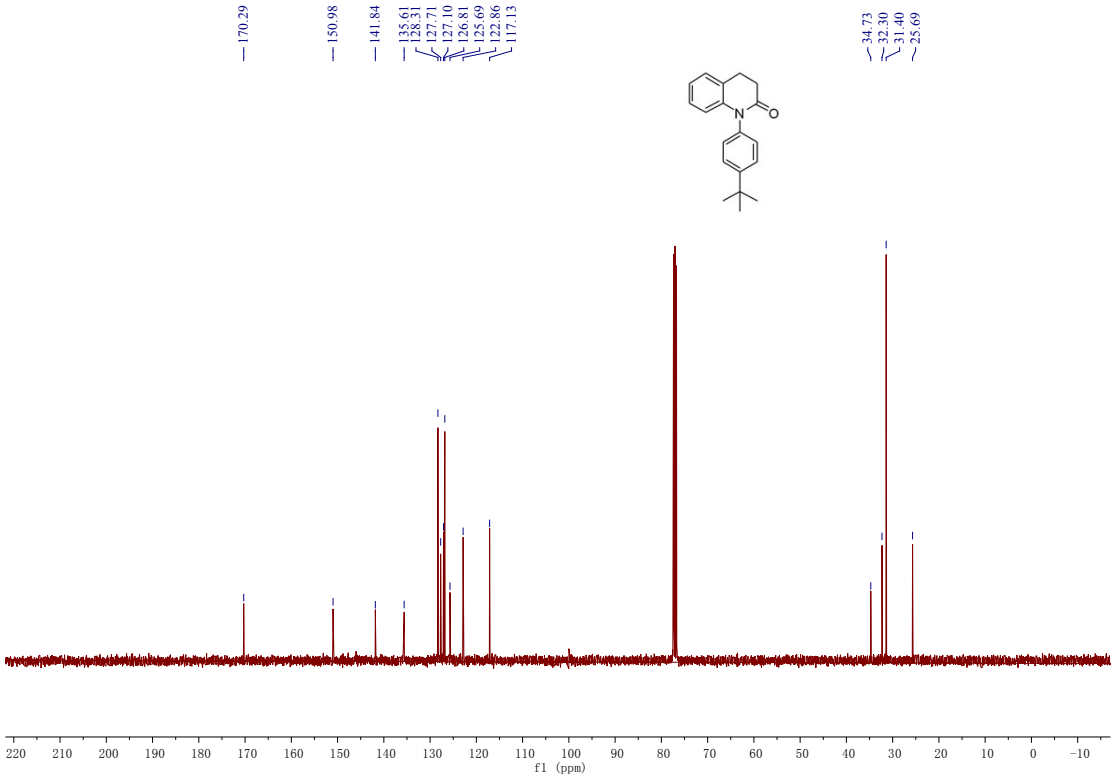
^{13}C NMR spectrum of compound **2e**



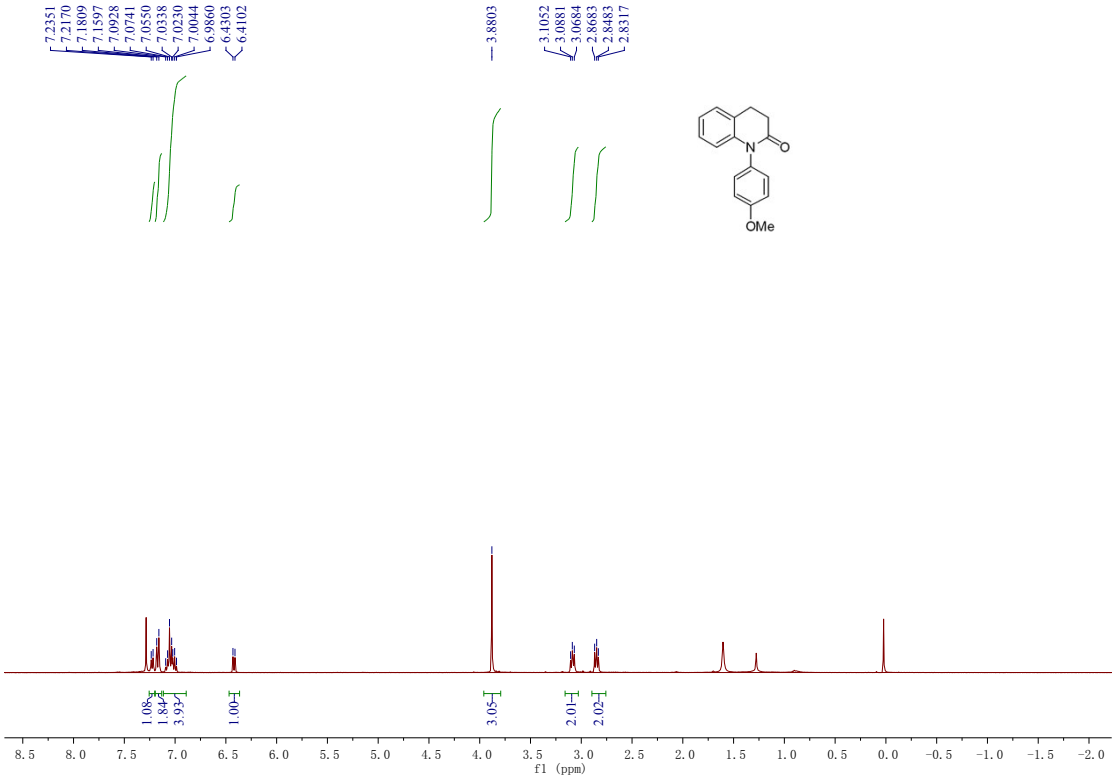
^{1}H NMR spectrum of compound **2f**



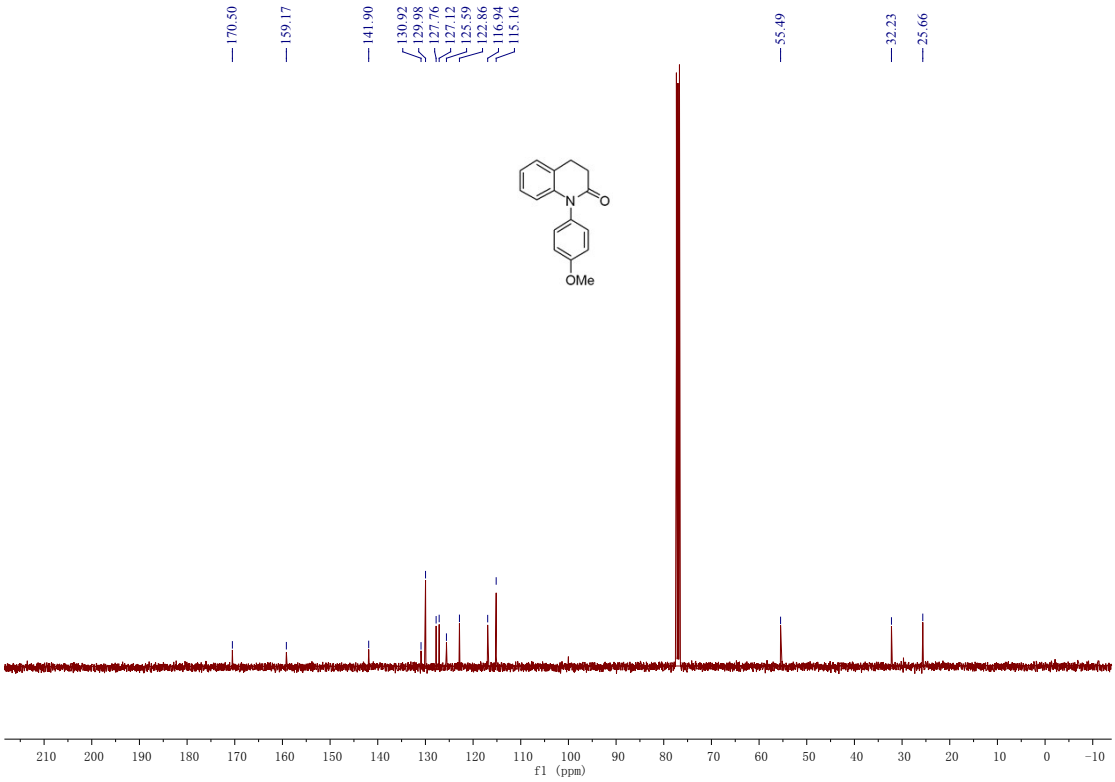
^{13}C NMR spectrum of compound **2f**



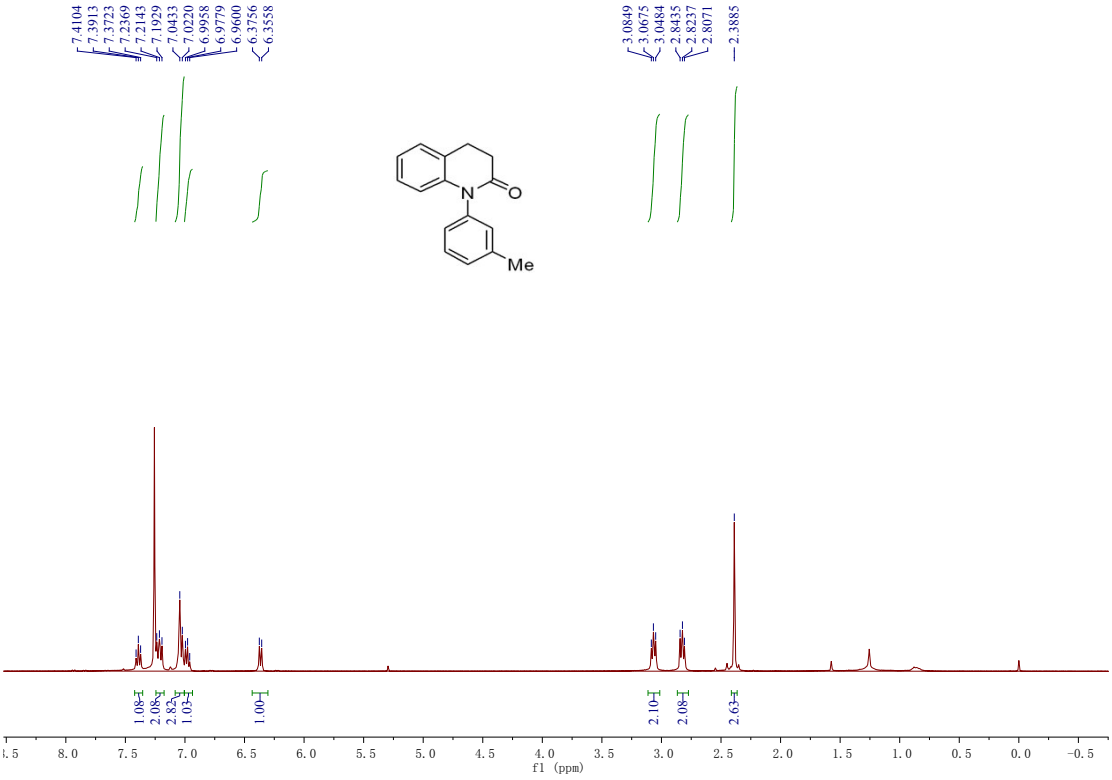
^{1}H NMR spectrum of compound **2g**



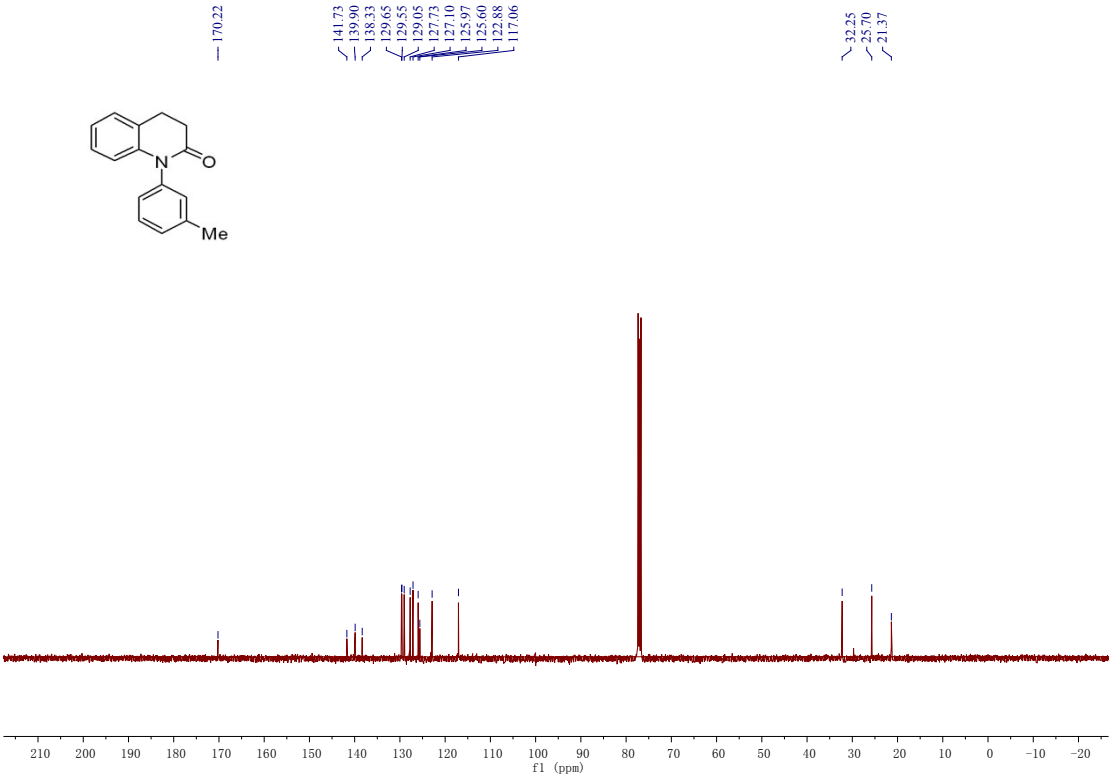
^{13}C NMR spectrum of compound **2f**



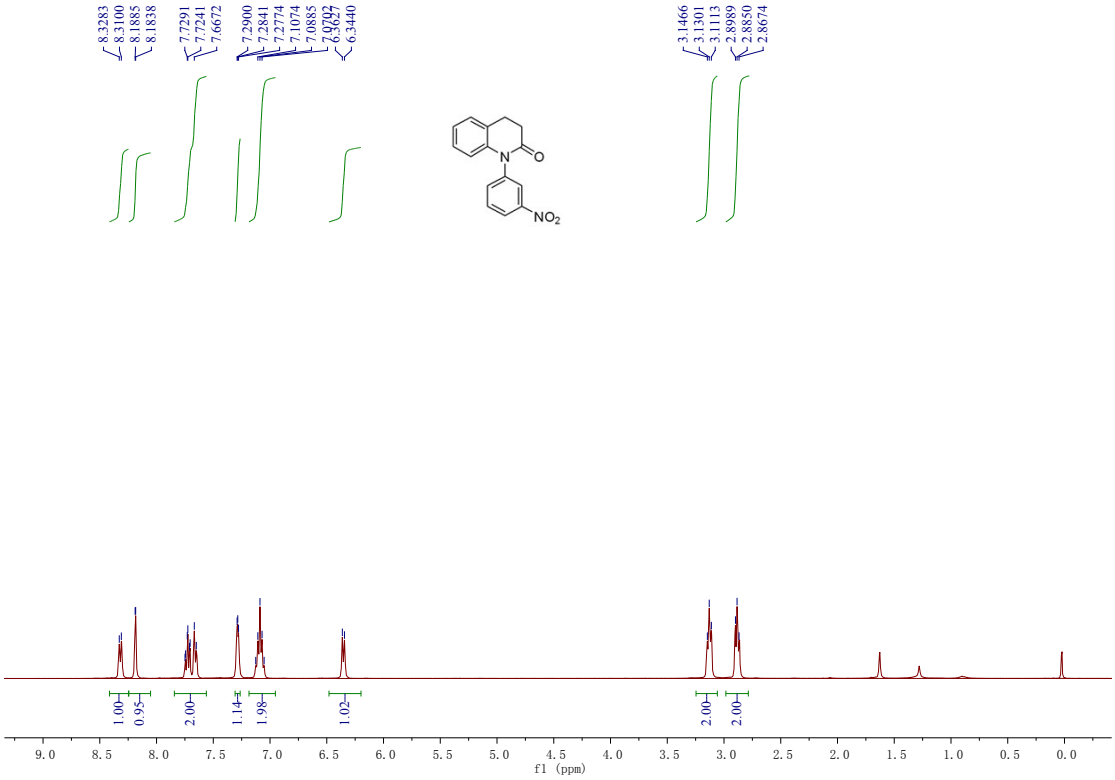
^{1}H NMR spectrum of compound **2j**



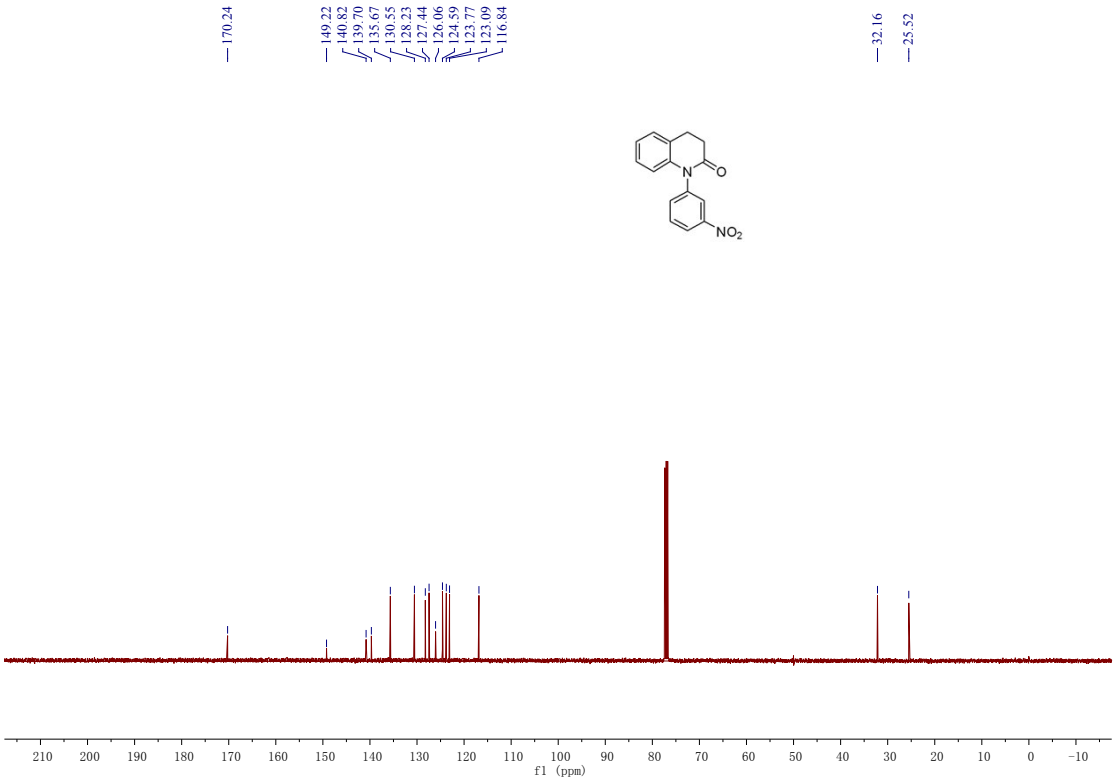
^{13}C NMR spectrum of compound **2j**



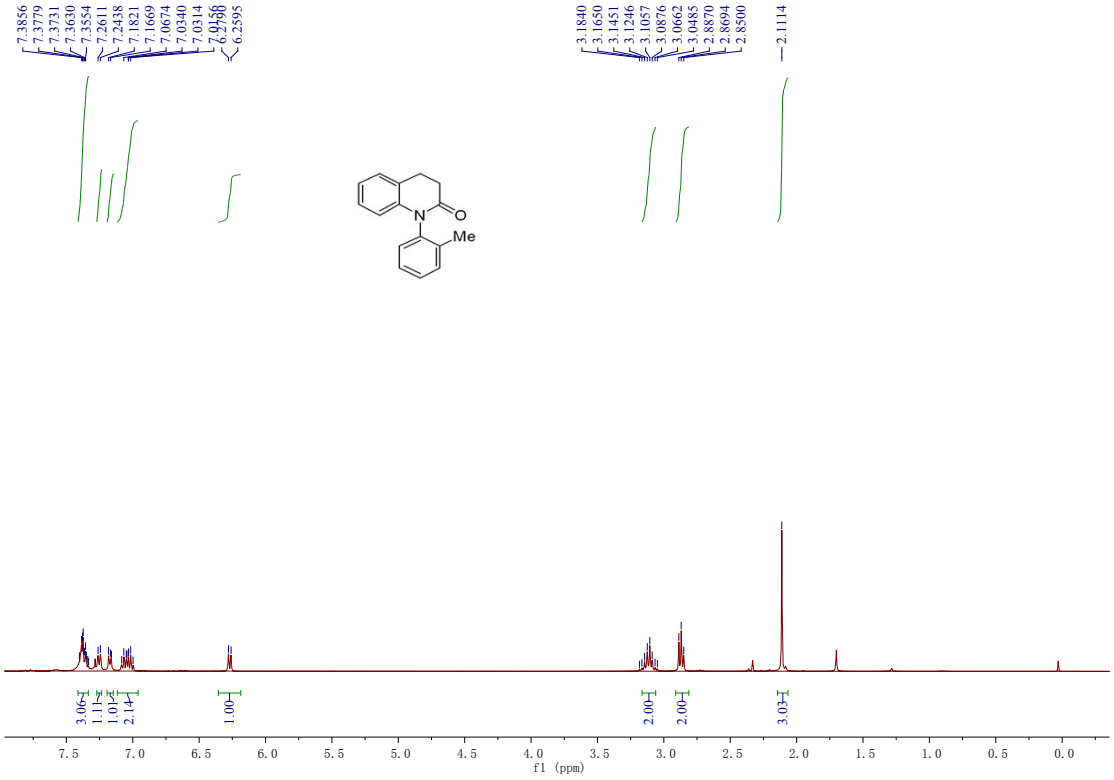
^{1}H NMR spectrum of compound **2g**



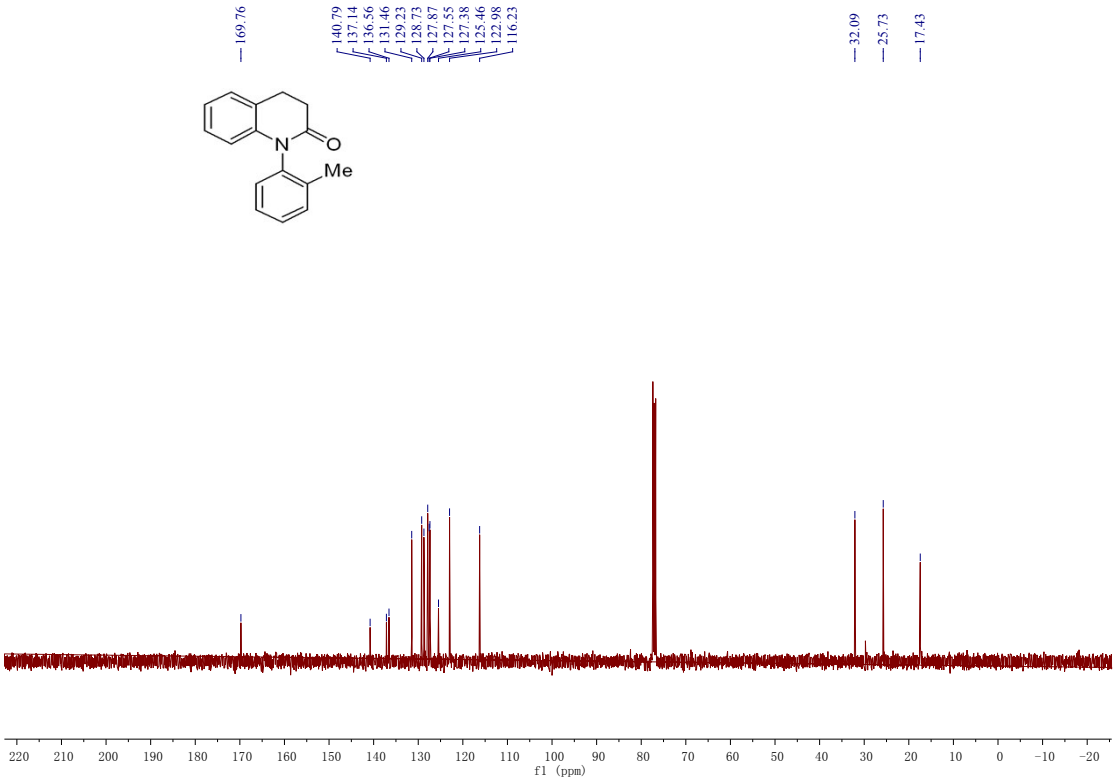
^{13}C NMR spectrum of compound **2g**



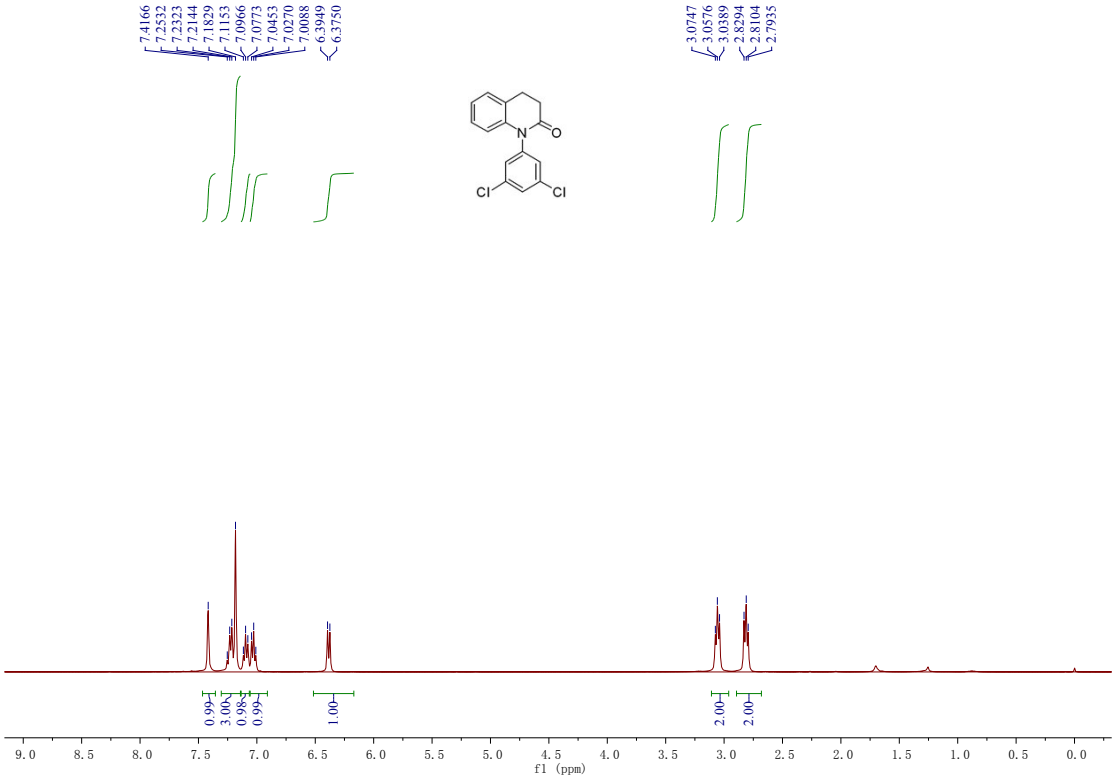
^{1}H NMR spectrum of compound **2j**



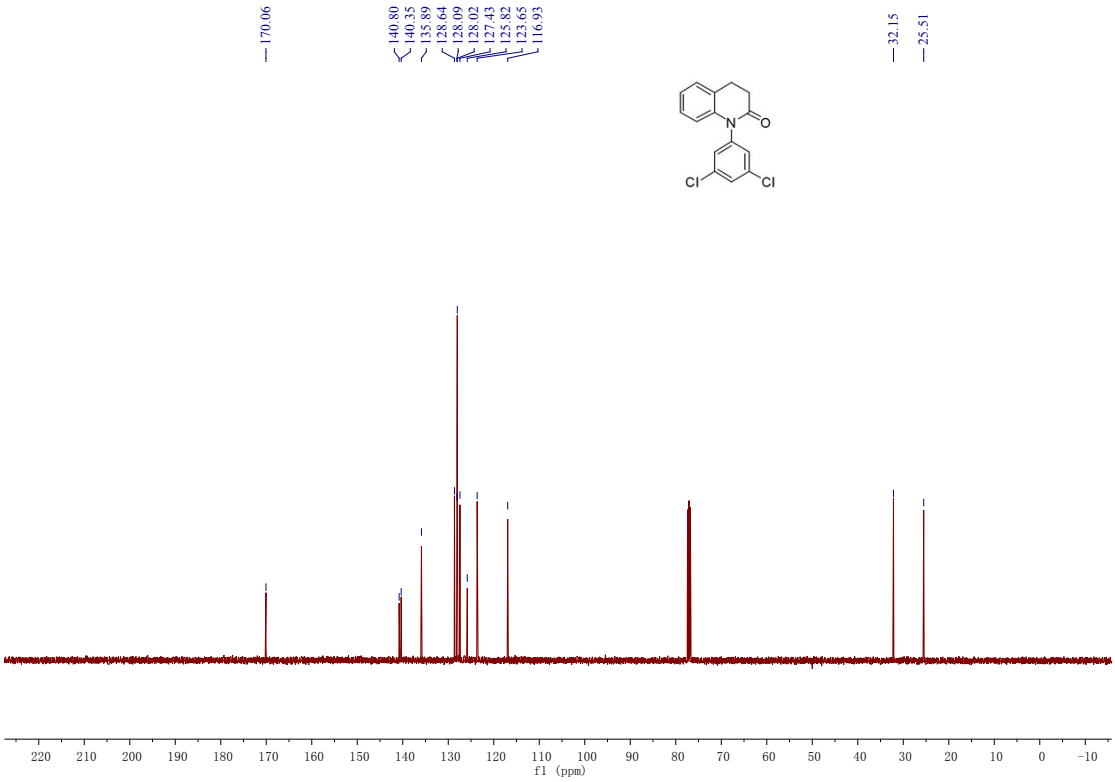
^{13}C NMR spectrum of compound **2j**



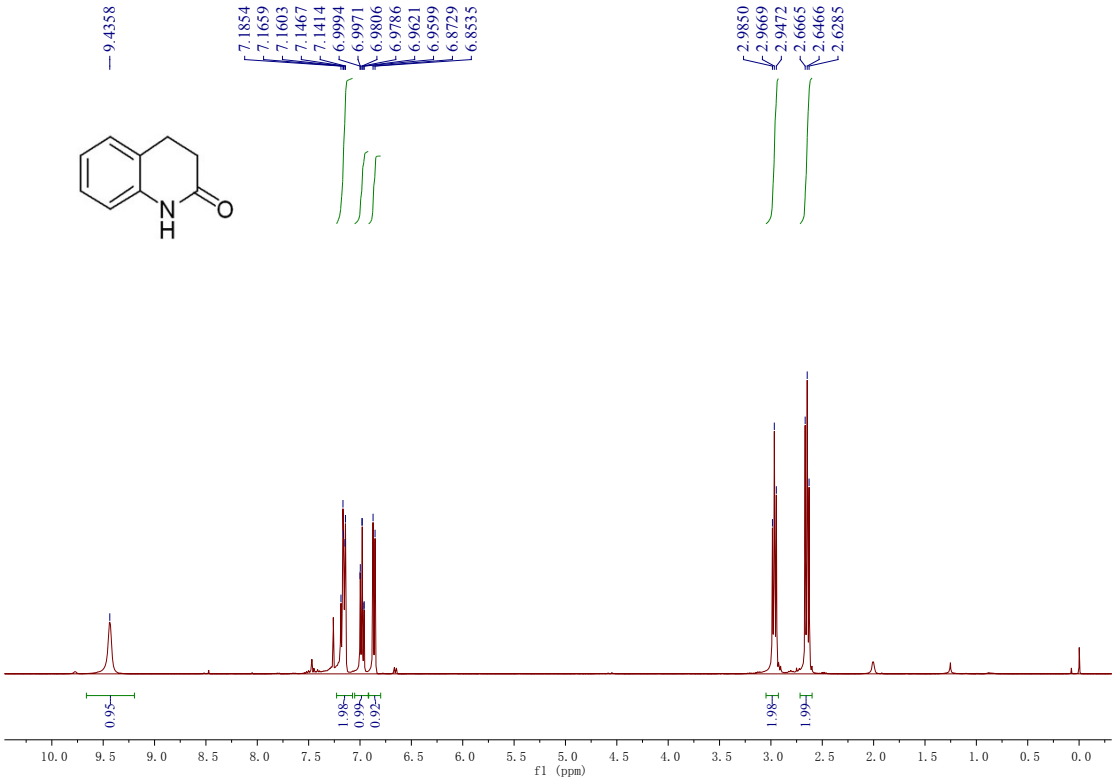
^{1}H NMR spectrum of compound **2k**



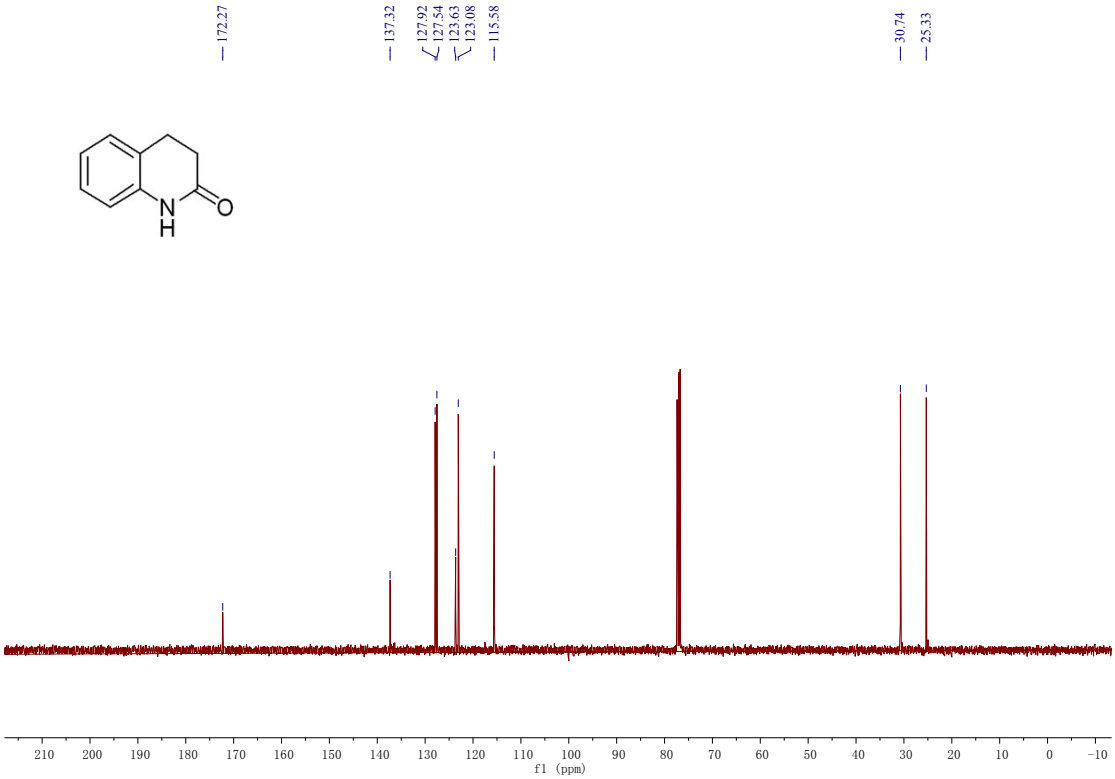
^{13}C NMR spectrum of compound **2h**



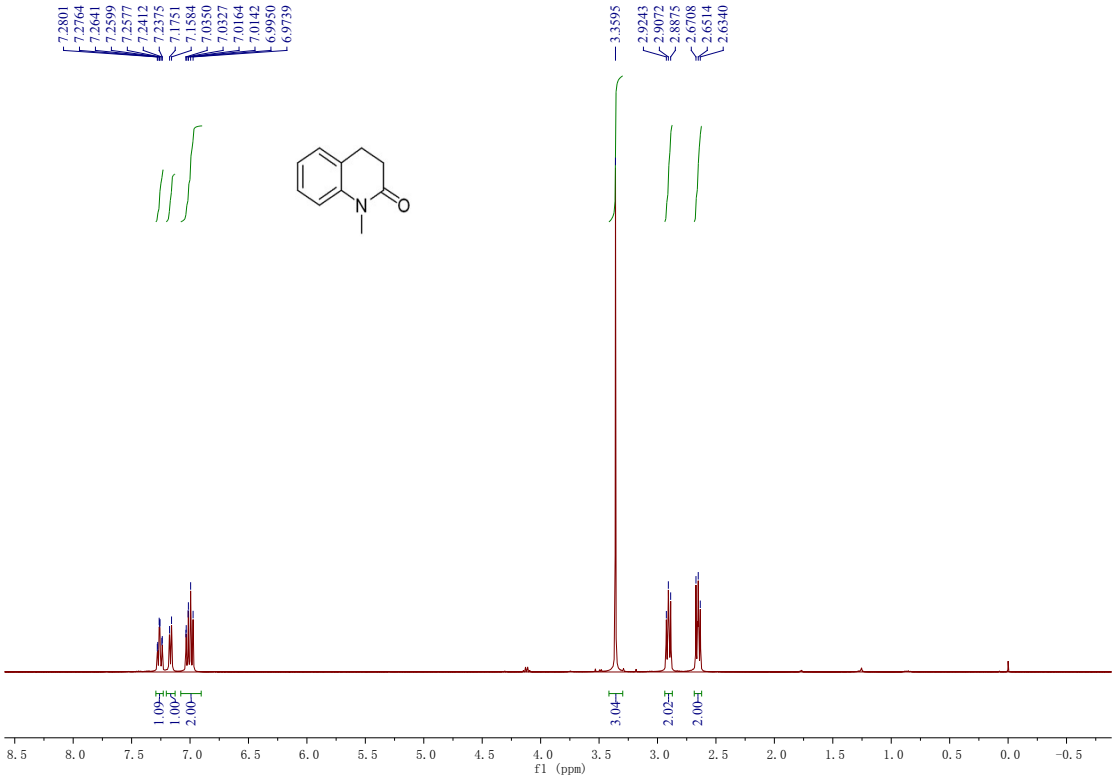
^{1}H NMR spectrum of compound **2l**



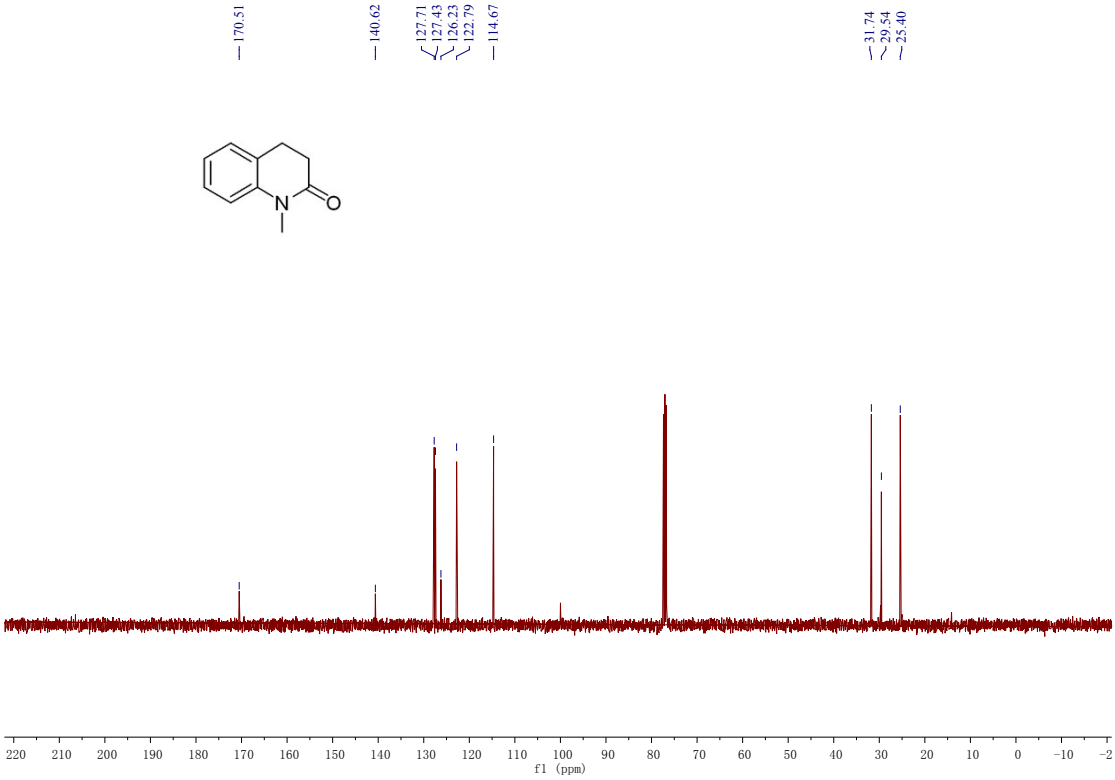
^{13}C NMR spectrum of compound **2l**



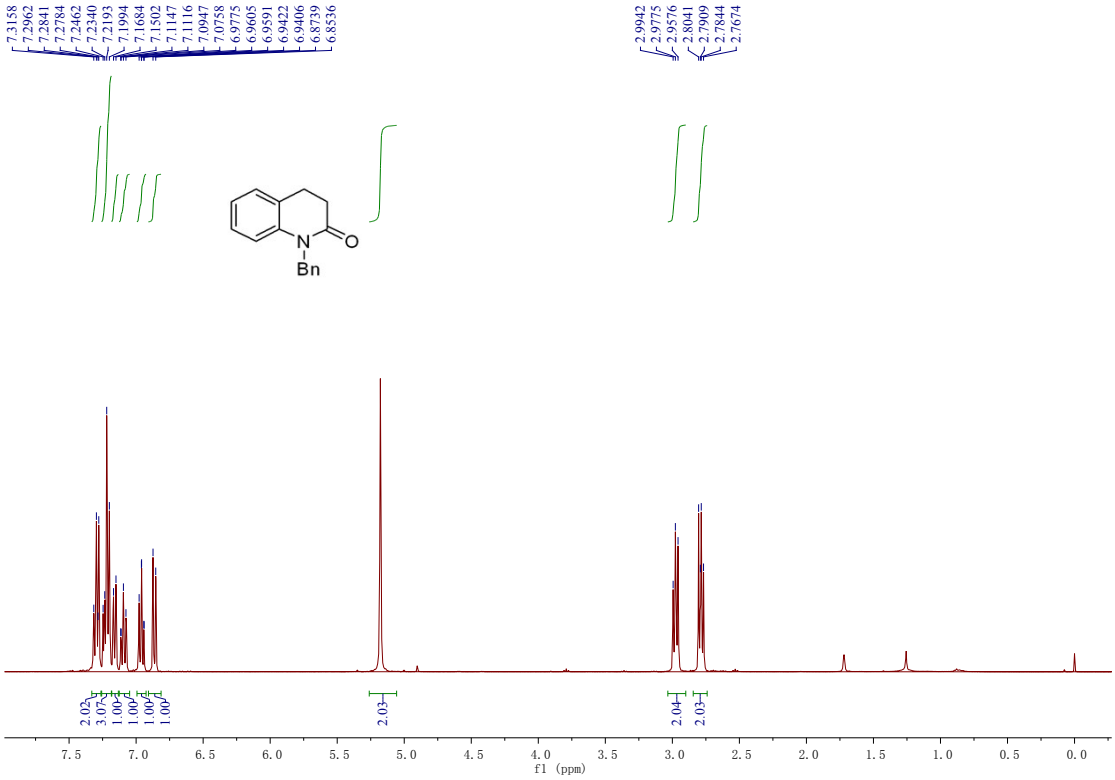
^{1}H NMR spectrum of compound **2m**



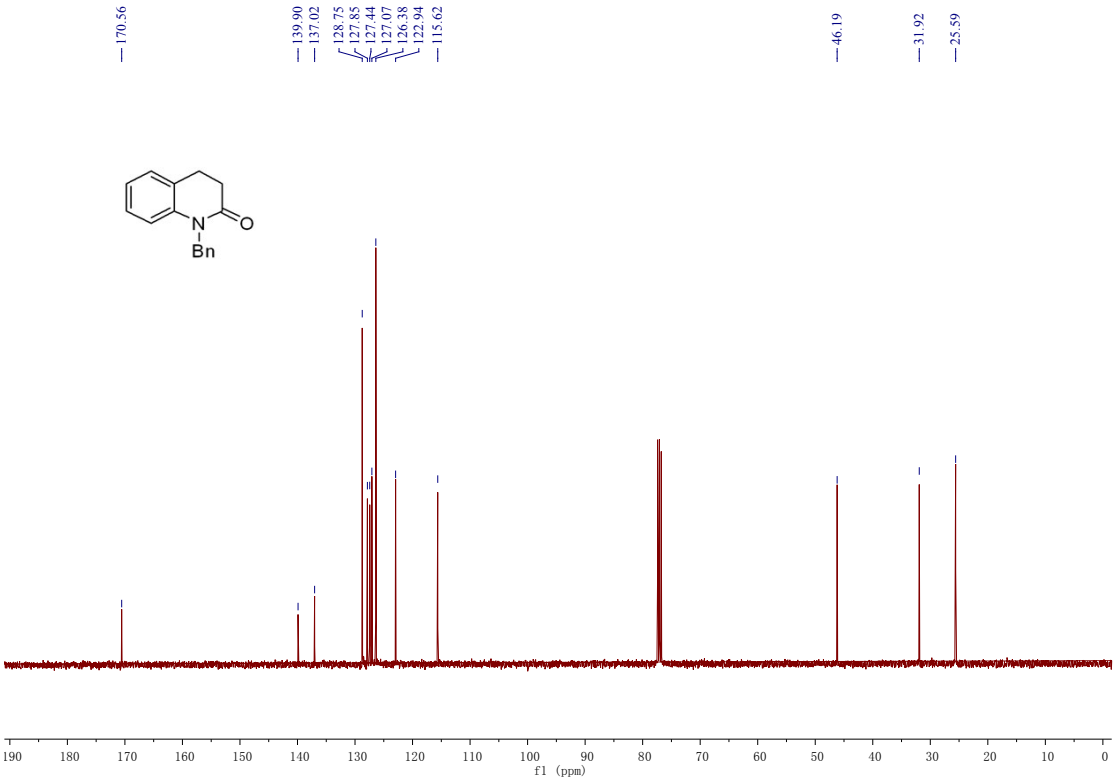
