Supplementary Information

Copper-catalyzed cyanoalkylarylation of activated alkenes with AIBN: a convenient and efficient approach to cyano-containing oxindoles

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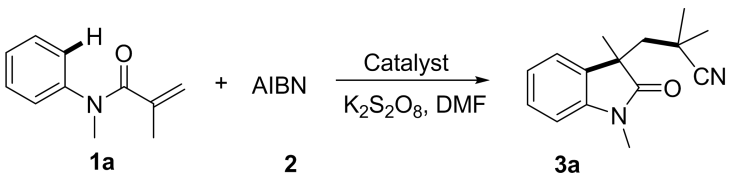
Contents

1. General information

All commercially available reagent grade chemicals were purchased from Aldrich, Acros, Alfa Aesar and Beijing Ouhe Chemical Company and used as received without further purification unless otherwise stated. All solvents were dried according to standard procedures. ^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ on a Bruker Avance III 400 spectrometer with TMS as internal standard (400 MHz ^{1}H, 100 MHz ^{13}C) at room temperature, the chemical shifts (δ) were expressed in ppm and J values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). Fourier-transform IR (FTIR) spectroscopy experiment was operated on a Nicolet IS5 spectrometer. Mass analyses and HRMS were obtained on a Finnigan-LCQDECA mass spectrometer and a Bruker Daltonics Bio-TOF-Q mass spectrometer by the ESI method, respectively. Column chromatography was performed on silica gel (200-300 mesh).

2. Optimization of the reaction conditions

Table S1. The reaction of **1a** and **2** in different conditions[a]



1a **2** **3a**

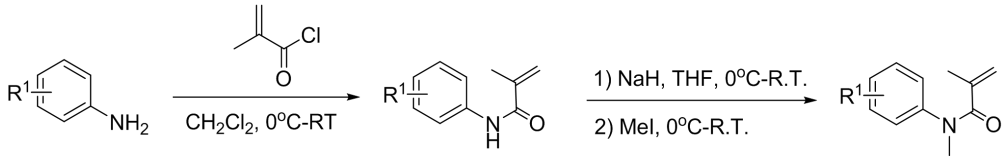
Entry	Catalyst	Oxidant	Yield (%)[b]
1	$Pd(OAc)_2$(5 mol%)	$K_2S_2O_8$ (2 equiv)	67
2	$FeCl_2·4H_2O$ (5 mol%)	$K_2S_2O_8$ (2 equiv)	26
3	$AgNO_3$(5 mol%)	$K_2S_2O_8$ (2 equiv)	48
4	$BiBr_3$ (5 mol%)	$K_2S_2O_8$ (2 equiv)	64
5	$InCl_3$ (5 mol%)	$K_2S_2O_8$ (2 equiv)	25
6	$NiCl_2$ (5 mol%)	$K_2S_2O_8$ (2 equiv)	30
7	$Cu(OAc)_2$ (5 mol%)	$K_2S_2O_8$ (2 equiv)	80
8	CuCl (5 mol%)	$K_2S_2O_8$ (2 equiv)	34
9	CuCN (5 mol%)	$K_2S_2O_8$ (2 equiv)	78
10	$Cu(OTf)_2$ (5 mol%)	$K_2S_2O_8$ (2 equiv)	63
11	CuI (5 mol%)	$K_2S_2O_8$ (2 equiv)	66
12	$Cu(CH_3CN)_4PF_6$(5 mol%)	$K_2S_2O_8$ (2 equiv)	54
13	CuO (5 mol%)	$K_2S_2O_8$ (2 equiv)	65
14	$CuCl_2$ (5 mol%)	$K_2S_2O_8$ (2 equiv)	48
15	CuBr (5 mol%)	$K_2S_2O_8$ (2 equiv)	83
16	CuBr (2.5 mol%)	$K_2S_2O_8$ (2 equiv)	60
17	CuBr (10 mol%)	$K_2S_2O_8$ (2 equiv)	77
18	CuBr (5 mol%)	$K_2S_2O_8$ (1 equiv)	54
19	CuBr (5 mol%)	$K_2S_2O_8$ (3 equiv)	84

[a] Reaction conditions: N-aryl acrylamide **1a** (0.25 mmol), AIBN **2** (1 mmol), catalyst (2-10 mol%), oxidant (1-3 equiv), DMF (1 mL), 80°C, 24 h. [b] Isolated yields based on **1a**.

3. Typical procedures for the synthesis of substrates

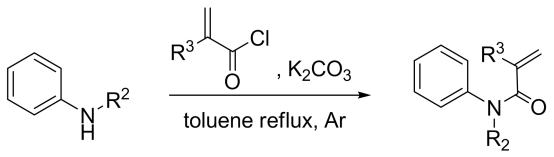
N-arylacrylamides **1** were prepared according to previous literatures.[S1,2]

Method A: substrate **1** was prepared according to previous literature.[S1]

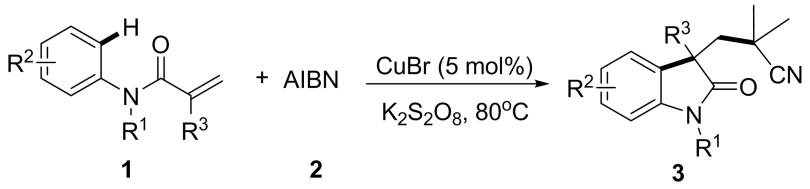


1

Method B: Substrate **1** was prepared according to previous literature.[S2]

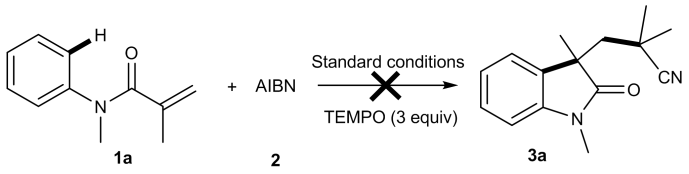


4. General procedure for direct cyanoalkylarylation of activated alkenes with AIBN.



To a mixture of N-arylacrylamide **1** (0.25 mmol), AIBN **2** (1 mmol), and $K_2S_2O_8$ (0.5 mmol) in a 25 mL round-bottomed flack at room temperature, was added the DMF (1 mL). The reaction vessel was allowed to stir at 80 °C for 24-36h. After the reaction, the solution was concentrated in vacuum. The resulting mixture purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **3**.

5. Preliminary mechanistic studies with TEMPO.



To a mixture of N-aryl acrylamide **1a** (0.25 mmol), AIBN **2** (0.75 mmol), TEMPO (0.75 mmol), $K_2S_2O_8$ (0.5 mmol), and DMF (1 mL) at room temperature. The reaction vessel was allowed to stir for 24 h at 80 °C. After the reaction, the solution was concentrated in vacuum, no desired product was detected.

6. The crystal structure of 3a.

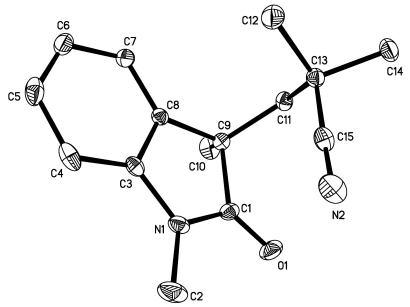


Figure S1 The crystal structure of **3a**. ORTEP drawing of $C_{15}H_{18}N_2O$ with 50% probability ellipsoids, showing the atomic numbering scheme.

Table S2. Crystal data and structure refinement for sad.

Identification code	sad
Empirical formula	C15H18N2O
Formula weight	242.31
Temperature	295(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P212121
Unit cell dimensions	a = 10.047(2) A alpha = 90 deg.
	b = 11.306(2) A beta = 90 deg.
	c = 12.199(2) A gamma = 90 deg.
Volume	1385.8(5) A^3
Z, Calculated density	4, 1.161 Mg/m^3
Absorption coefficient	0.074 mm^-1
F(000)	520
Crystal size	0.32 x 0.30 x 0.24 mm

Theta range for data collection	2.46 to 25.98 deg.
Limiting indices	-12<=h<=12, -13<=k<=13, -15<=l<=15
Reflections collected / unique	10664 / 2721 [R(int) = 0.0254]
Completeness to theta = 25.98	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9825 and 0.9768
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2721 / 0 / 167
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0434, wR2 = 0.1044
R indices (all data)	R1 = 0.0496, wR2 = 0.1083
Absolute structure parameter	0(2)
Largest diff. peak and hole	0.172 and -0.167 e.A^-3

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	11036(2)	9734(2)	8965(2)	51(1)
C(2)	12560(2)	10504(2)	10391(3)	91(1)
C(3)	10939(2)	8815(2)	10620(1)	46(1)
C(4)	11202(2)	8471(2)	11695(2)	67(1)
C(5)	10456(3)	7546(3)	12110(2)	79(1)
C(6)	9506(3)	6990(2)	11506(2)	75(1)
C(7)	9255(2)	7347(2)	10450(2)	59(1)

C(8)	9968(2)	8269(2)	10011(1)	42(1)
C(9)	9919(2)	8817(2)	8884(1)	43(1)
C(10)	10285(3)	7918(2)	7990(2)	70(1)
C(11)	8599(2)	9414(2)	8562(1)	48(1)
C(12)	7282(3)	9768(2)	10334(2)	79(1)
C(13)	7910(2)	10318(2)	9317(1)	48(1)
C(14)	6807(2)	10915(2)	8645(2)	67(1)
C(15)	8835(2)	11251(2)	9664(2)	55(1)
N(1)	11564(1)	9686(1)	9988(1)	54(1)
N(2)	9505(2)	11992(2)	9955(2)	84(1)
O(1)	11394(2)	10381(1)	8228(1)	80(1)

Table S4. Bond lengths [A] and angles [deg] for sad.

C(1)-O(1)	1.214(2)
C(1)-N(1)	1.357(3)
C(1)-C(9)	1.531(2)
C(2)-N(1)	1.449(2)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-C(8)	1.372(3)
C(3)-C(4)	1.394(3)
C(3)-N(1)	1.399(2)
C(4)-C(5)	1.383(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.359(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.374(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.374(3)
C(7)-H(7)	0.9300

C(8)-C(9)	1.508(2)
C(9)-C(10)	1.536(2)
C(9)-C(11)	1.539(2)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-C(13)	1.540(2)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.524(3)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(15)	1.468(3)
C(13)-C(14)	1.535(3)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-N(2)	1.132(3)
O(1)-C(1)-N(1)	126.11(19)
O(1)-C(1)-C(9)	125.32(19)
N(1)-C(1)-C(9)	108.56(15)
N(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
N(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(8)-C(3)-C(4)	121.26(19)
C(8)-C(3)-N(1)	109.69(15)
C(4)-C(3)-N(1)	129.03(18)
C(5)-C(4)-C(3)	116.9(2)
C(5)-C(4)-H(4)	121.6

C(3)-C(4)-H(4)	121.6
C(6)-C(5)-C(4)	122.2(2)
C(6)-C(5)-H(5)	118.9
C(4)-C(5)-H(5)	118.9
C(5)-C(6)-C(7)	120.1(2)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(6)-C(7)-C(8)	119.5(2)
C(6)-C(7)-H(7)	120.3
C(8)-C(7)-H(7)	120.3
C(3)-C(8)-C(7)	120.07(18)
C(3)-C(8)-C(9)	109.40(15)
C(7)-C(8)-C(9)	130.49(17)
C(8)-C(9)-C(1)	101.27(14)
C(8)-C(9)-C(10)	111.61(15)
C(1)-C(9)-C(10)	108.55(15)
C(8)-C(9)-C(11)	116.16(14)
C(1)-C(9)-C(11)	110.53(14)
C(10)-C(9)-C(11)	108.37(15)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-C(13)	121.73(14)
C(9)-C(11)-H(11A)	106.9
C(13)-C(11)-H(11A)	106.9
C(9)-C(11)-H(11B)	106.9
C(13)-C(11)-H(11B)	106.9
H(11A)-C(11)-H(11B)	106.7
C(13)-C(12)-H(12A)	109.5
C(13)-C(12)-H(12B)	109.5

H(12A)-C(12)-H(12B)	109.5
C(13)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(15)-C(13)-C(12)	108.73(17)
C(15)-C(13)-C(14)	107.18(16)
C(12)-C(13)-C(14)	108.37(17)
C(15)-C(13)-C(11)	111.37(15)
C(12)-C(13)-C(11)	113.67(16)
C(14)-C(13)-C(11)	107.26(15)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(2)-C(15)-C(13)	177.1(2)
C(1)-N(1)-C(3)	111.06(14)
C(1)-N(1)-C(2)	123.8(2)
C(3)-N(1)-C(2)	124.9(2)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters (A^2 x 10^3) for sad.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	45(1)	43(1)	64(1)	0(1)	18(1)	3(1)
C(2)	59(1)	64(1)	151(2)	-27(2)	-17(2)	-14(1)
C(3)	39(1)	47(1)	51(1)	-11(1)	-3(1)	12(1)
C(4)	62(1)	85(2)	56(1)	-23(1)	-16(1)	30(1)
C(5)	84(2)	101(2)	51(1)	21(1)	16(1)	43(2)

C(6)	67(1)	75(2)	82(2)	32(1)	20(1)	19(1)
C(7)	49(1)	52(1)	77(1)	13(1)	3(1)	2(1)
C(8)	37(1)	43(1)	47(1)	-1(1)	1(1)	4(1)
C(9)	47(1)	41(1)	42(1)	-5(1)	0(1)	-1(1)
C(10)	84(2)	68(1)	57(1)	-21(1)	0(1)	15(1)
C(11)	53(1)	49(1)	41(1)	-1(1)	-10(1)	0(1)
C(12)	79(2)	89(2)	70(1)	19(1)	27(1)	20(1)
C(13)	47(1)	51(1)	45(1)	2(1)	0(1)	4(1)
C(14)	56(1)	69(1)	76(2)	6(1)	-12(1)	13(1)
C(15)	59(1)	54(1)	52(1)	-12(1)	-6(1)	14(1)
N(1)	40(1)	46(1)	76(1)	-12(1)	-7(1)	-3(1)
N(2)	80(1)	71(1)	102(2)	-34(1)	-18(1)	9(1)
O(1)	74(1)	71(1)	94(1)	21(1)	34(1)	-6(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for sad.

	x	y	z	U(eq)
H(2A)	12904	10960	9791	137
H(2B)	13271	10070	10729	137
H(2C)	12163	11025	10920	137
H(4)	11849	8846	12115	81
H(5)	10608	7296	12825	94
H(6)	9026	6367	11808	90
H(7)	8607	6967	10035	71
H(10A)	11126	7561	8162	105
H(10B)	10346	8314	7296	105
H(10C)	9611	7317	7952	105
H(11A)	7962	8786	8427	57
H(11B)	8749	9805	7866	57
H(12A)	7968	9461	10802	119

H(12B)	6699	9136	10118	119
H(12C)	6782	10358	10721	119
H(14A)	6347	11478	9095	100
H(14B)	6191	10327	8391	100
H(14C)	7194	11313	8027	100

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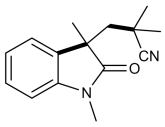
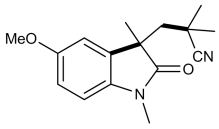
7. Characterization data of products 3a-3t



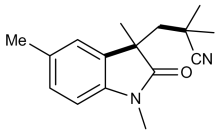
(3a)

Compound **3a** (white solid) was obtained in 83% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.35 (dt, J_1= 1.2 Hz, J_2 = 8.8 Hz, 2H), 7.13 (t, J = 7.5 Hz, 1H), 6.93 (d, J = 7.7 Hz, 1H), 3.27 (s, 3H), 2.36 (d, J = 14.6 Hz, 1H), 2.18 (d, J = 14.5 Hz, 1H), 1.38 (s, 3H), 1.19 (s, 3H), 1.11 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.6, 143.2, 131.0, 128.6, 124.7, 123.9, 122.5, 108.5, 47.0,46.6,30.7,29.7,27.4,26.7,26.4. IR (film, KBr) υ_{max}: 3059; 2967; 2936; 2234; 1714; 1609; 1493; 1470; 1377; 1296; 1021; 878 cm^{-1}. MS (ESI) calcd for $C_{15}H_{18}N_2ONa$ (M + Na)$^+$ 265.1317, found 265.1316.



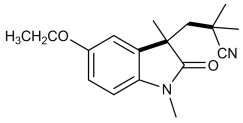
(3b)

Compound **3b** (white solid) was obtained in 69% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 6.95 (d, J = 2.4 Hz, 1H), 6.86 (dd, J_1 = 2.4 Hz, J_2 = 8.4 Hz, 1H), 6.81 (d, J = 8.4 Hz, 1H), 3.81 (s, 3H), 3.22 (s, 3H), 2.33 (d, J = 14.6 Hz, 1H), 2.15 (d, J = 14.6 Hz, 1H), 1.34 (s, 3H), 1.19 (s, 3H), 1.08 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.3, 156.0, 136.7, 132.2, 124.1, 113.2, 112.2, 108.8, 56.0, 47.4, 46.4, 30.7, 29.8, 27.5, 26.5, 26.4. IR (film, KBr) υ_{max}: 2976; 2900; 2230; 1707; 1575; 1453; 1425; 1383; 1285; 1042; 806cm^{-1}. HRMS (ESI) calcd for $C_{16}H_{20}N_2O_2Na$ (M + Na)$^+$ 295.1422, found 295.1422.



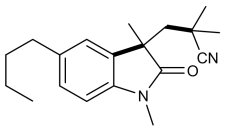
(3c)

Compound **3c** (white solid) was obtained in 75% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.12 (d, J = 8.4 Hz, 2H), 6.79 (d, J = 7.7 Hz, 1H), 3.22 (s, 3H), 2.36 (s, 3H), 2.31 (d, J = 14.6 Hz, 1H), 2.15 (d, J = 14.6 Hz, 1H), 1.34 (s 3H), 1.17 (s, 3H), 1.07 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.6, 140.8, 132.0, 130.9, 128.8, 125.6, 124.1, 108.2, 47.0, 46.5, 30.8, 29.7, 27.5, 26.5, 26.4, 21.2. IR (film, KBr) υ_{max}: 3066; 2965; 2926; 2233; 1715; 1596; 1497; 1451; 1373; 1288; 1125; 837 cm^{-1}. HRMS (ESI) calcd for $C_{16}H_{20}N_2ONa$ $(M + Na)^+$ 279.1473, found 279.1471.



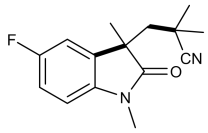
(3d)

Compound **3d** (white solid) was obtained in 81% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 6.95 (d, J = 2.4 Hz, 1H), 6.87 (dd, J_1 = 2.4 Hz, J_2 = 8.5 Hz, 1H), 6.81 (d, J = 8.4 Hz, 1H), 4.11-4.00 (m, 2H), 3.23 (s, 3H), 2.34 (d, J = 14.6 Hz, 1H), 2.15 (d, J = 14.6 Hz, 1H), 1.42 (t, J = 7.0 Hz, 3H), 1.36 (s, 3H), 1.20 (s, 3H), 1.10 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.3, 155.3, 136.6, 132.2, 124.1, 114.0, 112.8, 108.8, 64.3, 47.4, 46.5, 30.7, 29.7, 27.5, 26.6, 26.4, 14.9. IR (film, KBr) υ_{max}: 3069; 2980; 2910; 2231; 1709; 1596;1493; 1456; 1285; 1197; 1120; 1045; 804; 693cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{22}N_2O_2Na$ $(M + Na)^+$ 309.1579, found 309.1584.



