Supporting Information

Synthesis of *N*-alkyl isatins via oxidative cyclization of *N*-alkyl 2-bromo(chloro)acetanilides

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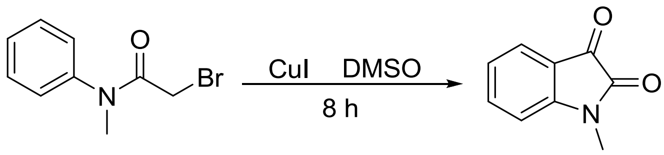
General information

All the solvents and commercially available reagents were purchased from commercial sources and used directly. ^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ at room temperature on the Varian INOVA-400 spectrometer (400 MHz ^{1}H). The chemical-shifts scale is based on internal TMS. The coupling constants, *J*, are reported in Hertz (Hz). Products were purified by flash column chromatography on 200-300 mesh silica gel, SiO2. ICP-MS data were obtained using a Perkin Elmer OPTIMA5300 DV. High-resolution mass spectra (HRMS) were performed using electron impact ionization.

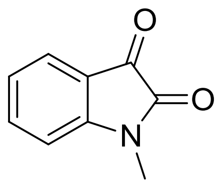
Experimental section



To a stirred solution of 3.0 ml of anhydrous DMSO was added CuI (0.025 mmol) and *N*-methyl-2-bromoacetanilide (0.5 mmol) at room temperature. The system was heated at 100^{o}C for 8 hours (open to air with a drying tube). After cooling to room temperature, the reaction mixture was diluted with diethyl ether (25 mL) and water (25 mL). The aqueous layer was extracted with diethyl ether (3x25 mL) and washed with brine. The organic layers were combined, dried with MgSO4, filtered, and the solvent was removed under reduced pressure. The residue was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate) to afford 68.5 mg of the desired product in 83% yield.

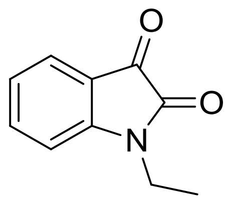
Analytical data of isatins

***N*-Methylindoline-2,3-dione (2a)**[1]



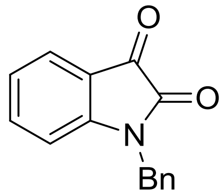
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 83% (Br)/ 78% (Cl);
red solid; m.p.: 121.7-124.5 ^{o}C;
IR(KBr)/cm^{-1}: 2930, 1749, 1615, 1486, 1253, 752;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.62 (m, 2 H), 7.14 (t, *J* = 7.9 Hz, 1 H), 6.90 (d, *J* = 7.7 Hz, 1 H), 3.26 (s, 3 H).
^{13}C NMR (100MHz, $CDCl_3$): δ 183.32, 158.21, 151.43, 138.38, 125.26, 123.81, 117.41, 109.89, 26.20.
MS (m/z) 161 (M^+).

***N*-Ethylindoline-2,3-dione (2b)**[2]



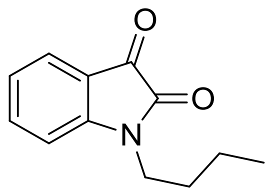
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 80% (Br)/74% (Cl);
red solid; m.p.: 122.5-124.8 °C;
IR(KBr)/cm^{-1}: 2932, 1731, 1609, 1408, 1349, 752;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.53 (m, 2 H), 7.05 (t, *J* = 7.5 Hz, 1 H), 6.85 (d, *J* = 8.2 Hz, 1 H), 3.72 (q, *J* = 7.2 Hz, 2 H), 1.25 (t, *J* = 7.2 Hz, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 183.66, 157.79, 150.57, 138.33, 125.41, 123.58, 117.49, 109.99, 34.87, 12.45;
MS (m/z) 175 (M^+).

***N*-Benzylindoline-2,3-dione (2c)** [1]



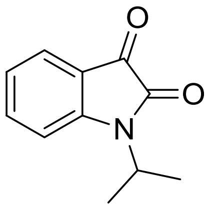
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 84% (Br)/77% (Cl);
red solid; m.p.: 127.8-129.2 °C;
IR(KBr)/cm^{-1}: 2932, 1731, 1611, 1449, 1332, 758;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.61 (d, *J* = 7.4 Hz, 1 H), 7.48 (d, *J* = 7.8 Hz, 1 H), 7.39 – 7.28 (m, 5H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.78 (d, *J* = 8.0 Hz, 1H), 4.94 (s, 2 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 183.21, 158.23, 150.68, 138.29, 134.45, 129.02, 128.13, 127.39, 125.39, 123.84, 117.63, 110.97, 44.01;
MS (m/z) 237 (M^+).

***N*-Butylindoline-2,3-dione(2d)** [3]



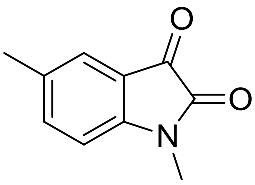
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 79%;
red solid; m.p.: 155.8-158.7 °C;
IR(KBr)/cm^{-1}: 2960, 1733, 1602, 1579, 1352, 767;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.52 (m, 2 H), 7.04 (t, *J* = 7.5 Hz, 1 H), 6.84 (m, 1 H), 3.65 (t, *J* = 7.3 Hz, 2 H), 1.61 (quint, *J* = 8.0 Hz, 2 H), 1.34 (sext, *J* = 8.0 Hz, 2 H), 0.90 (t, *J* = 7.3 Hz, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 183.62, 158.06, 150.99, 138.28, 125.34, 123.53, 117.48, 110.13, 39.93, 29.20, 20.06, 13.61;
MS (m/z) 203 (M^+).

N-Isopropylindoline-2,3-dione(2e)[3]



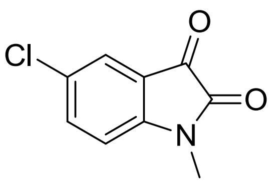
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 77% (Br)/75% (Cl);
red solid; m.p.: 124.4-125.7 °C;
IR(KBr)/cm^{-1}: 2978, 1732, 1609, 1468, 1349, 752;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.60 (m, 1H), 7.56 (d, *J* = 7.8 Hz, 1 H), 7.10 (t, *J* = 7.5 Hz, 1 H), 7.04 (d, *J* = 8.0 Hz, 1 H), 4.54 (m, 1 H), 1.53 (d, *J* = 7.0 Hz, 6 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 183.80, 157.80, 150.47, 138.08, 125.54, 123.22, 117.85, 111.29, 44.71, 19.31;
MS (m/z) 189 (M^+).

5-Methyl-N-methylindoline-2,3-dione (2f)[1]



TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 81% (Br)/77% (Cl);
red solid; m.p.: 150.1-151.6 °C;
IR(KBr)/cm^{-1}: 2973, 1755, 1625, 1595, 1448, 776;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.41 (m, 2 H), 6.79 (d, *J* = 8.5 Hz, 1 H), 3.23 (s, 3 H), 2.34 (s, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 183.59, 158.31, 149.24, 138.72, 133.62, 125.58, 117.40, 109.69, 26.17, 20.64;
MS (m/z) 175 (M^+).

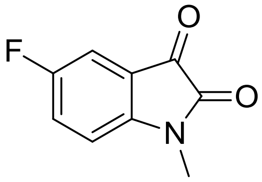
5-Chloro-N-methylindoline-2,3-dione (2g)[1]



TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 72%;
red solid; m.p.: 165.1-166.9 °C;
IR (KBr)/cm^{-1}: 2998, 1745, 1605, 1502, 1332, 722;
^{1}H NMR (400MHz, $CDCl_3$):δ 7.58 (m, 2H), 6.88 (d, *J* = 8.2 Hz, 1H), 3.26 (s, 3H);
^{13}C NMR (100MHz, $CDCl_3$): δ 182.29, 157.63, 149.65, 137.72, 129.63, 125.18, 118.18, 91.18, 26.34;

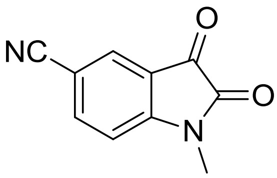
MS (m/z) 195 (M^+).

5-Fluoro-*N*-methylindoline-2,3-dione (2h) [1]



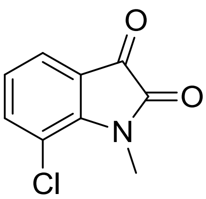
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 68%;
red solid; m.p.: 150.8-152.6 ^oC;
IR(KBr)/cm^{-1}: 2978, 1745, 1623, 1500, 1368, 779;
^1H NMR (400MHz, $CDCl_3$):δ 7.33 (m, 2 H), 6.89 (d, *J* = 8.5 Hz, 1 H), 3.26 (s, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 182.74, 160.56, 158.02, 157.93, 147.47, 124.76, 124.51, 117.98, 117.91, 112.46, 112.21, 111.08, 111.01, 26.30;
MS (m/z) 179 (M^+).

5-Cyan-*N*-methylindoline-2,3-dione (2i)



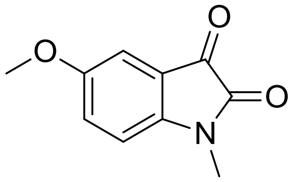
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 60%;
red solid; m.p.: 157.2-160.1 ^oC;
IR(KBr)/cm^{-1}: 2959, 1734, 1619, 1468, 1349, 752 ;
^1H NMR (400MHz, $CDCl_3$): δ 7.92 (m, 2H), 7.05 (d, *J* = 8.2 Hz, 1H), 3.33 (s, 3H);
^{13}C NMR (100MHz, $CDCl_3$): δ 181.11, 157.45, 153.96, 141.97, 128.66, 117.45, 117.34, 110.80, 107.64, 26.62;
HRMS m/z calcd for $C_{10}H_6N_2O_2$: 186.0429, found: 186.0425.

7-Chloro-*N*-methylindoline-2,3-dione (2j) [4]



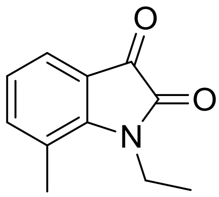
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 68%;
red solid; m.p.: 165.8-168.9 ^oC;
IR(KBr)/cm^{-1}: 2989, 1746, 1610,1489, 1352, 765;
^1H NMR (400MHz, $CDCl_3$): δ 7.47 (m, 2 H), 6.99 (d, *J* = 8.1 Hz, 1 H), 3.57 (s, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 182.66, 158.48, 146.78, 140.41, 134.14, 124.73, 123.94, 117.63, 29.69;
MS (m/z) 195 (M^+).

5-Methoxy-*N*-methylindoline-2,3-dione (2k) [1]



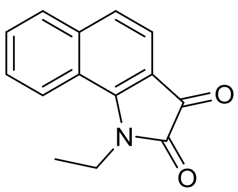
TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 85%;
red solid; m.p.: 171.4-172.2 °C;
IR(KBr)/cm^{-1}: 2956, 1750, 1620, 1488, 1329, 814;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.15 (m, 2 H), 6.82 (d, *J* = 8.4 Hz, 1 H), 3.81 (s, 3 H), 3.22 (s, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 183.68, 158.23, 156.50, 145.26, 124.51, 117.74, 110.84, 109.53, 55.91, 26.16;
MS (m/z) 191 (M^+).

7-Methyl-*N*-ethylindoline-2,3-dione (2l)



TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 70%;
red solid; m.p.: 167.5-168.3 °C;
IR(KBr)/cm^{-1}: 2973, 1727, 1653, 1595, 1449, 1355, 775;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.47 (d, *J* = 7.3 Hz, 1 H), 7.35 (d, *J* = 7.7 Hz, 1 H), 7.01 (t, *J* = 7.5 Hz, 1 H), 4.01 (q, *J* = 8.0 Hz, 2 H), 2.54 (s, 3 H), 1.34 (t, *J* = 7.1 Hz, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 184.12, 159.11, 148.33, 142.36, 123.67, 123.50, 121.35, 118.77, 36.85, 18.71, 14.55;
HRMS m/z calcd for $C_{11}H_{11}NO_2$: 189.0790, found: 189.0784.

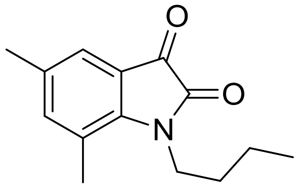
***N*-Ethyl-1H-benzo[g]indole-2,3-dione(2m)**



TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 63%;
red solid; m.p.: 198.2-200.2 °C;
IR(KBr)/cm^{-1}: 3055, 2978, 1744, 1628, 1592, 1575, 817, 758;
^{1}H NMR (400MHz, $CDCl_3$): δ 8.56 (d, *J* = 8.4 Hz, 1 H), 8.10 (d, *J* = 8.7 Hz, 1 H), 7.75 (d, *J* = 8.3 Hz, 1 H), 7.61 (t, *J* = 8.2 Hz, 1 H), 7.39 (t, *J* = 8.1 Hz, 1 H), 7.12 (d, *J* = 8.7 Hz, 1 H), 3.81 (q, *J* = 8.0 Hz, 2 H), 1.34 (t, *J* = 7.2 Hz, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 182.65, 158.48, 154.04, 140.48, 131.18, 129.95, 129.22, 128.88, 125.43, 123.14, 110.09, 108.97, 34.79, 13.04;

HRMS m/z calcd for $C_{14}H_{11}NO_2$: 225.0790, found: 225.0786.

5,7-Dimethyl-*N*-n-butylindoline-2,3-dione (2n)



TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 70%;

red solid; m.p.: 177.2-179.1 ^{o}C;

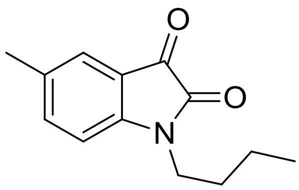
IR(KBr)/cm^{-1}: 2959, 2929, 2870, 1732, 1683, 1597, 1486, 722;

^{1}H NMR (400MHz, $CDCl_3$): δ 7.25 (s, 1 H), 7.15 (s, 1 H), 3.88 (t, *J* = 8.0 Hz, 2 H), 2.47 (s, 3 H), 2.27 (s, 3 H), 1.66 (m, 2 H), 1.42 (m, 2 H), 0.97 (t, *J* = 7.3 Hz, 3 H);

^{13}C NMR (100MHz, $CDCl_3$): δ 184.30, 159.30, 146.24, 142.82, 133.31, 123.70, 121.13, 118.85, 41.65, 31.28, 20.17, 19.82, 18.53, 13.64;

HRMS m/z calcd for $C_{14}H_{17}NO_2$: 231.1259, found: 231.1255.

5-Methyl-*N*-butyl-indoline-2,3-dione (2o) [3]



TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 70%;

red solid; m.p.: 174.2-176.4 ^{o}C;

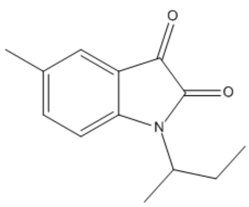
IR(KBr)/cm^{-1}: 2960, 2873, 1731, 1597, 1350, 767, 726;

^{1}H NMR (400MHz, $CDCl_3$): δ 7.38 (d, *J* = 7.3 Hz, 1 H), 7.26 (d, *J* = 7.7 Hz, 1 H), 6.93 (t, *J* = 7.5 Hz, 1 H), 3.85 (t, *J* = 8.0 Hz, 2 H), 2.44 (s, 3 H), 1.60 (quint, *J* = 8.0 Hz, 2 H), 1.35 (sext, *J* = 8.0 Hz, 2 H), 0.90 (t, *J* = 7.4 Hz, 3 H);

^{13}C NMR (100MHz, $CDCl_3$): δ 184.10, 159.22, 148.51, 142.40, 123.65, 123.47, 121.40, 118.76, 41.75, 31.40, 19.84, 18.75, 13.68;

MS (m/z) 217 (M^+).

5-Methyl-*N*-(sec-butyl)-indoline-2,3-dione(2p)



TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 73%;

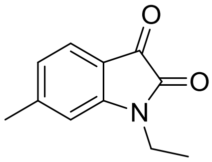
red solid; m.p.: 189.4-190.1 ^{o}C;

IR(KBr)/cm^{-1}: 2966, 2935, 2876, 1731, 1621, 1488, 1329, 813;

^{1}H NMR (400MHz, $CDCl_3$): δ 7.40 (m, 2 H), 6.96 (d, *J* = 8.0 Hz, 1 H), 4.32 (m, 1 H), 2.33 (s, 3 H), 2.03 (m, 1 H), 1.82 (m, 1 H), 1.49 (d, *J* = 8.0 Hz, 3 H), 0.93 (t, *J* = 7.4 Hz, 3 H);

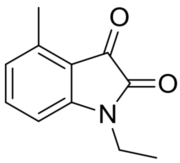
^{13}C NMR (100MHz, $CDCl_3$): δ 183.87, 158.01, 148.27, 138.48, 132.86, 125.57, 117.59, 111.21, 50.47, 26.10, 20.29, 17.35, 11.02;
HRMS m/z calcd for $C_{13}H_{15}NO_3$: 233.1052, found: 233.1050.

6-Methyl-*N*-ethylindoline-2,3-dione (2q)



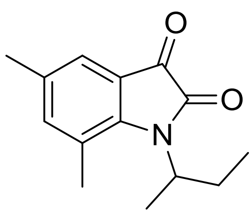
TLC (petroleum ether/ ethyl acetate, 2/1);
red solid; m.p.: 137.8-139.1 ^{o}C;
IR(KBr)/cm^{-1}: 2933, 1736, 1721, 1615, 1356, 755;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.49 (d, *J* = 7.6 Hz, 1 H), 6.91 (d, *J* = 7.6 Hz, 1 H), 6.71 (s, 1 H), 3.77 (q, *J* = 8.0 Hz, 2 H), 2.45 (s, 3 H), 1.31 (t, *J* = 7.2 Hz, 3 H);
^{13}C NMR (100MHz, $CDCl_3$): δ 184.18, 157.78, 150.67, 141.36, 137.41, 125.92, 115.76, 107.21, 34.81, 18.07, 12.58;
HRMS m/z calcd for $C_{14}H_{11}NO_2$: 189.0790, found: 189.0788.