^{13}C NMR spectrum of compound **2m**



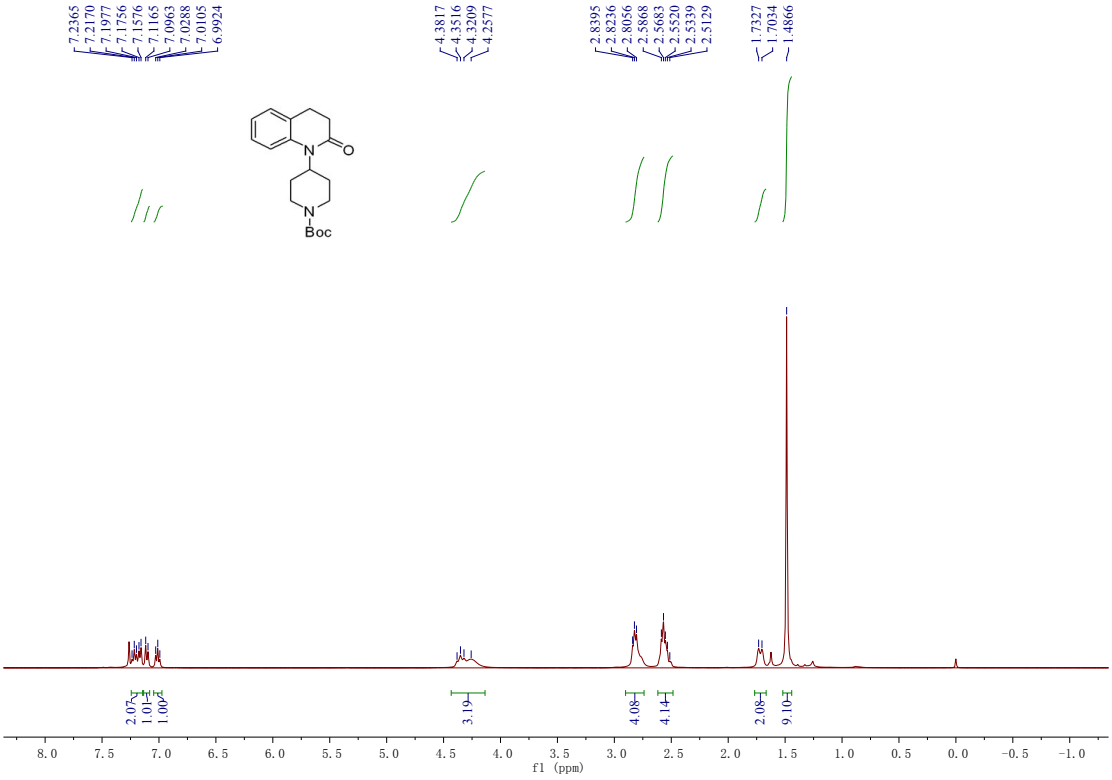
^{1}H NMR spectrum of compound **2n**



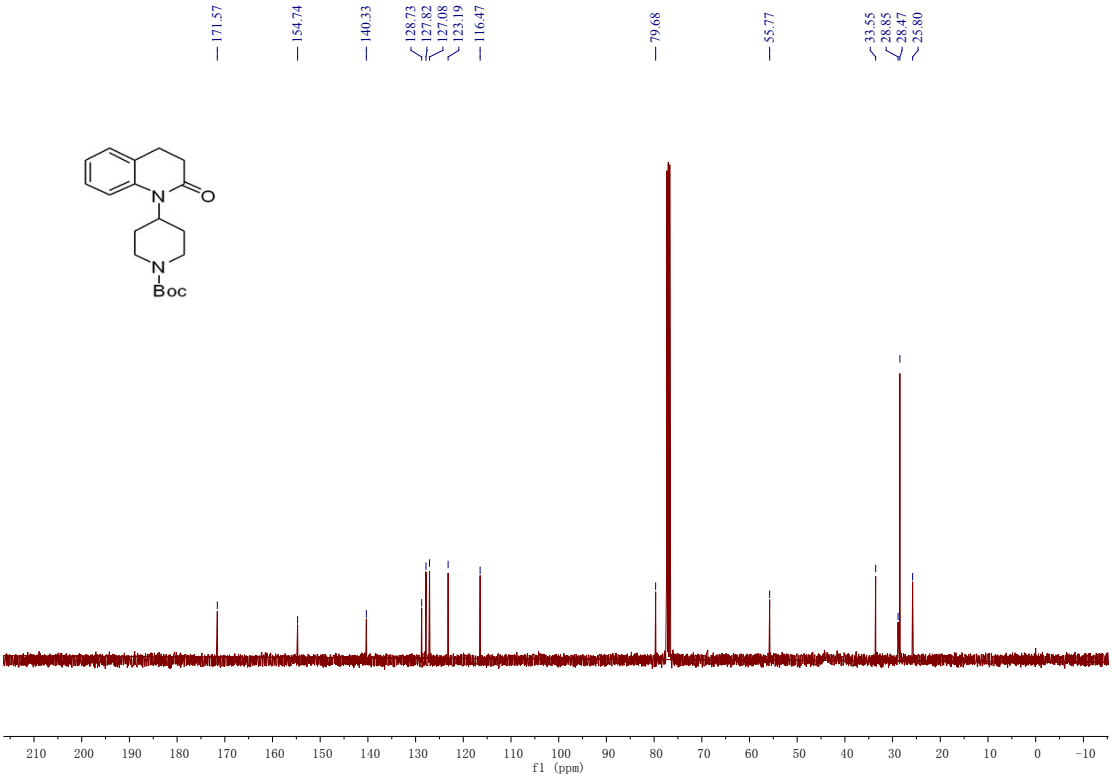
^{13}C NMR spectrum of compound **2n**



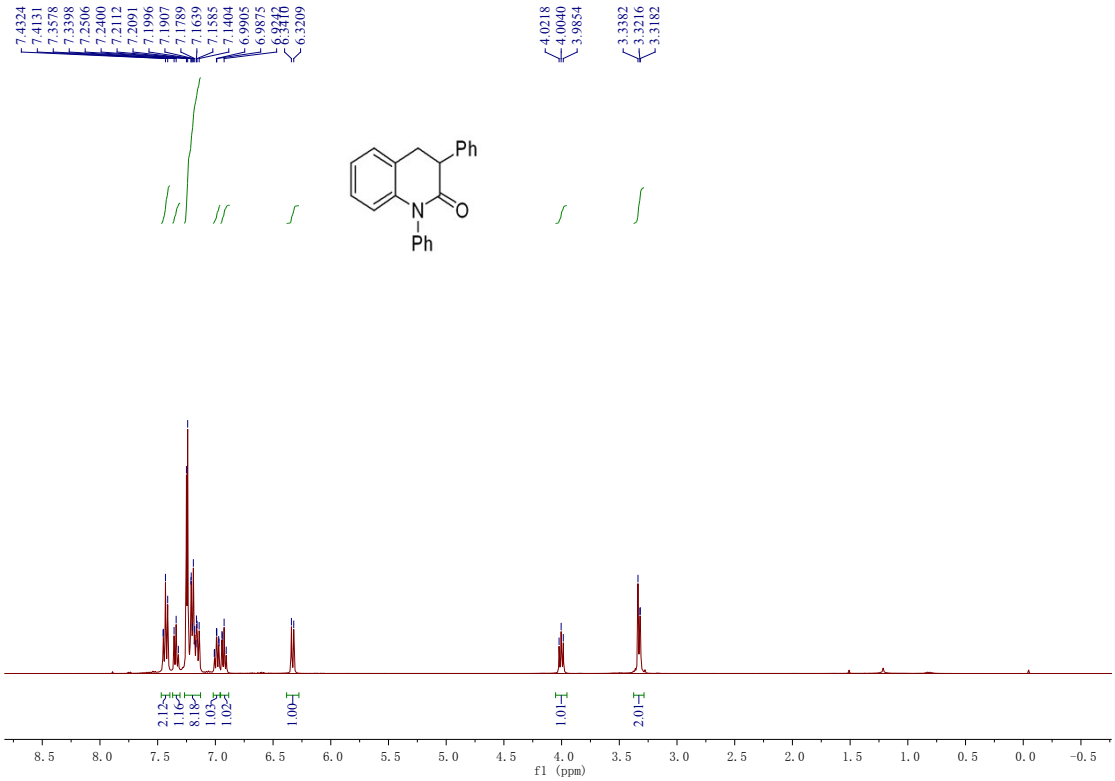
^{1}H NMR spectrum of compound **2o**



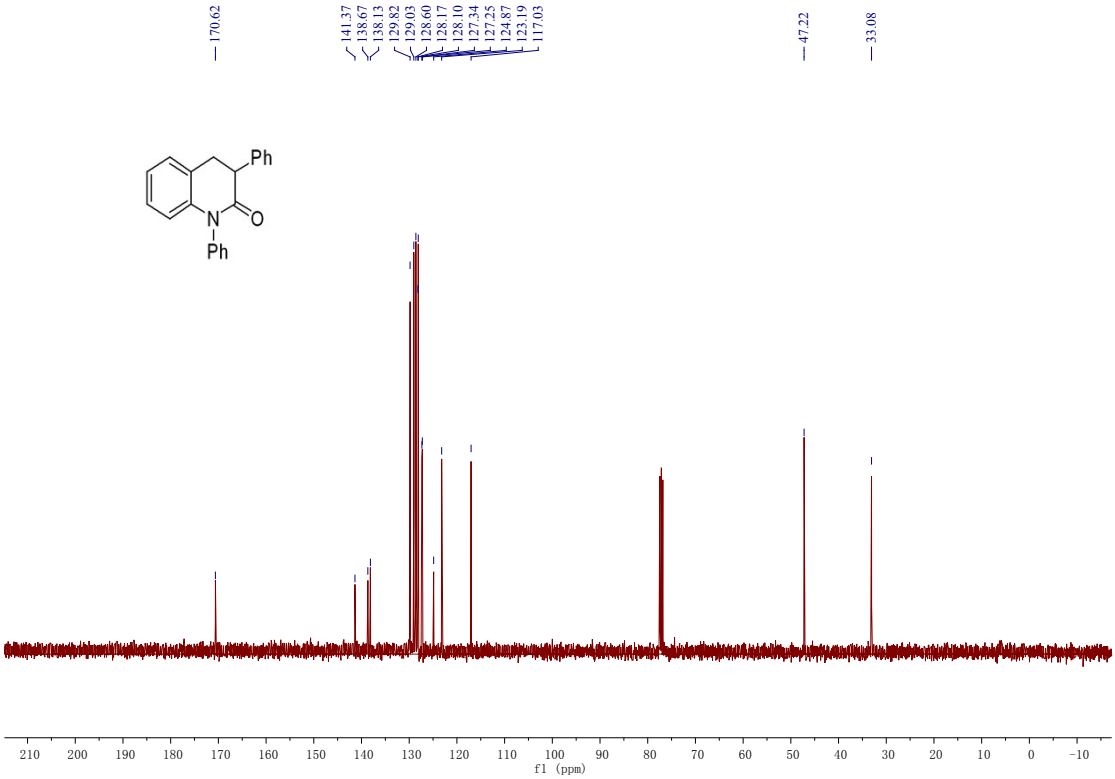
^{13}C NMR spectrum of compound **2o**



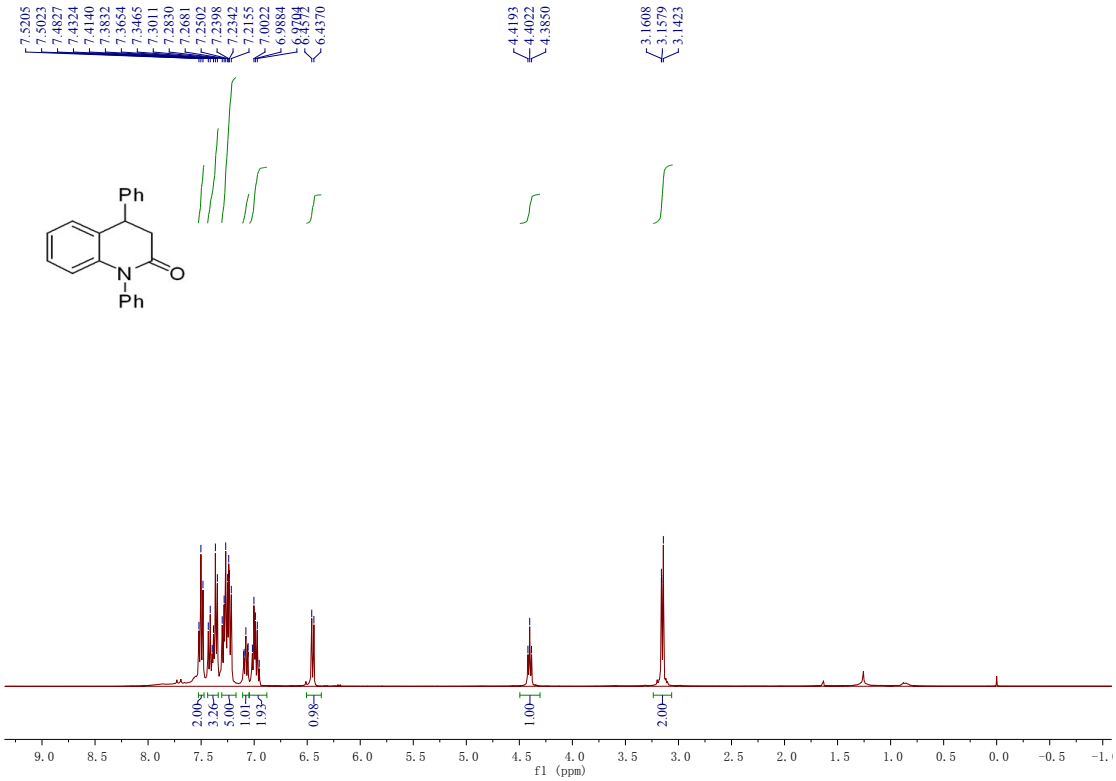
^{1}H NMR spectrum of compound **2p**



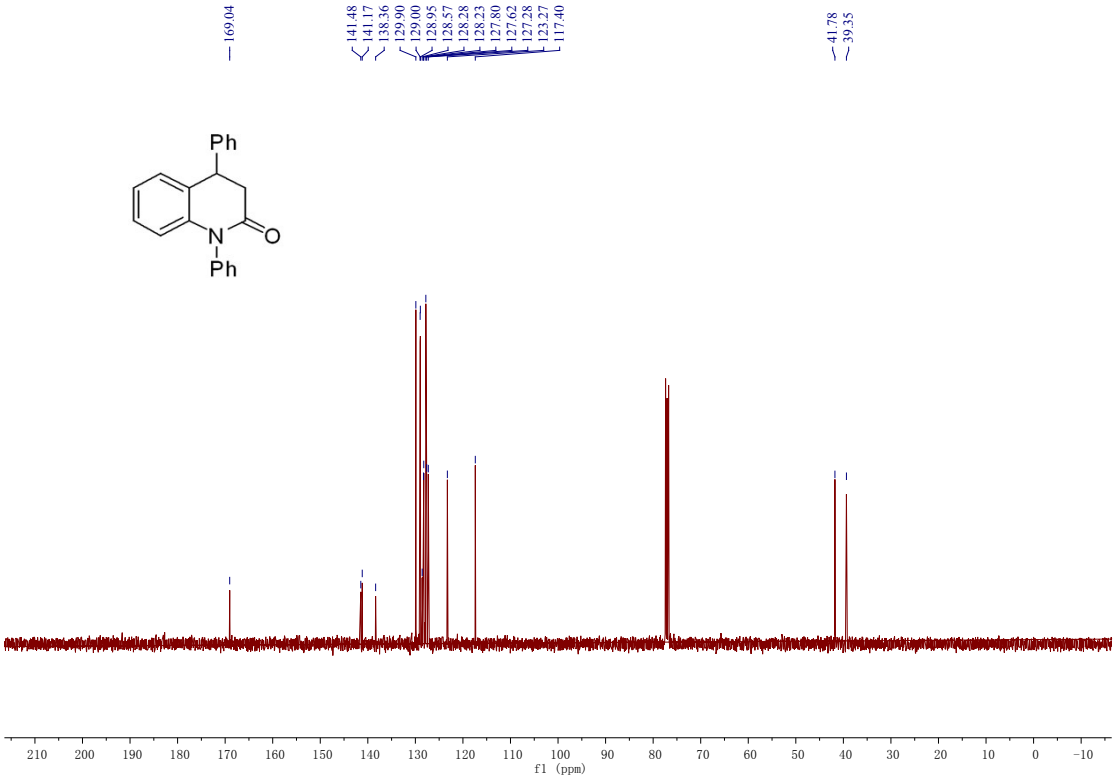
^{13}C NMR spectrum of compound **2p**



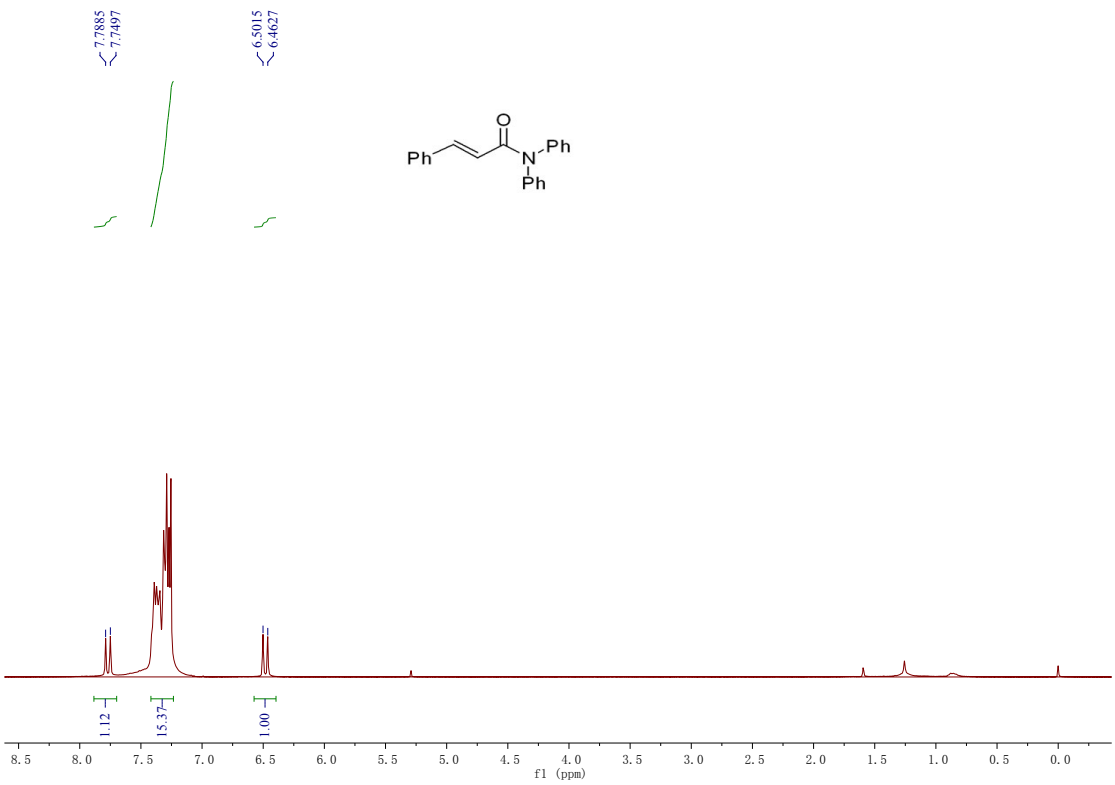
^{1}H NMR spectrum of compound **2q**



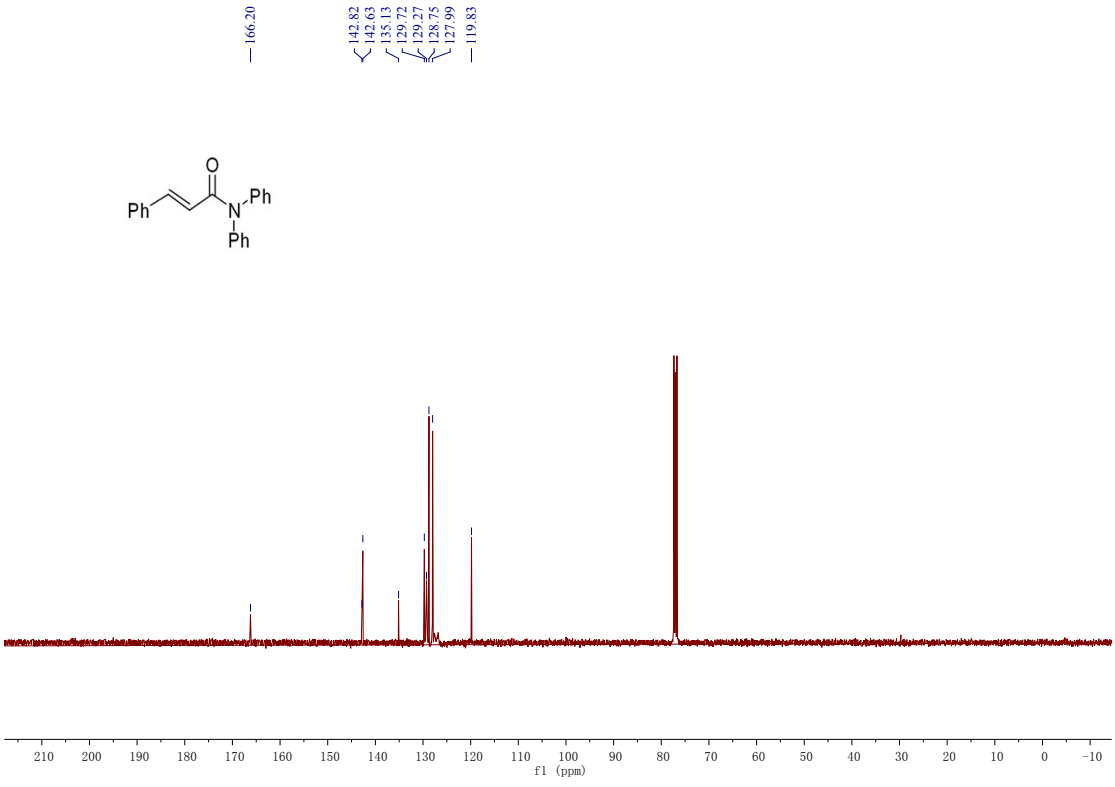
^{13}C NMR spectrum of compound **2q**



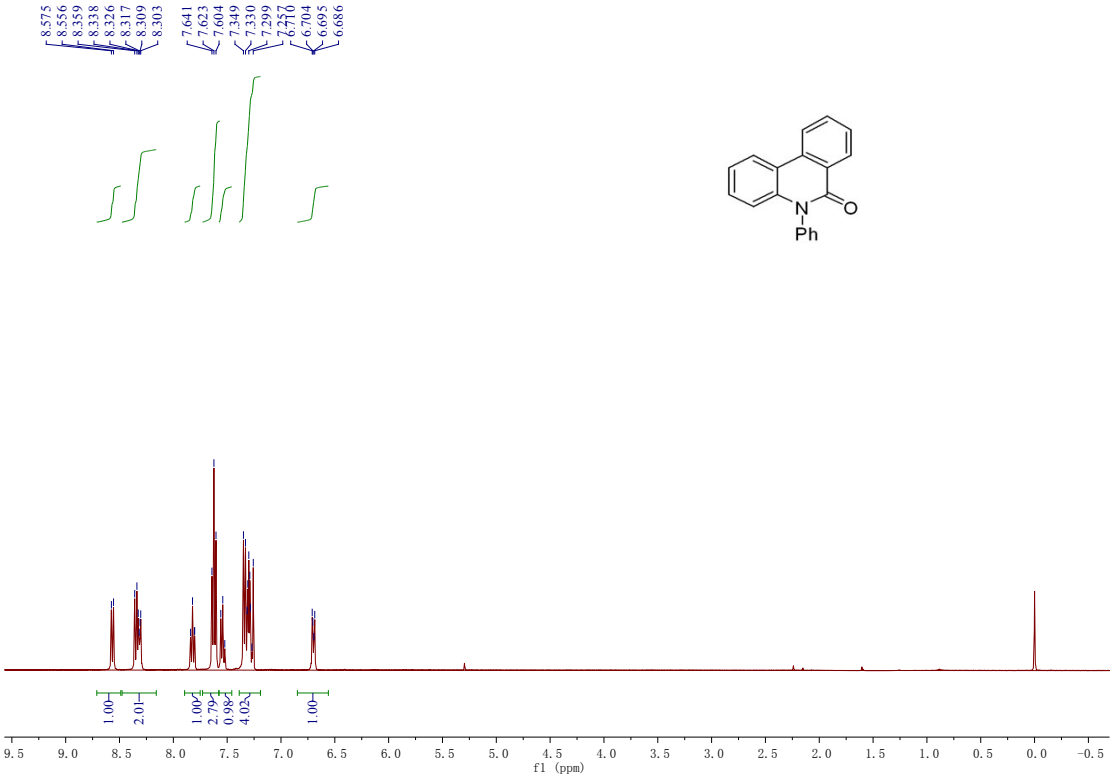
^{1}H NMR spectrum of compound **2q'**



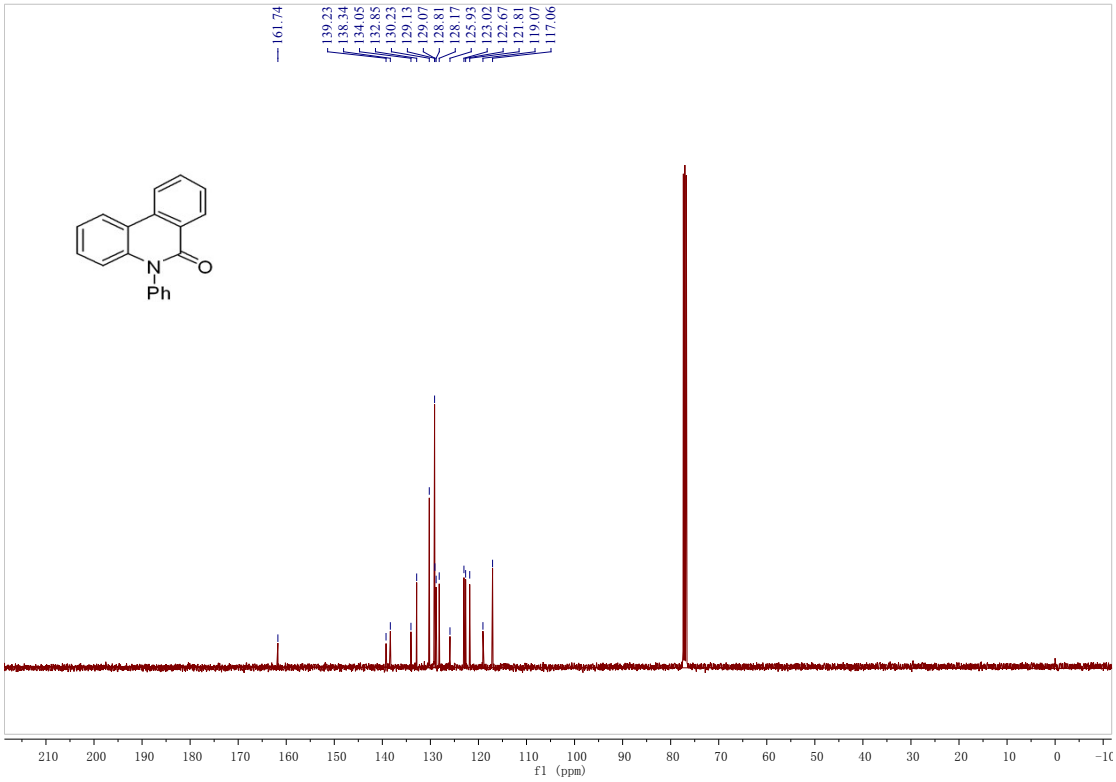
^{13}C NMR spectrum of compound **2q'**



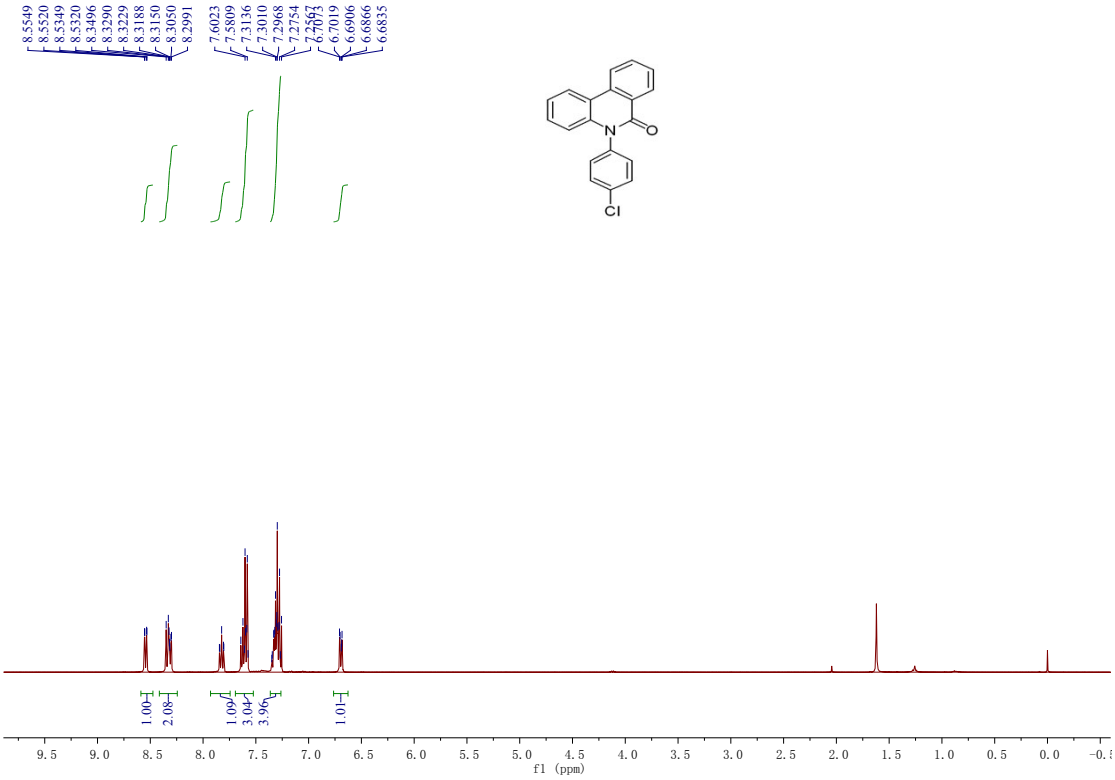
^{1}H NMR spectrum of compound **2r**



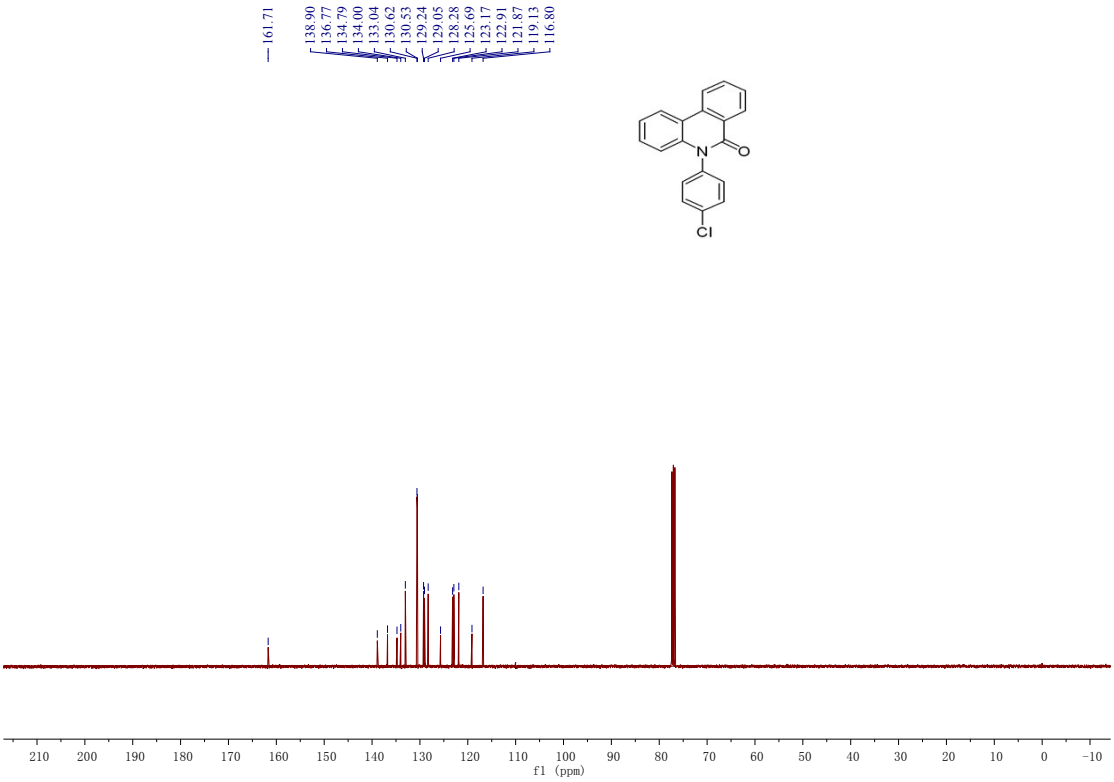
^{13}C NMR spectrum of compound **2r**



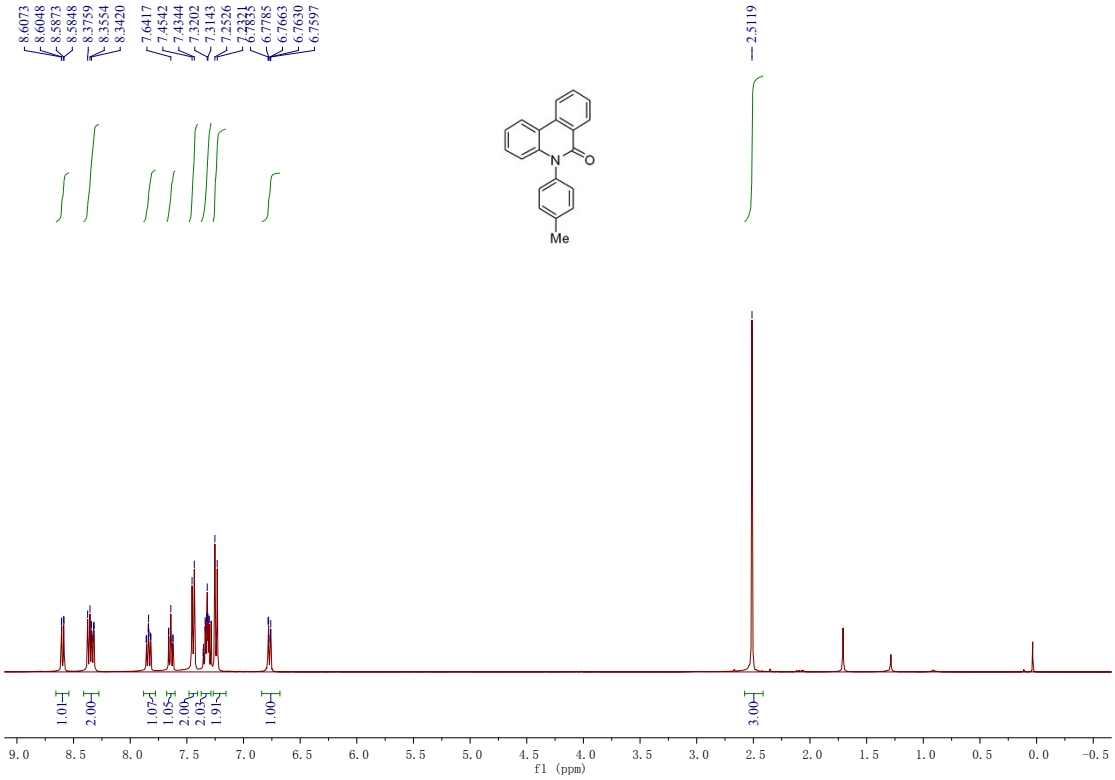
^{1}H NMR spectrum of compound **2s**



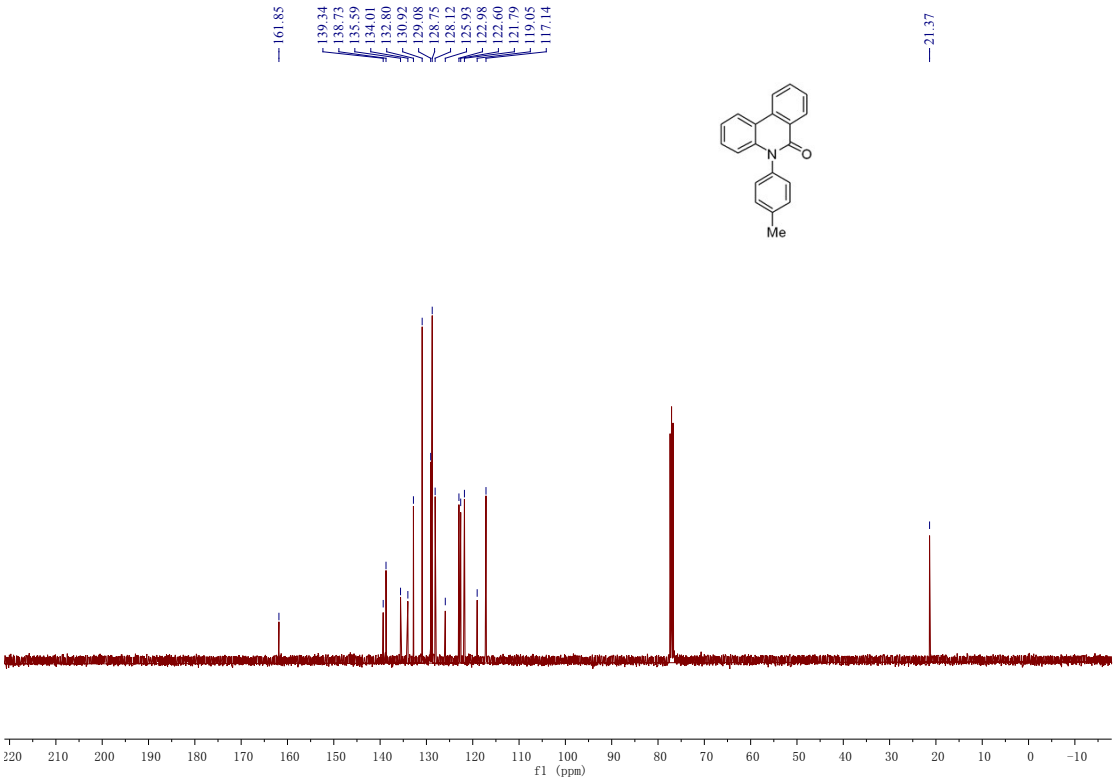
^{13}C NMR spectrum of compound **2s**



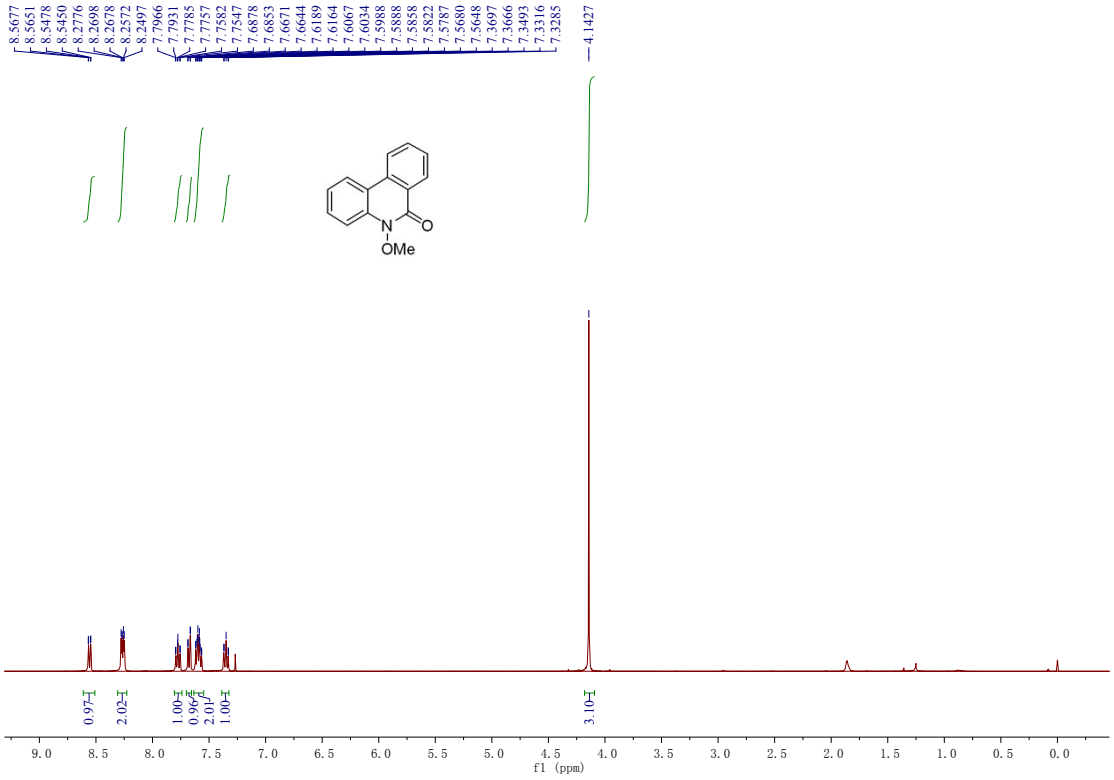
^{1}H NMR spectrum of compound **2t**



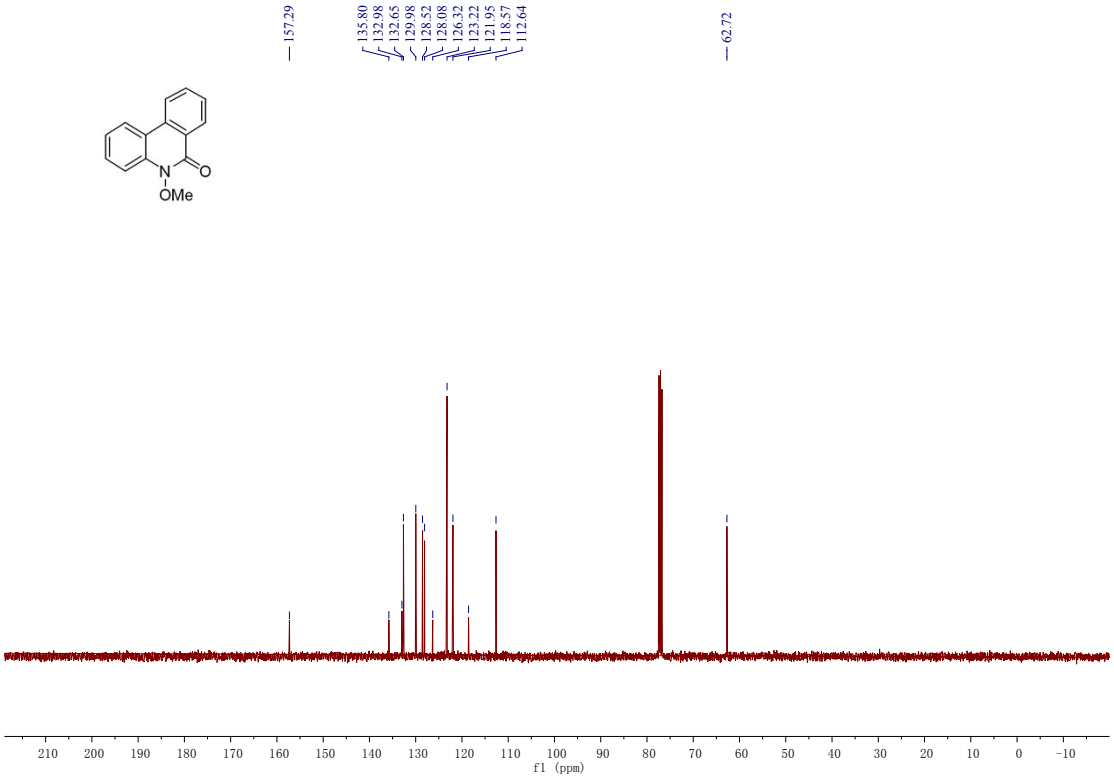
^{13}C NMR spectrum of compound **2t**