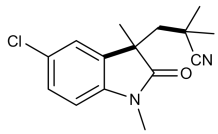
(3e)

Compound **3e** (yellow oil) was obtained in 84% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.15 (d, J = 6.8 Hz, 2H), 6.82 (d, J = 8.5 Hz, 1H), 3.24 (s, 3H), 2.62 (t, J = 7.9 Hz, 2H), 2.34 (d, J = 14.6 Hz, 1H), 2.16 (d, J = 14.6 Hz, 1H), 1.63-1.57 (m, 2H), 1.40-1.34 (m, 2H), 1.36 (s, 3H), 1.17 (s, 3H), 1.10 (s, 3H), 0.94 (t, J = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.7, 140.9, 137.3, 130.9, 128.3, 124.9, 124.1, 108.2, 47.1, 46.5, 35.4, 33.9, 30.8, 29.6, 27.5, 26.7, 26.4, 22.3, 13.9. IR (film, KBr) υ_{max}: 3063; 2976; 2931; 2228; 1712; 1613;1495; 1470; 1376; 1235; 1046; 752cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{26}N_2ONa$ $(M + Na)^+$ 321.1943, found 321.1943.



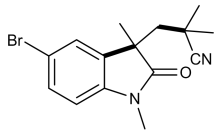
(3f)

Compound **3f** (yellow oil) was obtained in 71% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.09-7.02 (m, 2H), 6.86-6.82 (m, 1H), 3.24 (s, 3H), 2.34 (d, J = 14.6 Hz, 1H), 2.13 (d, J = 14.6 Hz, 1H), 1.36 (s, 3H), 1.19 (s, 3H), 1.12 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.2, 159.2 (d, J = 239.8 Hz), 139.1, 132.7 (d, J = 7.7 Hz), 123.7, 114.9 (d, J = 23.4 Hz), 112.7 (d, J = 24.6 Hz), 109.0 (d, J = 8.0 Hz), 47.4, 46.5, 30.6, 29.7, 27.3, 26.9, 26.5. IR (film, KBr) υ_{max}: 3057; 2971; 2932; 2236; 1716; 1606; 1576; 1496; 1378; 1271; 1112; 874 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{17}N_2ONaF$ $(M + Na)^+$ 283.1223, found 283.1222.



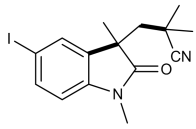
(3g)

Compound **3g** (yellow oil) was obtained in 76% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.34-7.30 (m, 2H), 6.84 (d, J = 8.2 Hz, 1H), 3.25 (s, 3H), 2.35 (d, J = 14.6 Hz, 1H), 2.13 (d, J = 14.6 Hz, 1H), 1.37 (s, 3H), 1.19 (s, 3H), 1.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.0, 141.8, 132.8, 128.5, 128.0, 125.0, 123.6, 109.4, 47.3, 46.6, 30.6, 29.6, 27.3, 27.1, 26.5. IR (film, KBr) υ_{max}: 3060; 2968; 2951; 2233; 1716; 1604; 1580; 1455; 1370; 1127; 843 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{17}N_2ONaCl$ $(M + Na)^+$ 299.0927, found 299.0930.



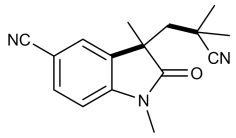
(3h)

Compound **3h** (white solid) was obtained in 81% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.47 (dd, J_1 = 1.8 Hz, J_2 = 8.3 Hz, 1H), 7.43 (d, J = 1.8 Hz, 1H), 6.80 (d, J = 8.2 Hz, 1H), 3.24 (s, 3H), 2.34 (d, J = 14.7 Hz, 1H), 2.12 (d, J = 14.6 Hz, 1H), 1.36 (s, 3H), 1.17 (s, 3H), 1.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 178.9, 142.3, 133.2, 131.4, 127.8, 123.6, 115.2, 110.0, 47.2, 46.6, 30.6, 29.6, 27.3, 27.2, 26.5. IR (film, KBr) υ_{max}: 3051; 2975; 2900; 2236; 1705; 1605; 1454; 1393; 1380; 1247; 1049; 879; 808 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{17}N_2ONaBr$ $(M + Na)^+$ 343.0422, found 343.0424.



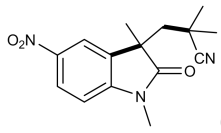
(3i)

Compound **3i** (light yellow solid) was obtained in 76% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.66 (dd, J_1= 1.7 Hz, J_2 = 8.2 Hz, 1H), 7.60 (d, J_1= 1.6 Hz, 1H), 6.70 (d, J = 8.2 Hz, 1H), 3.22 (s, 3H), 2.33 (d, J = 14.6 Hz, 1H), 2.11 (d, J = 14.6 Hz, 1H), 1.35 (s, 3H), 1.16 (s, 3H), 1.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 178.8, 143.0, 137.4, 133.6, 133.3, 123.6, 110.5, 84.9, 47.0, 46.6, 30.6, 29.6, 27.3, 27.2, 26.4. IR (film, KBr) υ_{max}: 2993; 2972; 2900; 2234; 1707; 1602; 1453; 1406; 1393; 1241; 1050; 879 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{17}N_2ONaI$ $(M + Na)^+$ 391.0283, found 391.0283.



(3j)

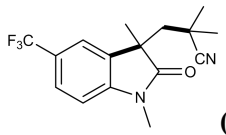
Compound **3j** (white solid) was obtained in 76% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.60 (dd, J_1 = 1.3 Hz, J_2 = 8.2 Hz, 1H), 7.49 (s, 1H), 6.91 (d, J = 8.1 Hz, 1H), 3.21 (s, 3H), 2.29 (d, J = 14.7 Hz, 1H), 2.08 (d, J = 14.7 Hz, 1H), 1.32 (s, 3H), 1.09 (s, 3H), 1.08 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.2, 147.2, 133.9, 132.2, 127.8, 123.3, 119.0, 109.0, 105.7, 46.9, 46.6, 30.5, 29.7, 27.5, 27.2, 26.6. IR (film, KBr) υ_{max}: 3055; 2971; 2215; 1719; 1610; 1497; 1459; 1341; 1182; 1049; 825 cm^{-1}. HRMS (ESI) calcd for $C_{16}H_{17}N_3ONa$ $(M + Na)^+$ 290.1269, found 290.1266.



(3k)

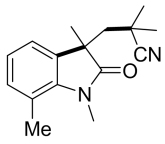
Compounds **3k** (white solid) was obtained in 69% yield according to the general procedure (24h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, J_1 = 2.2 Hz, J_2 = 8.6 Hz, 1H), 8.22 (d, J = 2.2 Hz, 1H), 7.01 (d, J = 8.6 Hz, 1H), 3.34 (s, 3H), 2.39 (d, J = 14.6 Hz, 1H), 2.23 (d, J = 14.6 Hz, 1H), 1.44 (s, 3H), 1.19 (s, 3H), 1.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.6, 148.9, 143.4, 132.0, 125.9, 123.3, 120.3, 108.2, 47.1, 46.6, 30.5, 29.7, 27.5, 27.2, 26.8. IR (film, KBr) υ_{max}: 3060; 2987; 2942; 2228; 1724; 1599; 1514; 1457; 1294; 1114; 1044; 831 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{17}N_3O_3Na$ $(M + Na)^+$ 310.1168,

found 310.1171.



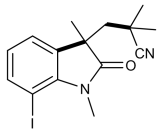
(3l)

Compounds **3l** (white solid) were obtained in 72% yield according to the general procedure (24h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.2 Hz, 1H), 7.55 (s, 1H), 7.00 (d, *J* = 8.2 Hz, 1H), 3.29 (s, 3H), 2.38 (d, *J* = 14.6 Hz, 1H), 2.18 (d, *J* = 14.6 Hz, 1H), 1.40 (s, 3H), 1.15 (s, 3H), 1.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.5, 146.2, 131.7, 126.3 (d, *J* = 4.0 Hz), 124.7 (d, *J* = 32.6 Hz), 124.4 (d, *J* = 269.9 Hz), 123.5, 121.6 (d, *J* = 4.3 Hz), 108.3, 47.0, 46.6, 30.6, 29.5, 27.3, 27.2, 26.6. IR (film, KBr) $\upsilon_{max:}$ 3029; 2979; 2931; 2236; 1715; 1605; 1506; 1455; 1326; 1173; 1057; 832 cm^{-1}. HRMS (ESI) calcd for $C_{16}H_{17}N_2F_3ONa$ $(M + Na)^+$ 333.1191, found 333.1190.



(3m)

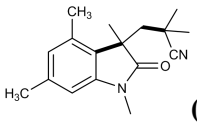
Compound **3m** (light yellow oil) was obtained in 61% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): *δ* 7.14 (d, *J* = 7.3 Hz, 1H), 7.07 (d, *J* = 7.2 Hz, 1H), 7.00 (t, *J* = 7.4 Hz, 1H), 3.54 (s, 3H), 2.62 (s, 3H), 2.34 (d, *J* = 14.5 Hz, 1H), 2.14 (d, *J* = 14.6 Hz, 1H), 1.34 (s, 3H), 1.16 (s, 3H), 1.12 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 180.3, 141.0, 132.3, 131.6, 123.9, 122.5, 122.3, 120.1, 46.8, 46.3, 30.7, 29.7, 29.6, 27.8, 26.9, 19.1. IR (film, KBr) υ_{max}: 2973; 2929; 2870; 2239; 1711; 1656; 1600; 1459; 1273; 1072; 748 cm^{-1}. HRMS (ESI) calcd for $C_{16}H_{20}N_2ONa$ $(M + Na)^+$ 279.1473, found 279.1471.



(3n)

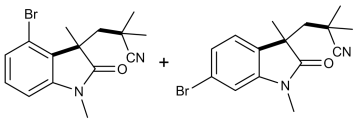
Compound **3n** (yellow oil) was obtained in 70% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): *δ* 7.75 (dd, J_1 = 1.1 Hz, J_2 = 8.1 Hz, 1H), 7.28 (dd, J_1 = 1.1 Hz, J_2 = 7.3 Hz, 1H), 6.83 (t, *J* = 7.9 Hz, 1H), 3.65 (s, 3H), 2.34 (d, *J* = 14.6 Hz, 1H), 2.17 (d, *J* = 14.6 Hz, 1H), 1.36 (s, 3H), 1.21 (s, 3H), 1.10 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 180.4, 143.5, 141.3, 133.9, 124.5, 124.2, 123.9, 71.9, 46.6, 46.5, 30.6, 30.4, 29.8, 27.8, 26.4. IR (film, KBr) υ_{max}: 2973; 2931; 2230; 1719; 1656; 1576;

1454; 1363; 1059; 1014; 764 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{17}N_2ONaI$ $(M + Na)^+$ 391.0283, found 391.0278.



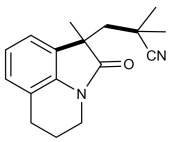
(3o)

Compounds **3o** (yellow oil) were obtained in 75% yield according to the general procedure (24h). ^1H NMR (400 MHz, $CDCl_3$) δ 6.71 (s, 1H), 6.60 (s, 1H), 3.22 (s, 3H), 2.42 (s, 3H), 2.38 (s, 3H), 2.36 (d, J = 15.2 Hz, 1H), 2.28 (d, J = 15.2 Hz, 1H), 1.41 (s, 3H), 1.21 (s, 3H), 1.11 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.0, 143.4, 138.6, 135.5, 125.9, 125.2, 123.6, 107.2, 47.4, 45.2, 30.9, 29.2, 26.4, 26.3, 24.8, 21.6, 18.8. IR (film, KBr) υ_{max}: 2985; 2932; 2875; 2233; 1716; 1606; 1578; 1455; 1381; 1126; 1058; 837 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{22}N_2ONa$ $(M + Na)^+$ 293.1630, found 293.1628.



(3p and **3p')**

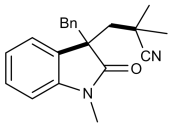
Compounds **3p** and **3p'** (light yellow oil) were obtained in 70% yield according to the general procedure (24h). ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.25 (d, J = 1.7 Hz, 0.33H), 7.22 (d, J = 3.0 Hz, 1H), 7.21(s, 1.33H), 7.07 (d, J = 1.6 Hz, 0.33H), 6.87 (dd, J_1 = 2.9 Hz, J_2 = 5.8 Hz, 1H), 3.25 (s, 3H), 3.24 (s, 1H), 2.70 (d, J = 14.5 Hz, 1H), 2.34 (d, J = 14.7 Hz, 0.33 H), 2.17 (d, J = 14.5 Hz, 1H), 2.16 (d, J = 14.7 Hz, 0.33H), 1.52 (s, 3H), 1.34 (s, 1H), 1.21 (s, 3H), 1.20 (s, 1H), 1.17 (s, 3H), 1.10 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.5, 178.8, 145.3, 144.5, 130.1, 129.4, 126.9, 126.0, 125.3, 123.9, 123.3, 122.2, 120.5, 112.1, 107.7, 49.0, 46.9, 46.3, 43.7, 30.7, 30.6, 28.3, 28.1, 27.4, 26.6, 26.5, 25.8, 23.5, 22.9. IR (film, KBr) υ_{max}: 2962; 2928; 2858; 2236; 1722; 1604; 1545; 1456; 1287; 1072; 764 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{17}N_2OBrNa$ $(M + Na)^+$ 343.0422, found 343.0428.



(3q)

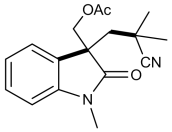
Compound **3q** (yellow oil) was obtained in 77% yield according to the general procedure (36h). ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.17 (d, J = 7.3 Hz, 1H), 7.10 (d, J = 7.6 Hz, 1H), 7.01 (d, J = 7.5 Hz, 1H), 3.80-3.72 (m, 2H), 2.88-2.78 (m, 2H), 2.35 (d, J = 14.6 Hz,

1H), 2.16 (d, J = 14.6 Hz, 1H), 2.08-2.02 (m, 2H), 1.38 (s, 3H), 1.20 (s, 3H), 1.14 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 178.5, 139.0, 129.5, 127.3, 124.0, 122.6, 121.8, 120.6, 48.3, 46.5, 39.0, 30.8, 29.6, 27.2, 26.9, 24.6, 21.1. IR (film, KBr) υ_{max}: 2973; 2929; 2875; 2230; 1710; 1600; 1482; 1454; 1354; 1241; 1168; 751 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{20}N_2O$ Na $(M + Na)^+$ 291.1473, found 291.1472.



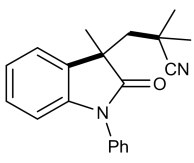
(3r)

Compound **3r** (white solid) was obtained in 72% yield according to the general procedure (36h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.37 (d, J = 7.2 Hz, 1H), 7.26 (t, J = 8.3 Hz, 1H), 7.14-7.02 (m, 4H), 6.74 (d, J = 7.1 Hz, 2H), 6.62 (d, J = 7.7 Hz, 1H), 3.06 (d, J = 12.5 Hz, 1H), 2.97 (d, J = 12.9 Hz, 1H), 2.94 (s, 3H), 2.48 (d, J = 14.6 Hz, 1H), 2.37 (d, J = 14.6 Hz, 1H), 1.27 (s, 3H), 1.11(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 178.1, 143.8, 134.3, 130.0, 128.7, 127.8, 127.4, 126.7, 126.0, 124.3, 121.9, 108.1, 53.1, 46.8, 45.1, 30.8, 30.0, 26.5, 25.9. IR (film, KBr) υ_{max}: 3058; 2973; 2931; 2228; 1706; 1612; 1495; 1471; 1377; 1259; 1184; 1086; 916; 879 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{22}N_2ONa$ $(M + Na)^+$ 341.1630, found 341.1624.



(3s)

Compound **3s** (yellow oil) was obtained in 74% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.40-7.36 (m, 2H), 7.11 (dt, J_1 = 0.8 Hz, J_2 = 7.6 Hz, 1H), 6.93 (d, J = 8.3 Hz, 1H), 4.37 (d, J = 10.6 Hz, 1H), 4.02 (d, J = 10.6 Hz, 1H), 3.27 (s, 3H), 2.31 (s, 2H), 1.93 (s, 3H), 1.20 (s, 3H), 1.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 176.4, 170.2, 144.0, 129.4, 126.4, 125.9, 123.7, 122.5, 108.6, 68.5, 51.0, 41.7, 30.4, 29.8, 26.8, 26.5, 20.5. IR (film, KBr) υ_{max}: 2973; 2920; 2853; 2236; 1716; 1577; 1494; 1471; 1375; 1234; 1045; 755 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{20}N_2O_3Na$ $(M + Na)^+$ 323.1372, found 323.1377.



(3t)

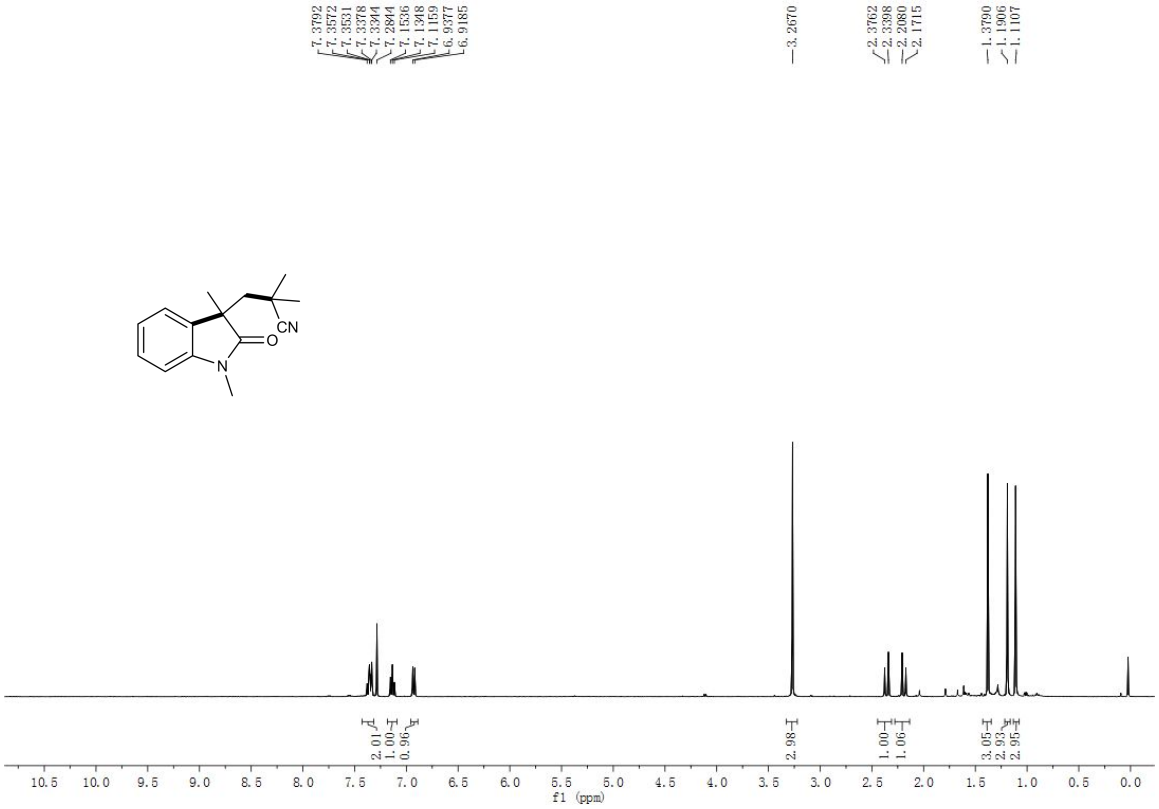
Compound **3t** (white solid) was obtained in 75% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.55 (t, J = 7.8 Hz, 2H), 7.48-7.22 (m, 4H), 7.29 (dt, J_1= 1.2 Hz, J_2= 7.8 Hz, 1H), 7.18 (dt, J_1= 0.8 Hz, J_2= 7.5 Hz, 1H), 6.92 (d, J = 7.9 Hz, 1H), 2.45 (d, J = 14.7 Hz, 1H), 2.32 (d, J = 14.7 Hz, 1H), 1.51 (s, 3H), 1.31 (s, 3H), 1.23 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): 179.0, 143.3, 134.5, 130.7, 129.6, 128.5, 128.1, 126.3, 125.1, 124.2, 122.9, 109.9, 47.2, 46.5, 30.9, 29.9, 28.3, 26.5. IR (film, KBr) υ_{max}: 3052; 2979; 2912; 2233; 1705; 1609; 1502; 1466; 1368; 1208; 1024; 755 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{20}N_2ONa$ $(M + Na)^+$ 327.1473, found 327.1471.