4-Methyl-*N*-ethylindoline-2,3-dione (2q')



TLC (petroleum ether/ ethyl acetate, 2/1);
red solid; m.p.: 137.8-139.1 ^{o}C;
IR(KBr)/cm^{-1}: 2920, 1742, 1718, 1610, 1355, 738;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.43 (t, *J* = 7.8 Hz, 1 H), 6.88 (d, *J* = 7.8 Hz, 1 H), 6.71 (d, *J* = 7.8 Hz, 1 H), 3.77 (q, *J* = 8.0 Hz, 2 H), 2.57 (s, 3 H), 1.30 (t, *J* = 7.2 Hz, 3 H).
^{13}C NMR (100MHz, $CDCl_3$): δ 182.96, 158.50, 151.04, 150.61, 125.50, 124.26, 115.47, 110.71, 34.82, 22.59, 12.59;
HRMS m/z calcd for $C_{14}H_{11}NO_2$: 189.0790, found: 189.0784.

5,7-Dimethyl-*N*-(sec-butyl)indoline-2,3-dione(2r)



TLC (petroleum ether/ ethyl acetate, 2/1); Yield: 68%;
red solid; m.p.: 174.2-176.2 ^{o}C;
IR(KBr)/cm^{-1}: 2967, 2875, 1729, 1620, 1592, 1487, 779;
^{1}H NMR (400MHz, $CDCl_3$): δ 7.27 (s, 1 H), 7.12 (s, 1 H), 4.27 (m, 1 H), 2.47 (s, 3 H), 2.26 (s, 3 H), 1.85 (m, 2 H), 1.55 (d, *J* = 8.0 Hz, 3 H), 0.94 (t, *J* = 7.4 Hz, 3 H);

^{13}C NMR (100MHz, $CDCl_3$): δ 184.66, 159.60, 148.01, 143.36, 133.08, 124.01, 120.95, 119.25, 54.32, 26.46, 20.57, 20.14, 18.10, 11.52;

HRMS m/z calcd for $C_{14}H_{17}NO_2$: 231.1259, found: 231.1256.

Result of ICP-MS analysis of DMSO solvent

1	sample	element	concentration	unit
2	DMSO	Al	0.301	mg/L
3	DMSO	B	0.046	mg/L
4	DMSO	Ca	1.008	mg/L
5	DMSO	Cd	0.041	mg/L
6	DMSO	Co	0.03	mg/L
7	DMSO	Cu	0.088	mg/L
8	DMSO	K	0.21	mg/L
9	DMSO	Li	0.212	mg/L
10	DMSO	Mg	0.072	mg/L
11	DMSO	Na	0.723	mg/L

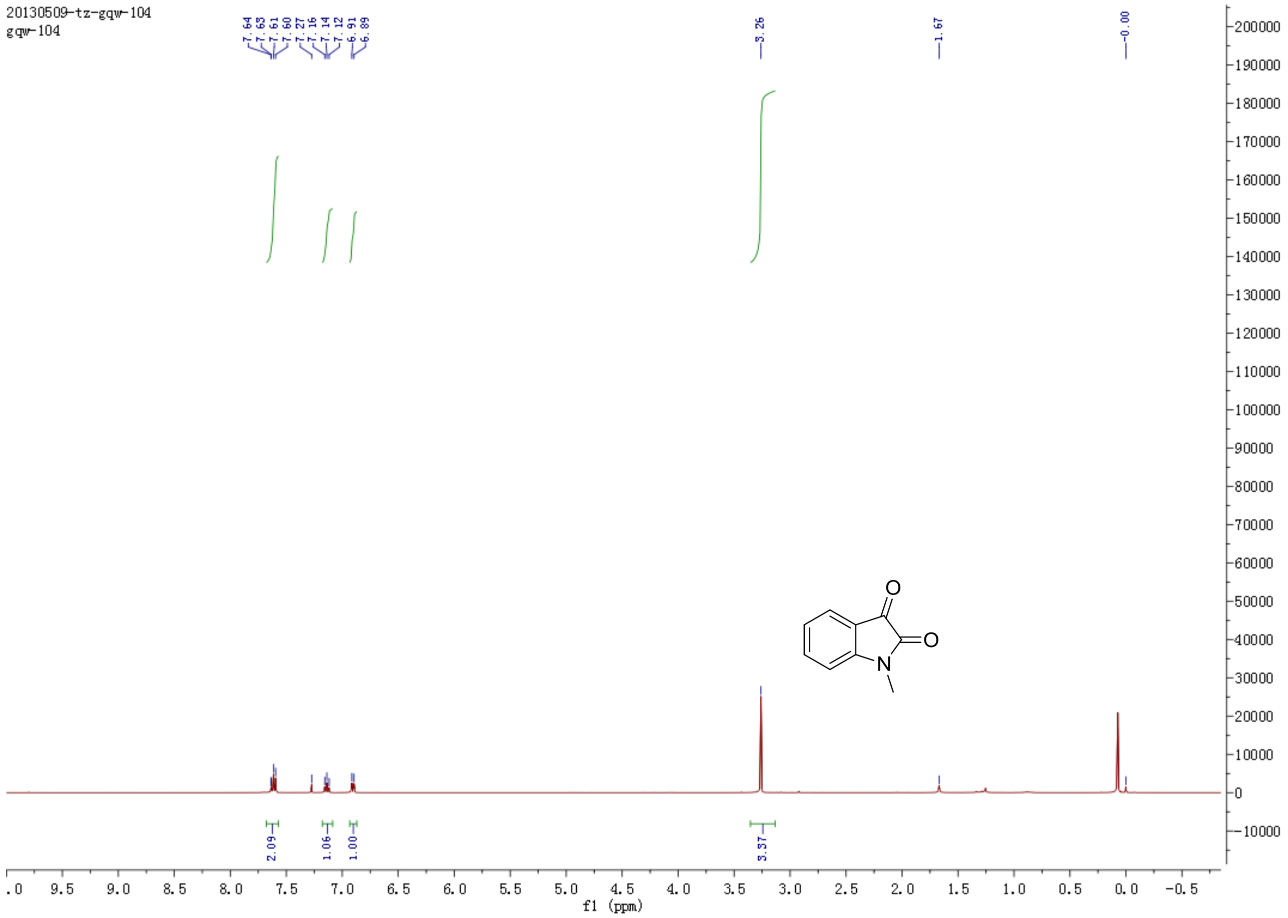
References

(1) B. X. Tang, R. J. Song, C. Y. Wu, Y. Liu, M. B. Zhou, W. T. Wei, G. B. Deng, D. L. Yin and J. H. Li, *J. Am. Chem. Soc.* 2010, **132**, 8900.

(2) M. S. Shmidt, I. A. Perillo, M. Gonzalez and M. M. Blanco, *Tetrahedron lett.* 2012, **53**, 2514.

(3) T. Liu, H. J. Yang, Y. Y. Jiang and H. Fu, *Adv. Synth. Catal.* 2013, **355**, 1169