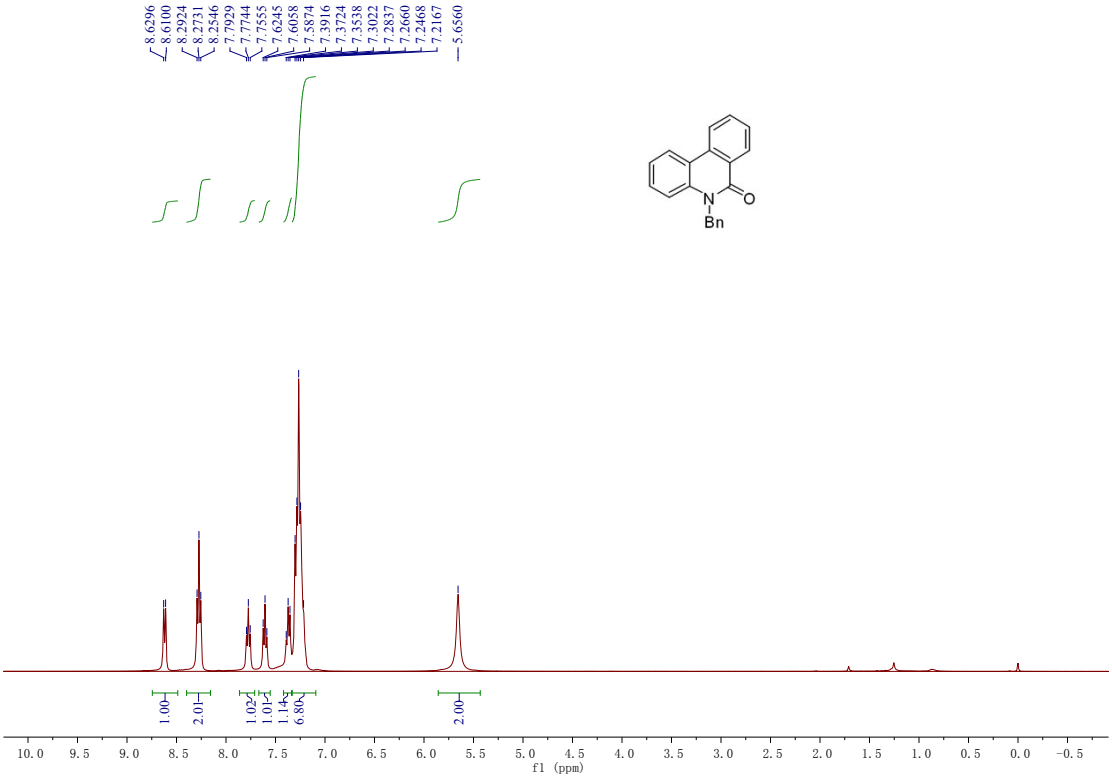
^{1}H NMR spectrum of compound **2u**



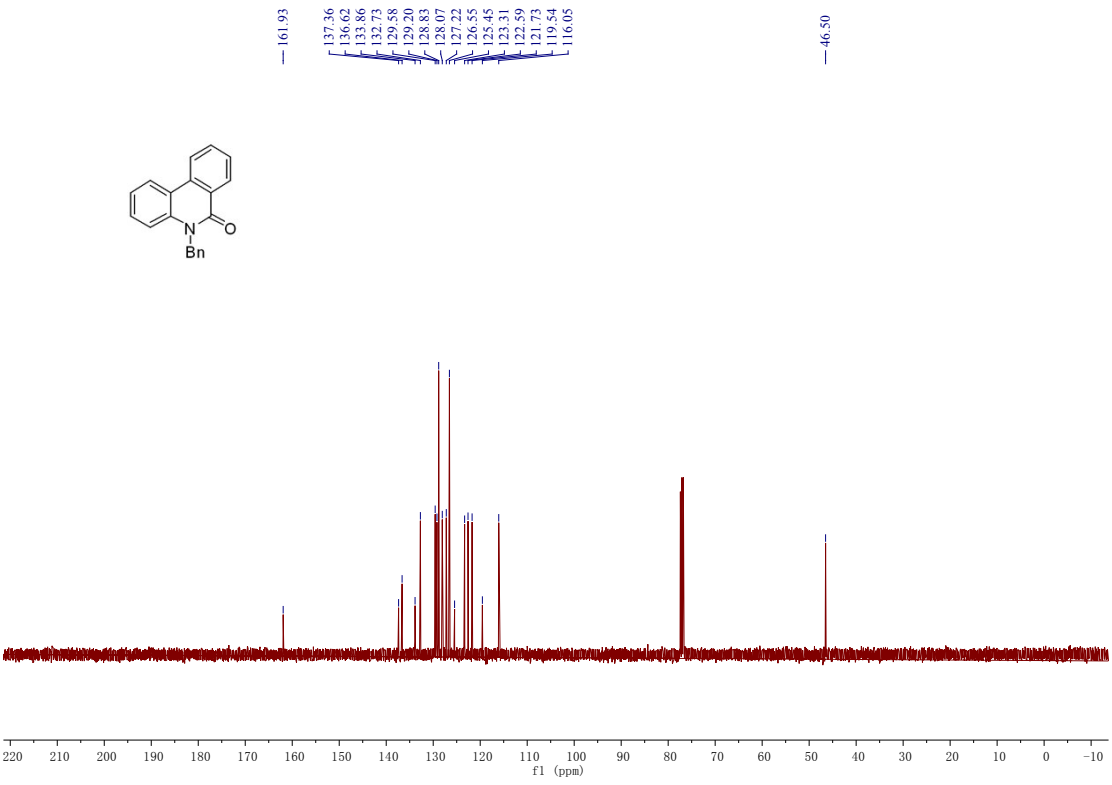
^{13}C NMR spectrum of compound **2u**



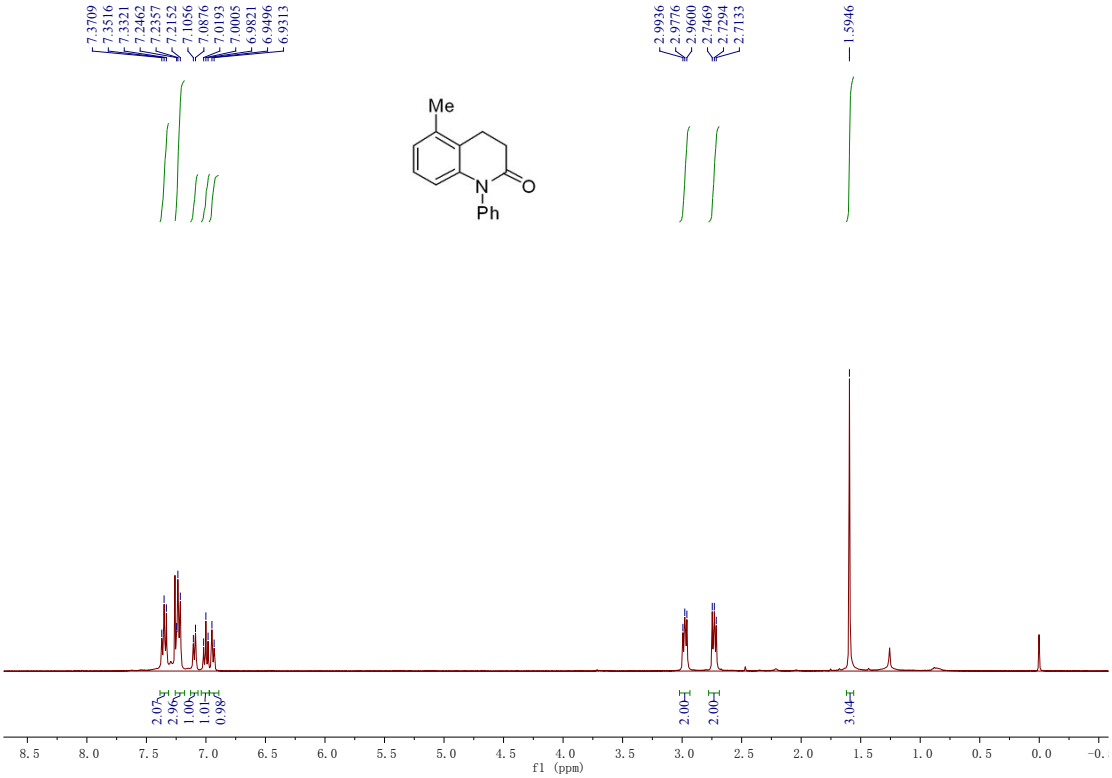
^{1}H NMR spectrum of compound **2v**



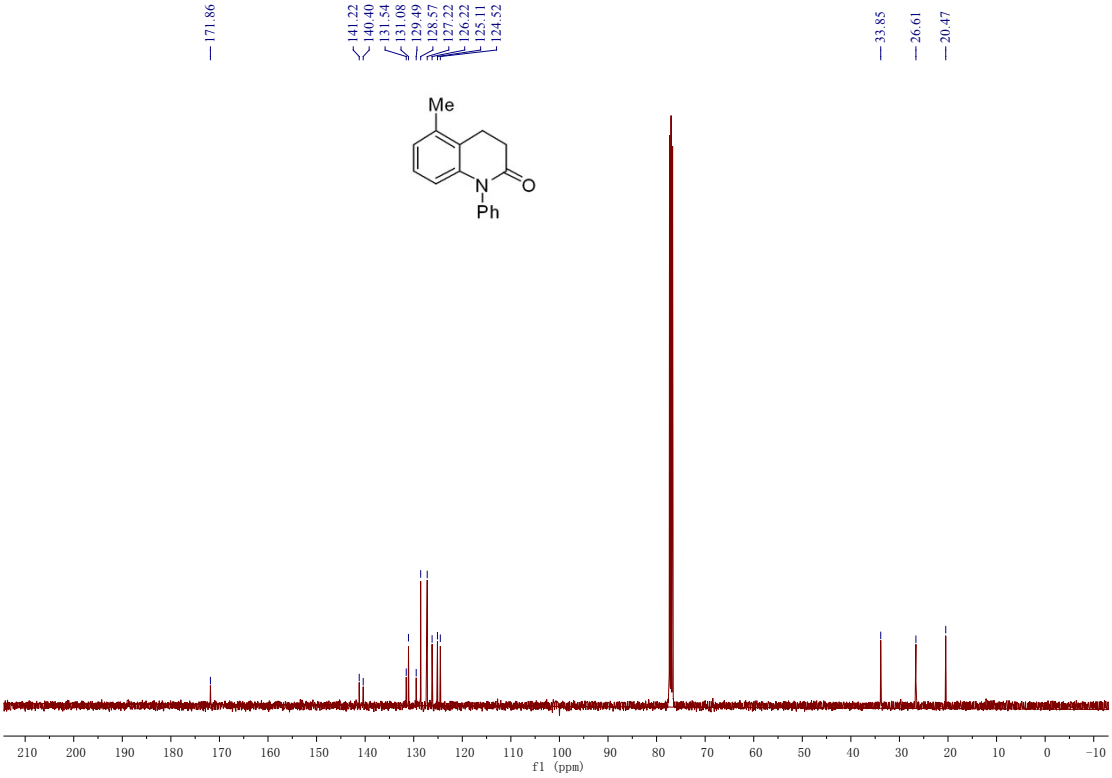
^{13}C NMR spectrum of compound **2v**



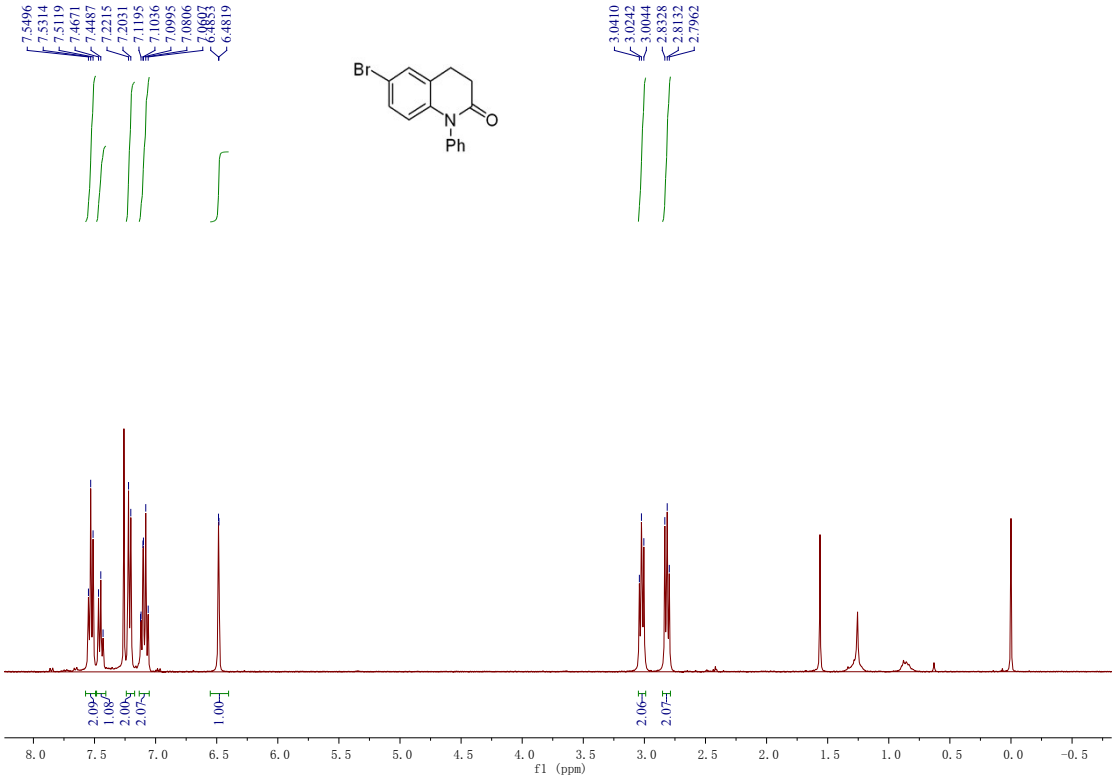
^{1}H NMR spectrum of compound **2w**



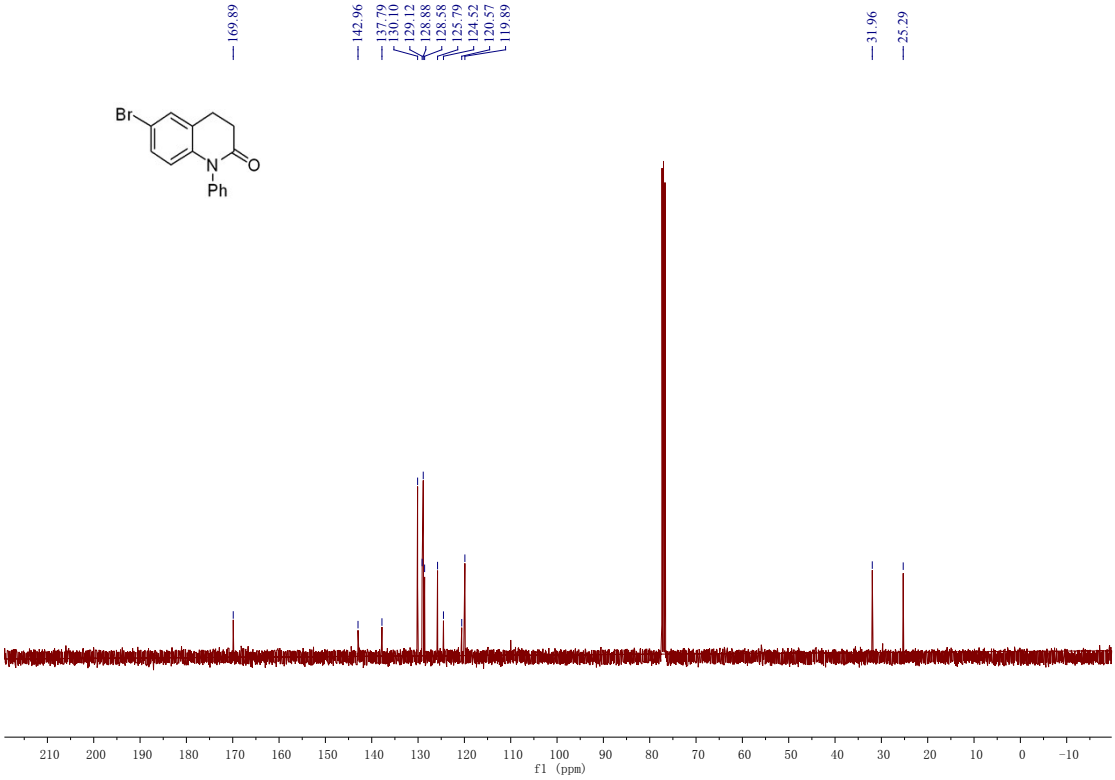
^{13}C NMR spectrum of compound **2w**



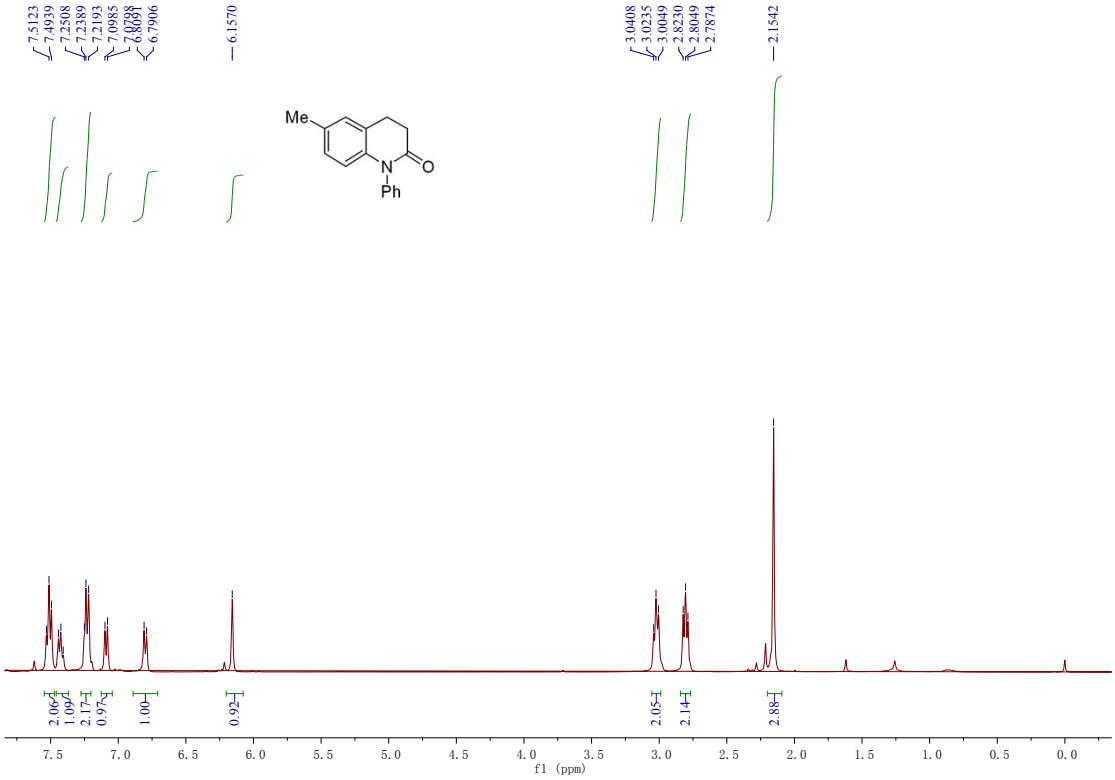
^{1}H NMR spectrum of compound **2x**



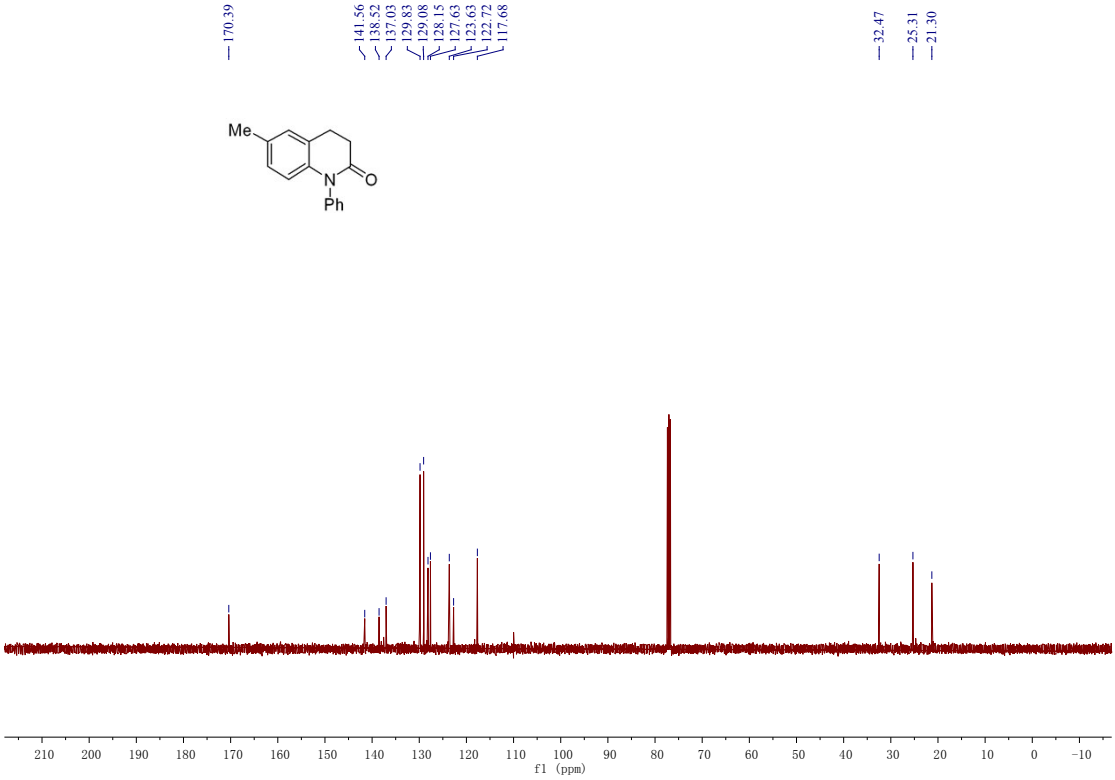
^{13}C NMR spectrum of compound **2x**



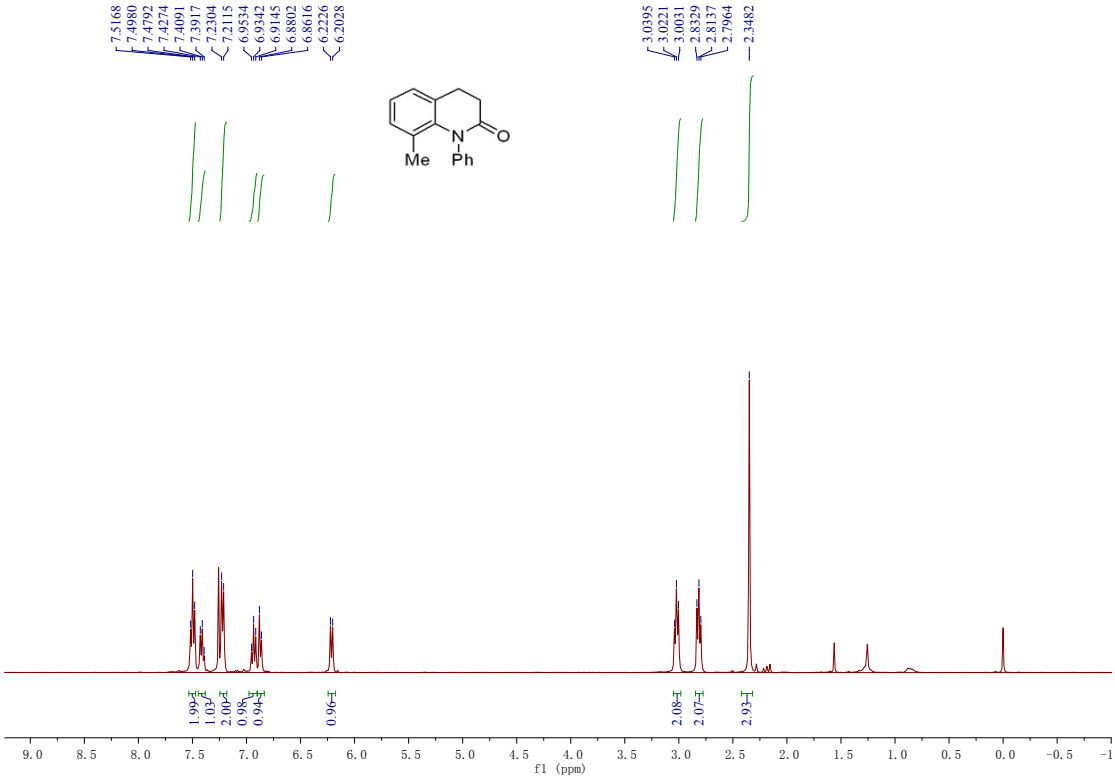
^{1}H NMR spectrum of compound **2y**



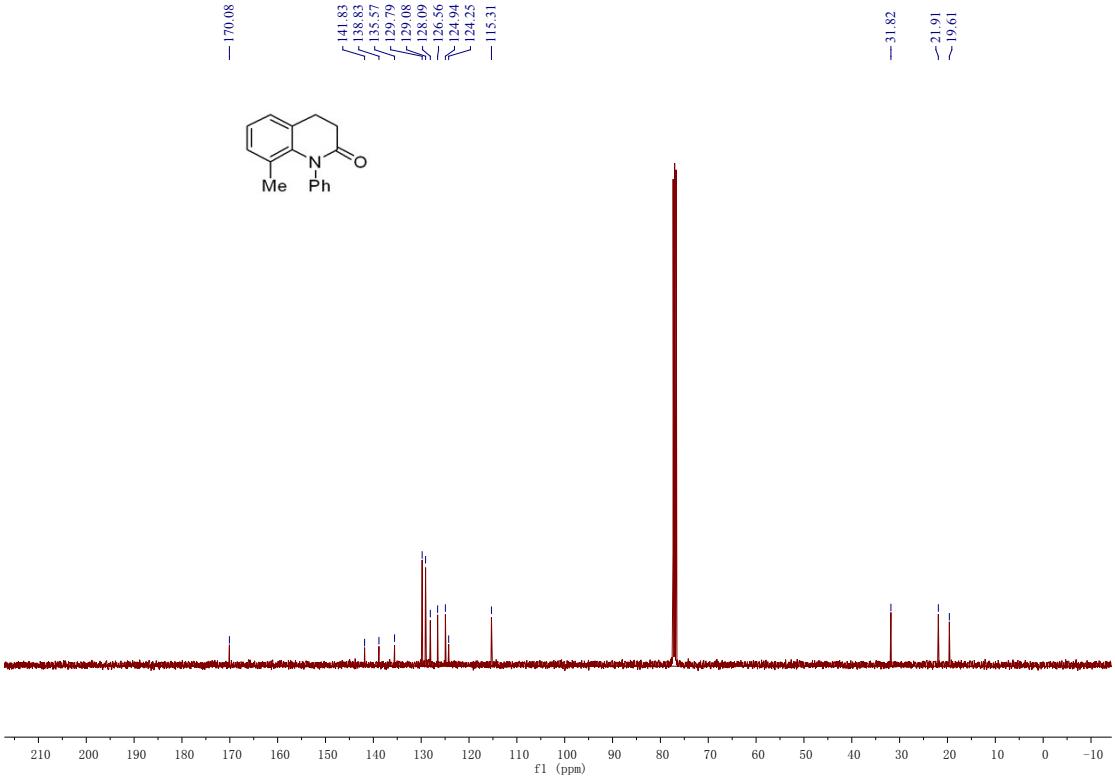
^{13}C NMR spectrum of compound **2y**



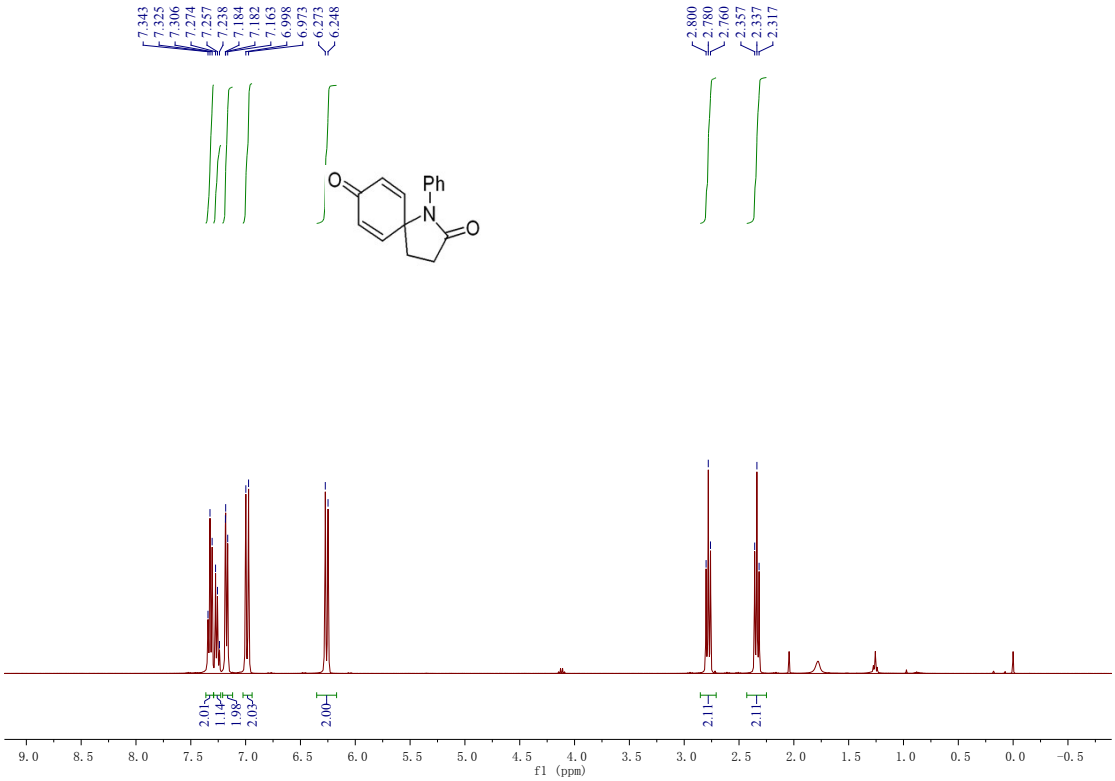
^{1}H NMR spectrum of compound **2y'**



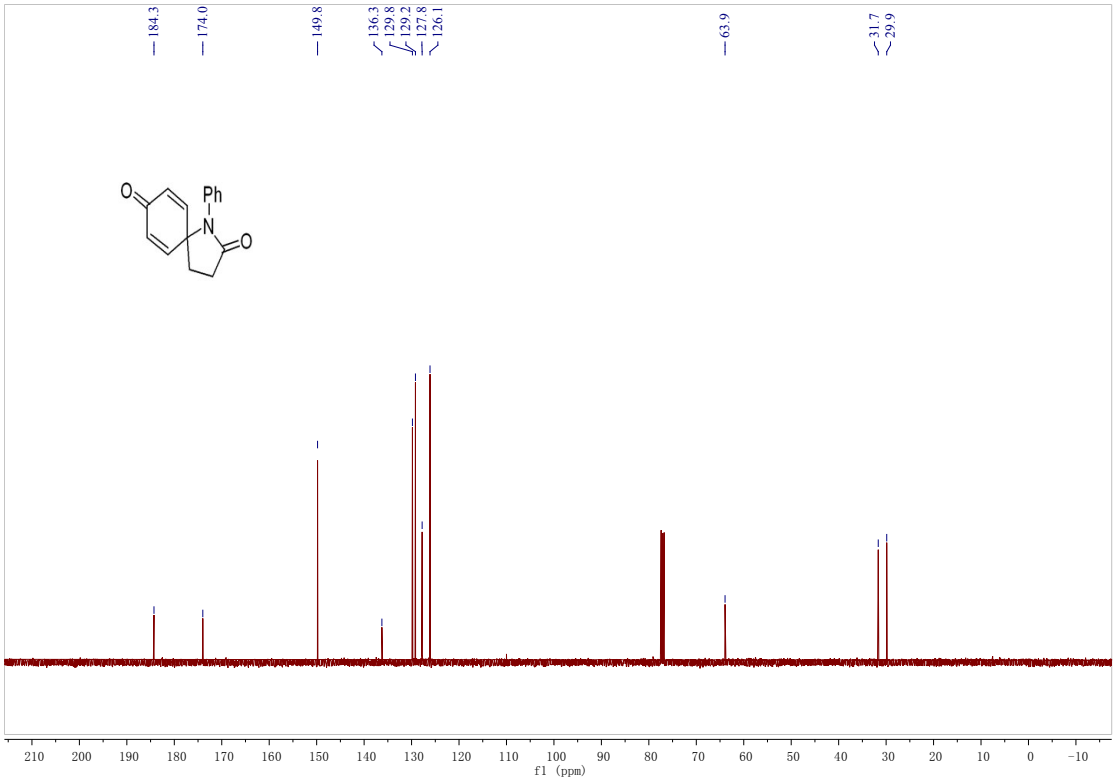
^{13}C NMR spectrum of compound **2y'**



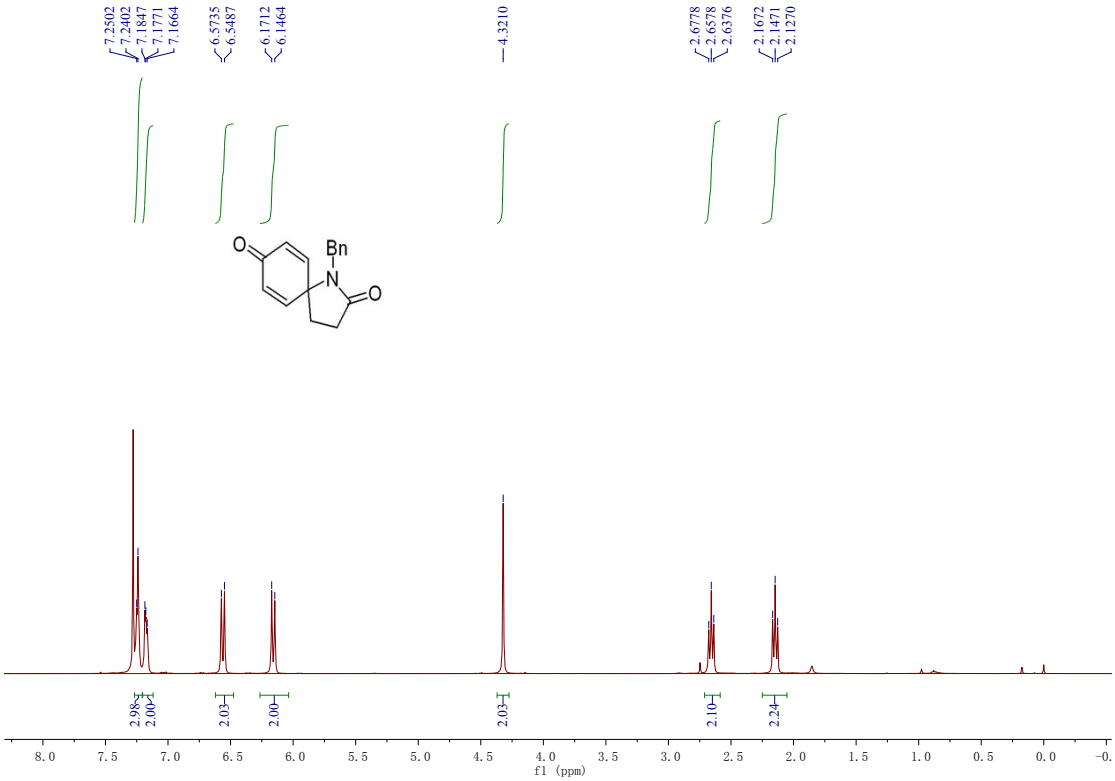
^{1}H NMR spectrum of compound **2aa**



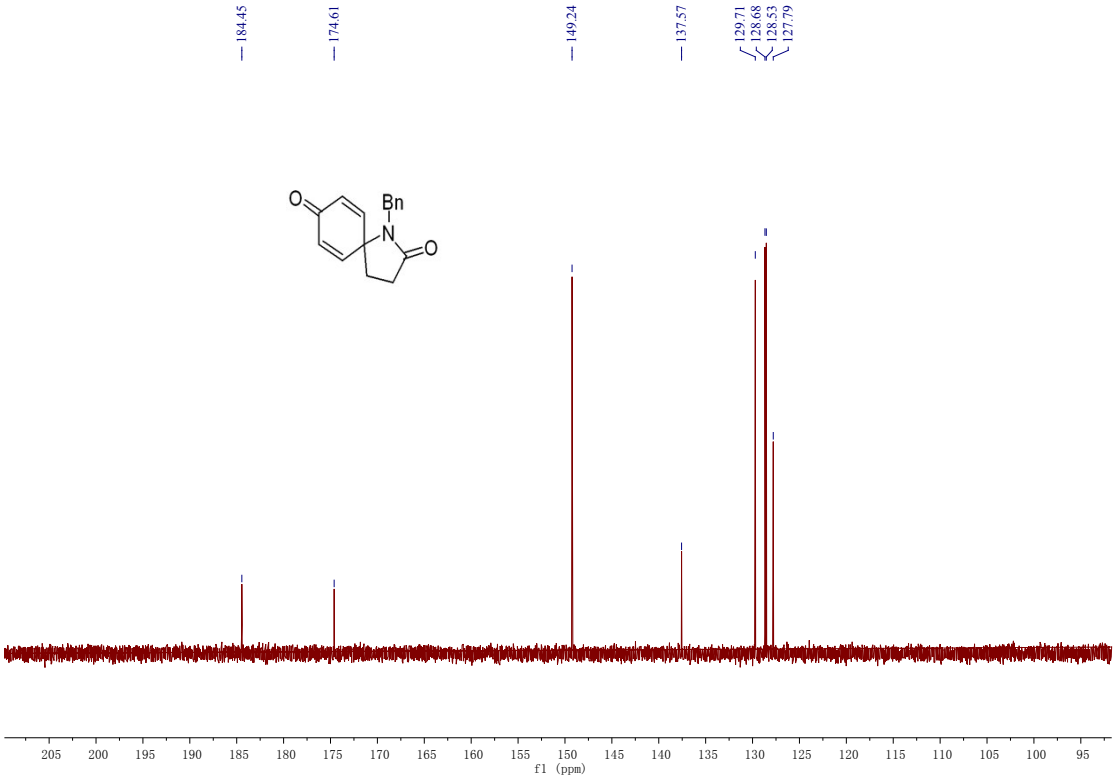
^{13}C NMR spectrum of compound **2aa**



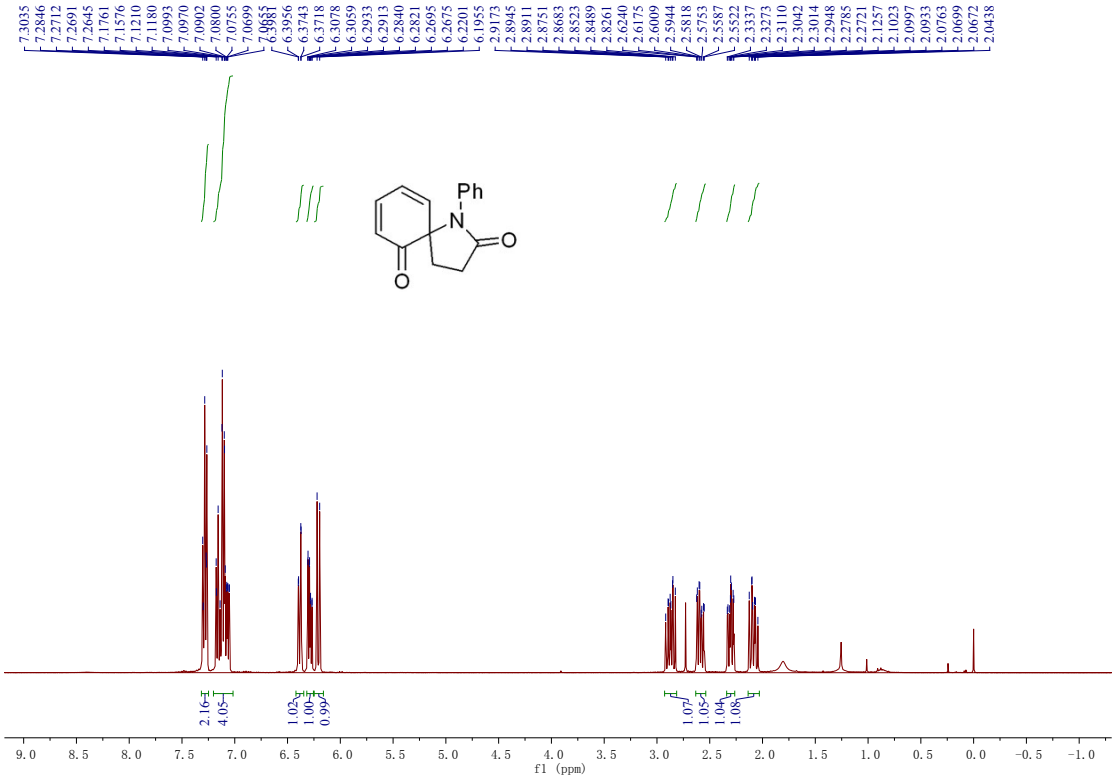
^{1}H NMR spectrum of compound **2ab**



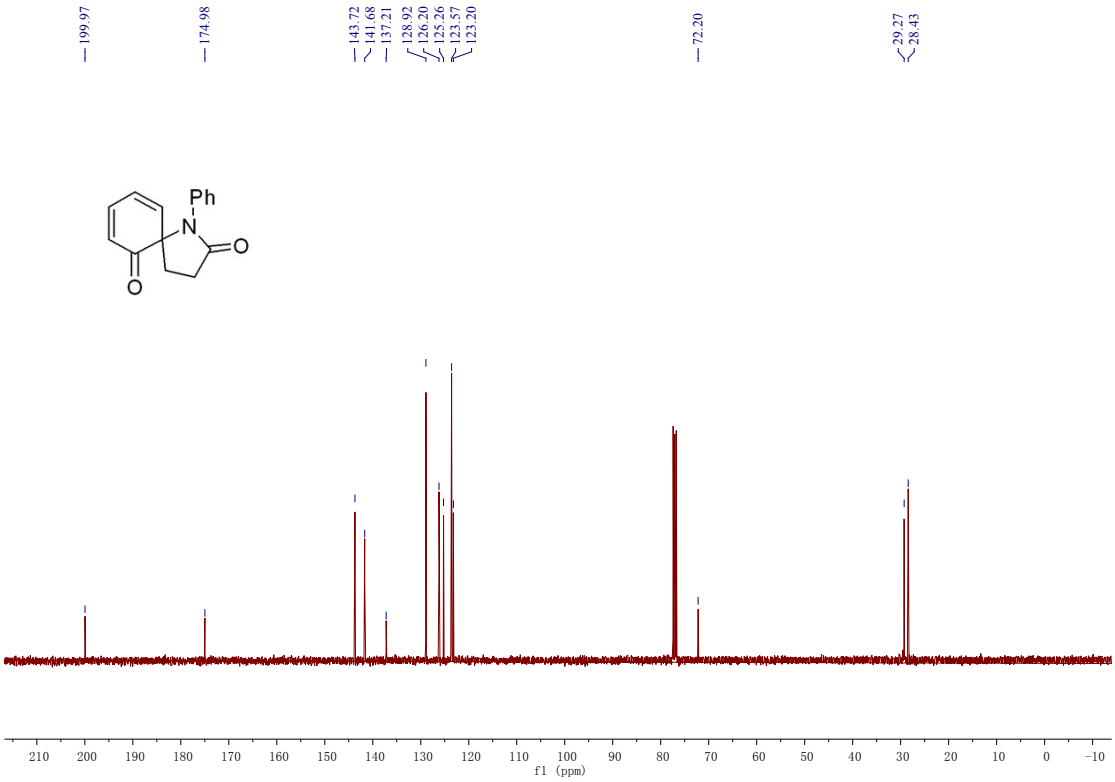
^{13}C NMR spectrum of compound **2ab**