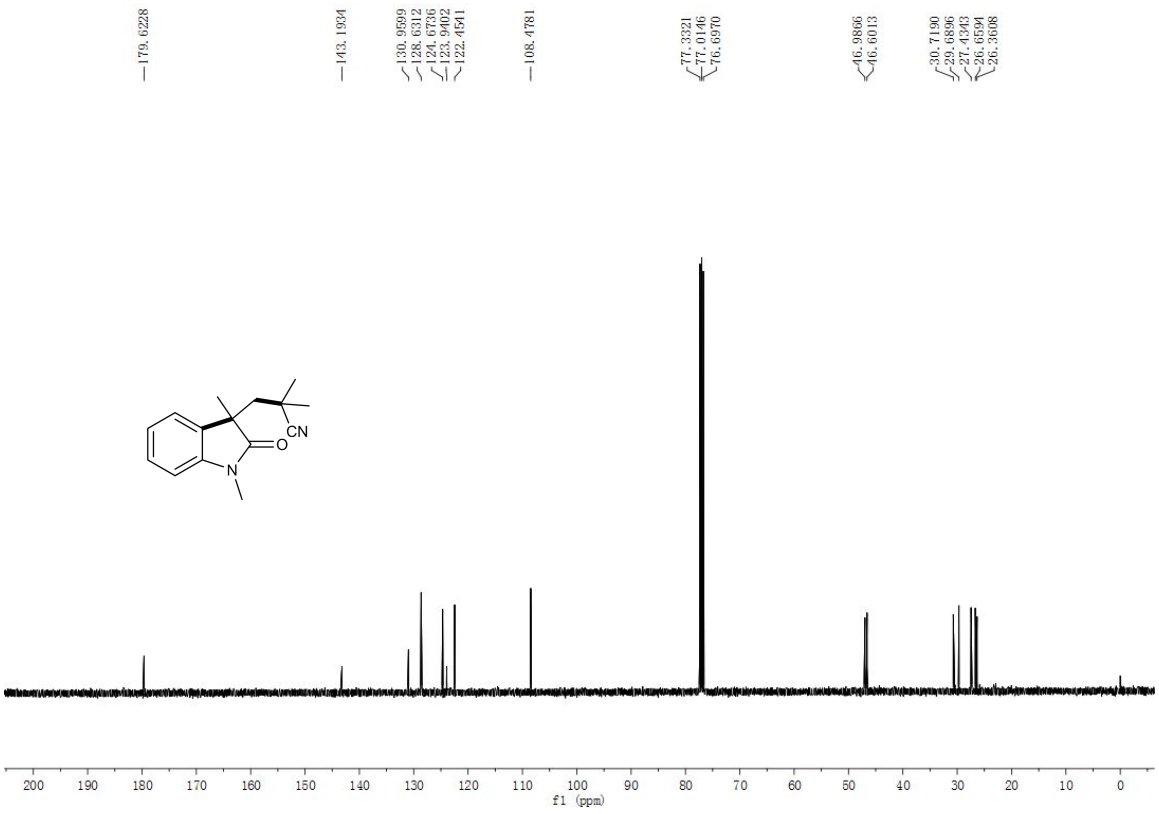
8. Reference

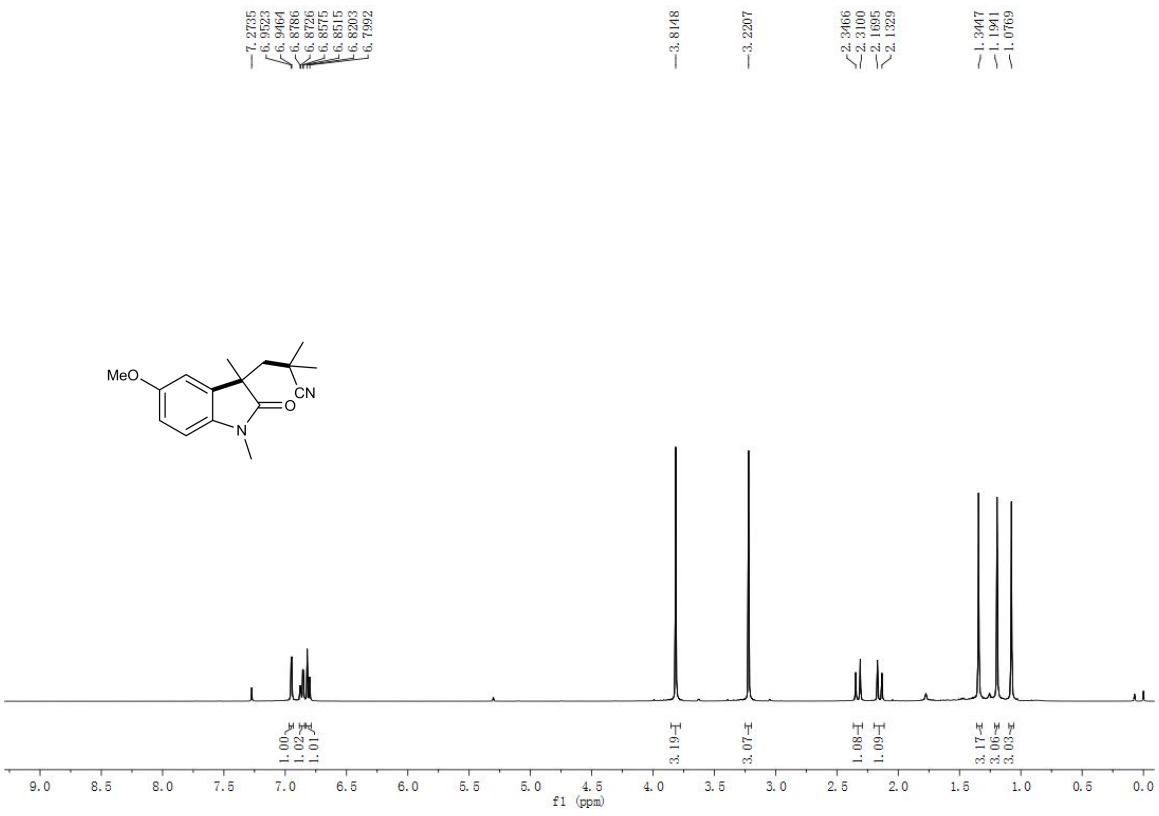
[S1] A. Pinto, Y. Jia, L. Neuville, J. Zhu, *Chem. Eur. J.* **2007**, *13*, 961.

[S2] A. A.-L. Ayitou, J. Sivaguru, *Chem. Commun.* **2011**, *47*, 2568.