(4) Y. Ferandin, K. Bettayeb, M. Kritsanida, O. Lozach, P. Polychronopoulos, P. Magiatis, A. L. Skaltsounis and L. Meijer, *J. Med. Chem*, 2006, **49**, 4638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f1 (ppm)
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O
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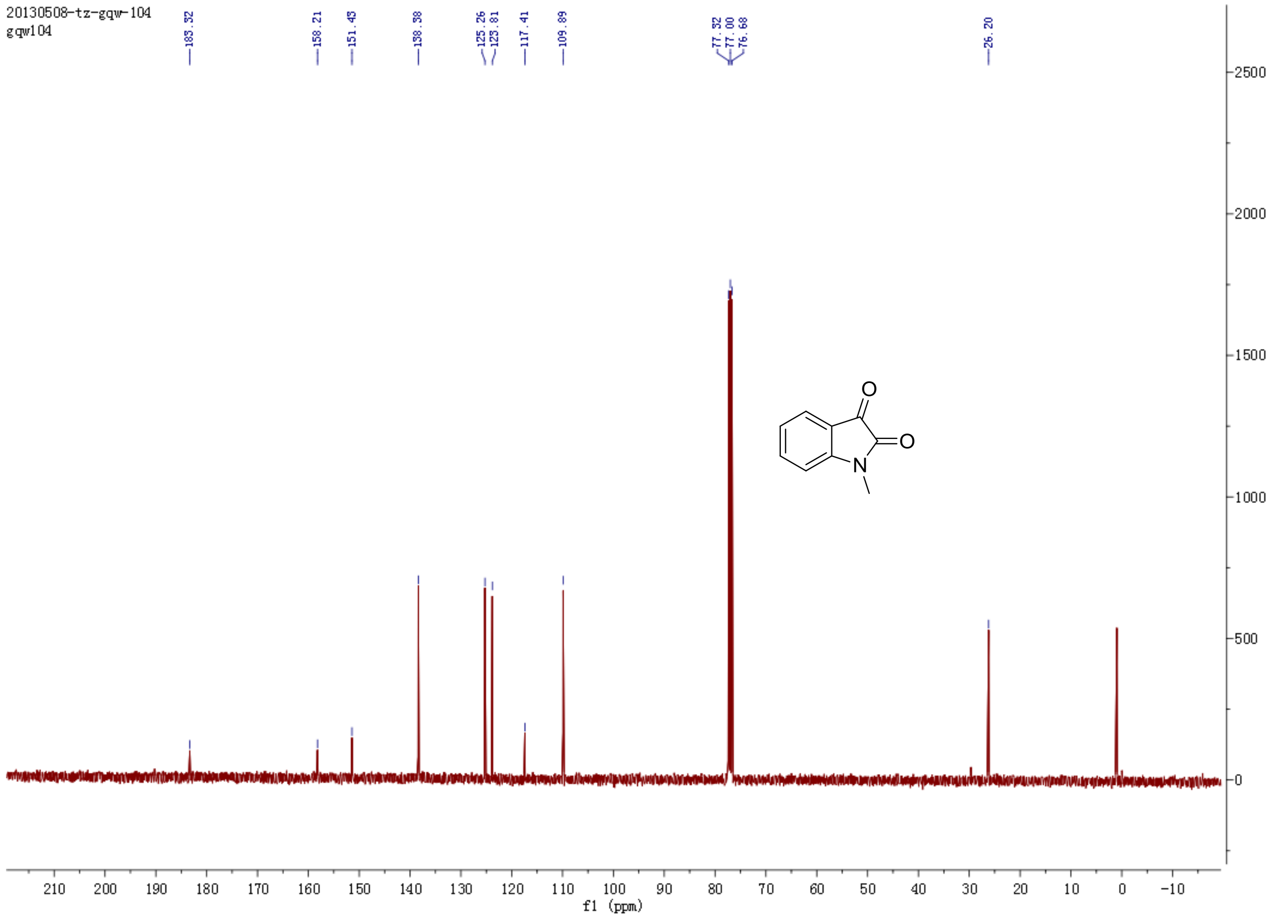
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f1 (ppm)
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O
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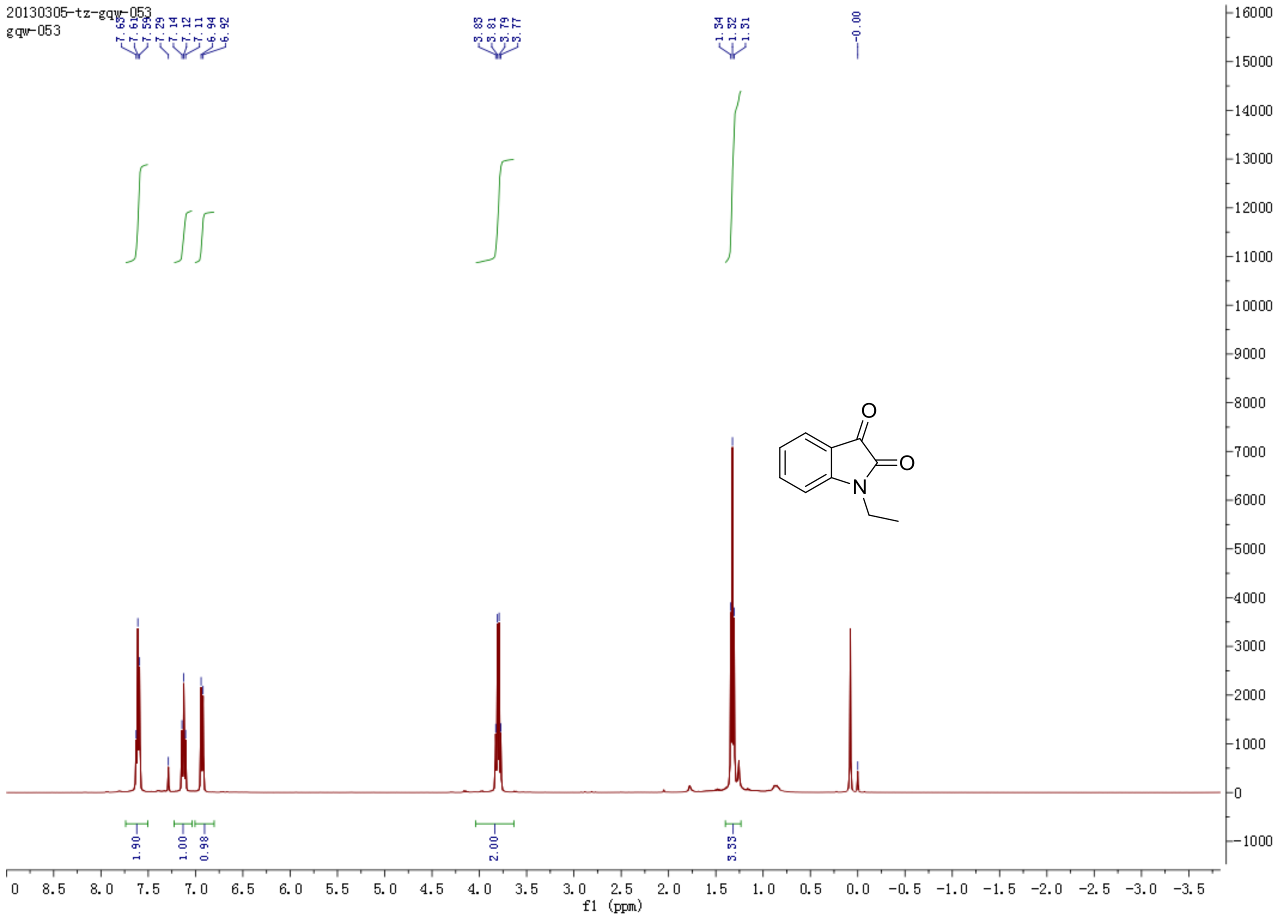
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6.92
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3.81
3.79
3.77
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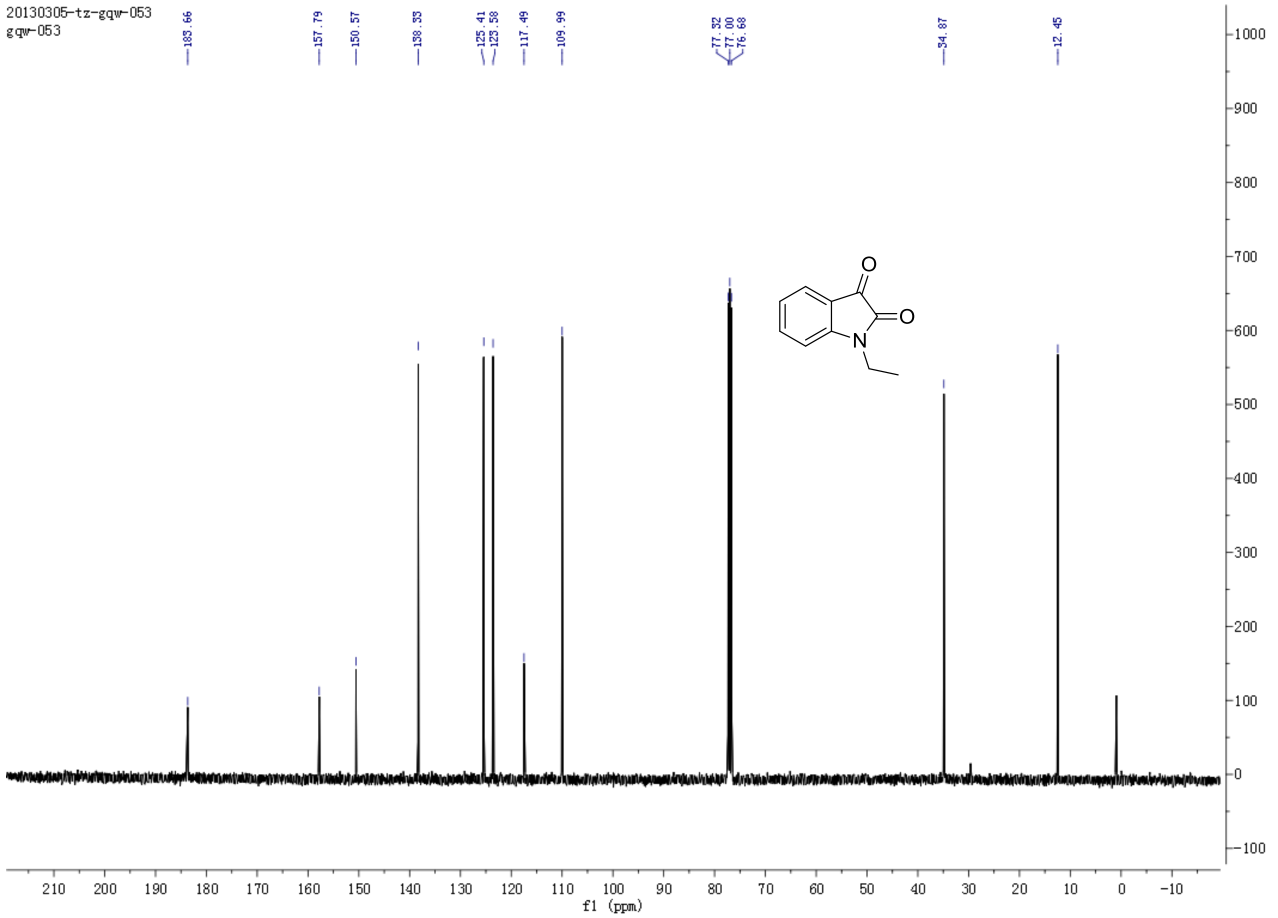
O
N
f1 (ppm)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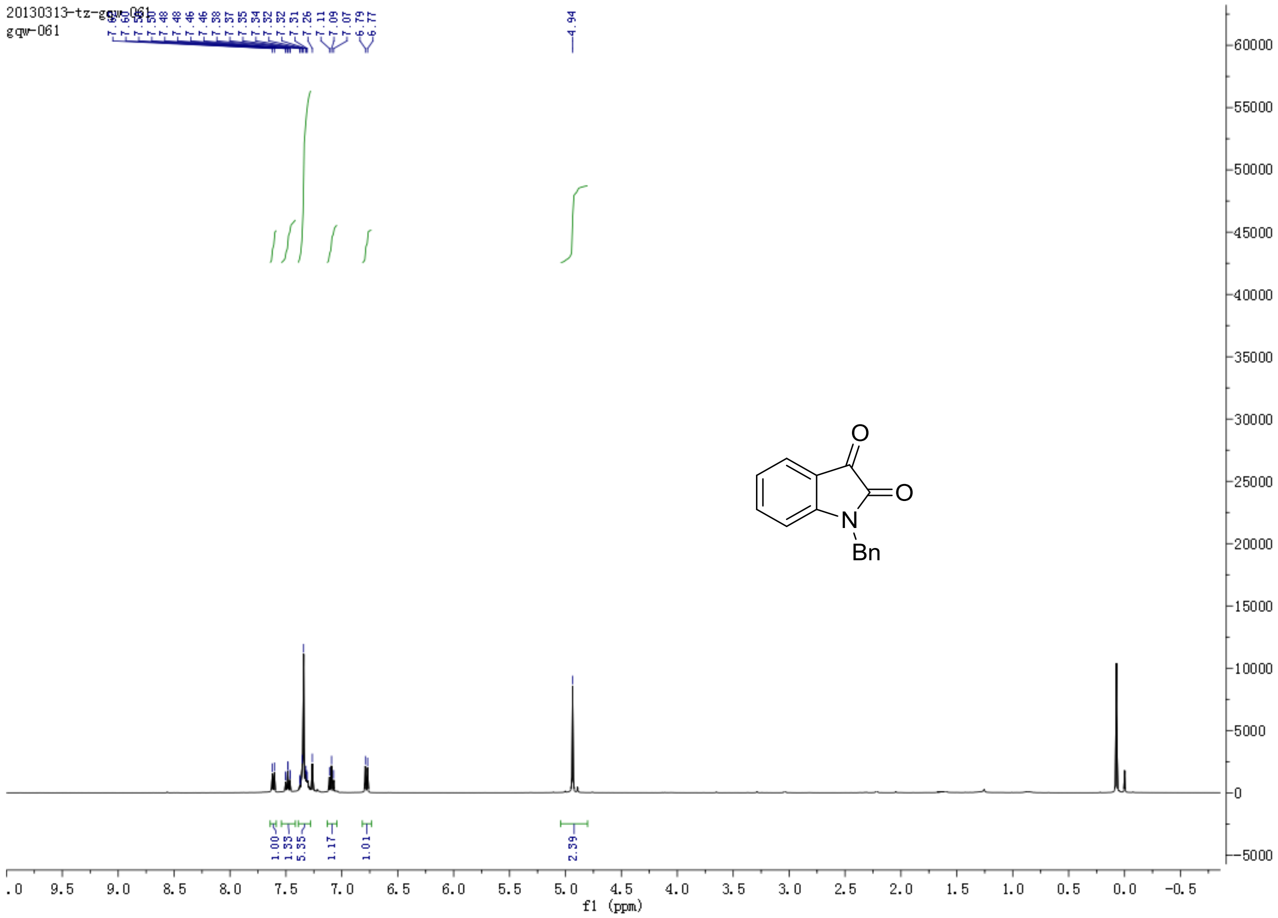
f1 (ppm)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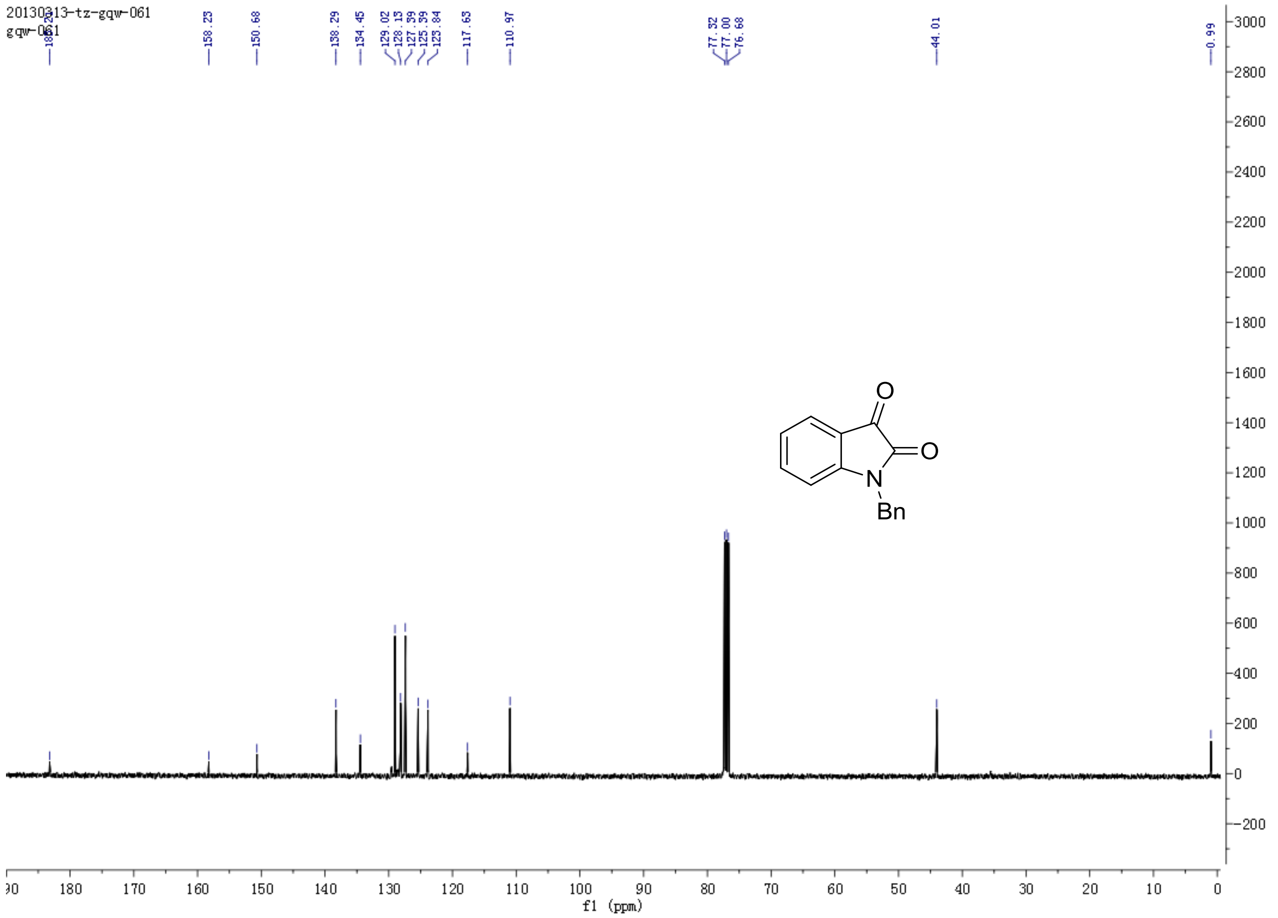
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f1 (ppm)
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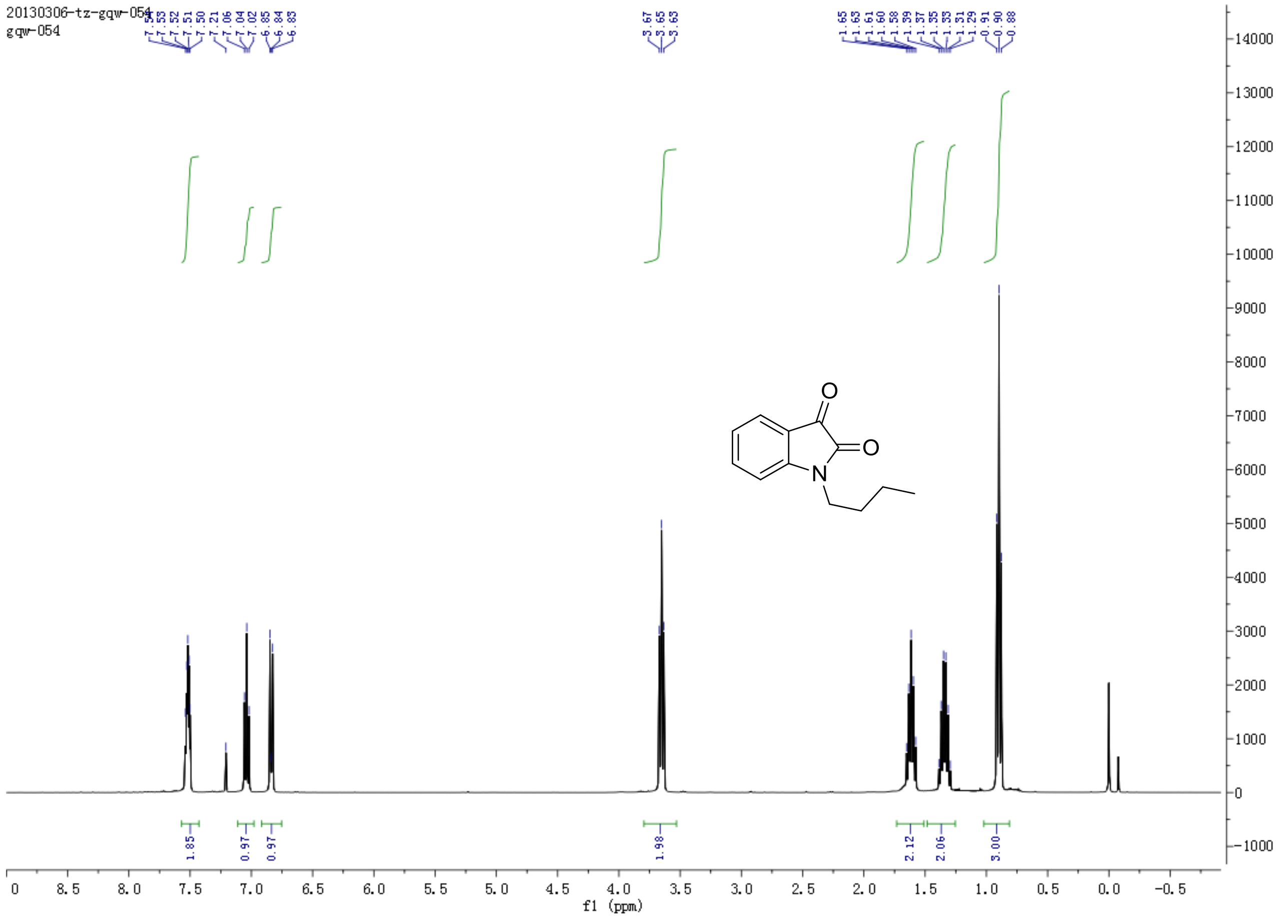
O
N
Bn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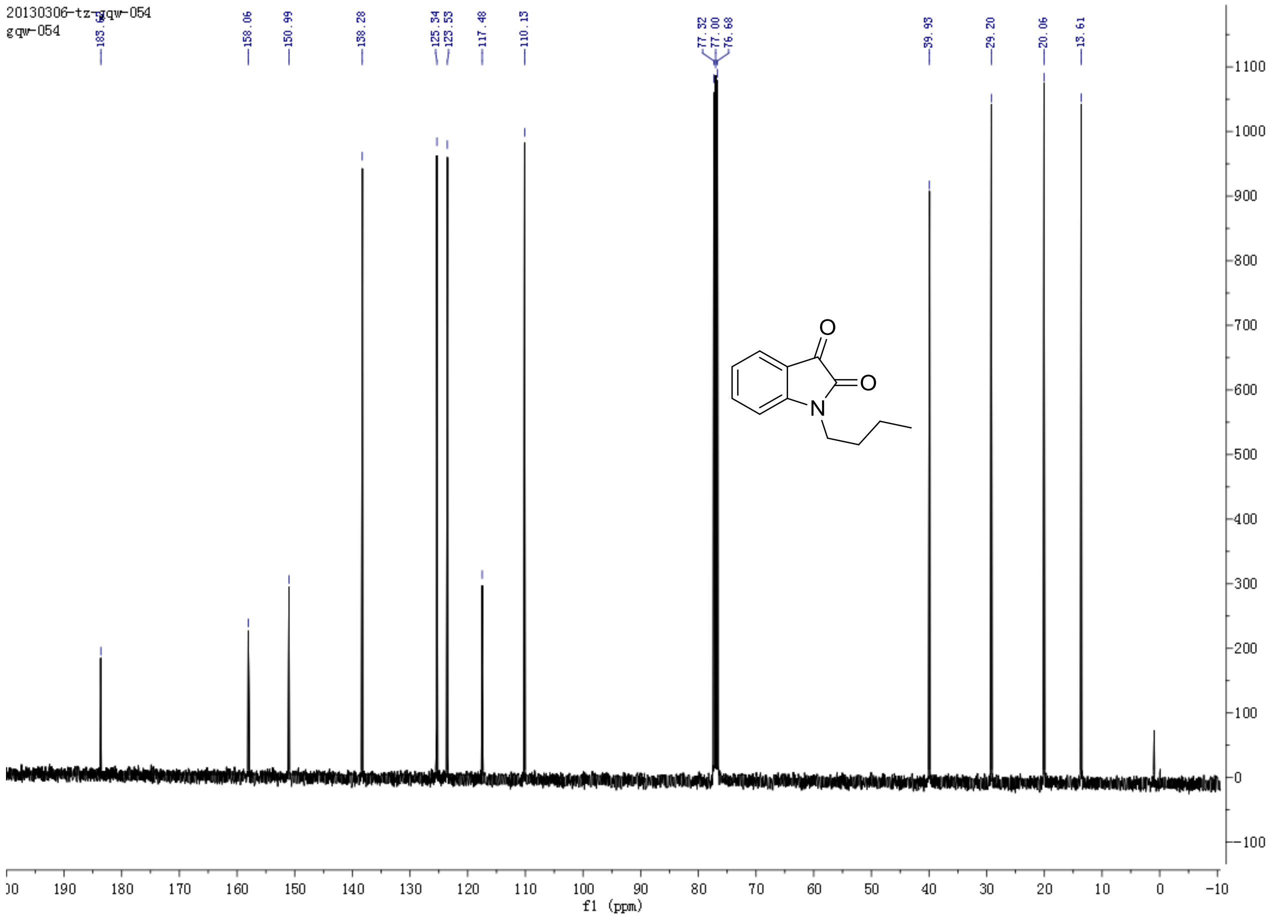