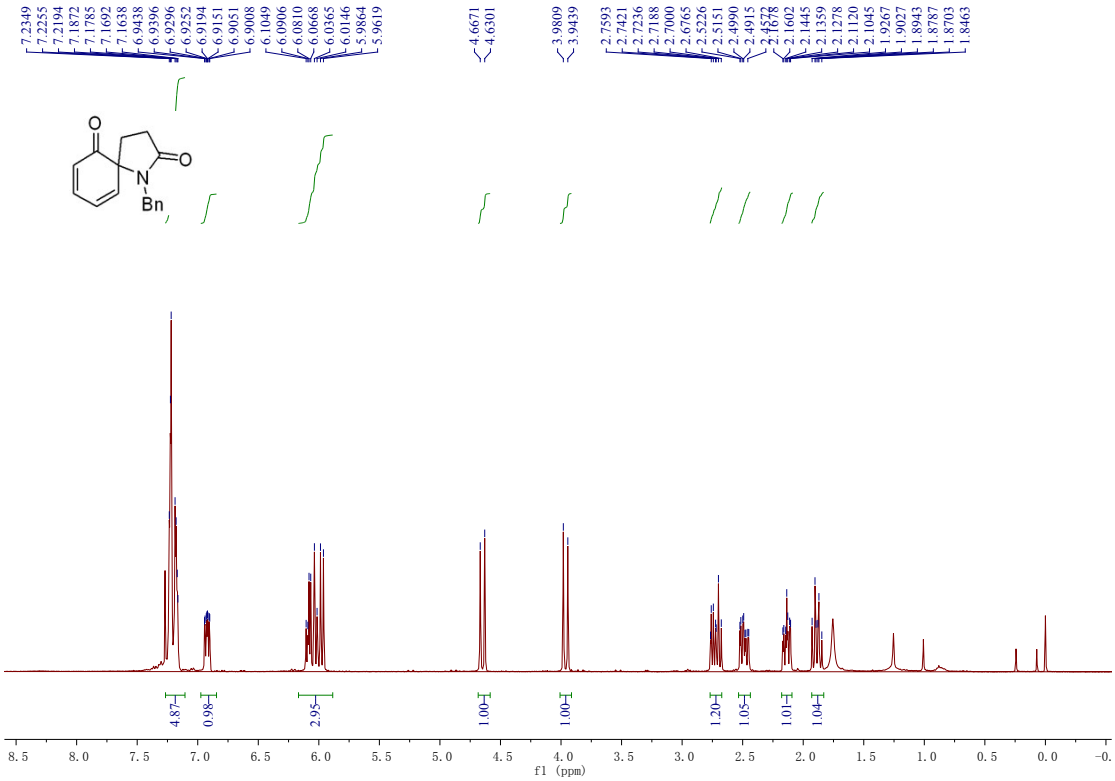
^{1}H NMR spectrum of compound **2ac**



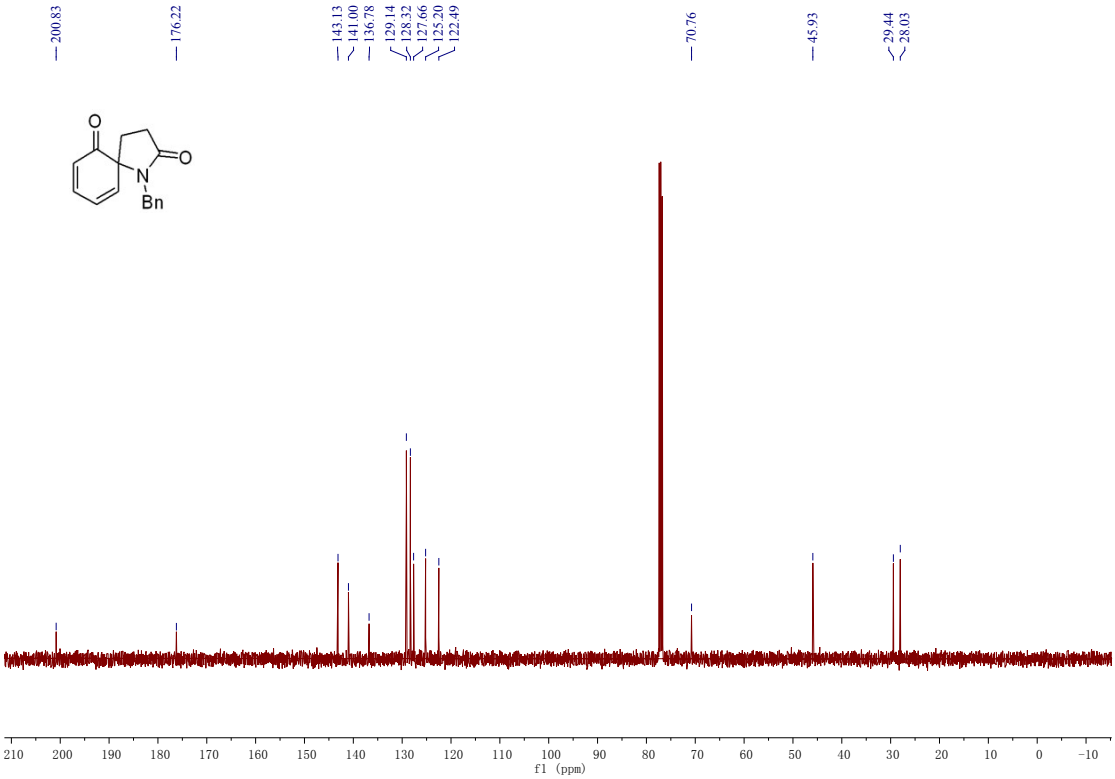
^{13}C NMR spectrum of compound **2ac**



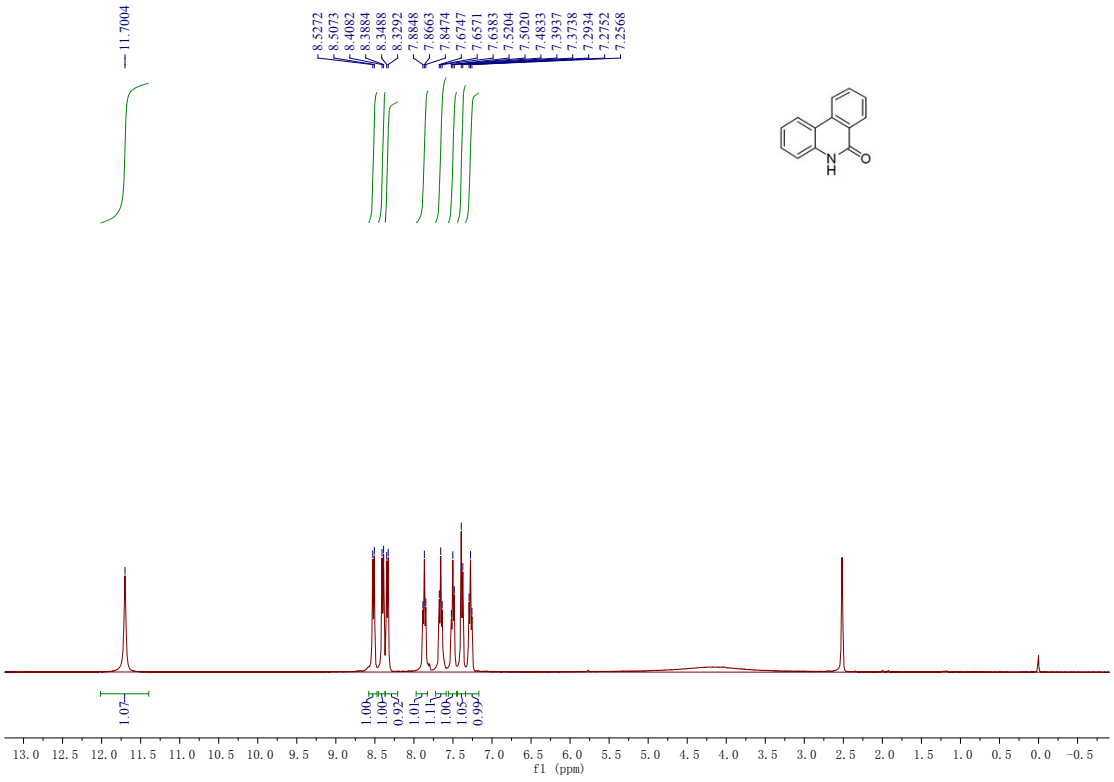
^{1}H NMR spectrum of compound **2ad**



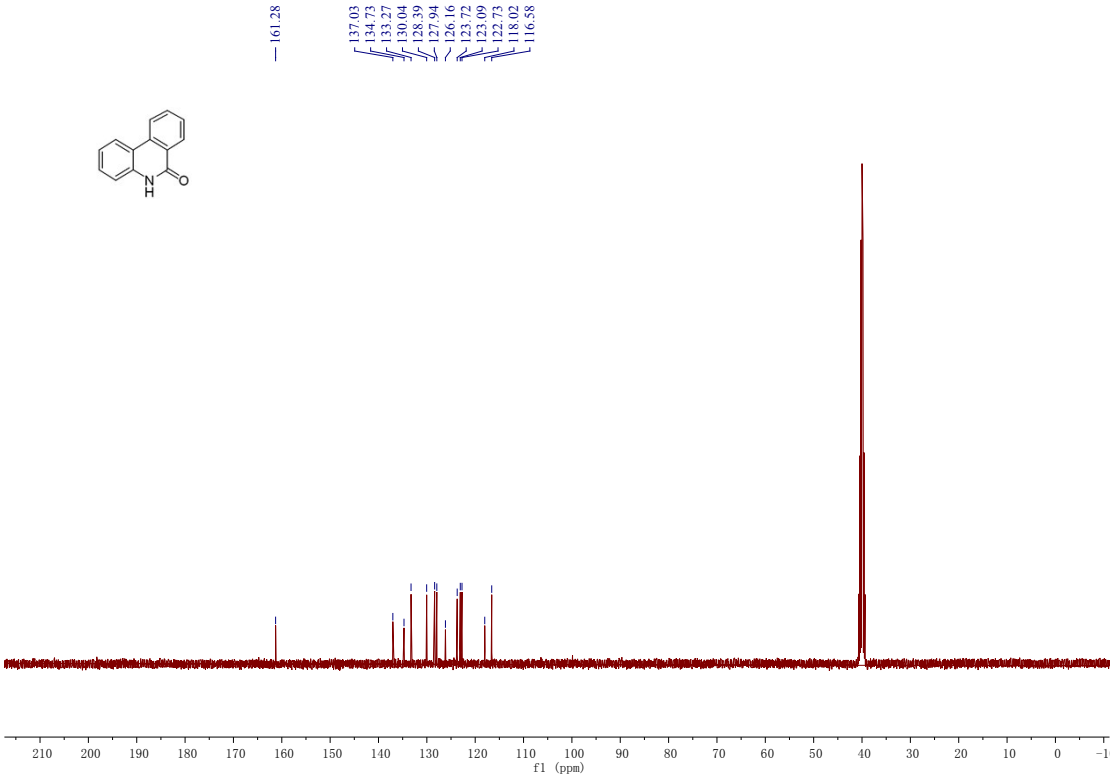
^{13}C NMR spectrum of compound **2ad**



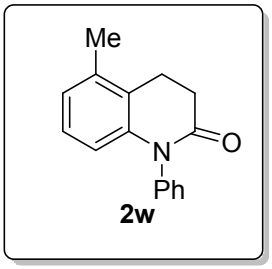
^{1}H NMR spectrum of compound **3**



^{13}C NMR spectrum of compound **3**



4. X-ray single crystal data for product



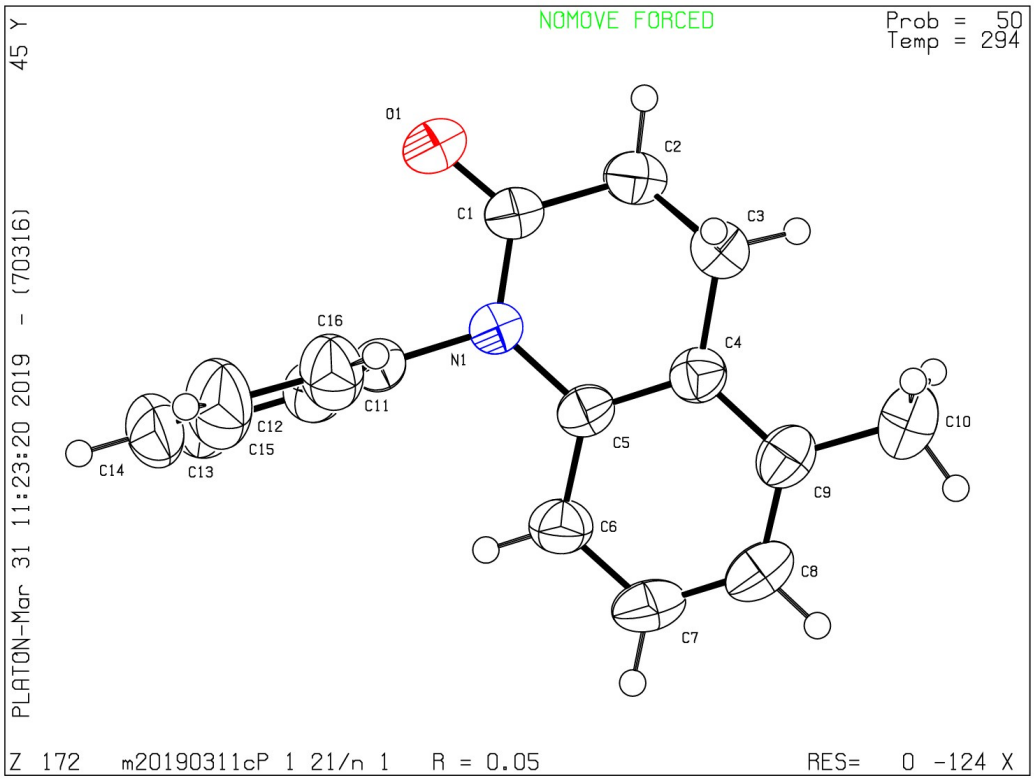


Table 1 Crystal data and structure refinement for 2q.

Identification code	**2w**
Empirical formula	$C_{16}H_{15}NO$
Formula weight	237.29
Temperature/K	294.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.7435(14)
b/Å	7.1127(9)
c/Å	15.6205(15)
α/°	90
β/°	95.141(9)

γ/°	90
Volume/Å^3	1299.5(3)
Z	4
ρ_{calc}g/cm^3	1.213
μ/mm^{-1}	0.076
F(000)	504.0
Crystal size/mm^3	0.24 × 0.22 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.704 to 56.558
Index ranges	-14 ≤ h ≤ 15, -8 ≤ k ≤ 9, -20 ≤ l ≤ 20
Reflections collected	19218
Independent reflections	3232 [R_{int} = 0.0669, R_{sigma} = 0.0513]
Data/restraints/parameters	3232/0/164
Goodness-of-fit on F^2	1.016
Final R indexes [I>=2σ (I)]	R_1 = 0.0514, wR_2 = 0.1214
Final R indexes [all data]	R_1 = 0.1112, wR_2 = 0.1472
Largest diff. peak/hole / e Å^{-3}	0.25/-0.15