9.Copies of NMR Spectra for 3a−3t



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O
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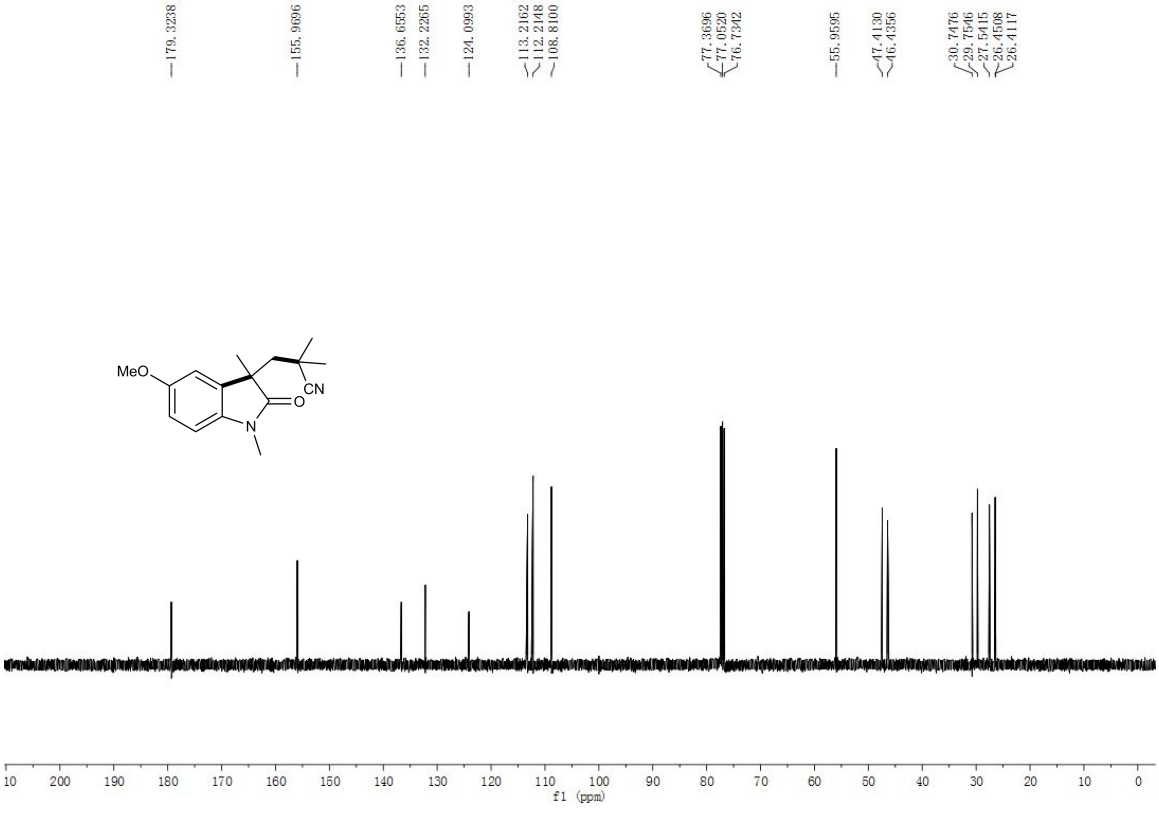
3.03
f1 (ppm)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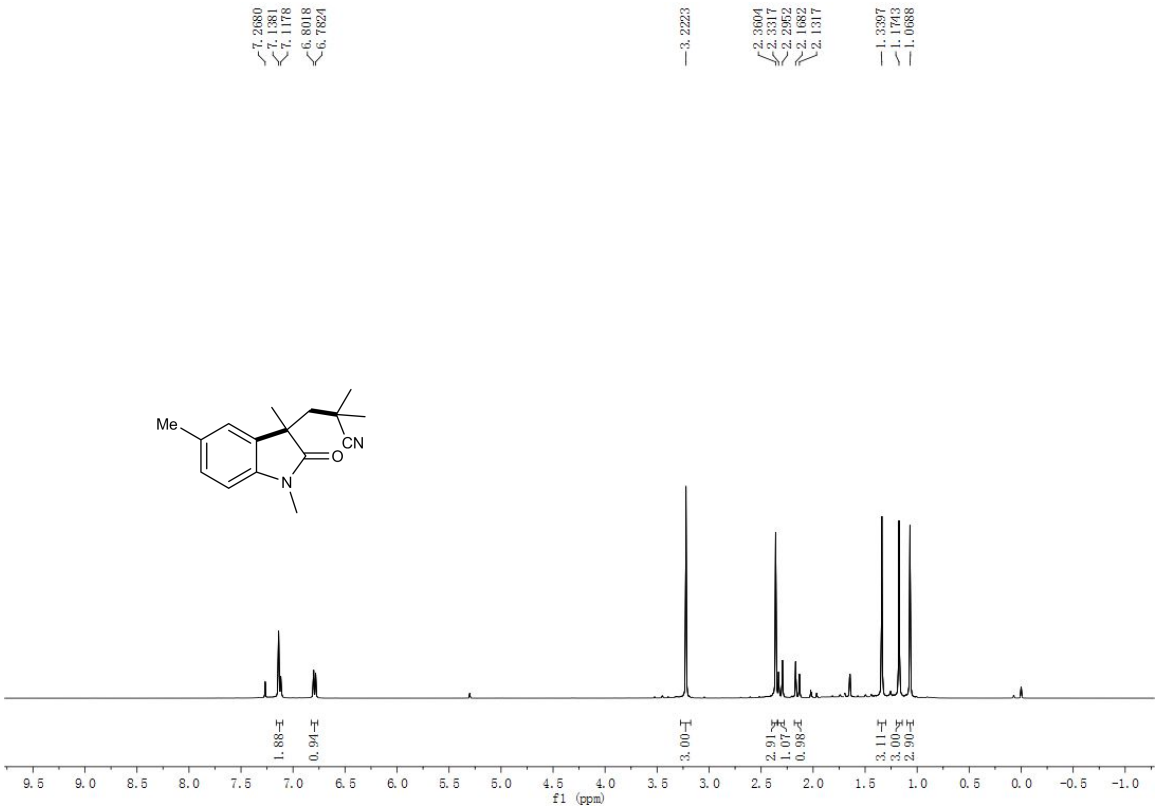
f1 (ppm)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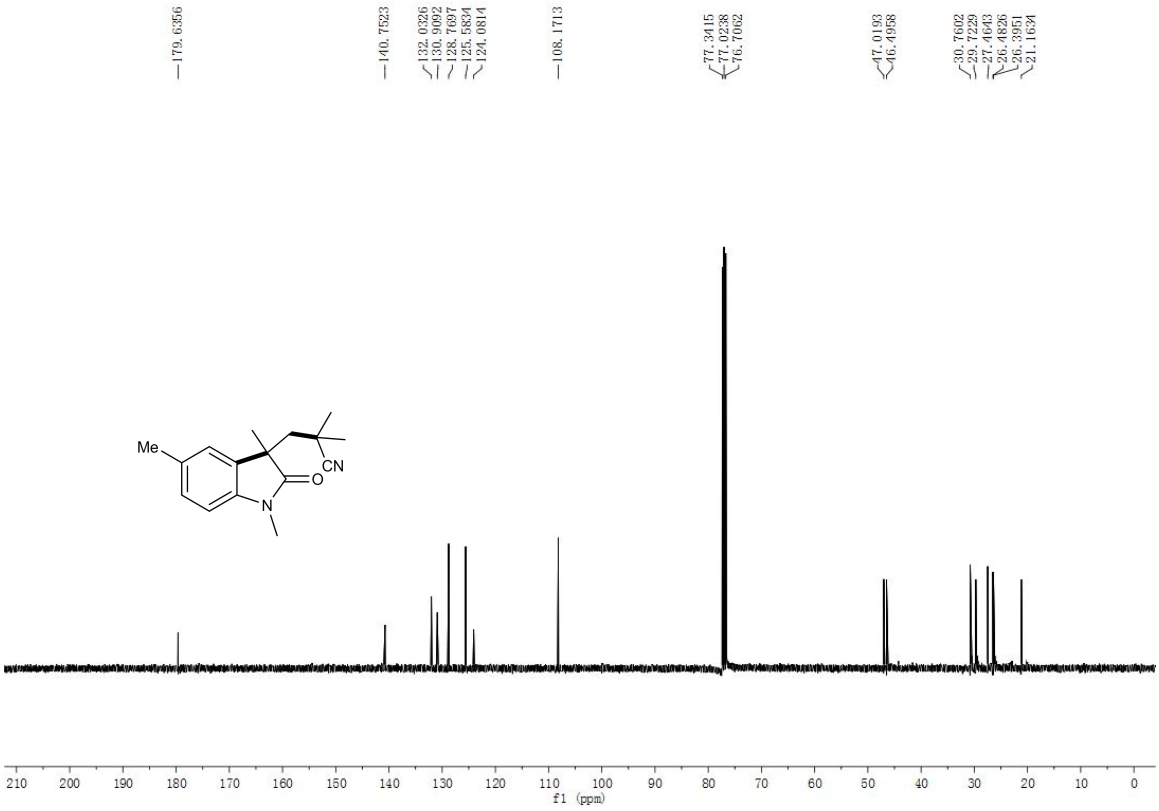
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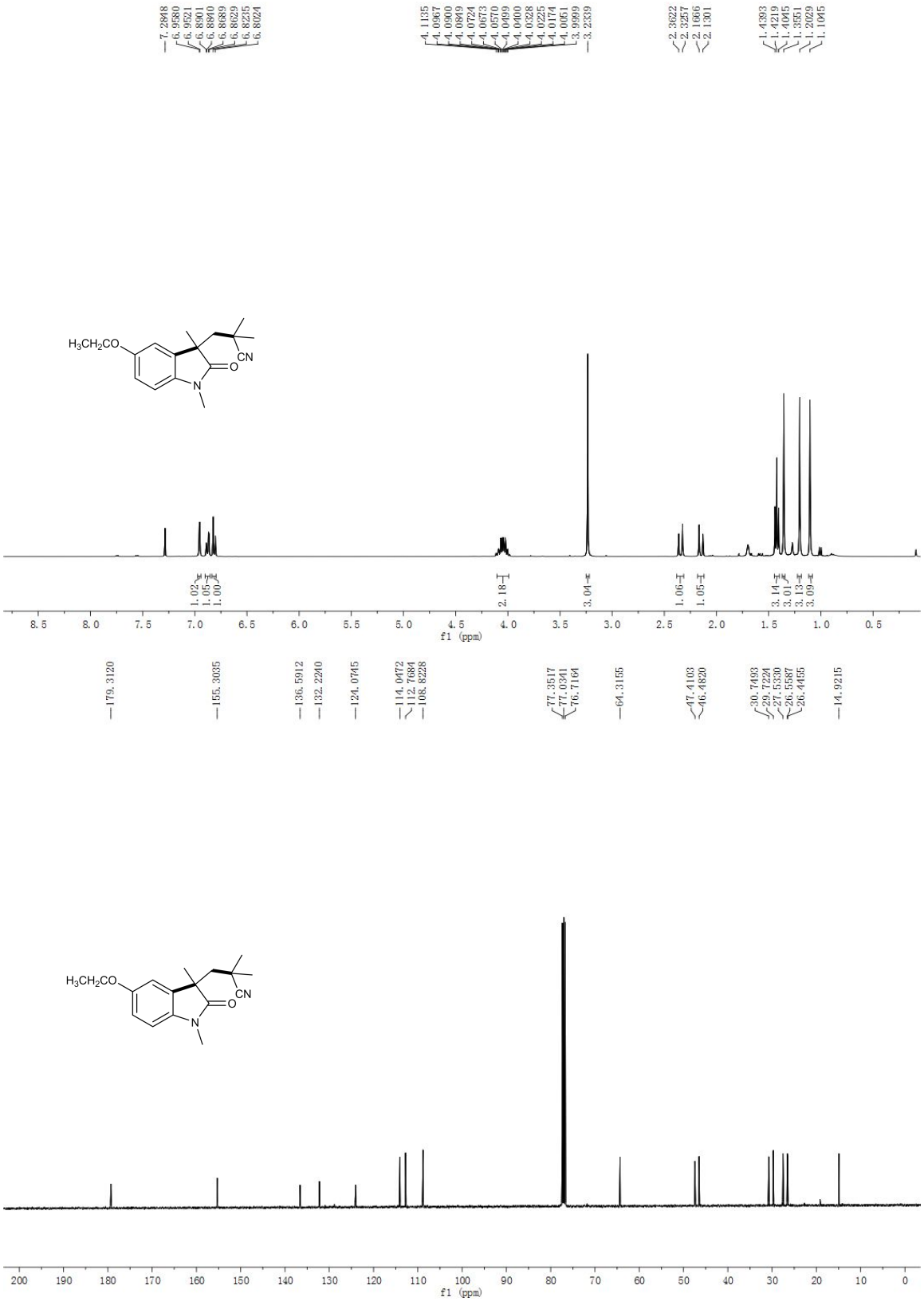
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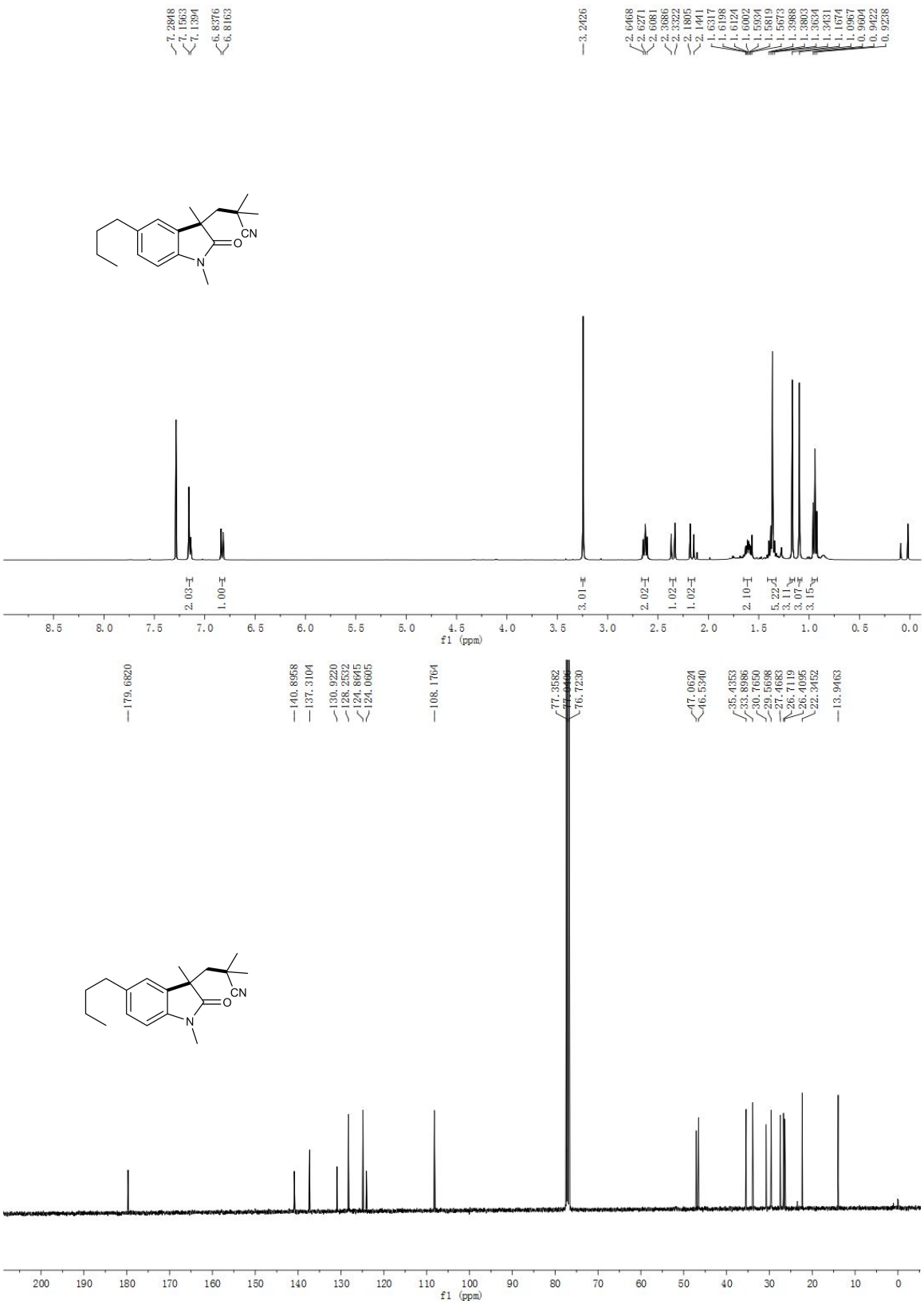
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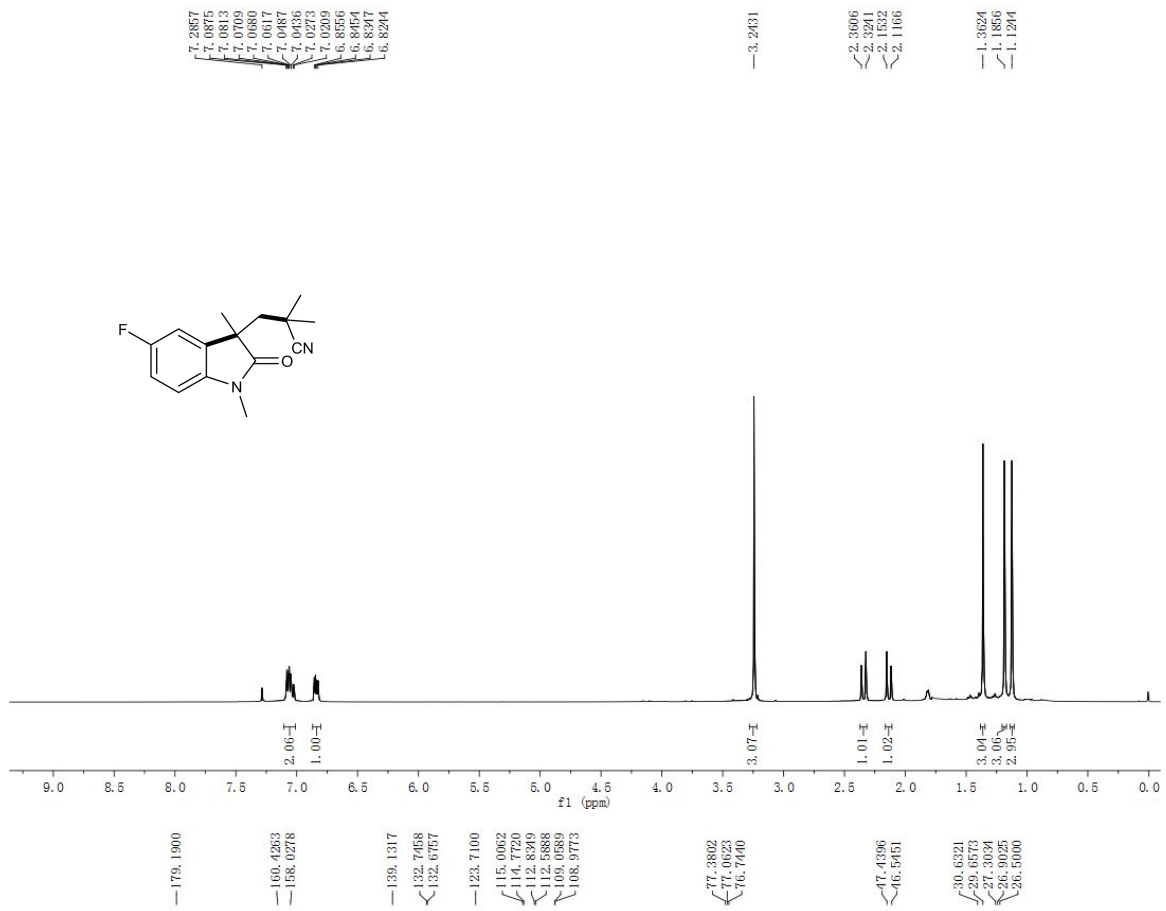
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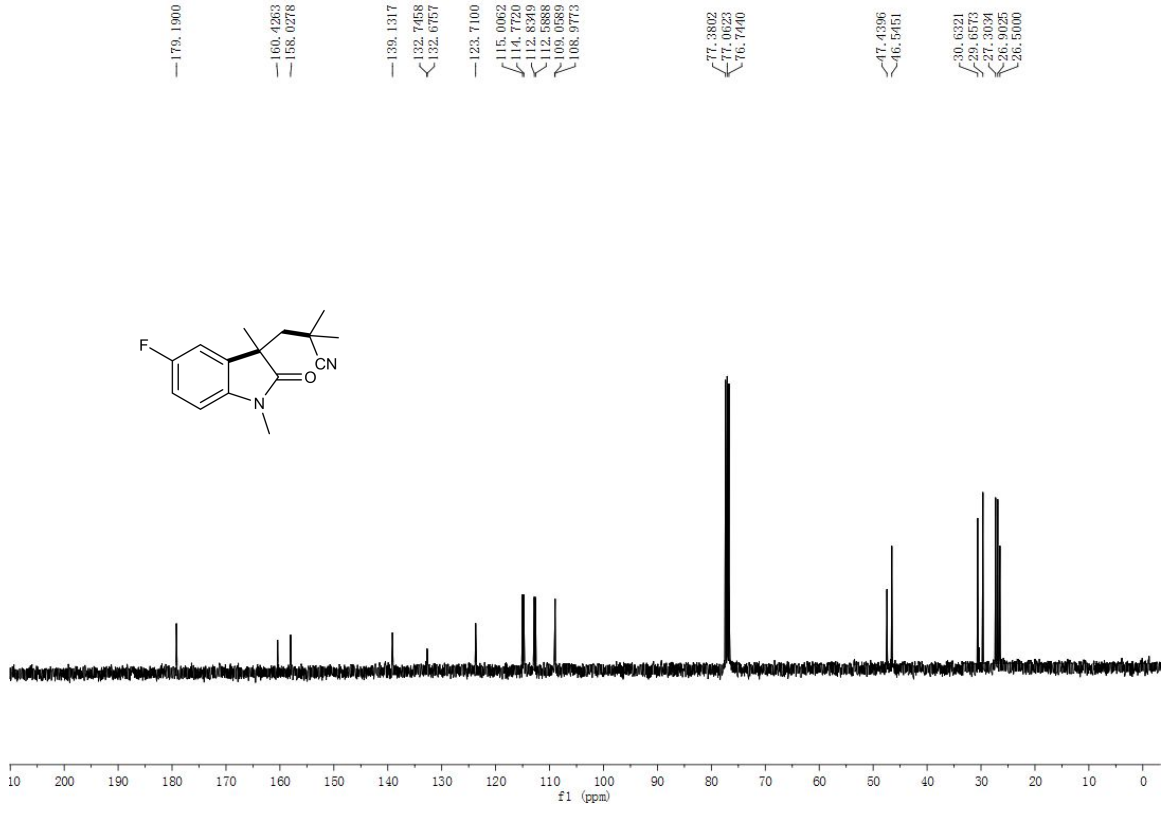
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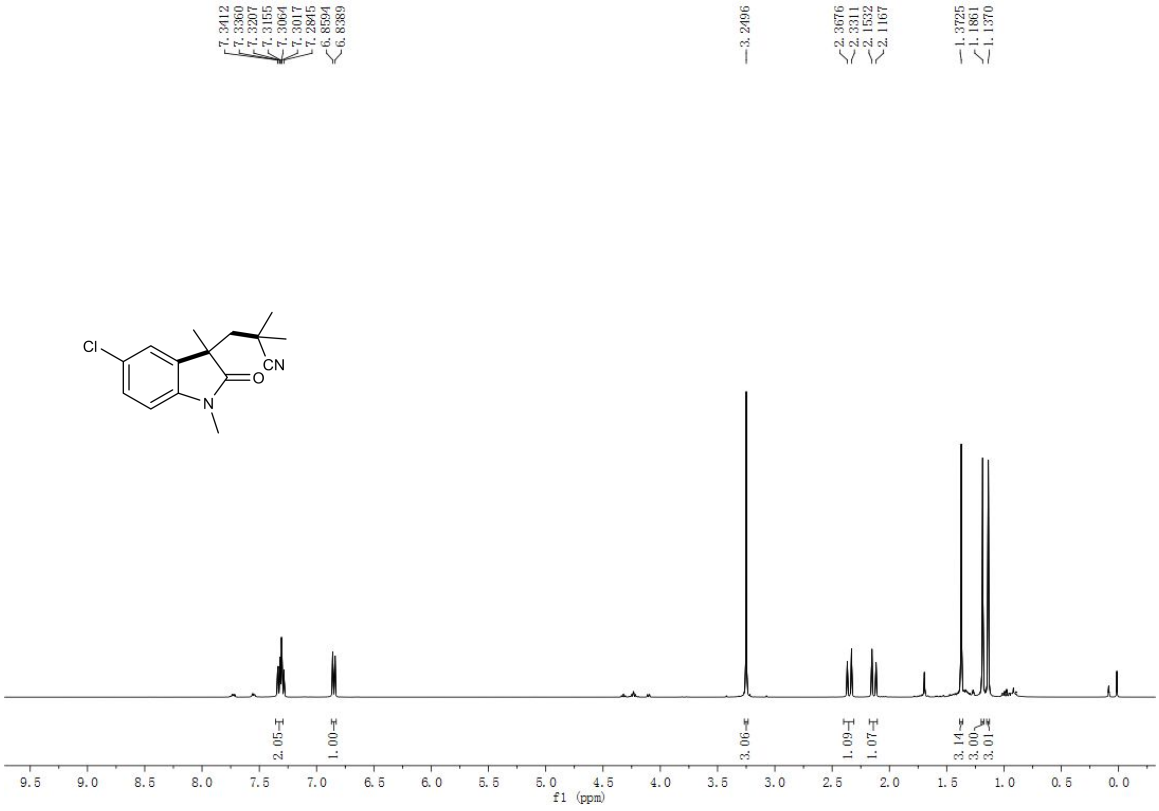
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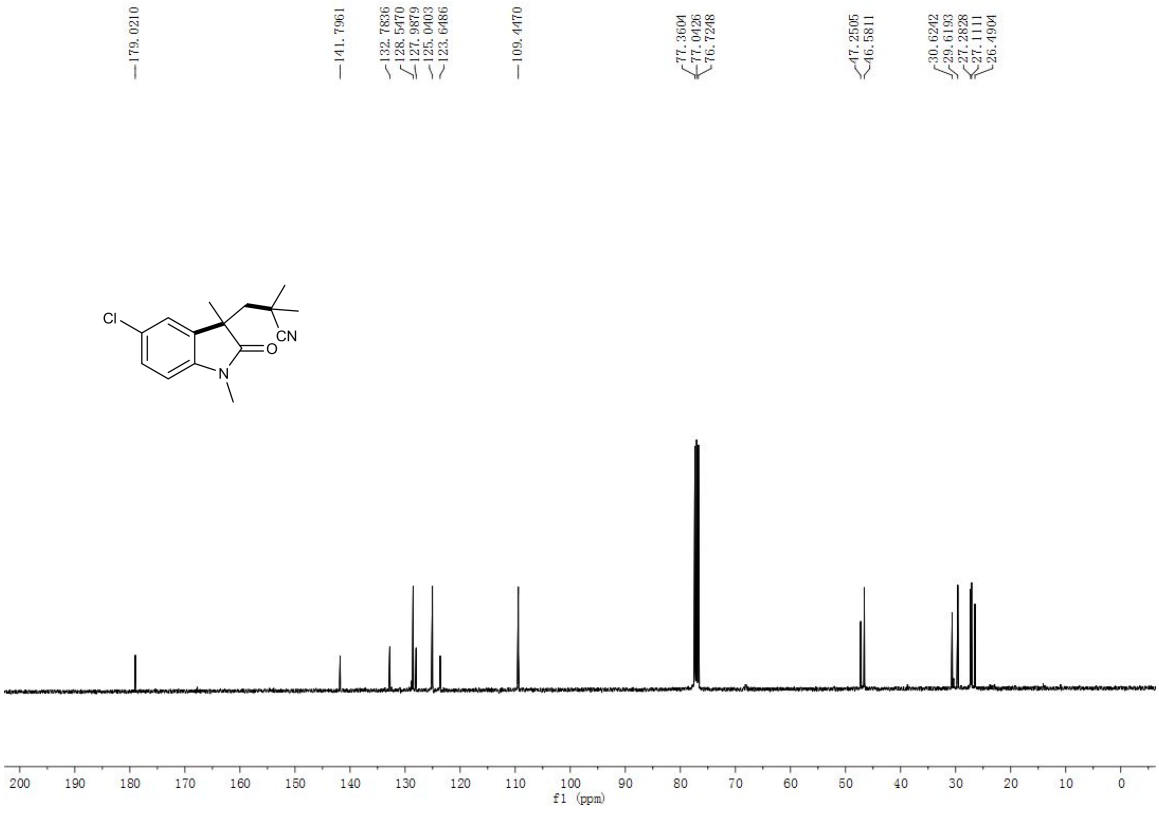
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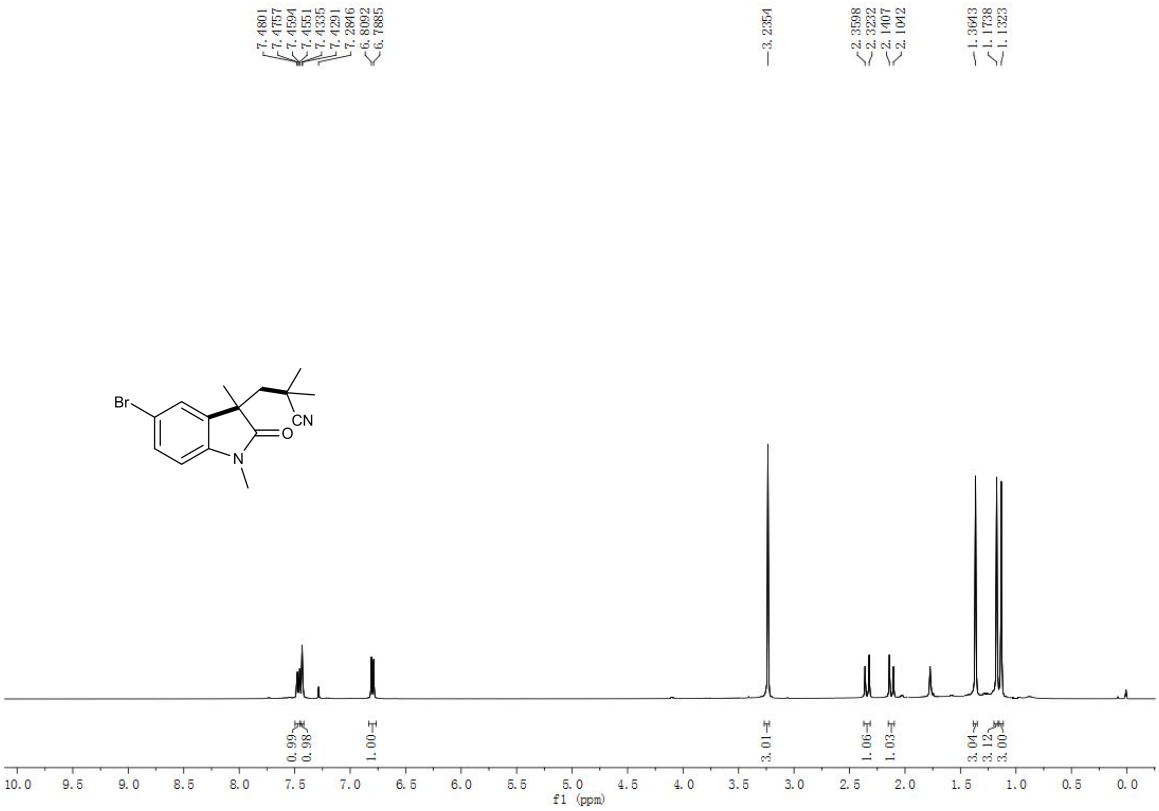
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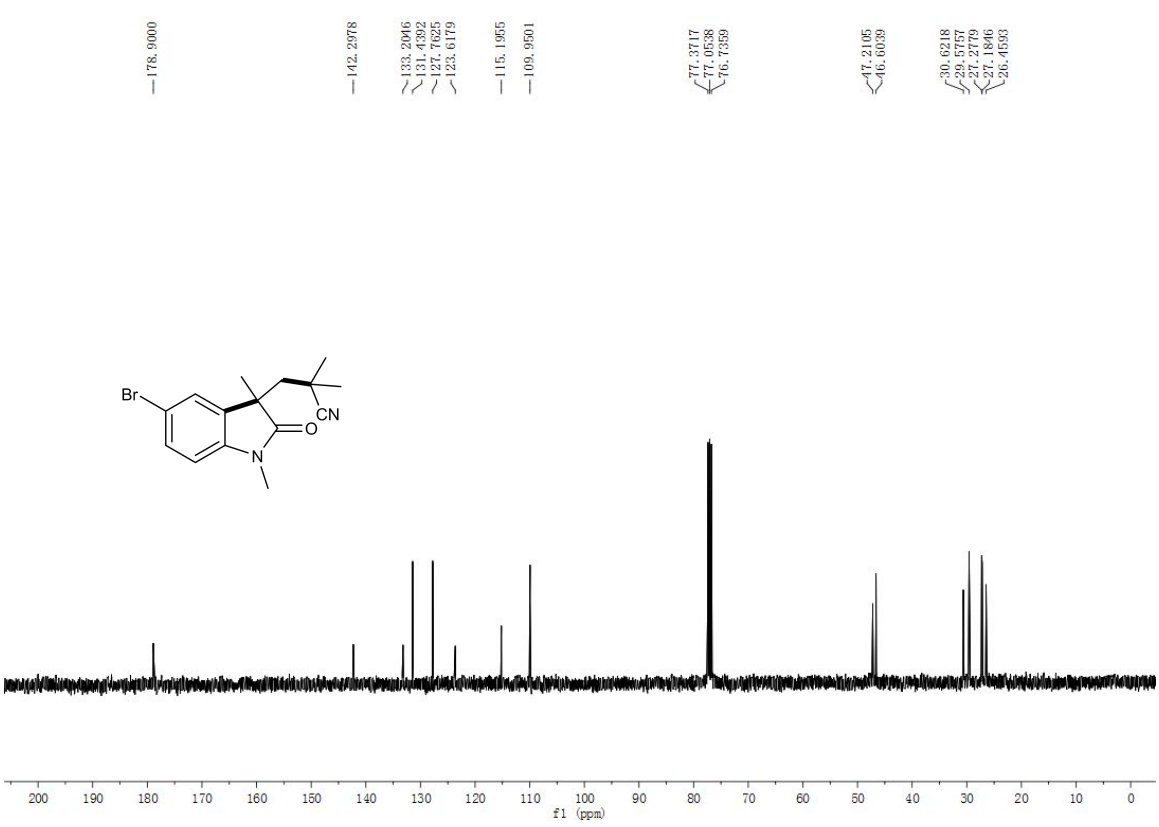