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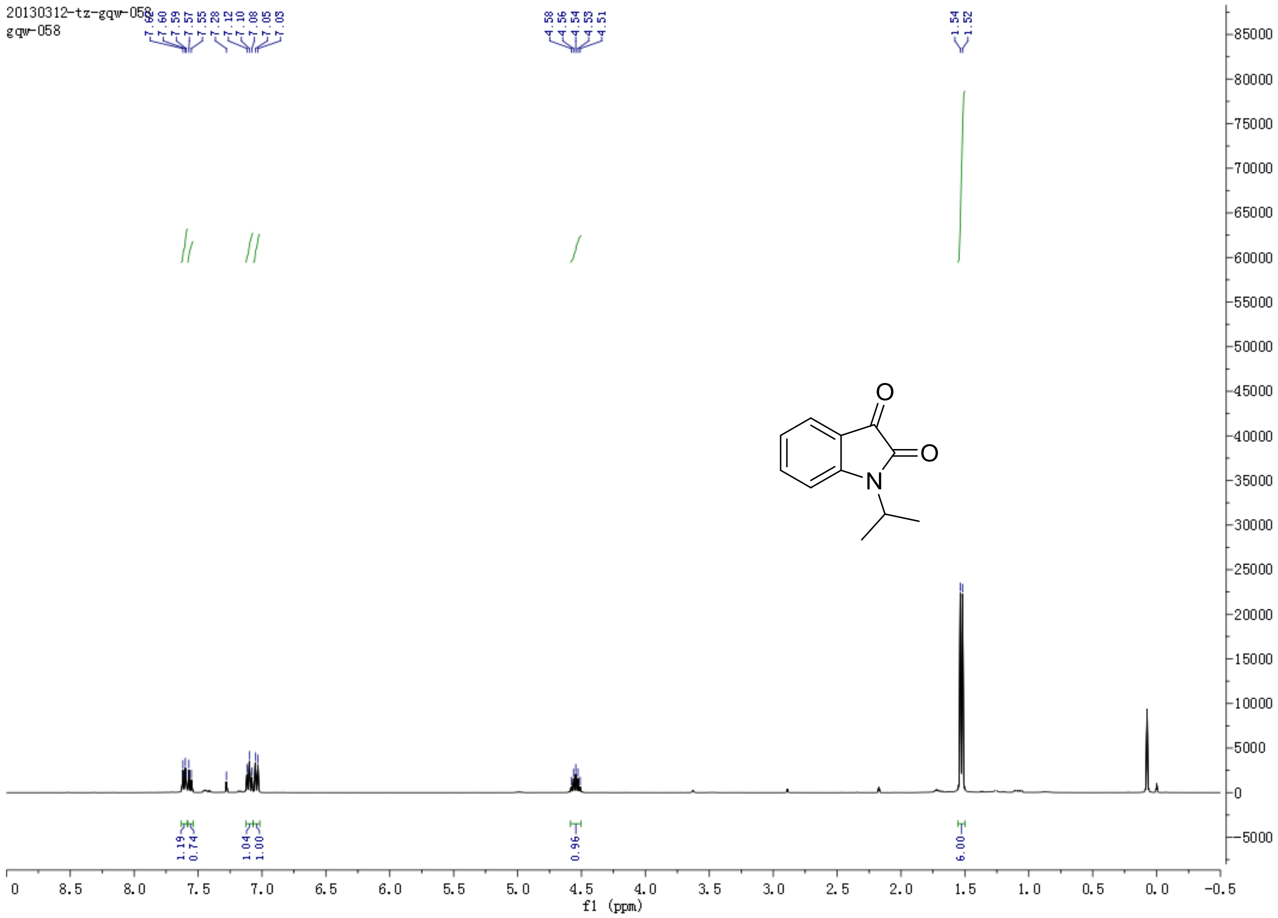
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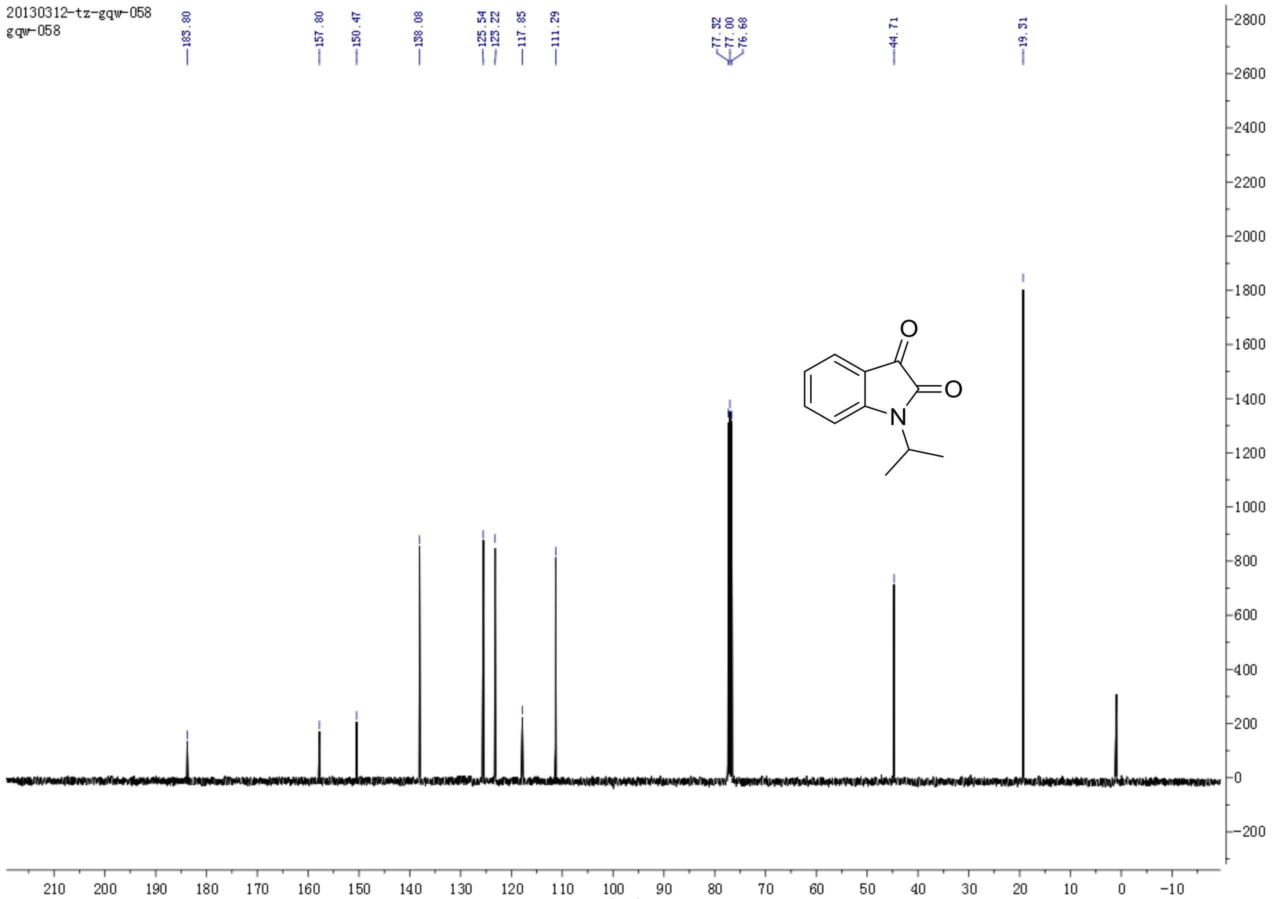
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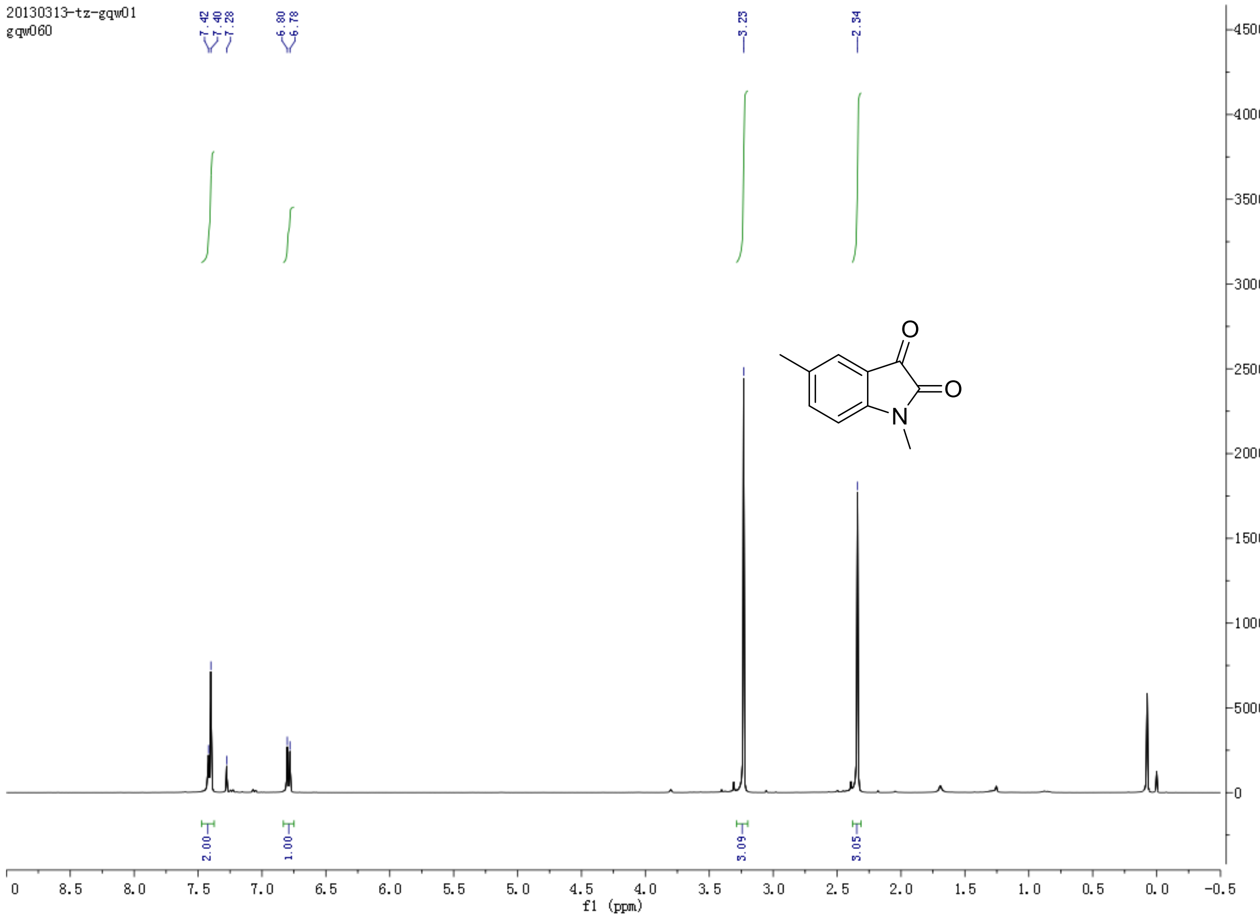
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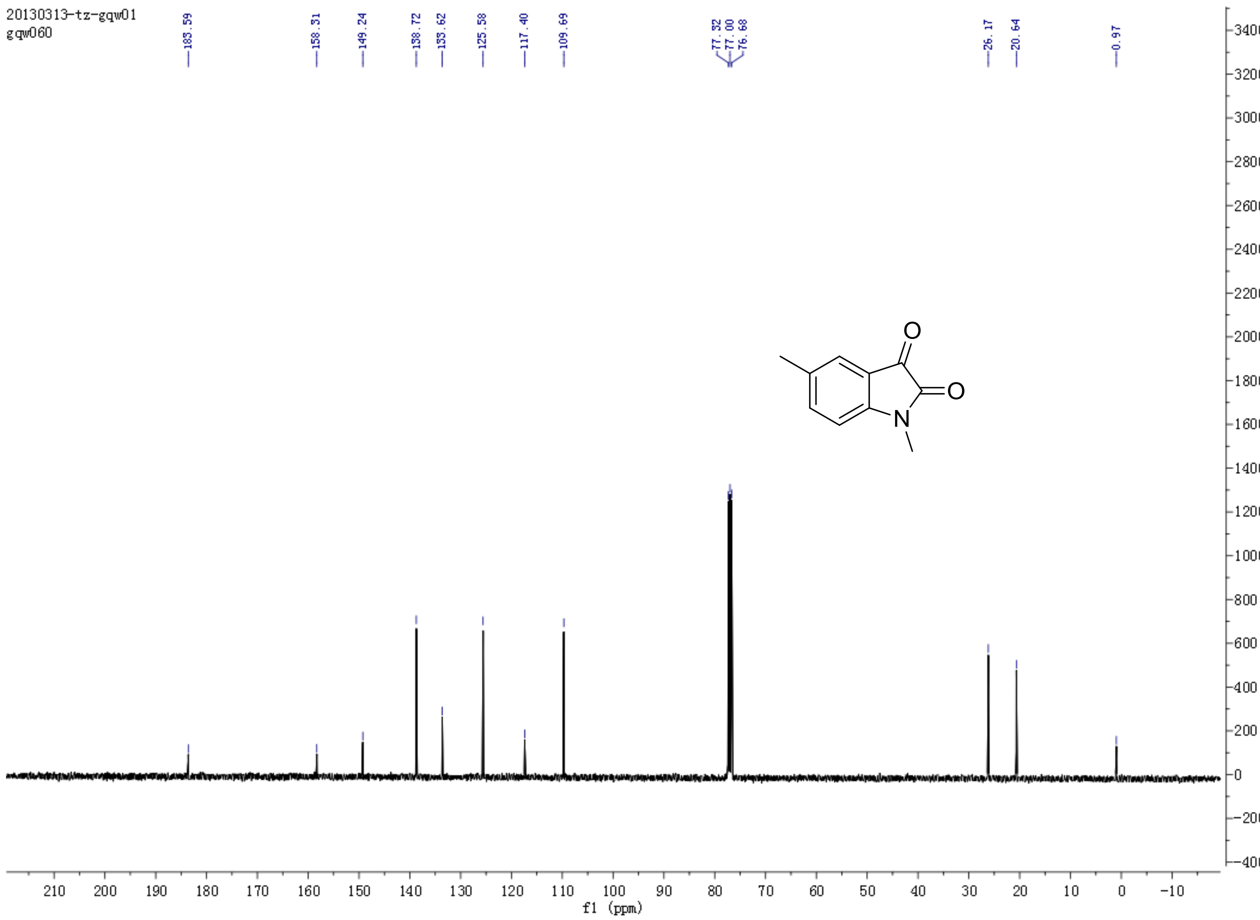
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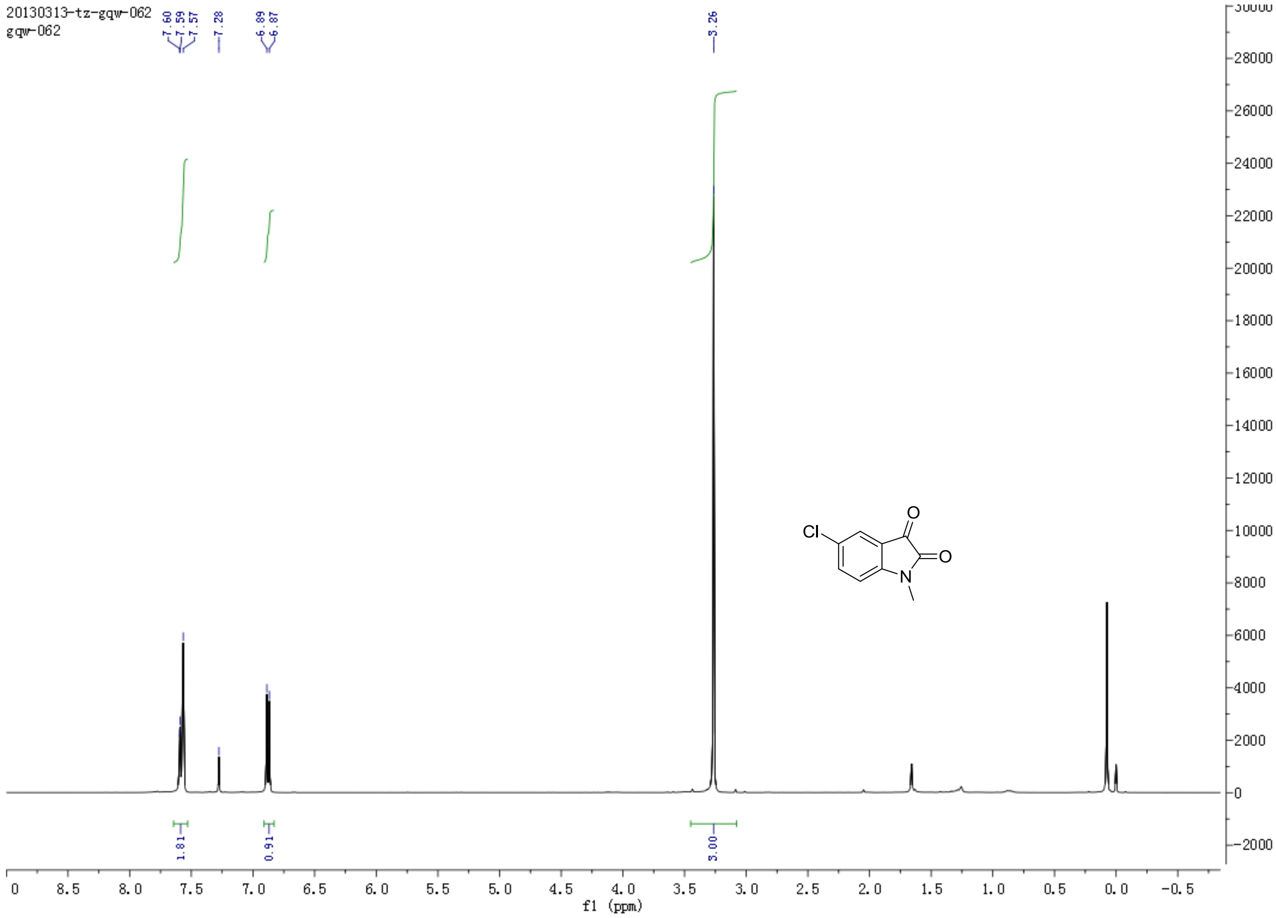
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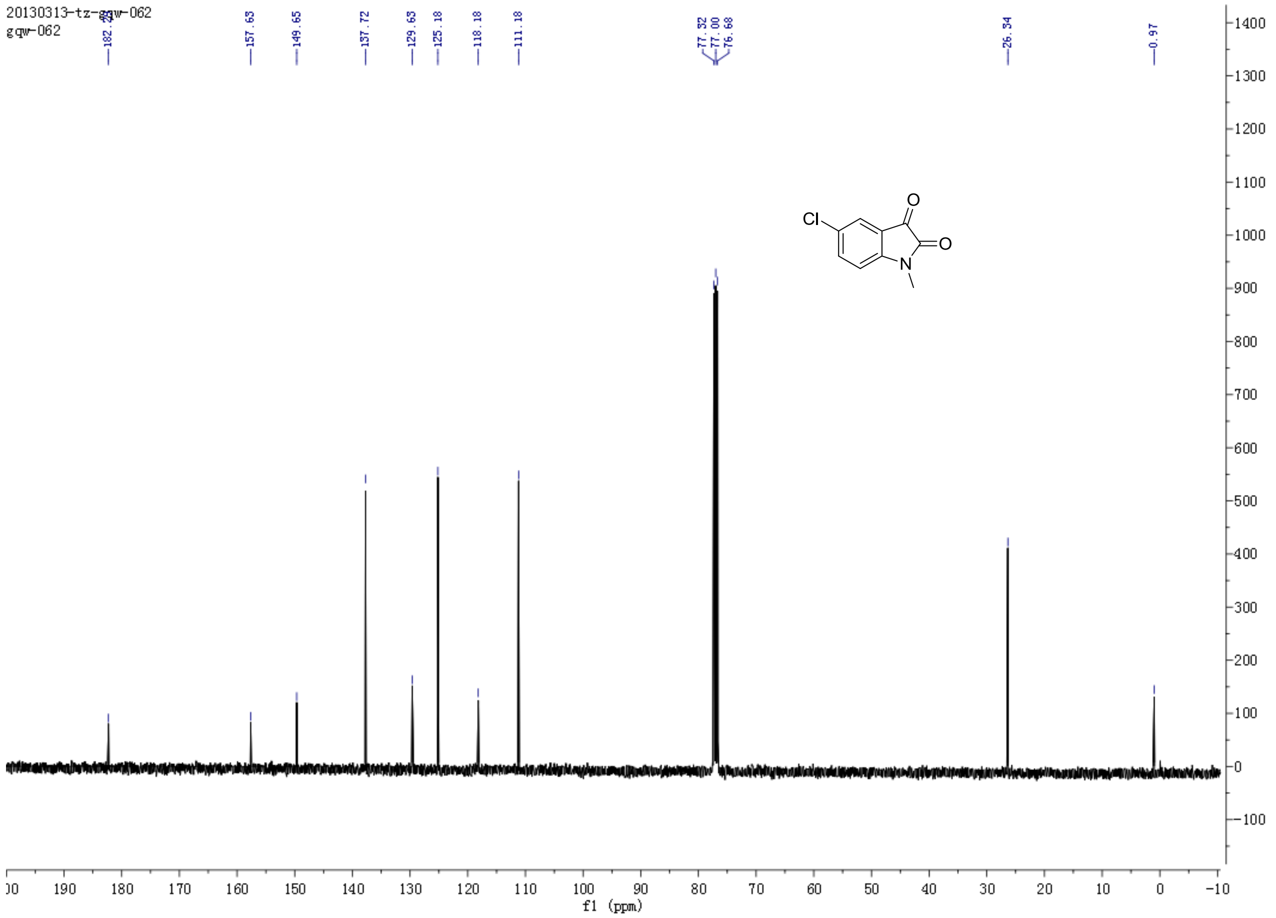
f1 (ppm)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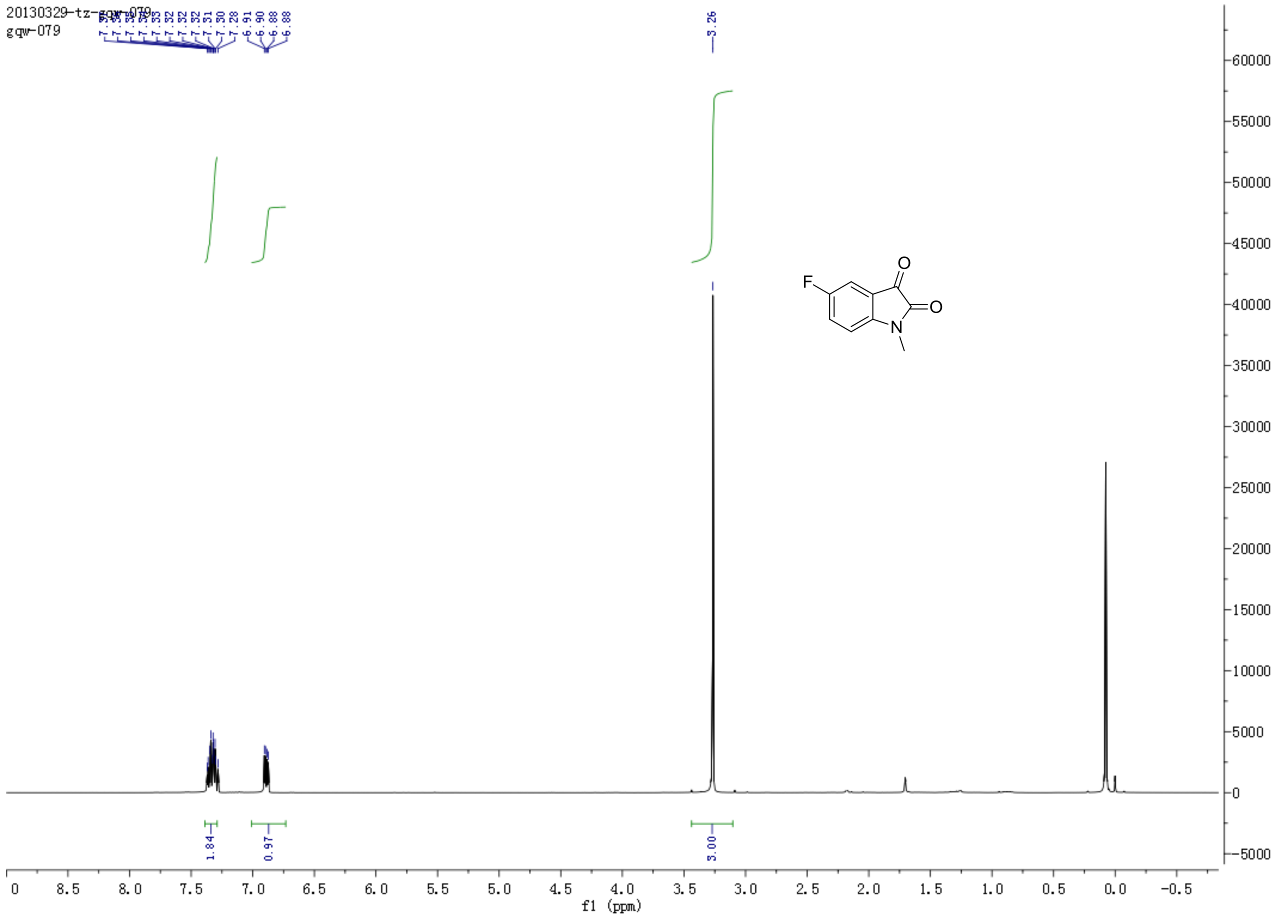
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O
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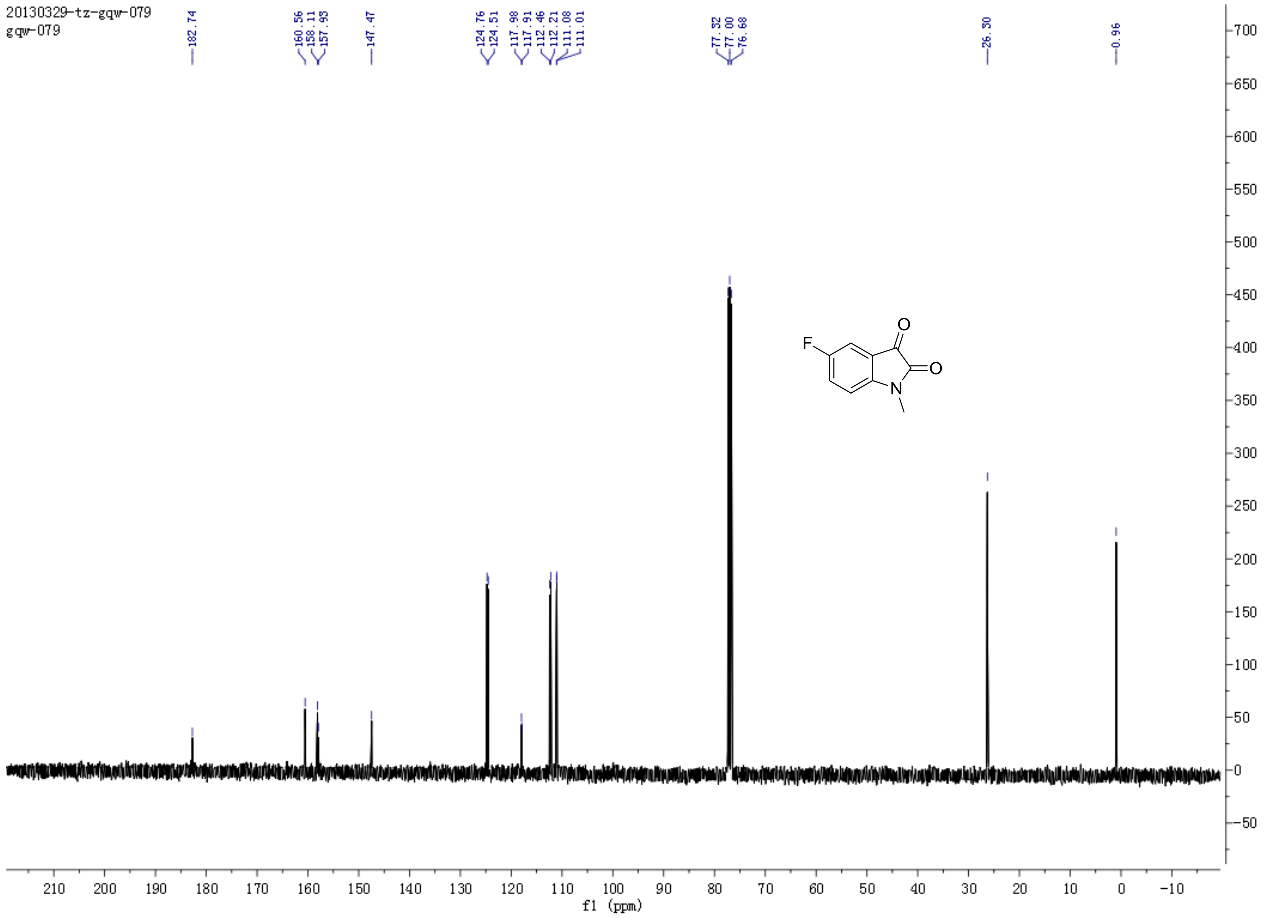
f1 (ppm)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N
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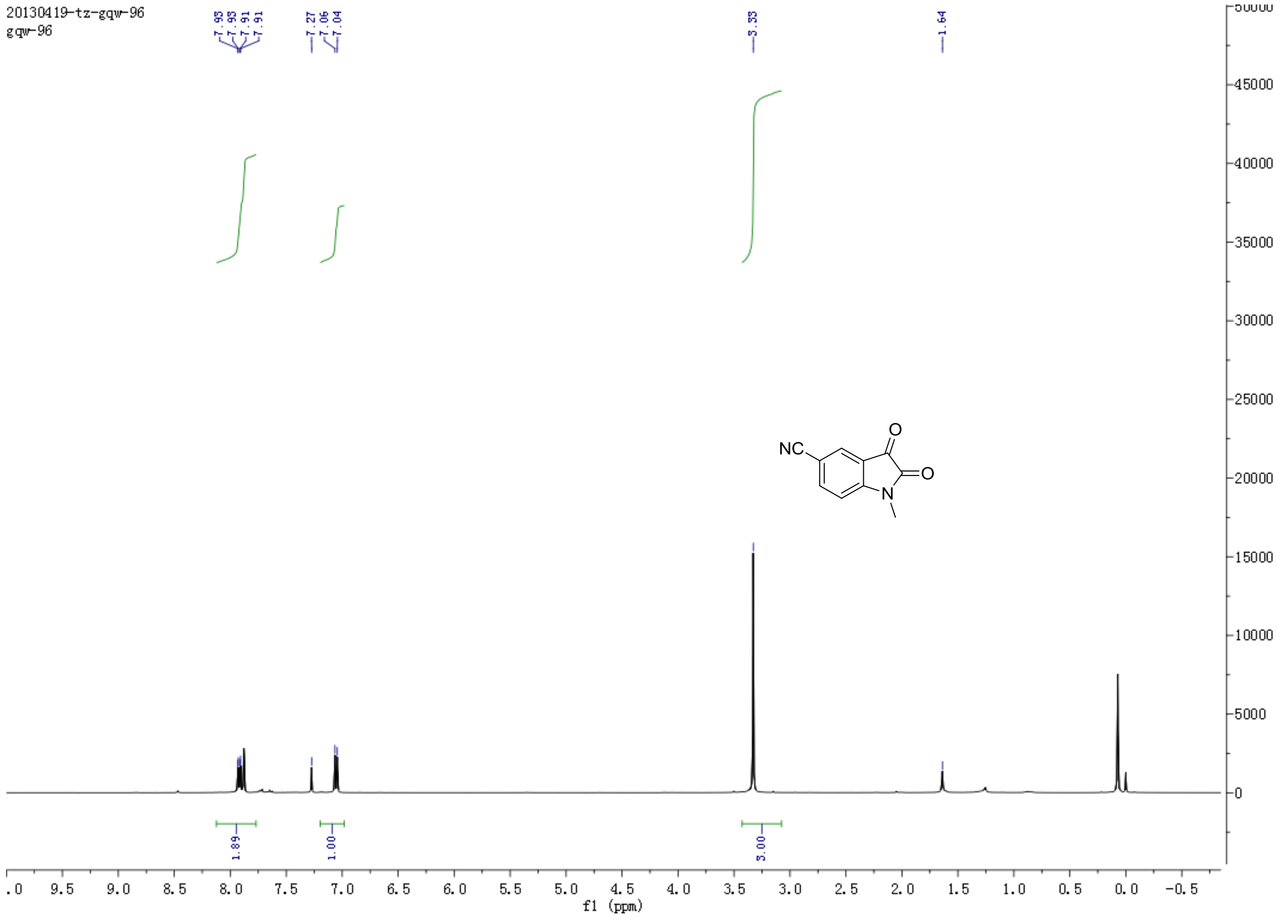
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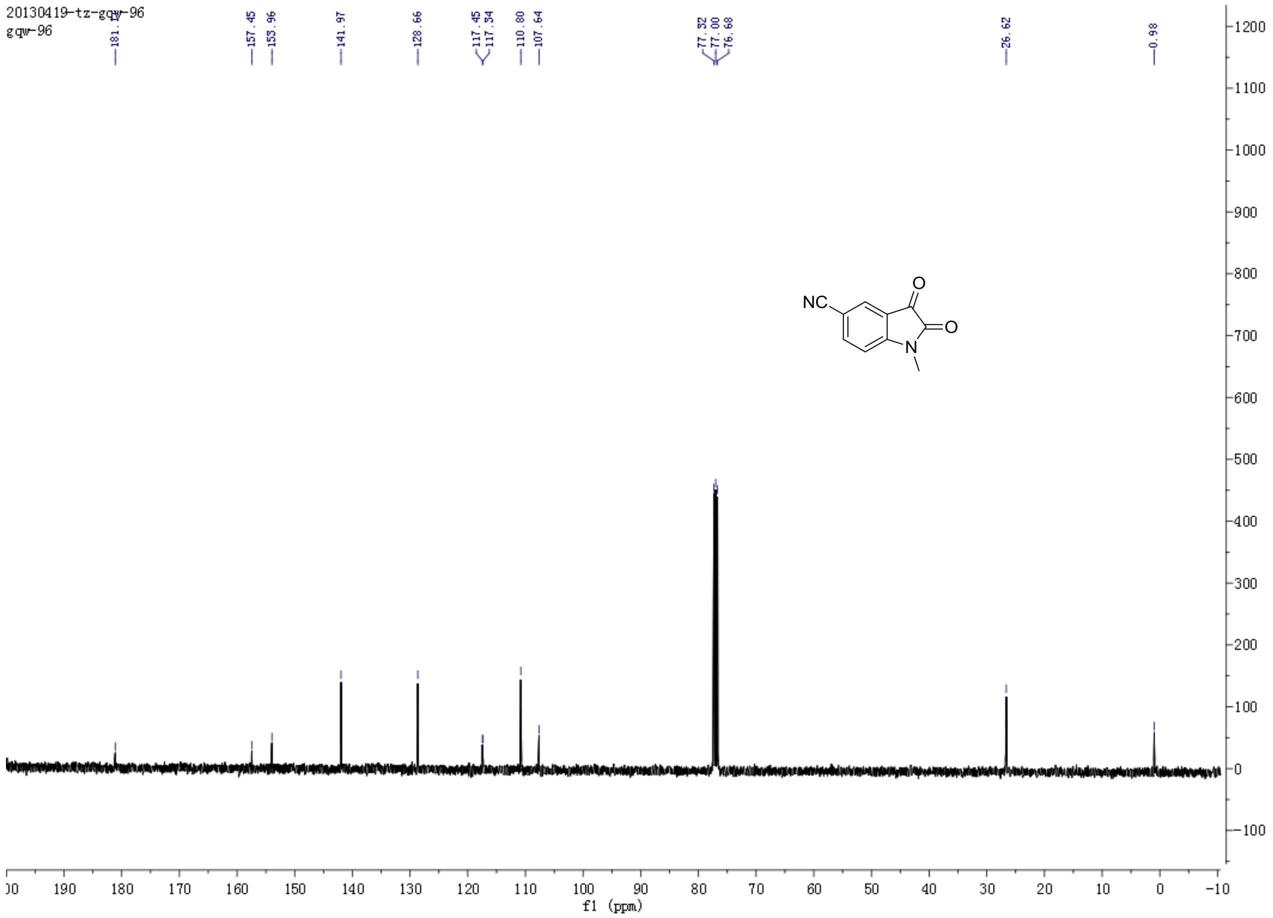
f1 (ppm)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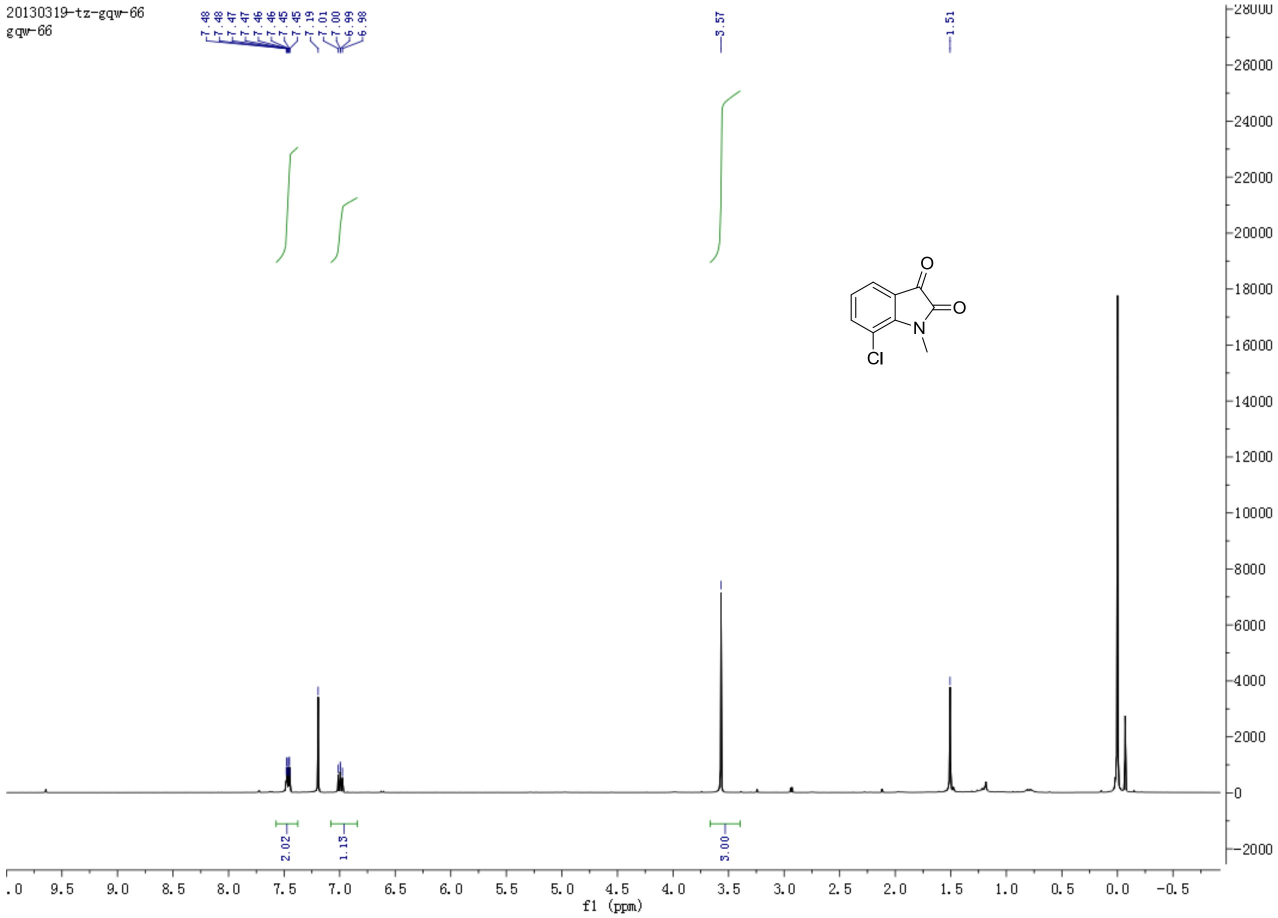
f1 (ppm)