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for m20190311c. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	5735.0(12)	7814(2)	4644.9(8)	75.2(5)
N1	5401.7(11)	6503(2)	3334.8(8)	45.9(4)
C1	5146.0(15)	7736(3)	3963.2(11)	51.6(4)
C2	4096.5(16)	8901(3)	3764.4(11)	57.9(5)
C3	3938.3(17)	9489(3)	2831.6(11)	58.1(5)
C4	4022.8(13)	7826(2)	2246.2(10)	44.3(4)
C5	4749.0(13)	6362(2)	2523.8(10)	42.4(4)
C6	4864.2(16)	4792(3)	2004.5(11)	53.5(5)
C7	4262.0(17)	4718(3)	1202.6(12)	60.4(5)
C8	3560.9(16)	6178(3)	918.4(11)	59.6(5)
C9	3427.4(15)	7739(3)	1429.0(11)	52.6(5)
C10	2652.9(19)	9318(4)	1099.6(14)	79.5(7)
C11	6364.3(15)	5266(3)	3538.3(10)	49.3(4)
C12	6205.3(19)	3555(3)	3920.0(12)	64.4(5)
C13	7141(3)	2404(4)	4118.2(13)	85.7(8)
C14	8208(3)	2968(5)	3948.5(16)	99.1(10)

C15	8359(2)	4682(5)	3577.7(17)	98.5(9)
C16	7432.3(17)	5831(4)	3361.0(13)	71.5(6)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for m20190311c. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	81.4(10)	87.3(11)	52.9(8)	-24.8(7)	-16.6(7)	21.7(8)
N1	48.2(8)	48.6(9)	40.0(7)	-6.0(6)	-1.3(6)	6.4(6)
C1	55.4(10)	52.5(11)	45.7(9)	-10.7(8)	-1.5(8)	3.7(9)
C2	58.3(11)	59.9(12)	54.9(10)	-16.7(9)	1.9(8)	7.8(9)
C3	61.1(11)	54.1(12)	57.9(11)	-7.5(9)	-2.1(8)	11.3(9)
C4	41.7(9)	45.4(10)	45.7(9)	-2.1(7)	2.7(7)	-3.9(7)
C5	42.8(9)	44.6(10)	39.6(8)	-3.1(7)	2.7(6)	-5.7(7)
C6	63.1(11)	45.8(11)	51.3(10)	-6.7(8)	3.7(8)	-1.3(9)