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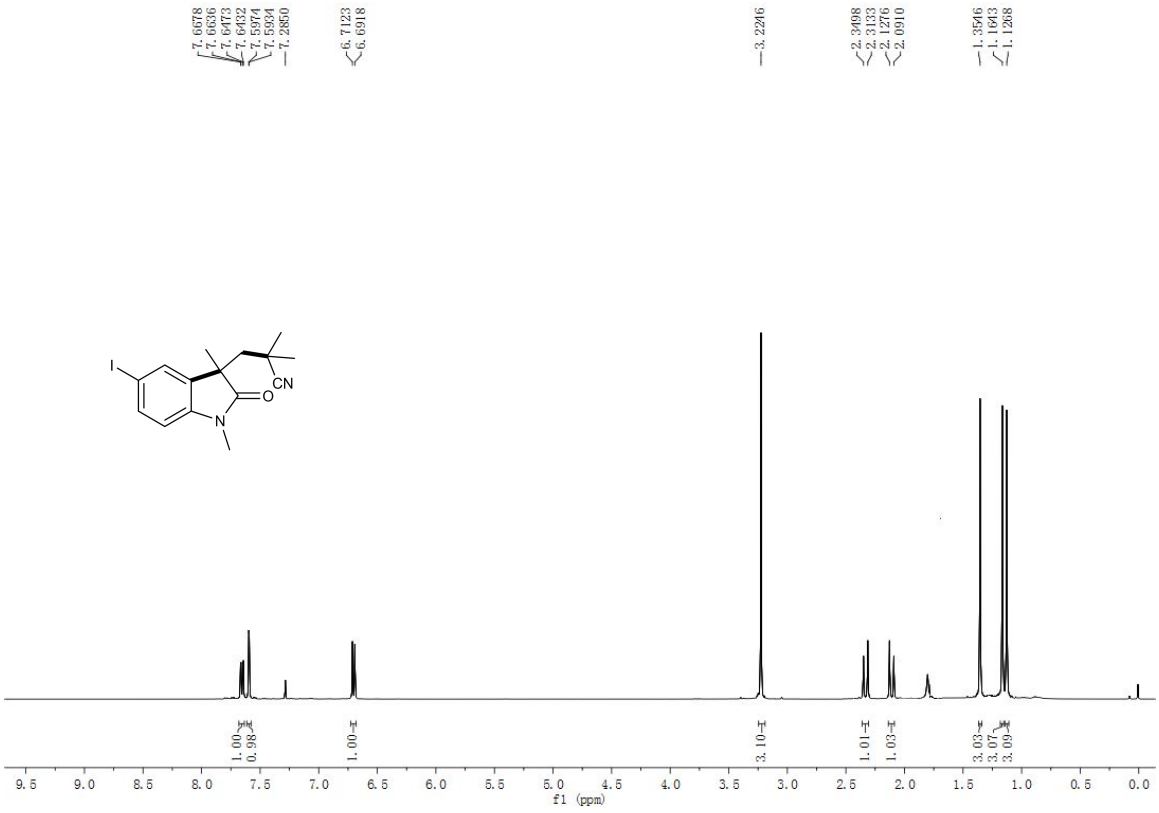
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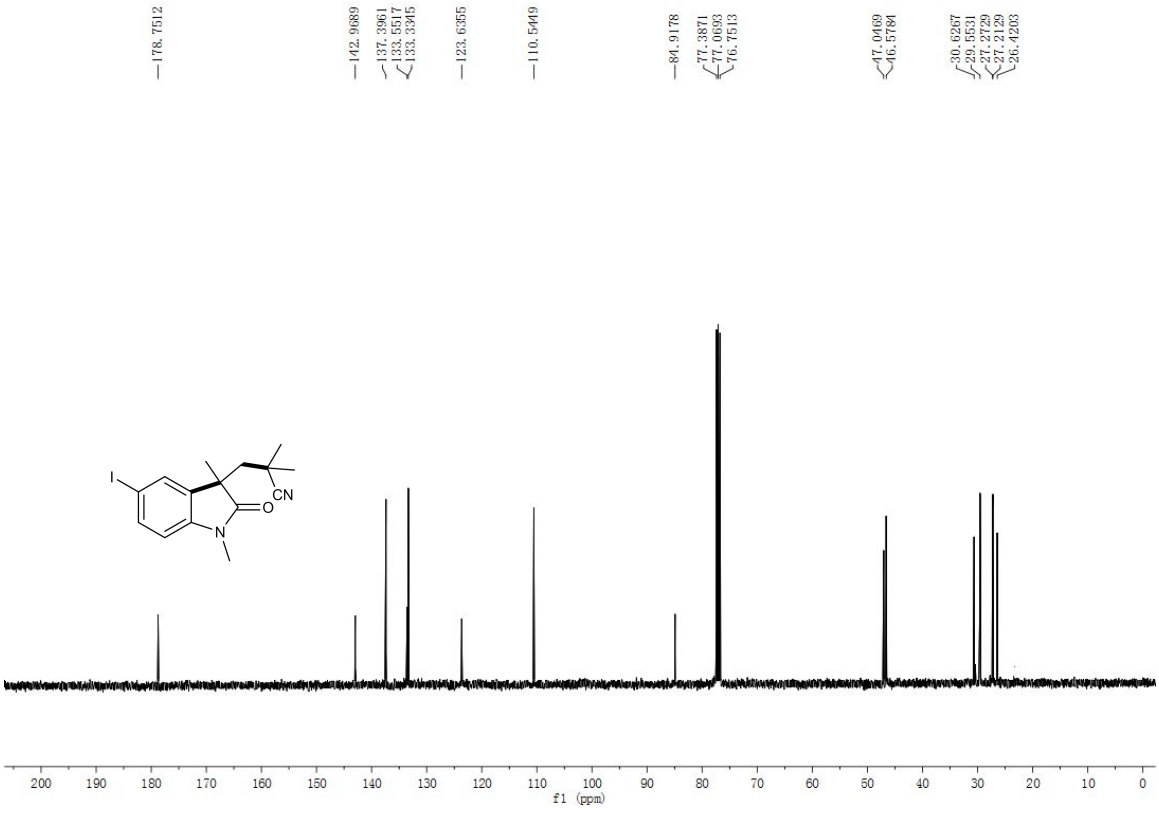
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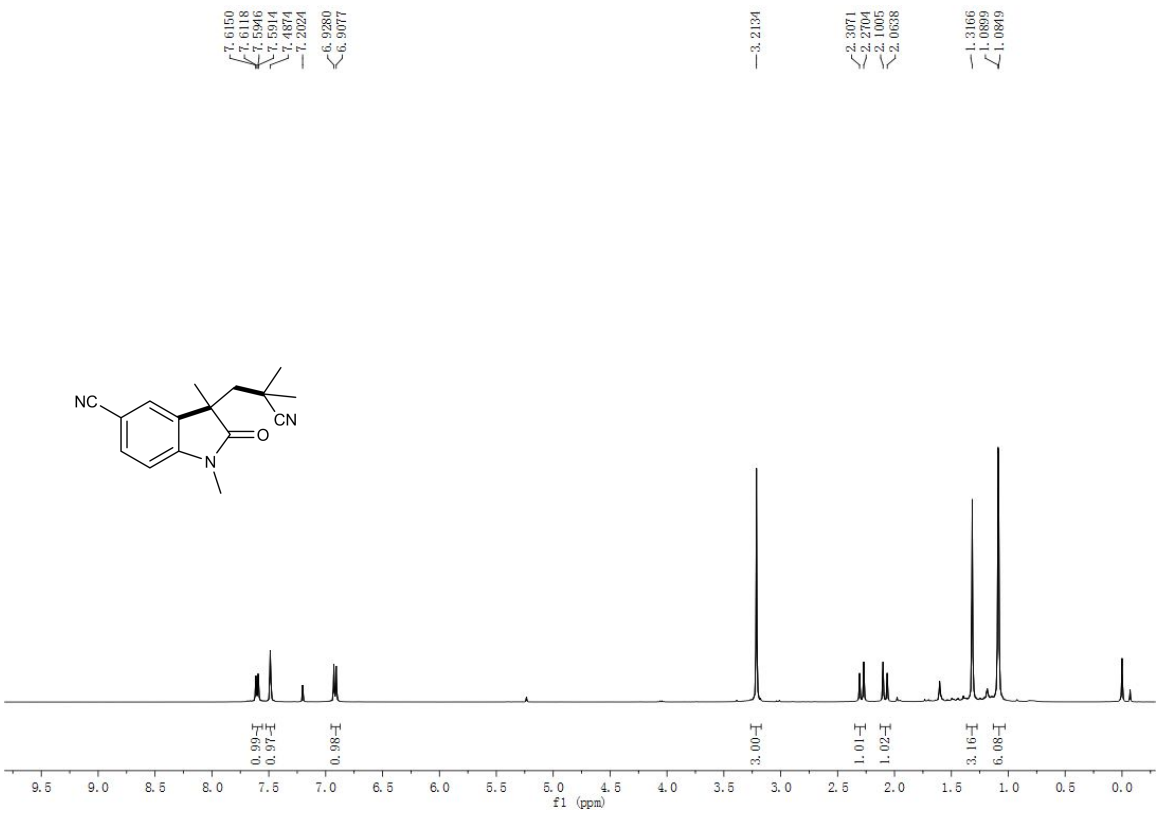
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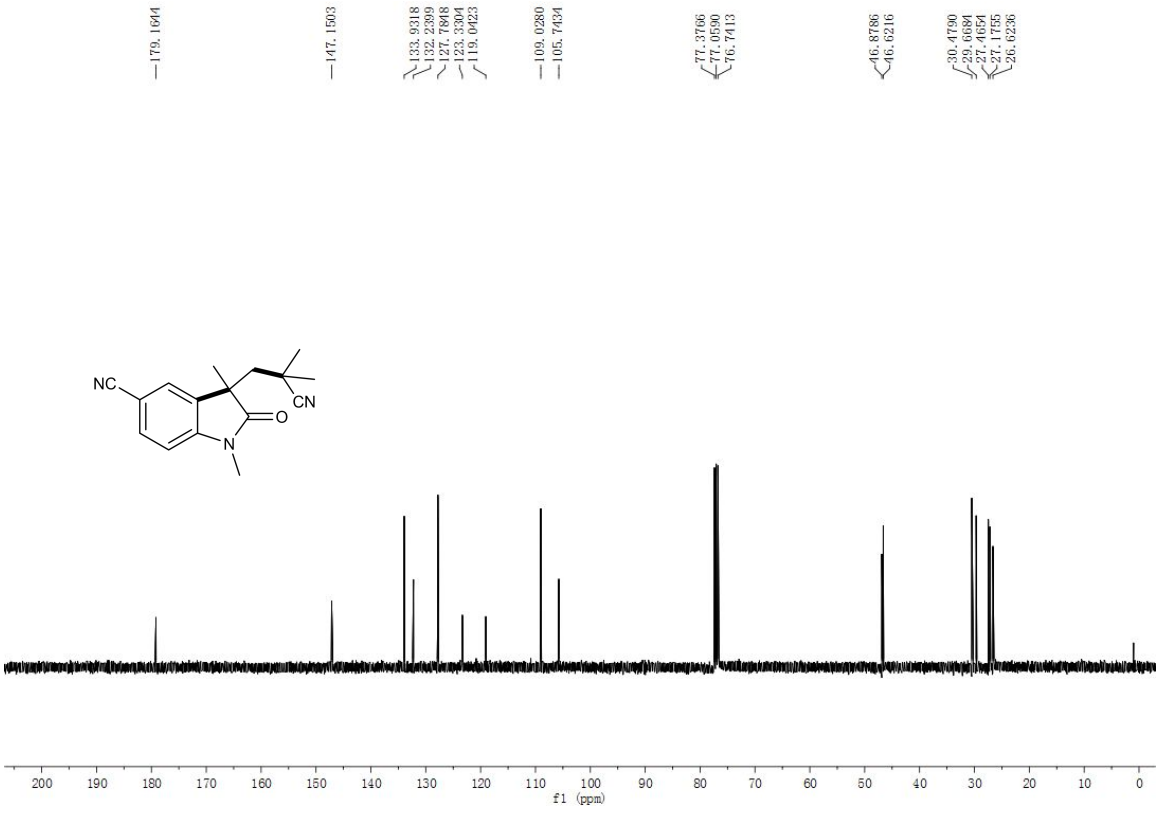
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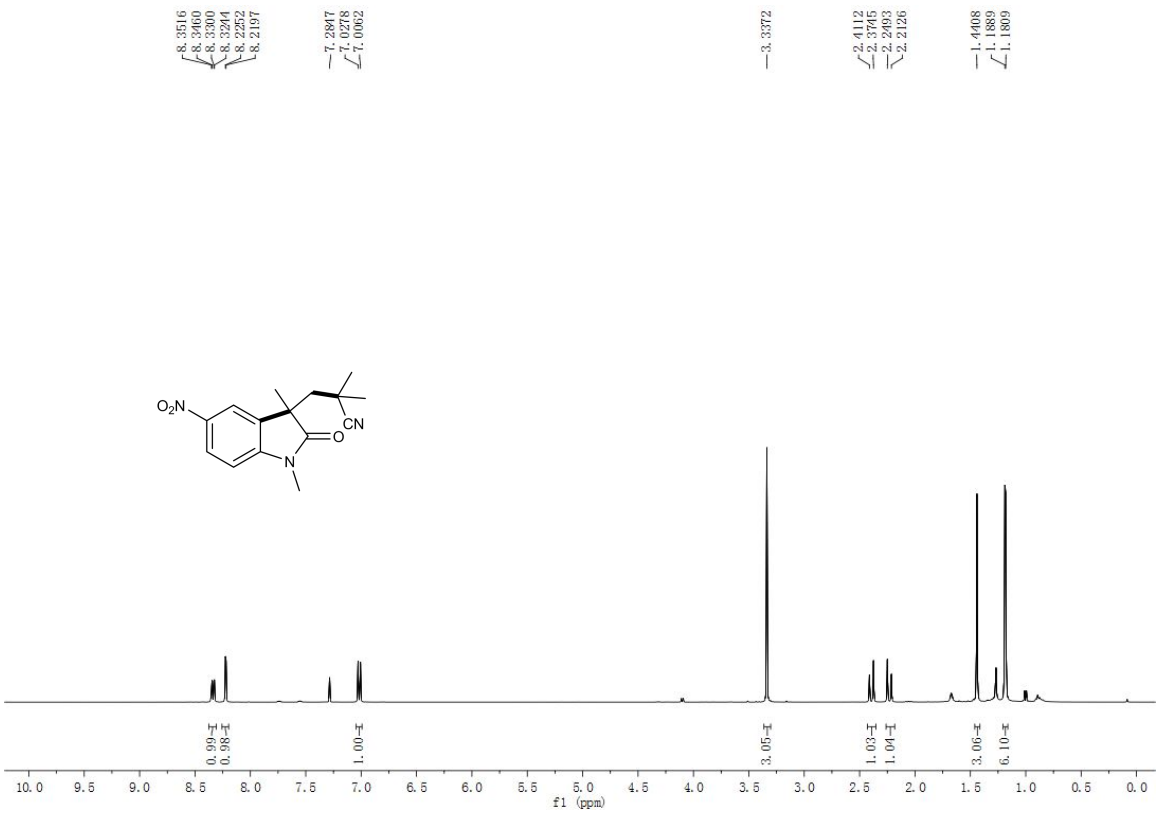
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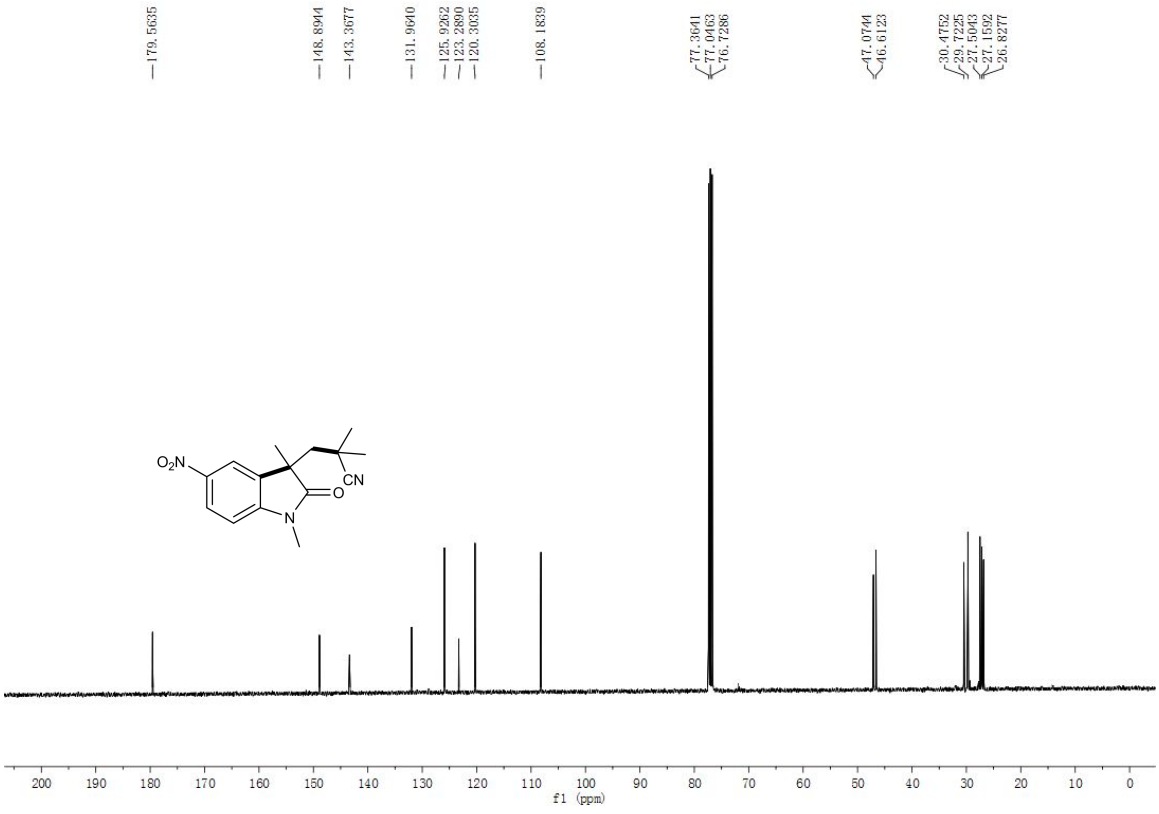
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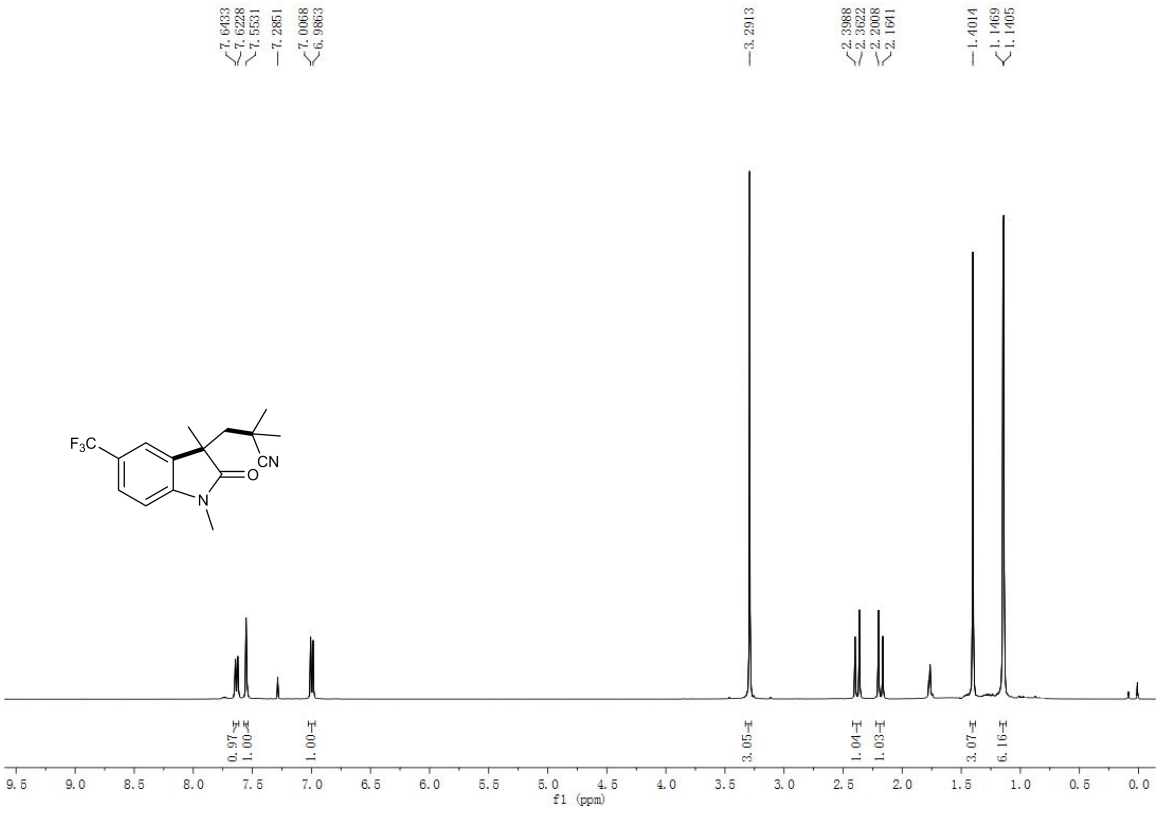
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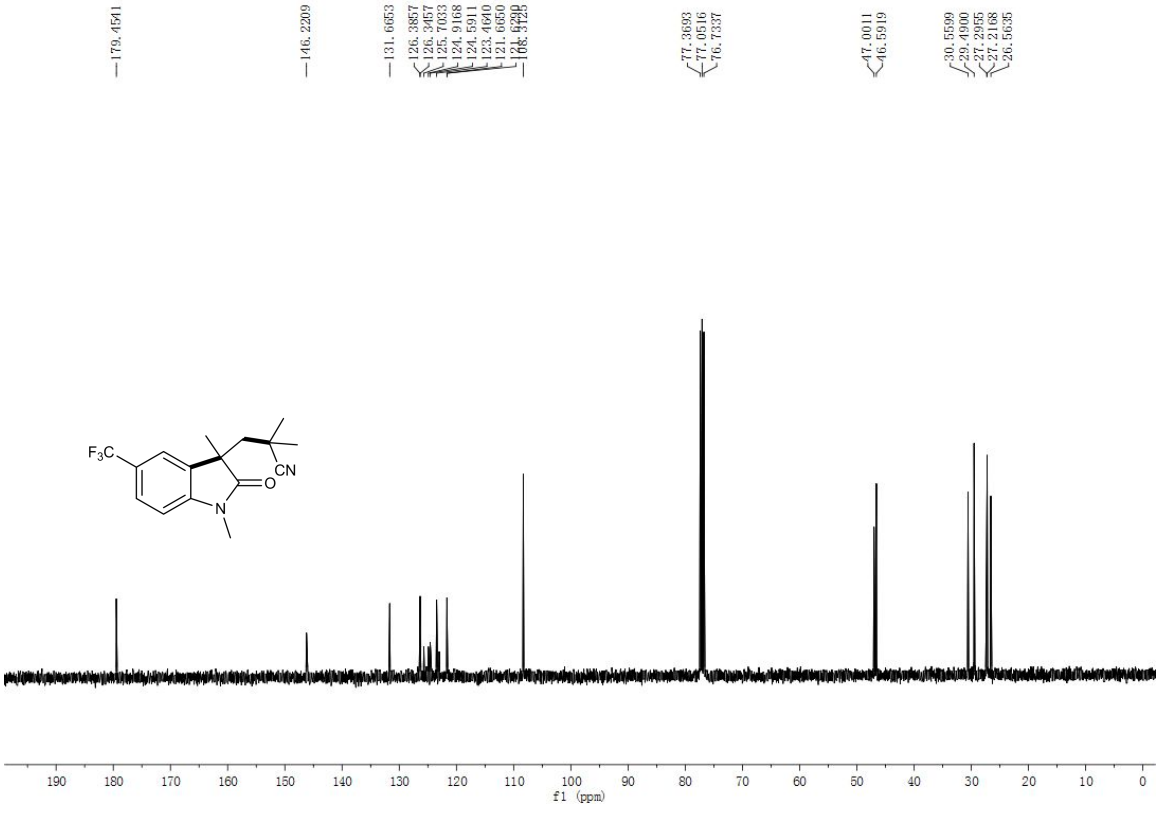
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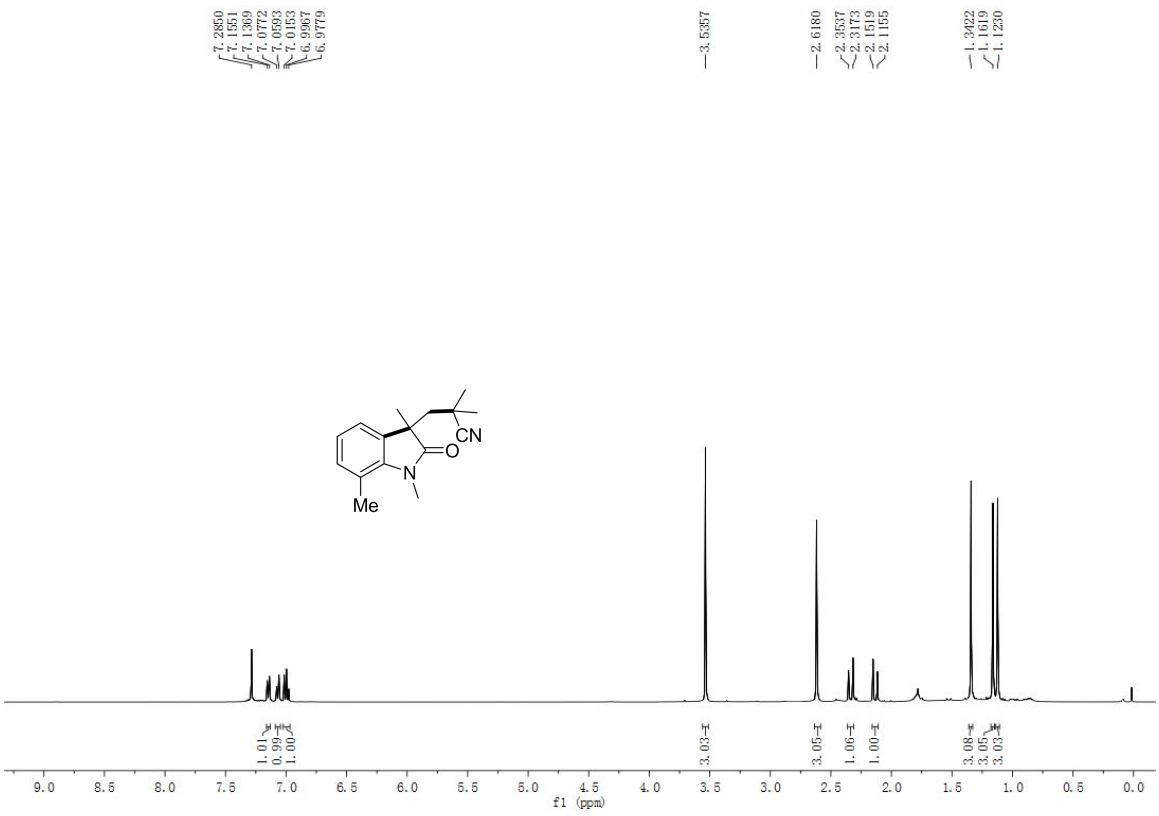
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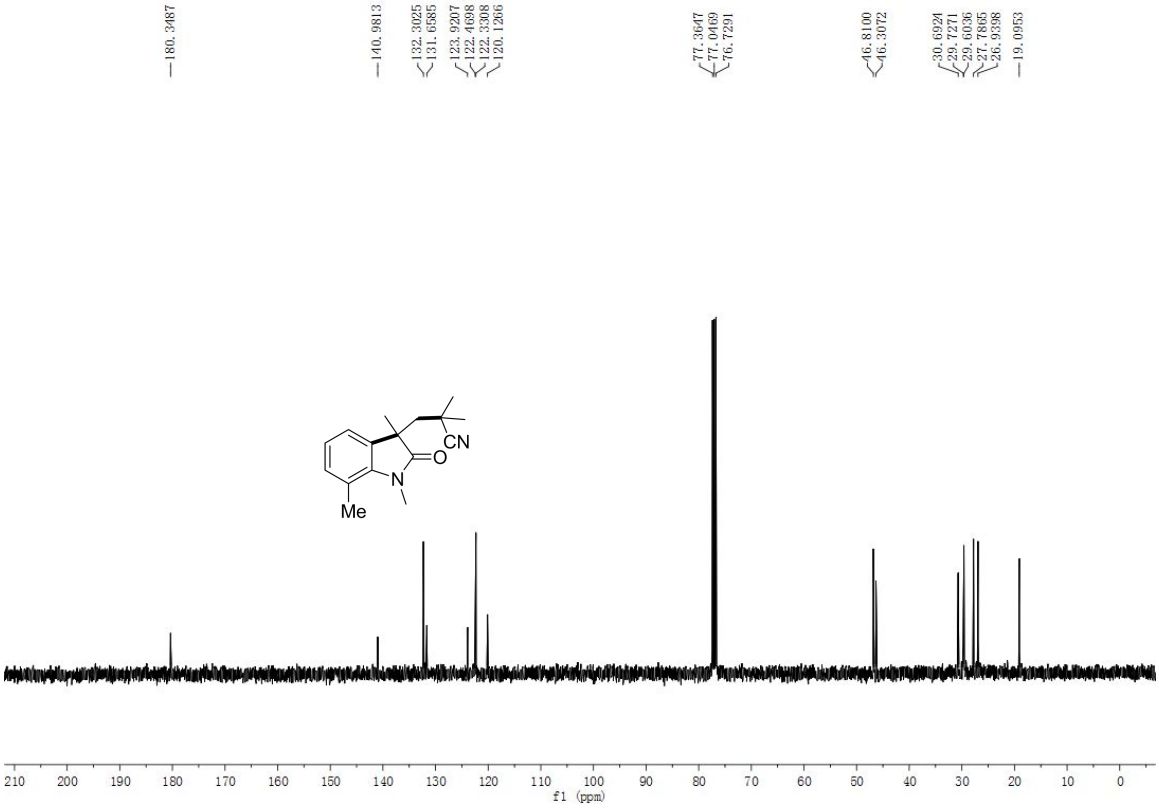
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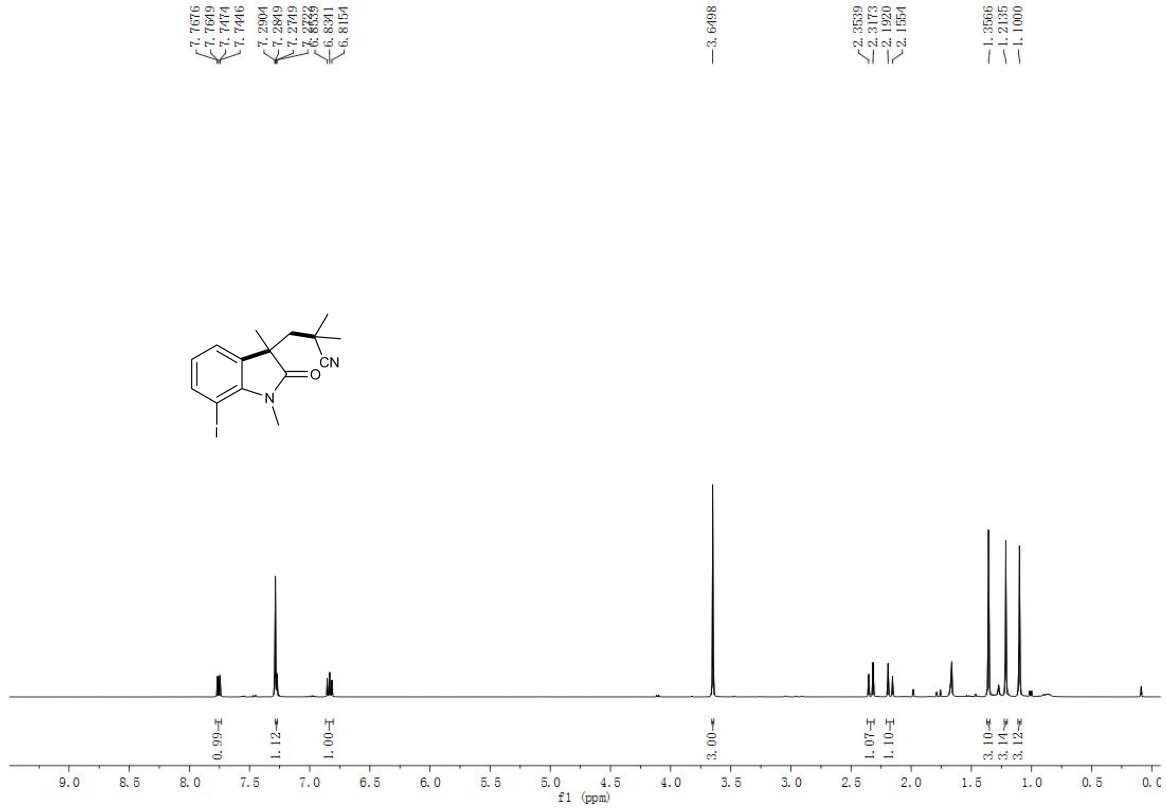
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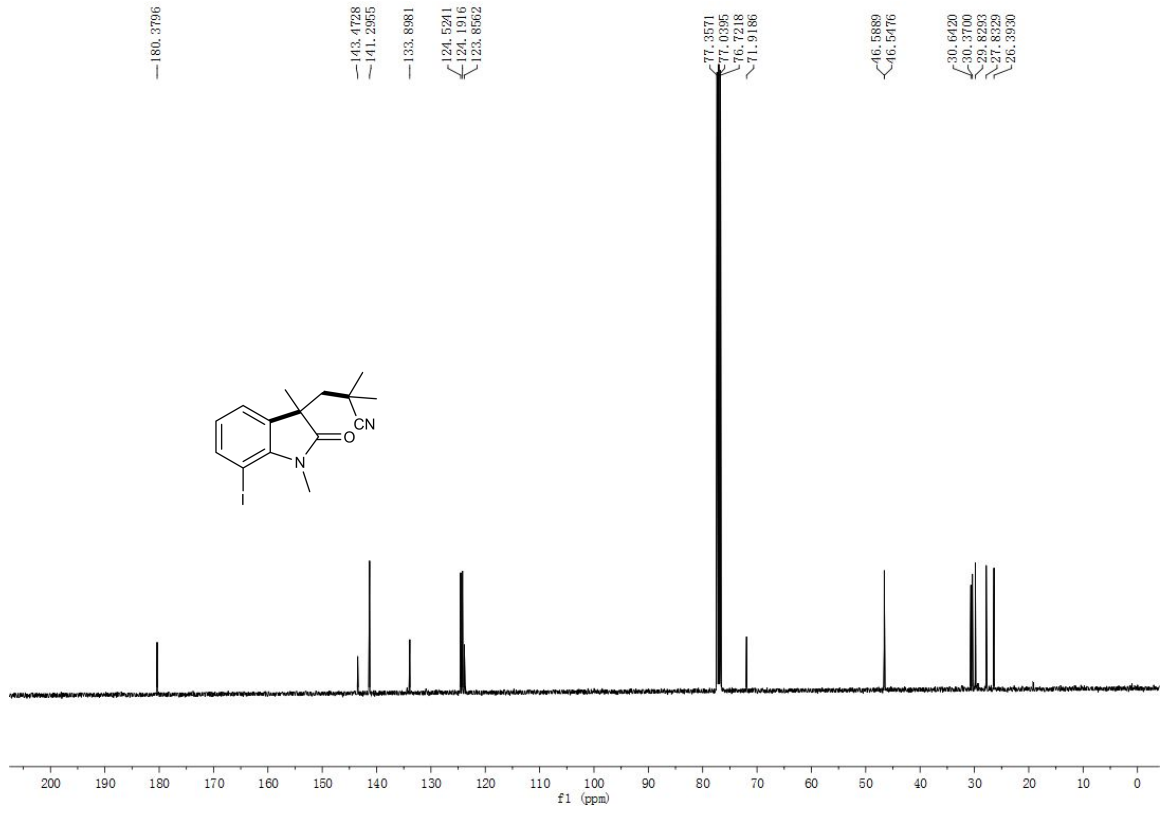
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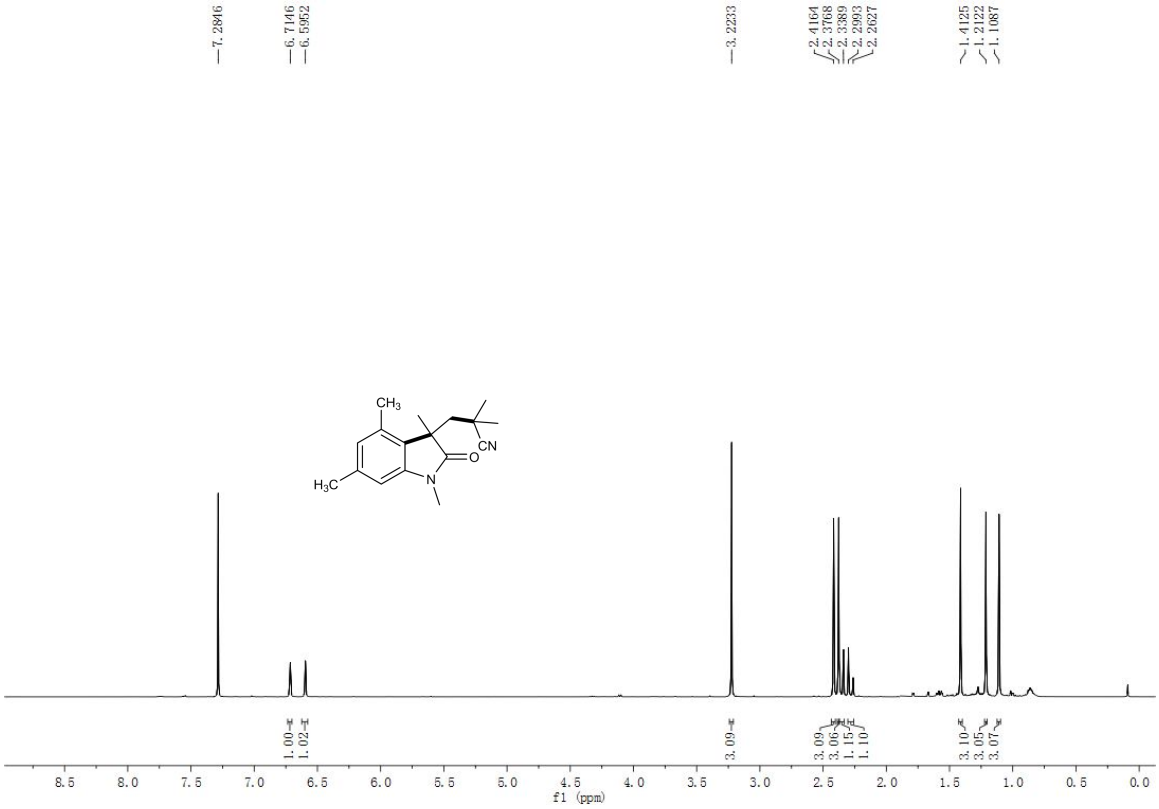
O
N
I