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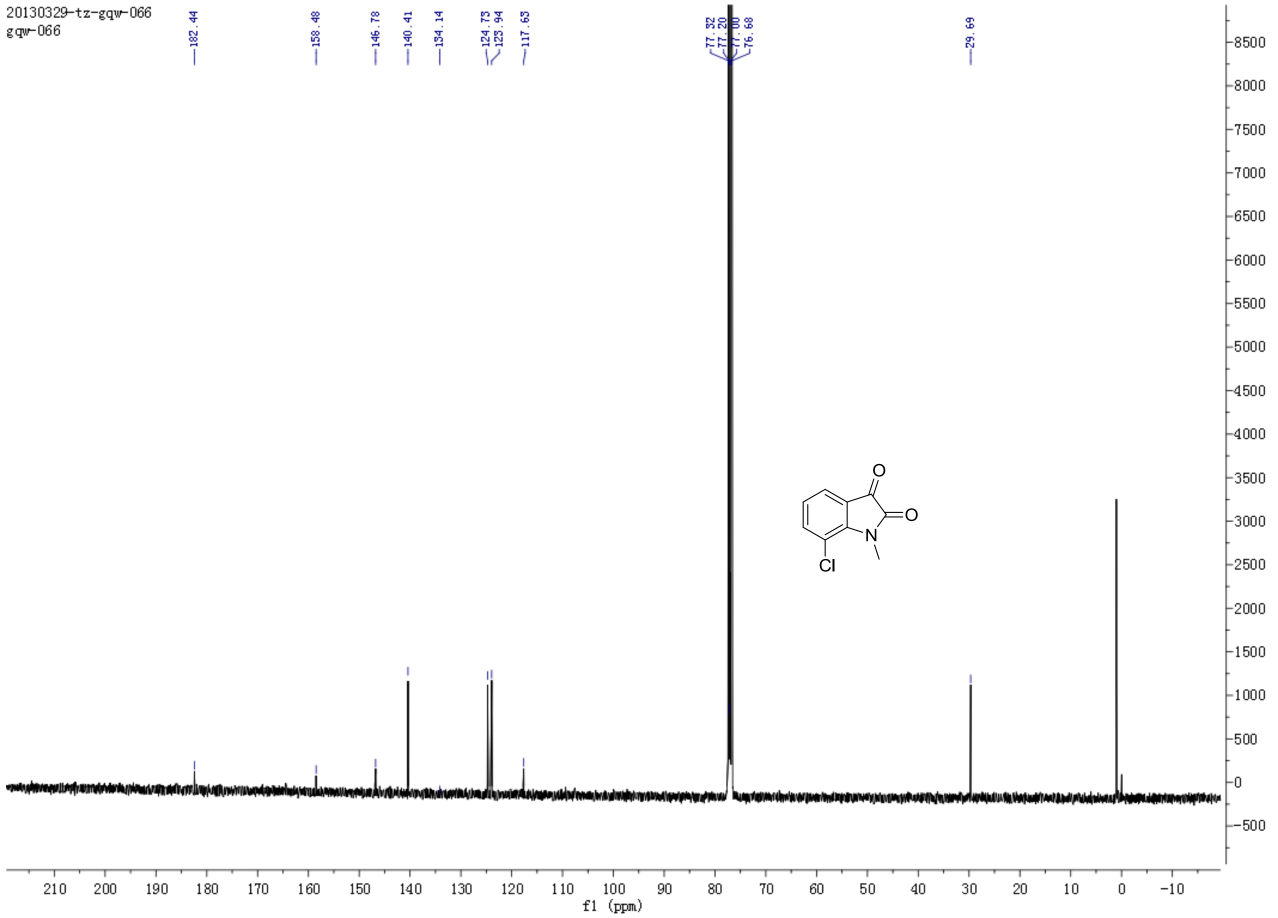
f1 (ppm)