C7	74.6(13)	56.0(12)	49.9(10)	-15.5(9)	2.0(9)	-14.6(11)
C8	61.7(12)	69.5(14)	45.7(10)	-6.4(9)	-5.9(8)	-16.4(10)
C9	47.2(10)	58.4(12)	51(1)	1.0(9)	-3.4(7)	-8.6(9)
C10	77.5(15)	88.0(18)	68.4(13)	3.3(12)	-19.3(11)	11.9(13)
C11	54.7(11)	55.2(11)	37.4(8)	-3.1(8)	1.1(7)	11.6(9)
C12	81.2(14)	58.8(13)	52.1(10)	2.8(9)	0.2(9)	9.2(11)
C13	132(2)	69.1(16)	54.0(12)	7.1(11)	-4.0(13)	36.2(16)
C14	101(2)	132(3)	63.0(14)	-4.6(15)	0.7(13)	70(2)
C15	66.6(15)	144(3)	86.8(17)	15.3(18)	18.9(12)	39.6(17)
C16	59.4(13)	87.5(16)	68.9(13)	10.4(12)	13.4(10)	15.3(12)

Table 4 Bond Lengths for m20190311c.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.218(2)	C6	C7	1.383(3)
N1	C1	1.369(2)	C7	C8	1.374(3)
N1	C5	1.424(2)	C8	C9	1.384(3)
N1	C11	1.445(2)	C9	C10	1.506(3)
C1	C2	1.494(3)	C11	C12	1.375(3)
C2	C3	1.511(3)	C11	C16	1.369(3)
C3	C4	1.504(2)	C12	C13	1.383(3)
C4	C5	1.390(2)	C13	C14	1.364(4)
C4	C9	1.401(2)	C14	C15	1.368(4)
C5	C6	1.394(2)	C15	C16	1.378(3)

Table 5 Bond Angles for m20190311c.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C1	N1	C5	123.19(14)	C7	C6	C5	119.30(18)
C1	N1	C11	116.72(13)	C8	C7	C6	120.42(18)
C5	N1	C11	120.06(13)	C7	C8	C9	121.05(16)
O1	C1	N1	120.80(16)	C4	C9	C10	121.01(17)
O1	C1	C2	123.33(16)	C8	C9	C4	119.16(18)
N1	C1	C2	115.84(14)	C8	C9	C10	119.83(17)
C1	C2	C3	112.43(14)	C12	C11	N1	120.00(17)