f1 (ppm)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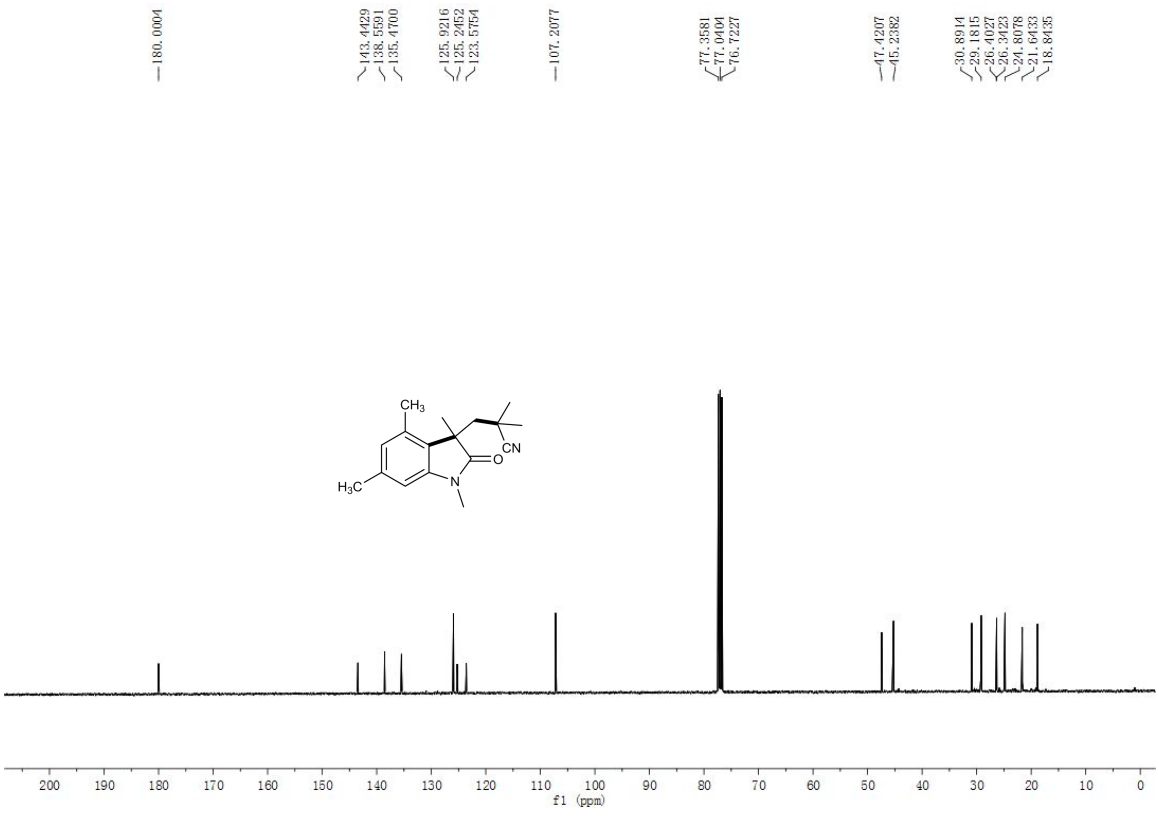
6.5952
3.2233
2.4164
2.3768
2.3389
2.2993
2.2627
1.4125
1.2122
1.1087
CH3
CN
O
H3C
N
1.00
1.02
3.09
3.09
3.06
1.15
1.10
3.10
3.05
3.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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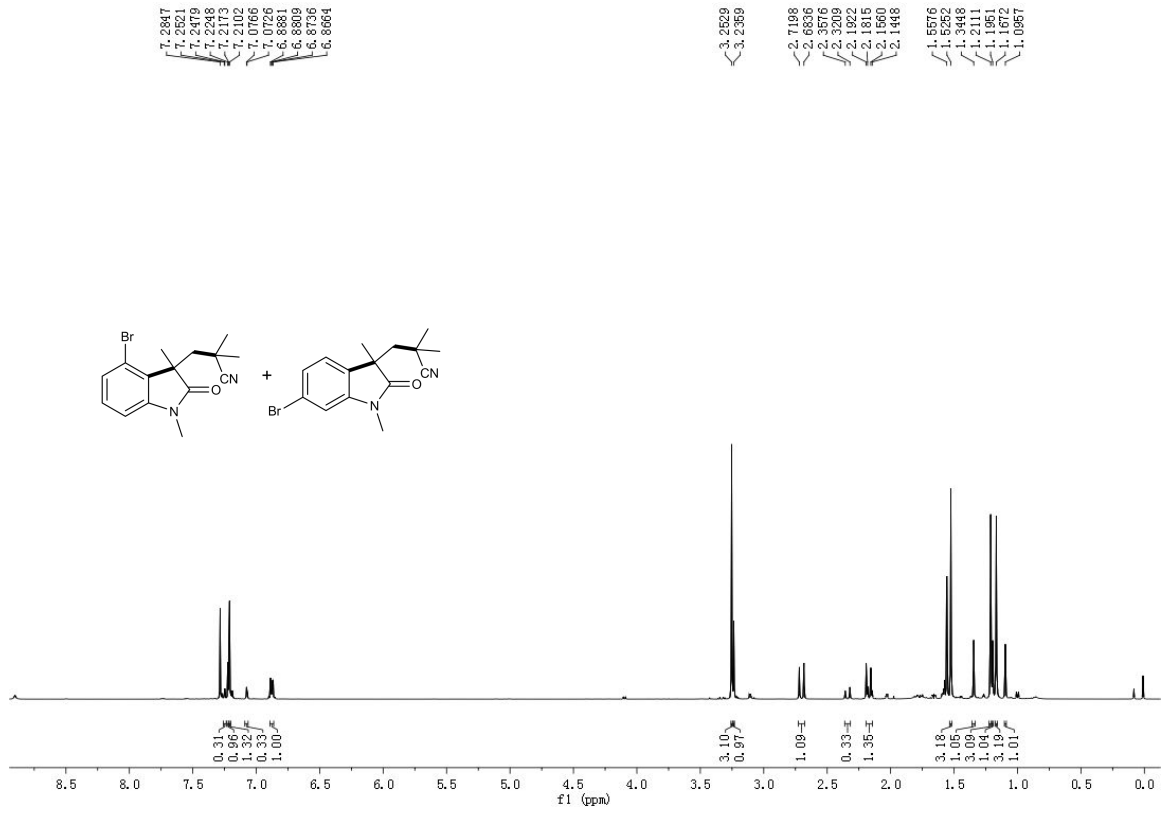
138.5591
135.4700
125.9216
125.2452
123.5754
107.2077
77.3581
77.0404
76.7227
47.4207
45.2382
30.8914
29.1815
26.4027
26.3423
24.8078
21.6433
18.8435
CH3
CN
O
H3C
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.2479
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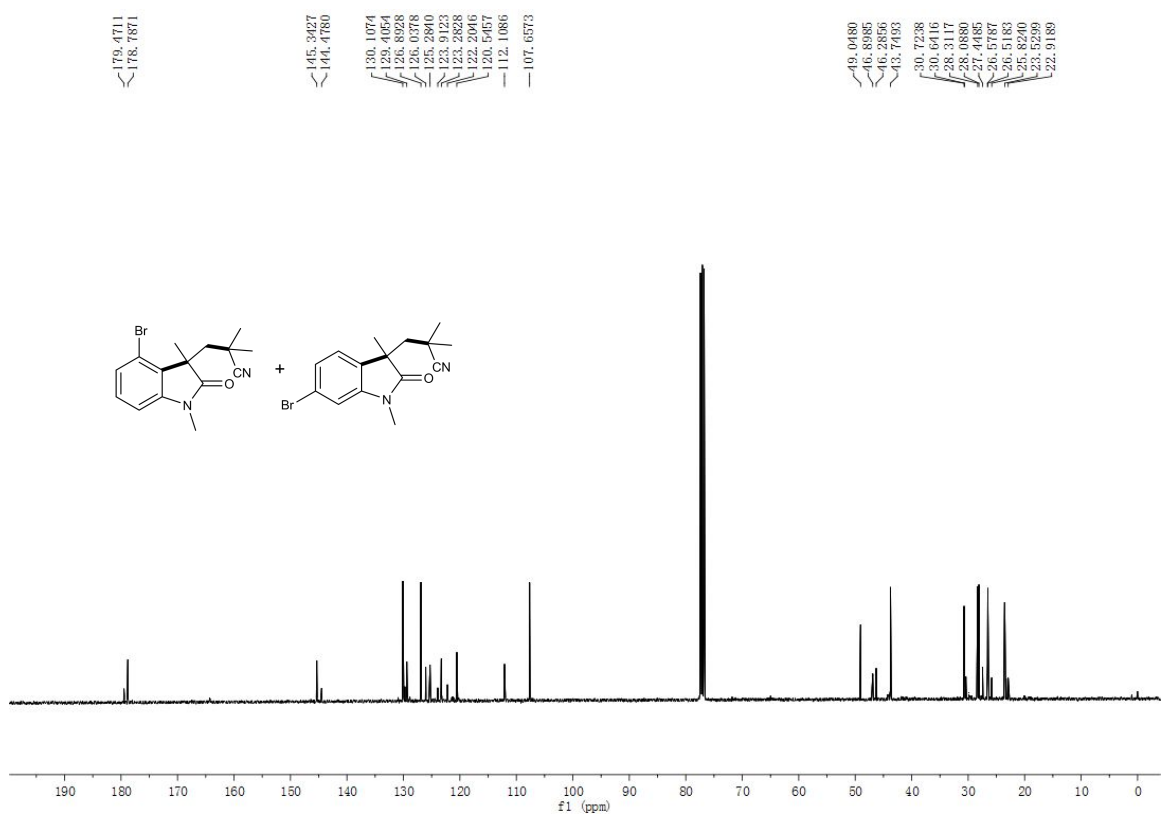
7.2173
7.2102
7.0766
7.0726
6.8881
6.8809
6.8736
6.8664
3.2629
3.2359
2.7198
2.6836
2.3676
2.3209
2.1922
2.1815
2.1560
2.1448
1.5576
1.5252
1.3448
1.2111
1.1961
1.1672
1.0967
Br
CN
O
N
+
0.31
0.96
1.32
0.33
1.00
3.10
0.97
1.09
0.33
1.35
3.18
1.05
3.09
1.04
3.19
1.01
f1 (ppm)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178.7871
145.3427
144.4780
130.1074
129.4654
126.8928
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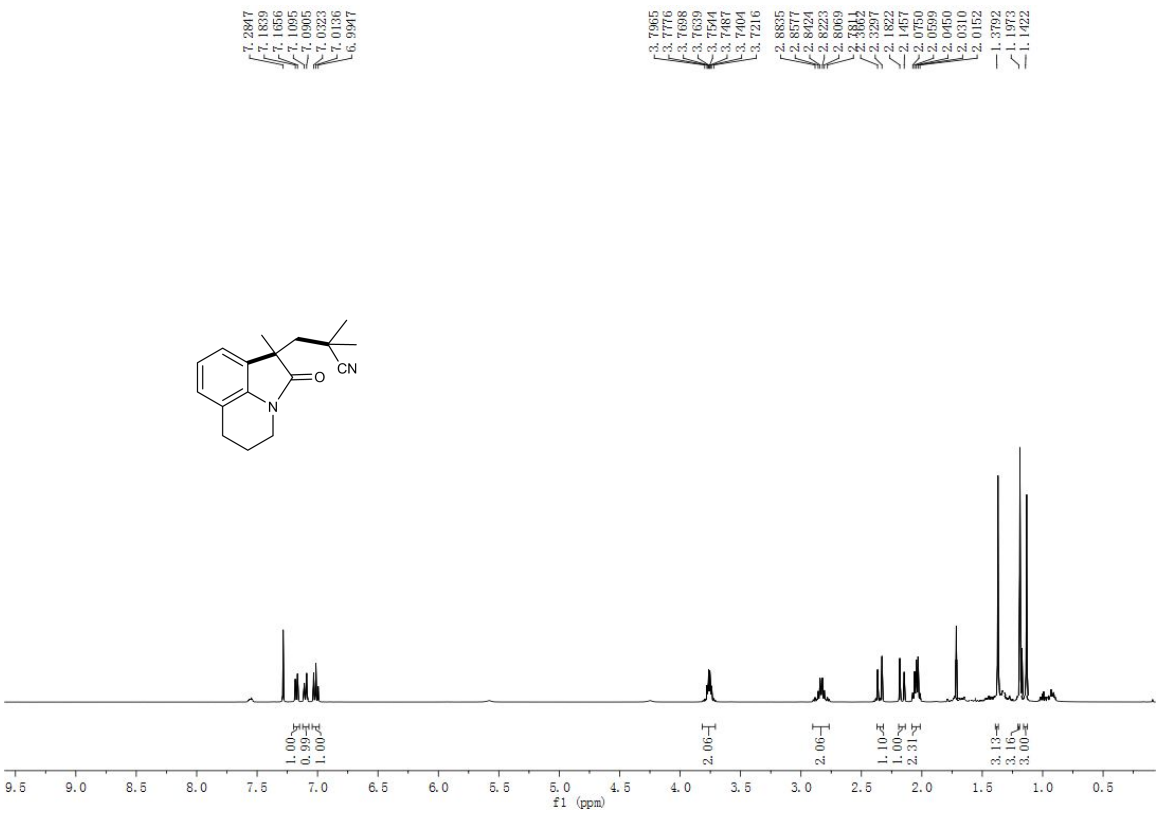
125.2840
123.9123
123.2828