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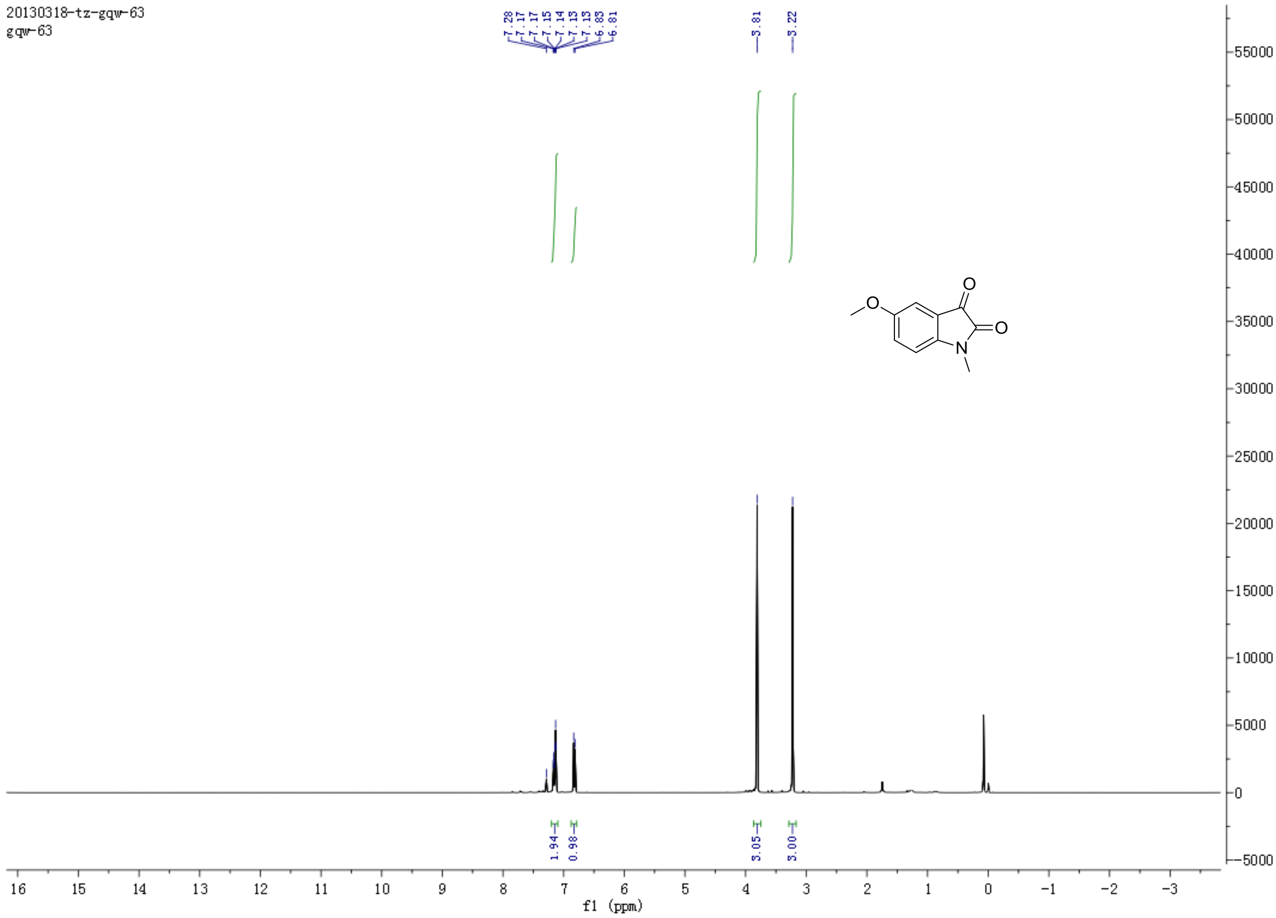
Cl
f1 (ppm)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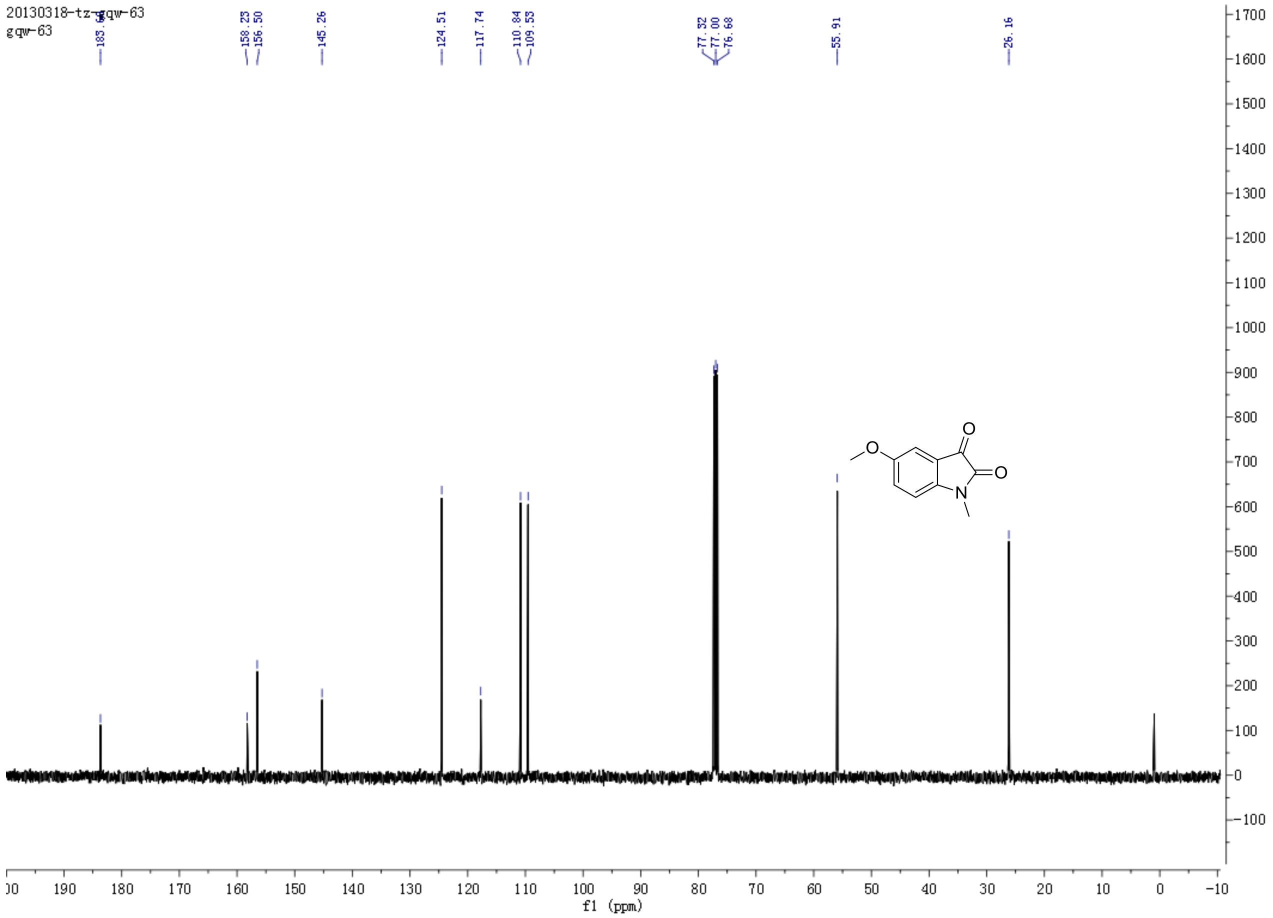
f1 (ppm)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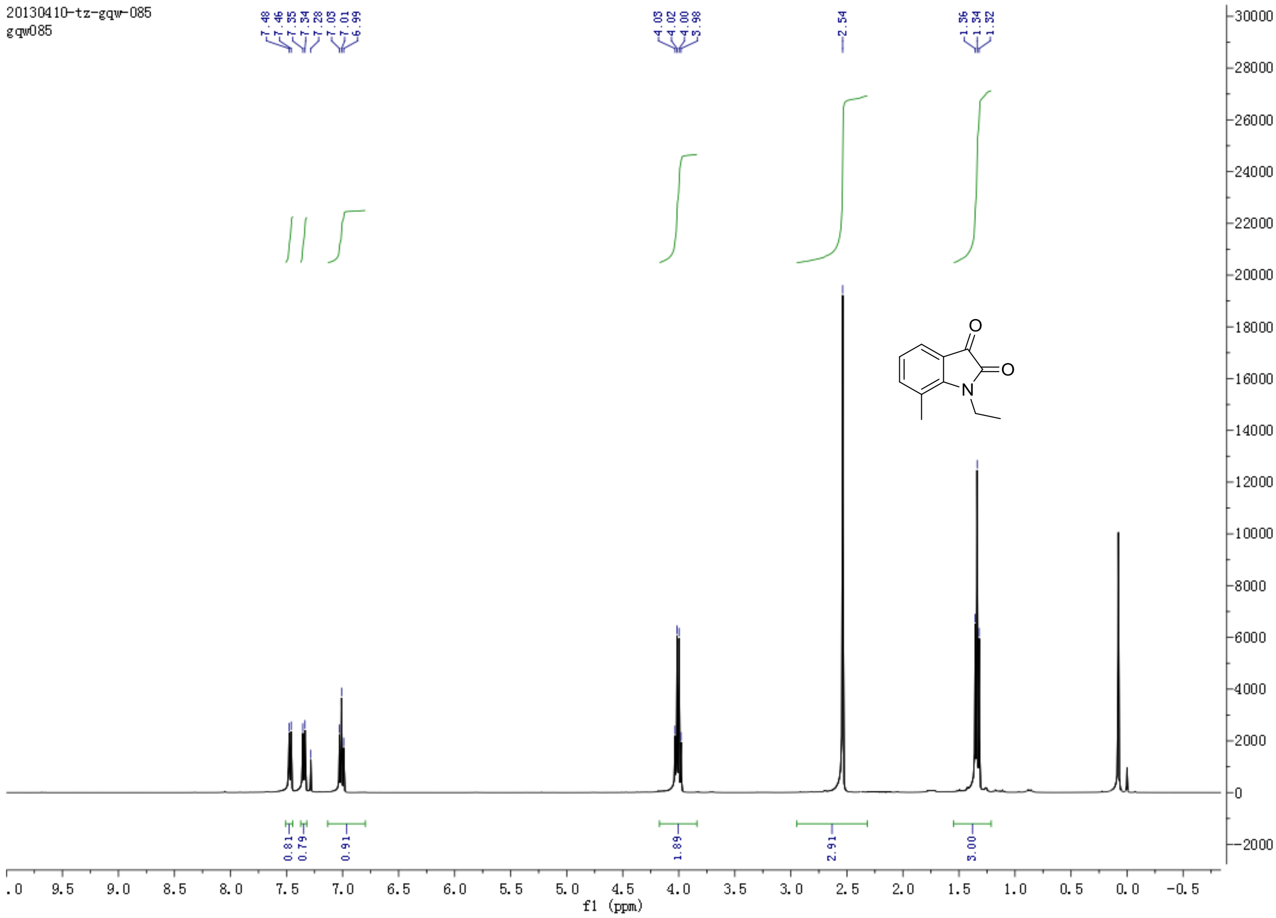
f1 (ppm)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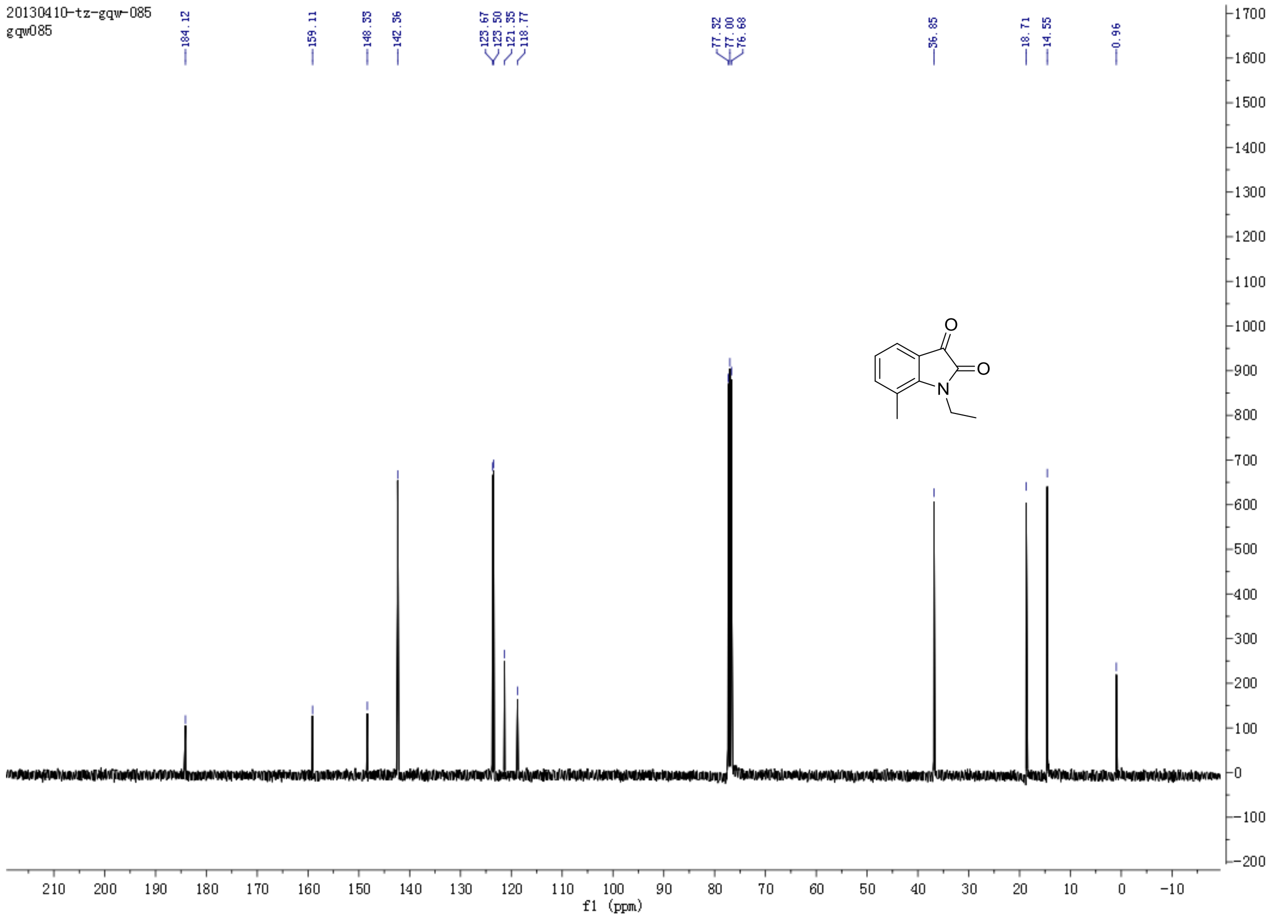
f1 (ppm)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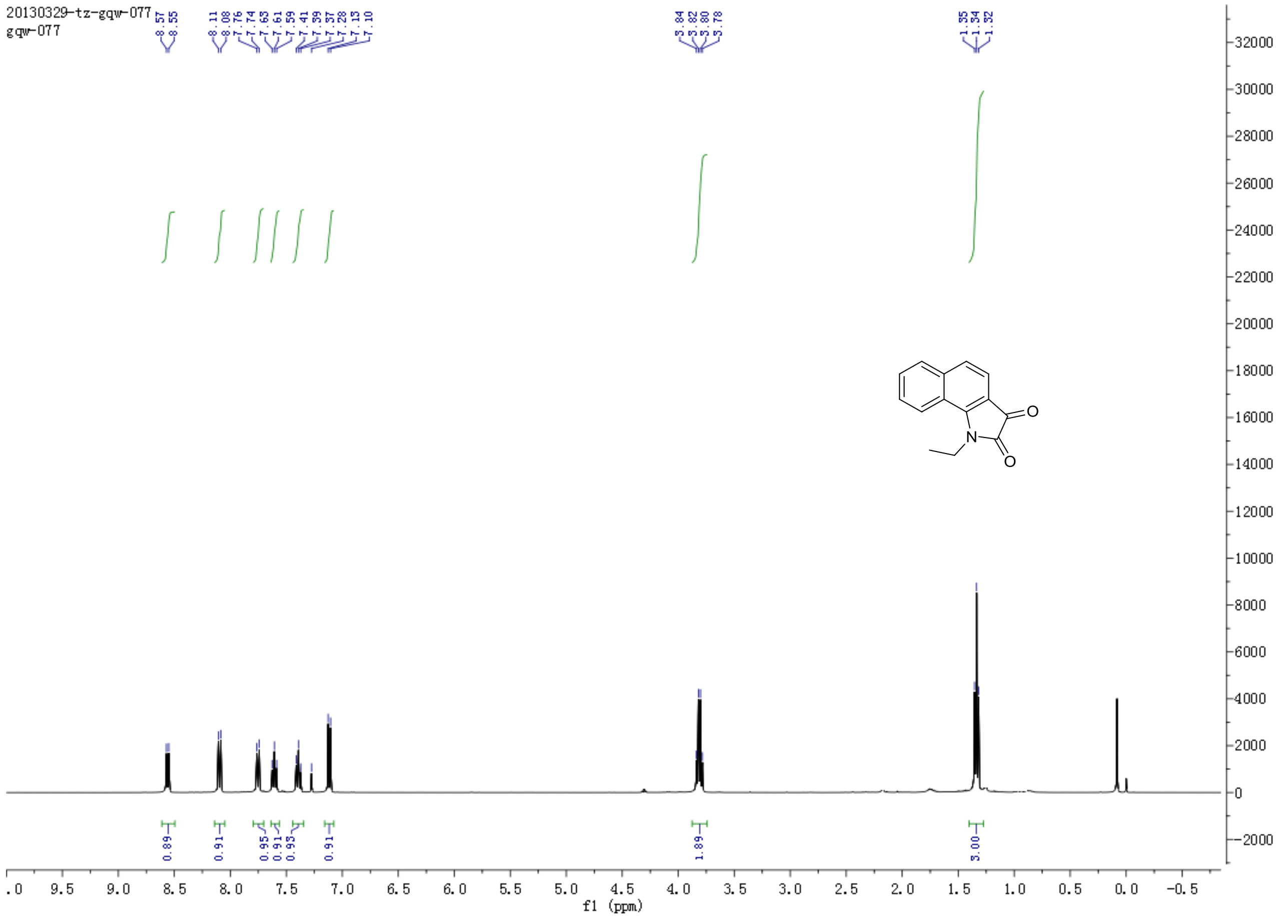