C4	C3	C2	111.07(16)	C16	C11	N1	119.33(17)
C5	C4	C3	118.12(14)	C16	C11	C12	120.66(19)
C5	C4	C9	119.57(16)	C11	C12	C13	119.0(2)
C9	C4	C3	122.27(16)	C14	C13	C12	120.5(2)
C4	C5	N1	119.42(14)	C13	C14	C15	120.0(2)
C4	C5	C6	120.47(15)	C14	C15	C16	120.2(3)
C6	C5	N1	120.09(15)	C11	C16	C15	119.6(2)

Table 6 Torsion Angles for m20190311c.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
O1	C1	C2	C3	144.9(2)	C5	N1	C11	C16	91.9(2)
N1	C1	C2	C3	-37.0(2)	C5	C4	C9	C8	1.0(2)
N1	C5	C6	C7	-177.14(16)	C5	C4	C9	C10	-178.67(17)
N1	C11	C12	C13	-179.25(16)	C5	C6	C7	C8	0.3(3)
N1	C11	C16	C15	178.02(19)	C6	C7	C8	C9	-0.9(3)
C1	N1	C5	C4	18.2(2)	C7	C8	C9	C4	0.3(3)
C1	N1	C5	C6	-163.59(16)	C7	C8	C9	C10	179.99(19)
C1	N1	C11	C12	88.8(2)	C9	C4	C5	N1	176.50(15)
C1	N1	C11	C16	-90.0(2)	C9	C4	C5	C6	-1.7(2)
C1	C2	C3	C4	50.8(2)	C11	N1	C1	O1	2.5(3)
C2	C3	C4	C5	-32.2(2)	C11	N1	C1	C2	-175.60(16)
C2	C3	C4	C9	149.91(16)	C11	N1	C5	C4	-163.89(15)
C3	C4	C5	N1	-1.4(2)	C11	N1	C5	C6	14.3(2)
C3	C4	C5	C6	-179.64(16)	C11	C12	C13	C14	0.9(3)
C3	C4	C9	C8	178.89(17)	C12	C11	C16	C15	-0.8(3)
C3	C4	C9	C10	-0.8(3)	C12	C13	C14	C15	-0.1(4)
C4	C5	C6	C7	1.1(3)	C13	C14	C15	C16	-1.1(4)
C5	N1	C1	O1	-179.47(18)	C14	C15	C16	C11	1.6(4)

C5	N1	C1	C2	2.4(2)	C16	C11	C12 C13	-0.4(3)
C5	N1	C11	C12	-89.23(19)			

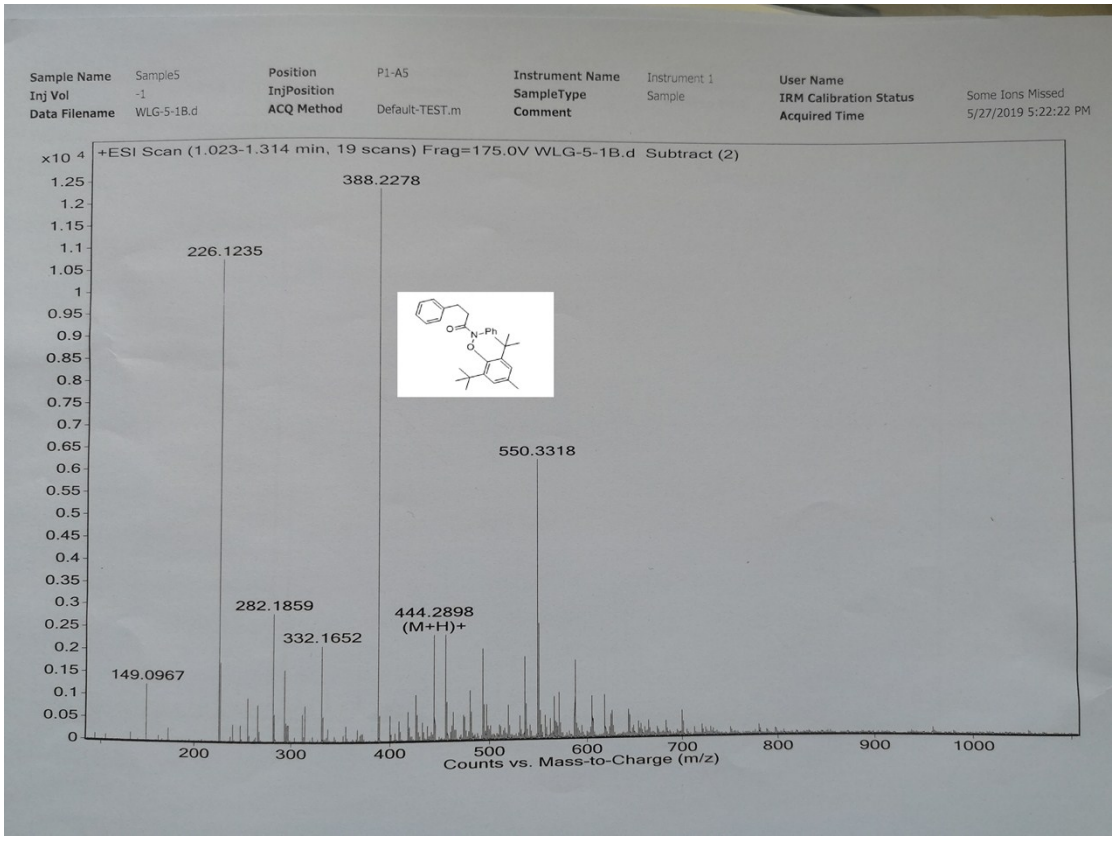
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for m20190311c.