122.2046
120.5457
112.1086
107.6573
49.0480
46.8985
46.2856
43.7493
30.7238
30.6416
28.3117
28.0880
27.4485
26.5787
26.5183
25.8240
23.5299
22.9189
Br
CN
O
N
+
f1 (ppm)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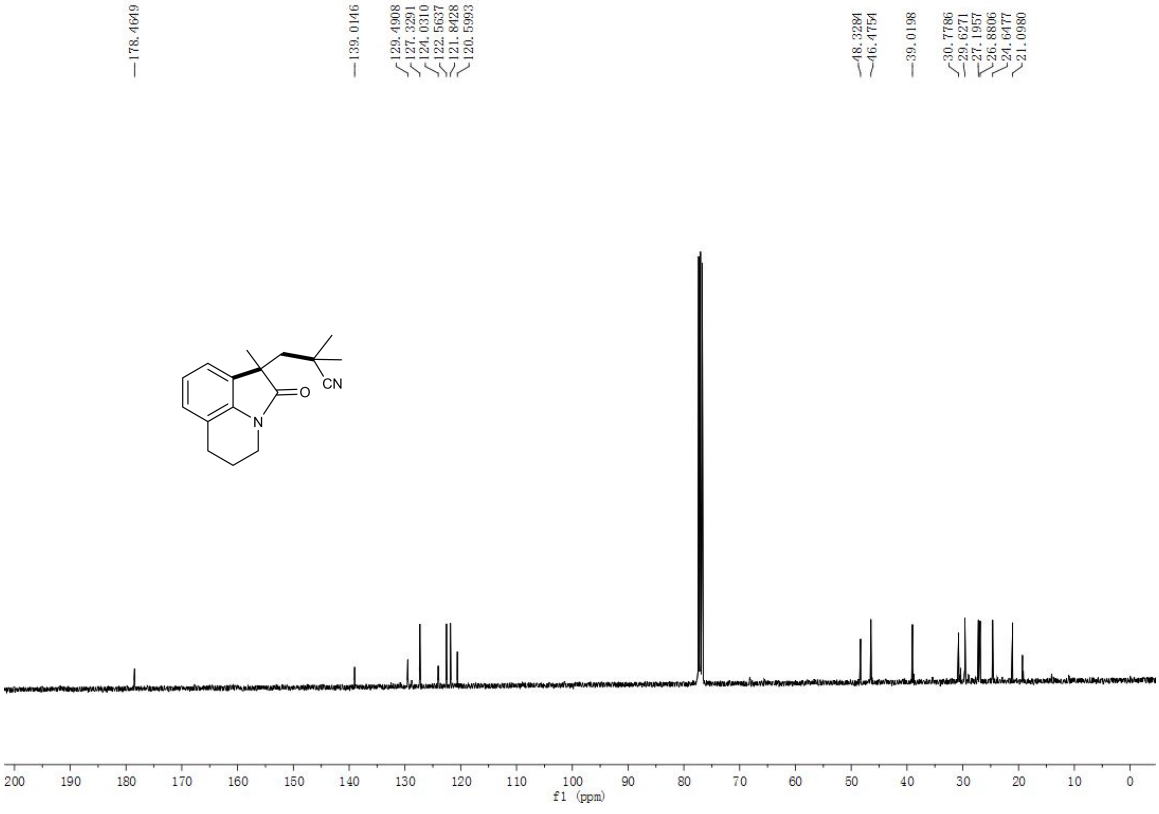
7.1656
7.1095
7.0905
7.0323
7.0136
6.9947
3.7965
3.7776
3.7698
3.7639
3.7594
3.7487
3.7404
3.7216
2.8835
2.8577
2.8424
2.8223
2.8069
2.3862
2.3297
2.1822
2.1457
2.0750
2.0599
2.0450
2.0310
2.0152
1.3792
1.1973
1.1422
CN
O
N
1.00
0.99
1.00
2.06
2.06
1.10
1.00
2.31
3.13
3.16
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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129.4908
127.3291
124.0310
122.5637
121.8428
120.5993
48.3284
46.4754
39.0198
30.7786
29.6271
27.1957
26.8806
24.6477
21.0980
CN
O
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.3817
7.3636
7.2837
7.2629
7.2440
7.1421
7.1237
7.1046
7.0958
7.0684
7.0511
7.0330
7.0160
6.7559
6.7382
6.6301
6.6109
3.0767
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2.9613
2.9395
2.5031
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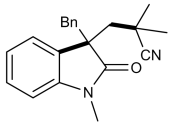
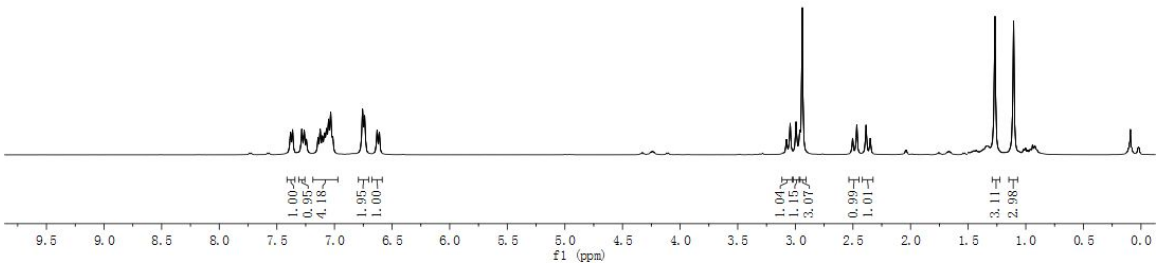
2.3861
2.3496
1.2675
1.1058