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7.13
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3.80
3.78
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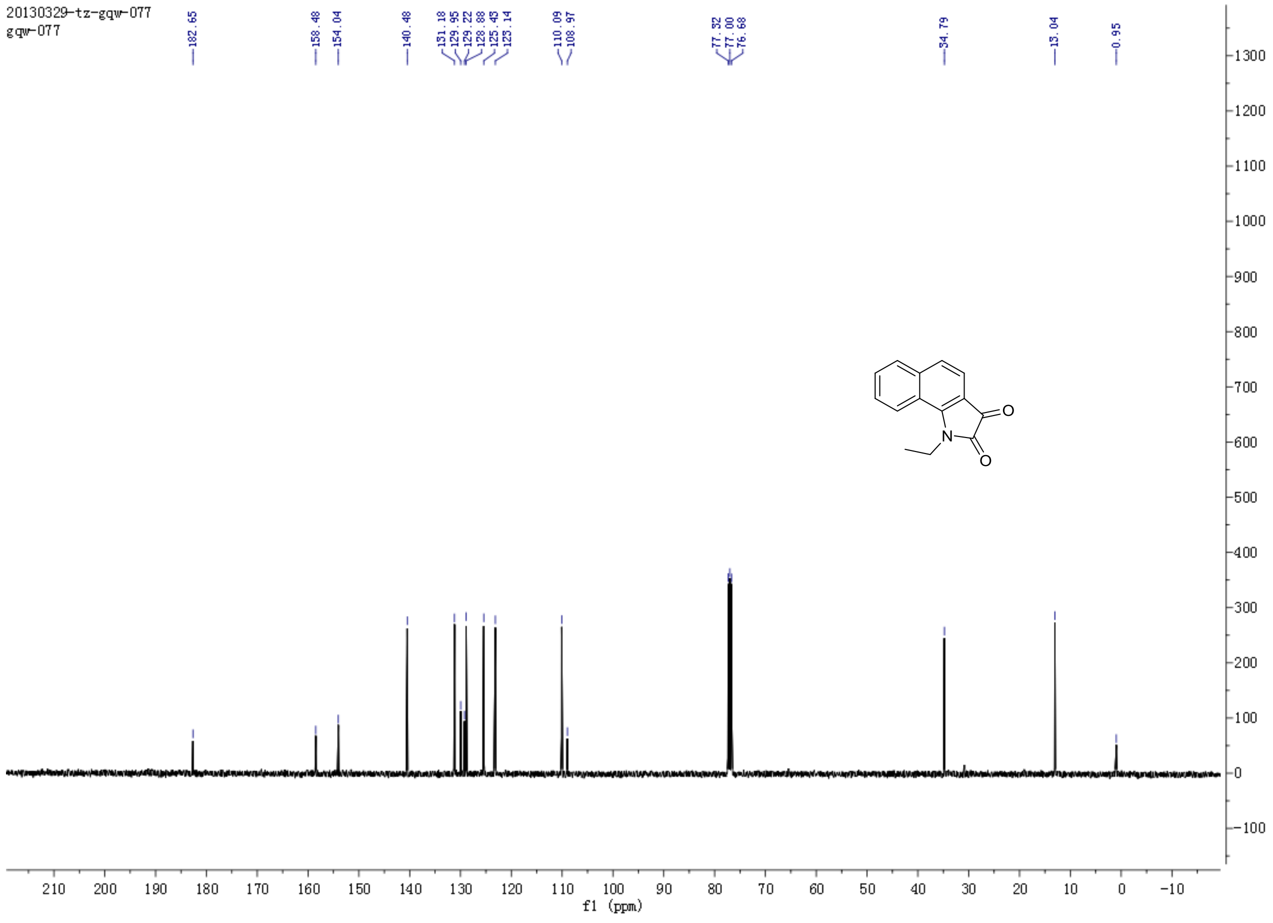