Atom	*x*	*y*	*z*	U(eq)
H2A	4145.89	10015.38	4123.64	69
H2B	3433.18	8187.35	3902.48	69
H3A	3196.06	10078.76	2714.3	70
H3B	4518.71	10404.48	2719.31	70
H6	5340.89	3805.64	2195.14	64
H7	4332.04	3672.52	853.49	72
H8	3169.97	6116.57	374.42	72
H10A	2044.48	9459.39	1466.11	119
H10B	2337.56	9035.33	525.77	119
H10C	3083.02	10465.41	1097.16	119
H12	5479.38	3177.98	4042.98	77
H13	7041.42	1236.55	4369.09	103
H14	8832.63	2186.5	4084.9	119
H15	9088.36	5073.3	3471.62	118
H16	7532.39	6982.96	3096.09	86

5. Analytical data of HRMS

When 2.0 eq TEMPO or BHT was added to the above reaction mixture, the reaction was inhibited. When 2.0 eq BHT was added to the reaction of **1a**, the reaction was monitored by mass spectrometry experiment. The HRMS showed a peak at 444.2898, which corresponds to the product of the radical captured by BHT. So we think this is a radical mechanism.

The mass spectra of the reaction of 1a with NIS.


Sample Name Sample5
Inj Vol -1
Data Filename WLG-5-1B.d
Position P1-A5
InjPosition
ACQ Method Default-TEST.m
Instrument Name Instrument 1
SampleType Sample
Comment
User Name
IRM Calibration Status Some Ions Missed
Acquired Time 5/27/2019 5:22:22 PM
+ESI Scan (1.023-1.314 min, 19 scans) Frag=175.0V WLG-5-1B.d Subtract (2)
x10 4
388.2278
226.1235
550.3318
282.1859
444.2898
(M+H)+
332.1652
149.0967
N-Ph
O
Counts vs. Mass-to-Charge (m/z)