Bn
CN
O
N


1.00
0.95
4.18
1.95
1.00
1.04
1.15
3.07
0.99
1.01
3.11
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


178.1440
143.7735
134.2603
129.9649
128.7379
128.6221
127.3696
126.7428
125.9916
124.2691
121.9221
108.1165
77.3571
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76.7218
53.0639
46.8113
45.0898
30.7629
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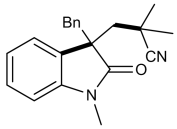
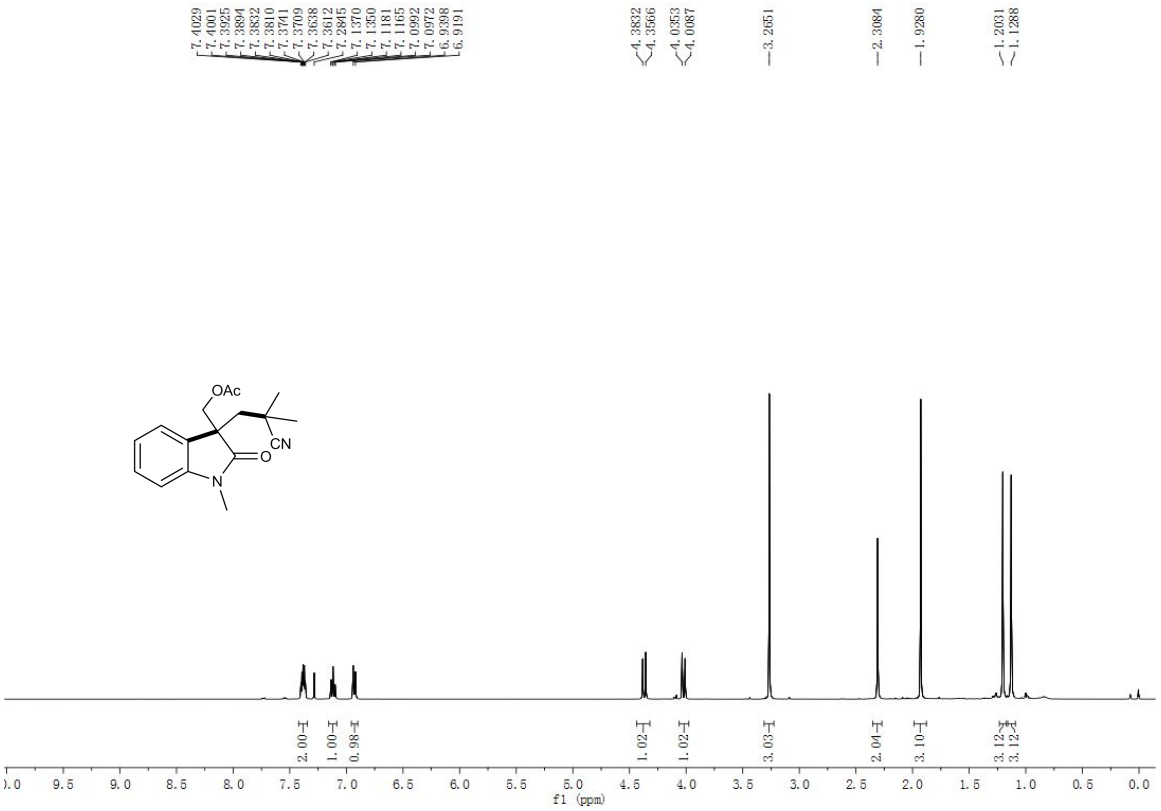
26.4762
25.9075


Bn
CN
O
N

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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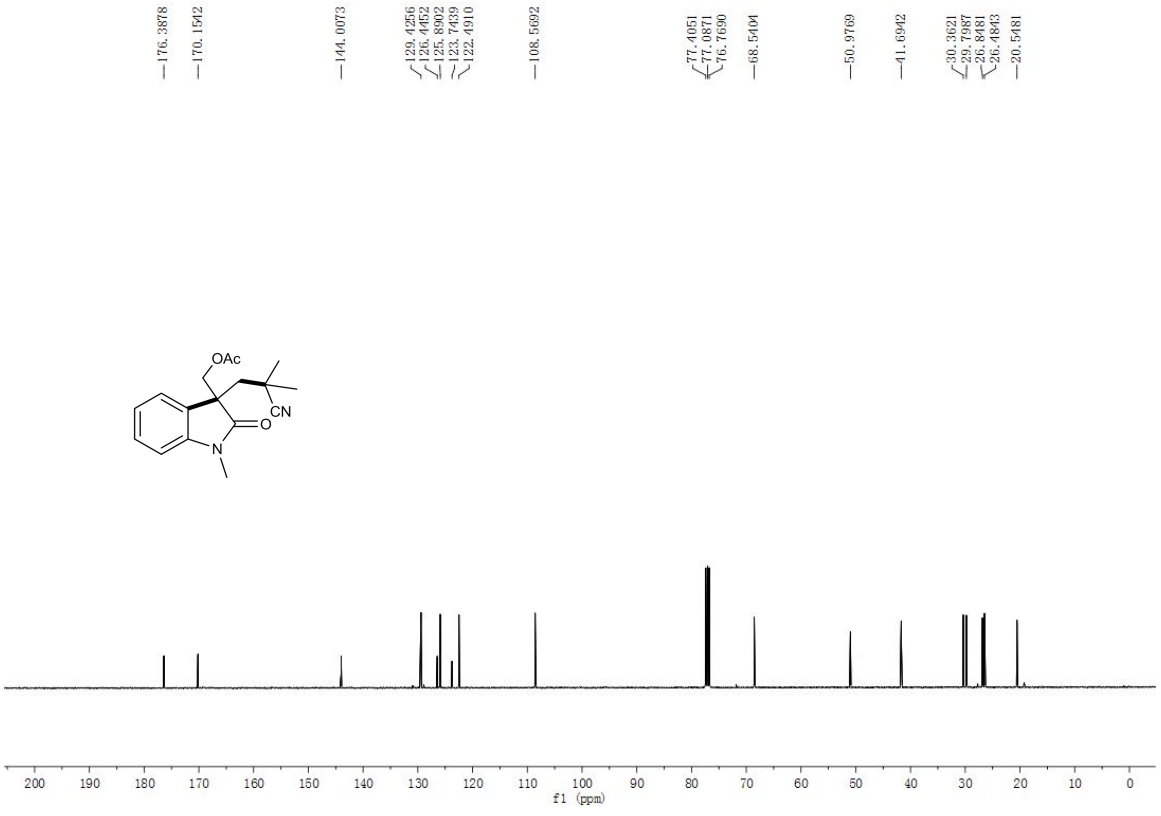
7.4001
7.3925
7.3894
7.3832
7.3810
7.3741
7.3709
7.3638
7.3612
7.2845
7.1370
7.1350
7.1181
7.1165
7.0992
7.0972
6.9398
6.9191
4.3832
4.3566
4.0353
4.0087
3.2651
2.3084
1.9280
1.2031
1.1288
OAc
CN
O
N
2.00
1.00
0.98
1.02
1.02
3.03
2.04
3.10
3.12
3.12
f1 (ppm)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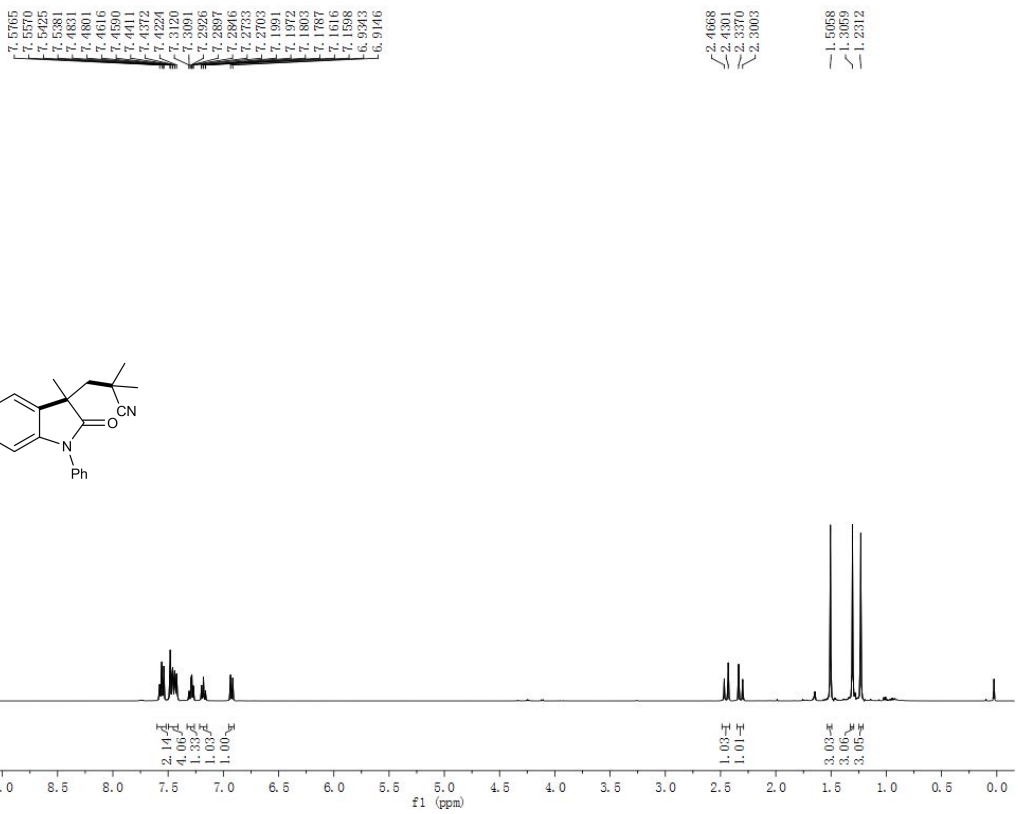
170.1542
144.0073
129.4256
126.4452
125.8902
123.7439
122.4910
108.5692
77.4051
77.0871
76.7690
68.5404
50.9769
41.6942
30.3621
29.7987
26.8481
26.4843
20.5481
OAc
CN
O
N
f1 (ppm)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7.5425
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7.4831
7.4801
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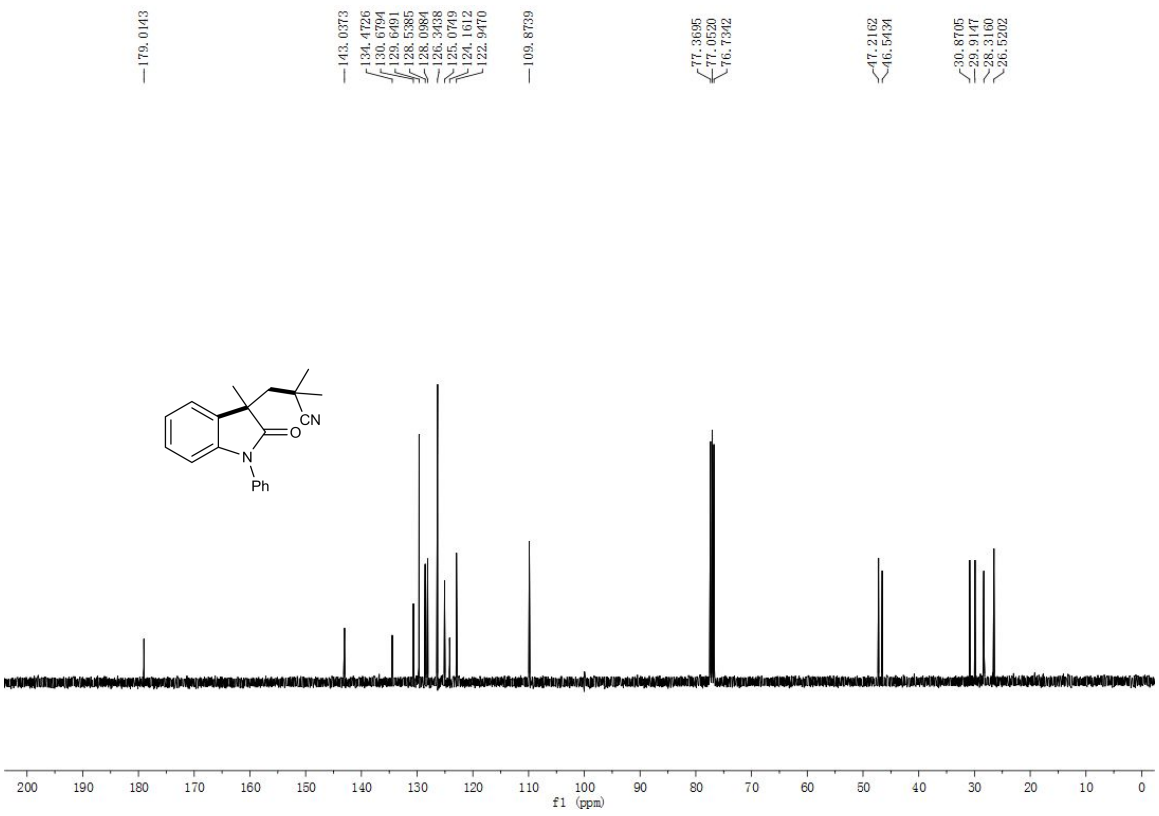
7.4590
7.4411
7.4372
7.4224
7.3120
7.3091
7.2926
7.2897
7.2846
7.2733
7.2703
7.1991
7.1972
7.1803
7.1787
7.1616
7.1598
6.9343
6.9146
2.4668
2.4301
2.3370
2.3003
1.5058
1.3059
1.2312
CN
O
N
Ph
2.14
4.06
1.33
1.03
1.00
1.03
1.01
3.03
3.06
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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134.4726
130.6794
129.6491
128.5385
128.0984
126.3938
125.0749
124.1612
122.9470
109.8739
77.3695
77.0520
76.7342
47.2162
46.5434
30.8705
29.9147
28.3160
26.5202
CN
O
N
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)