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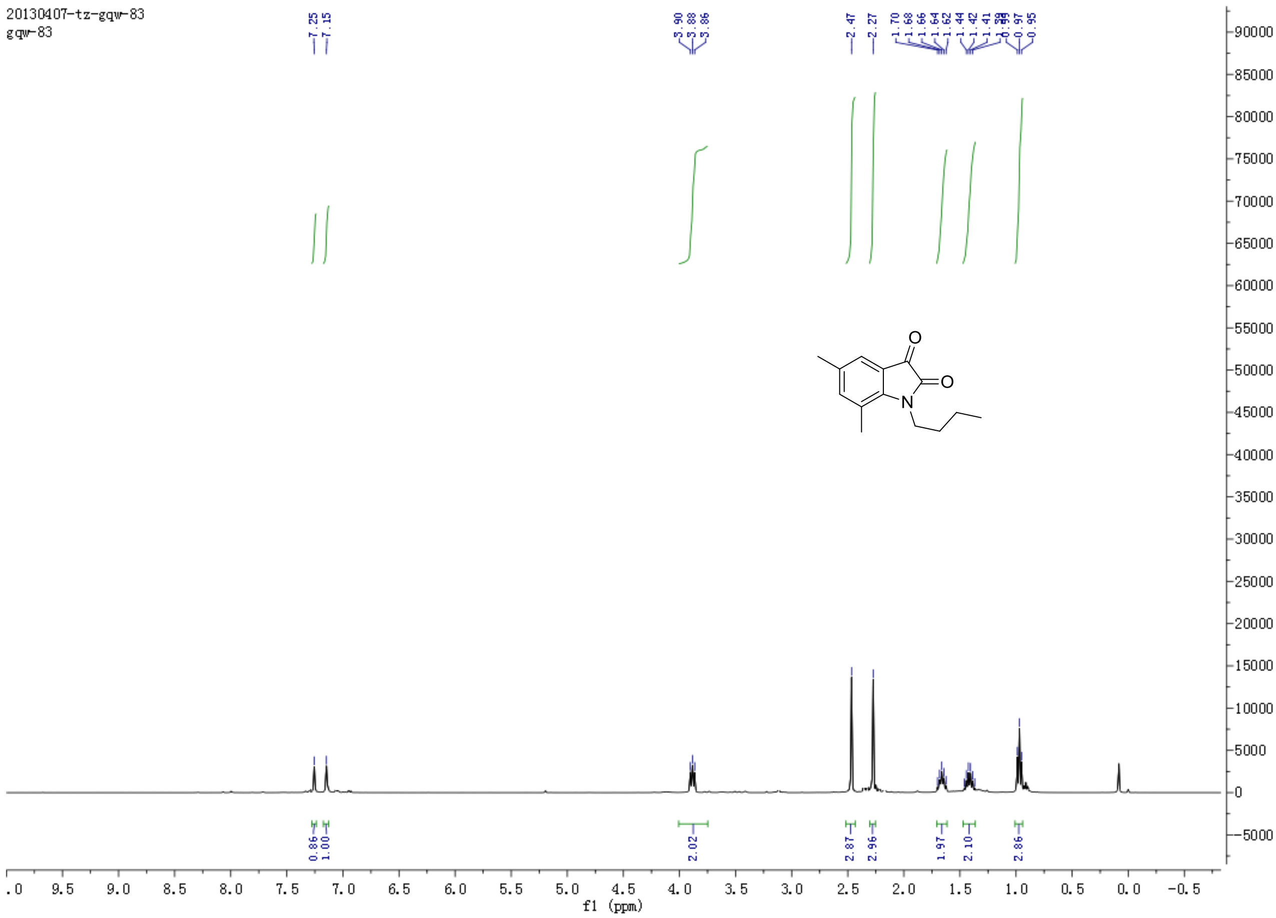
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1.41
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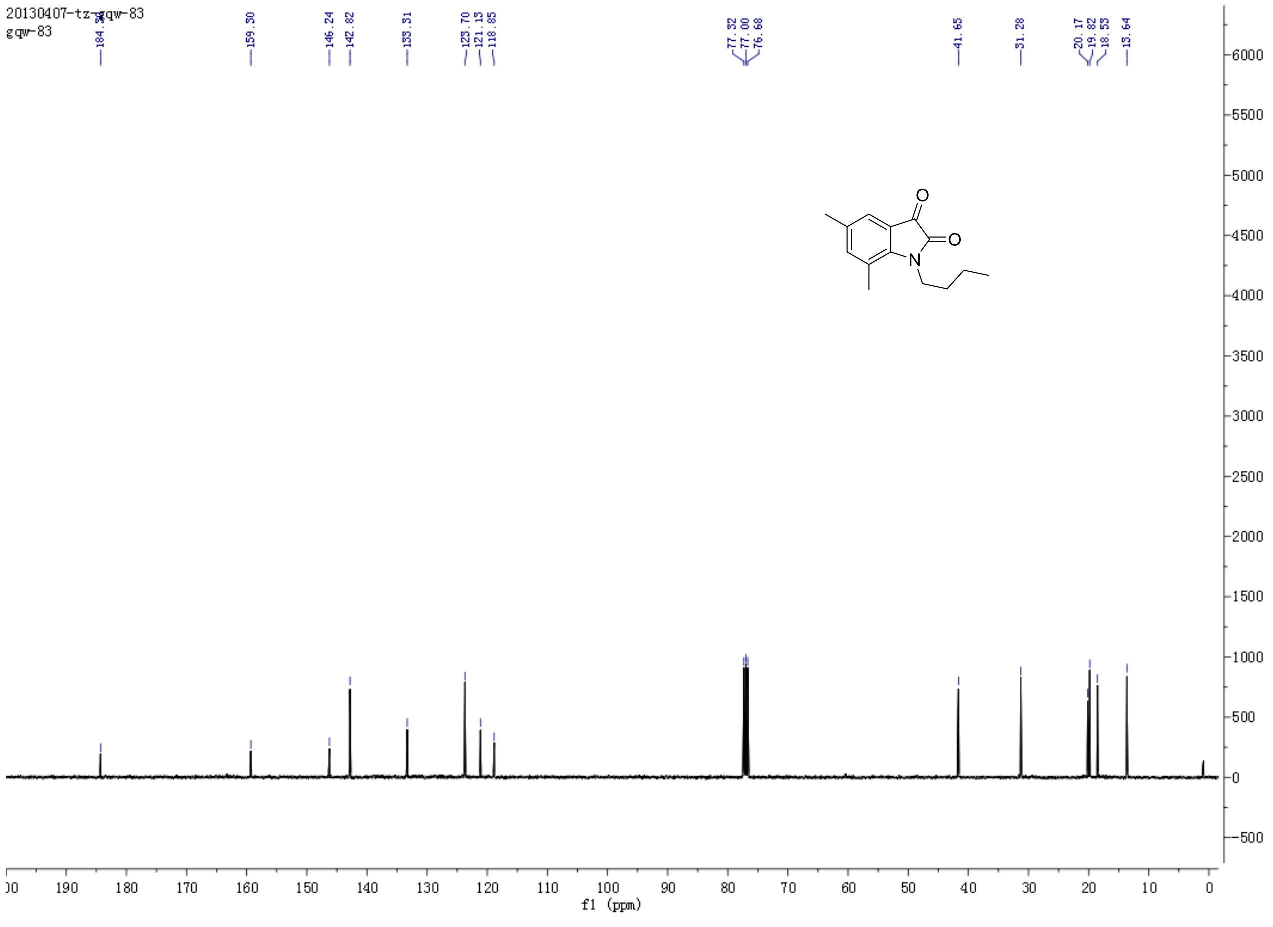
f1 (ppm)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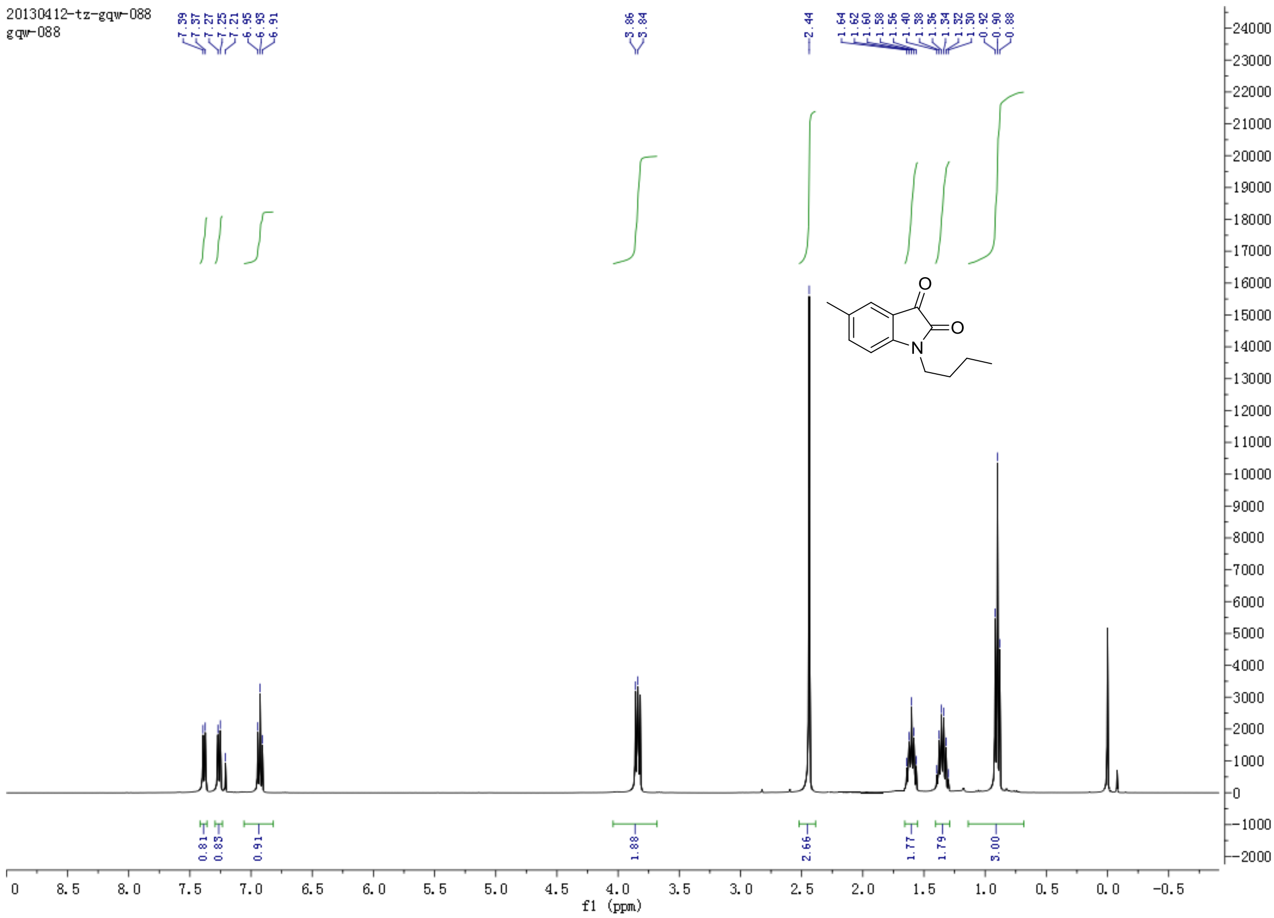
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1.38
1.36
1.34
1.32
1.30
0.92
0.90
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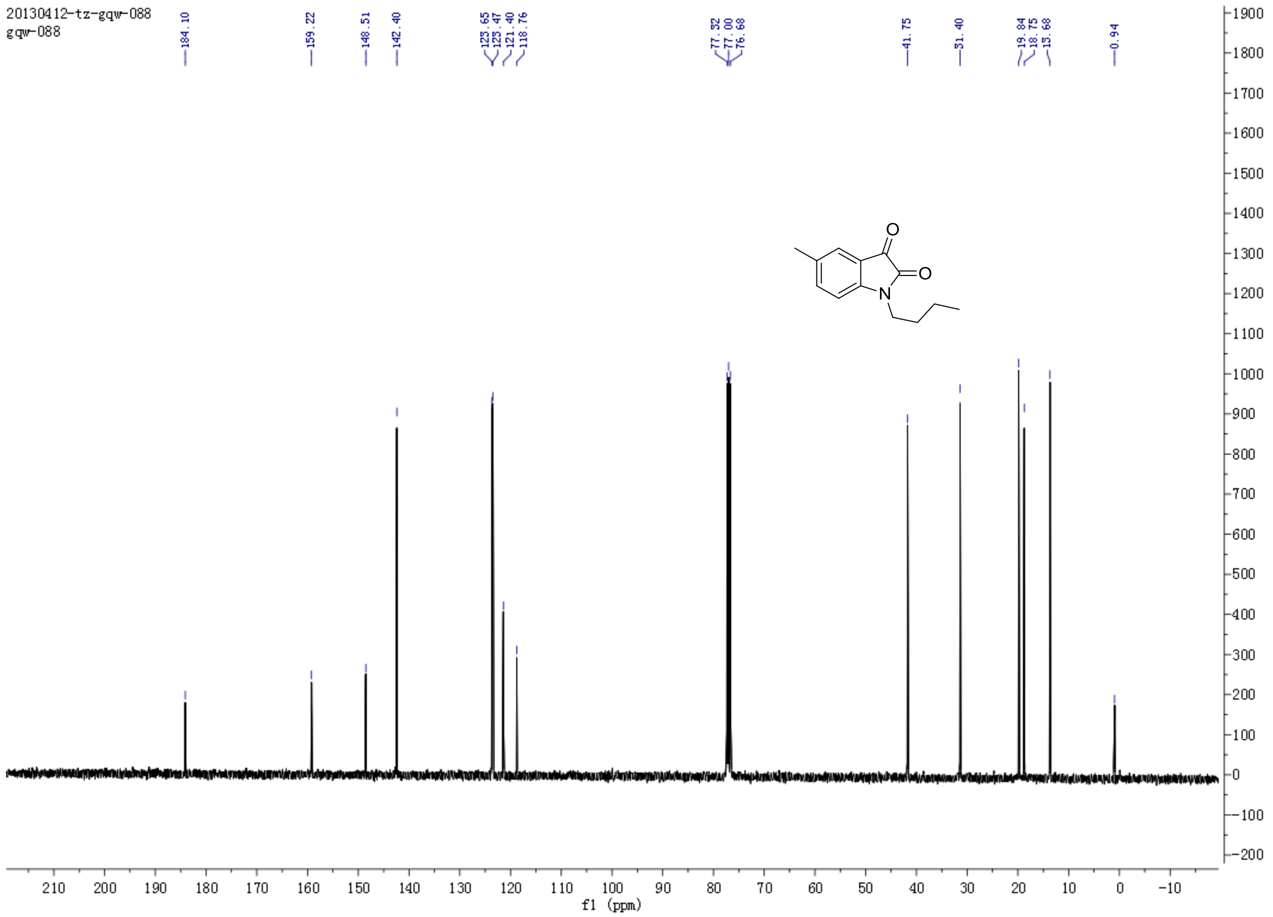
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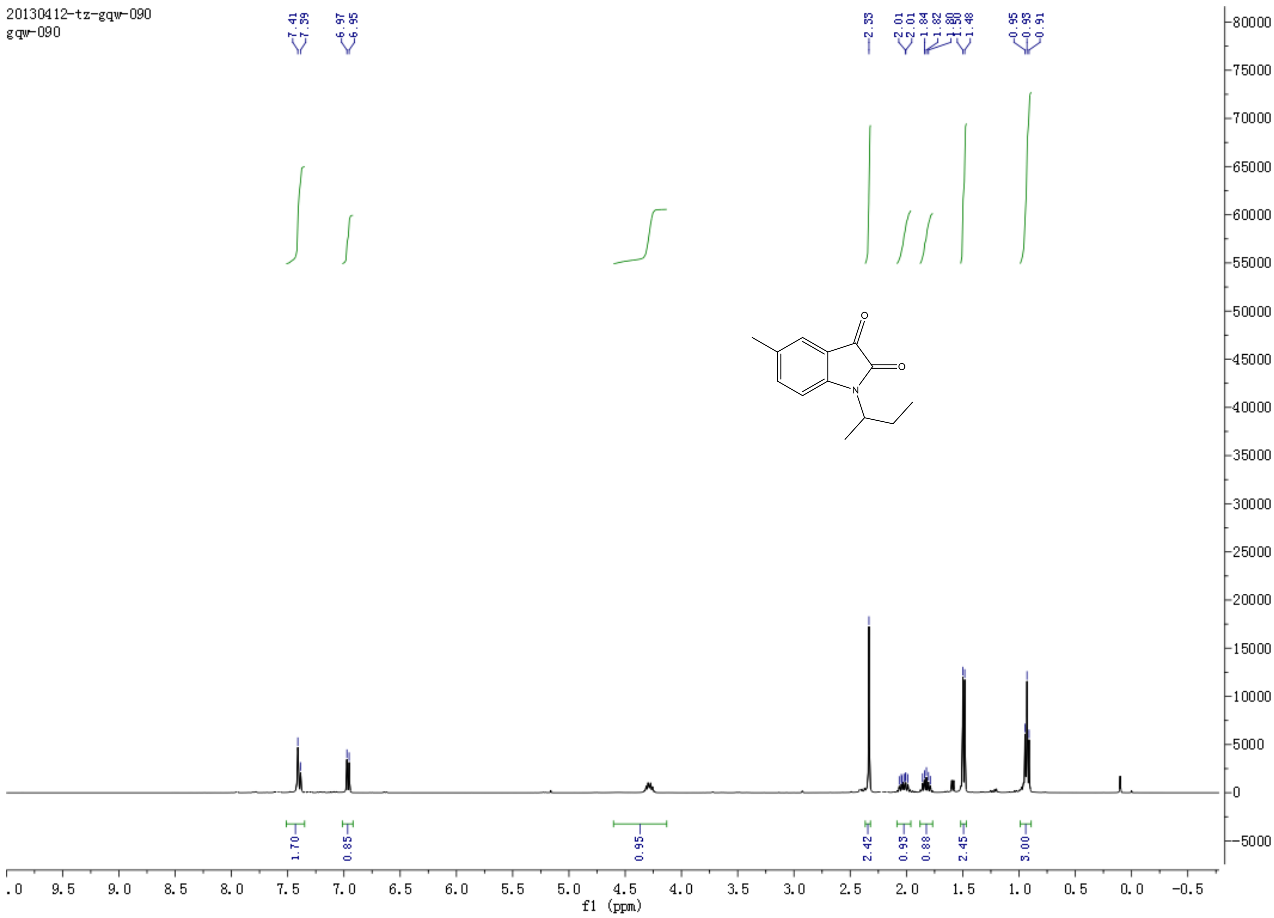
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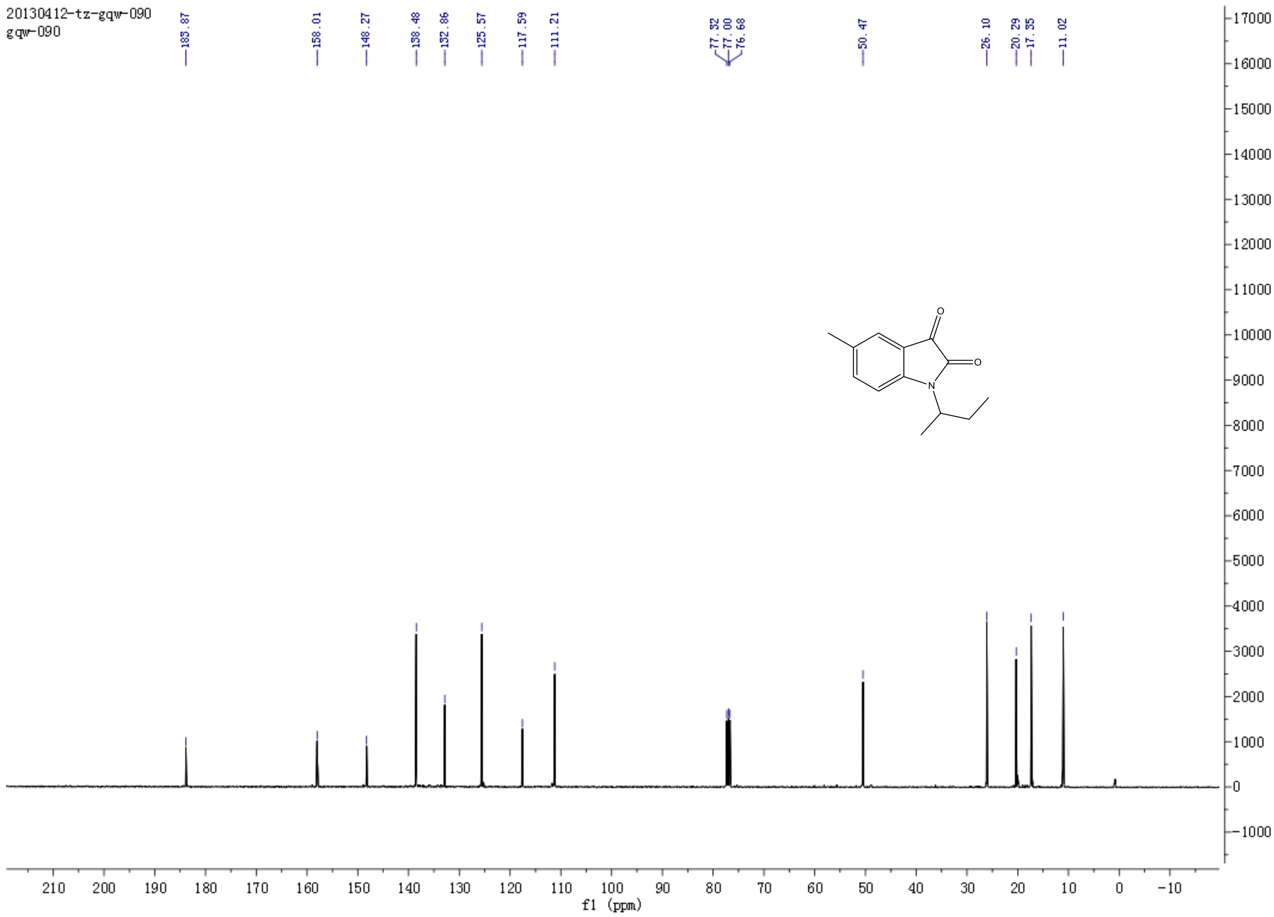
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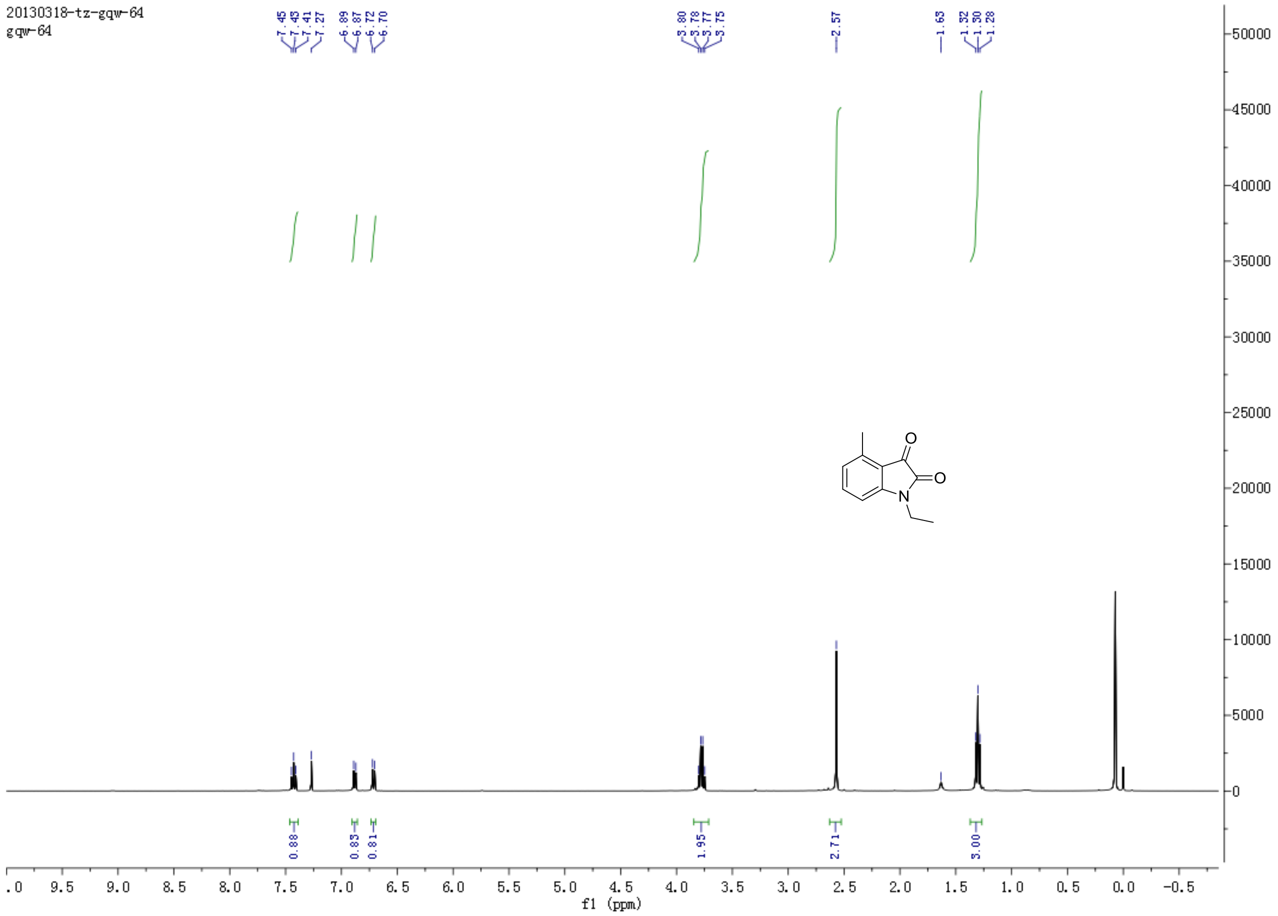
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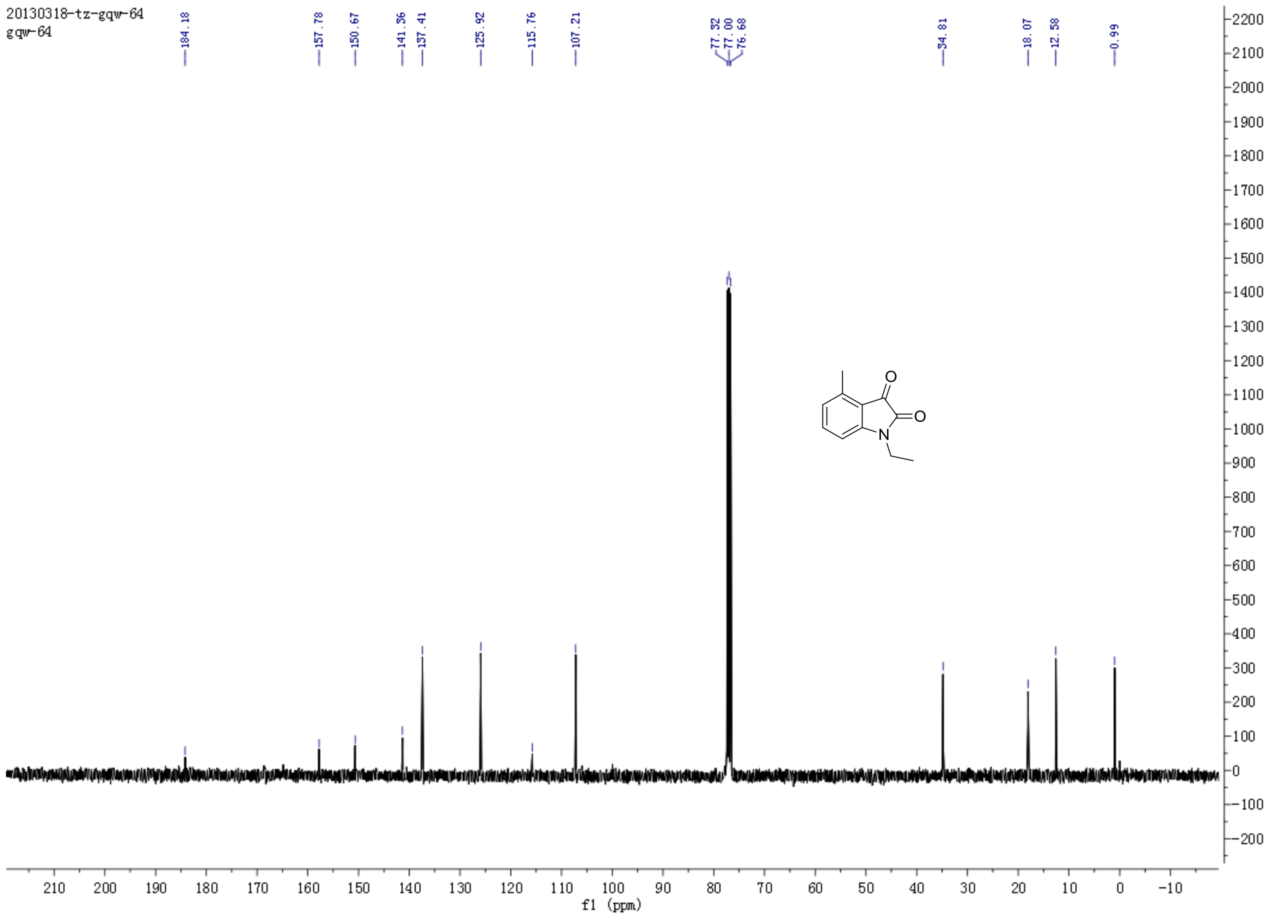
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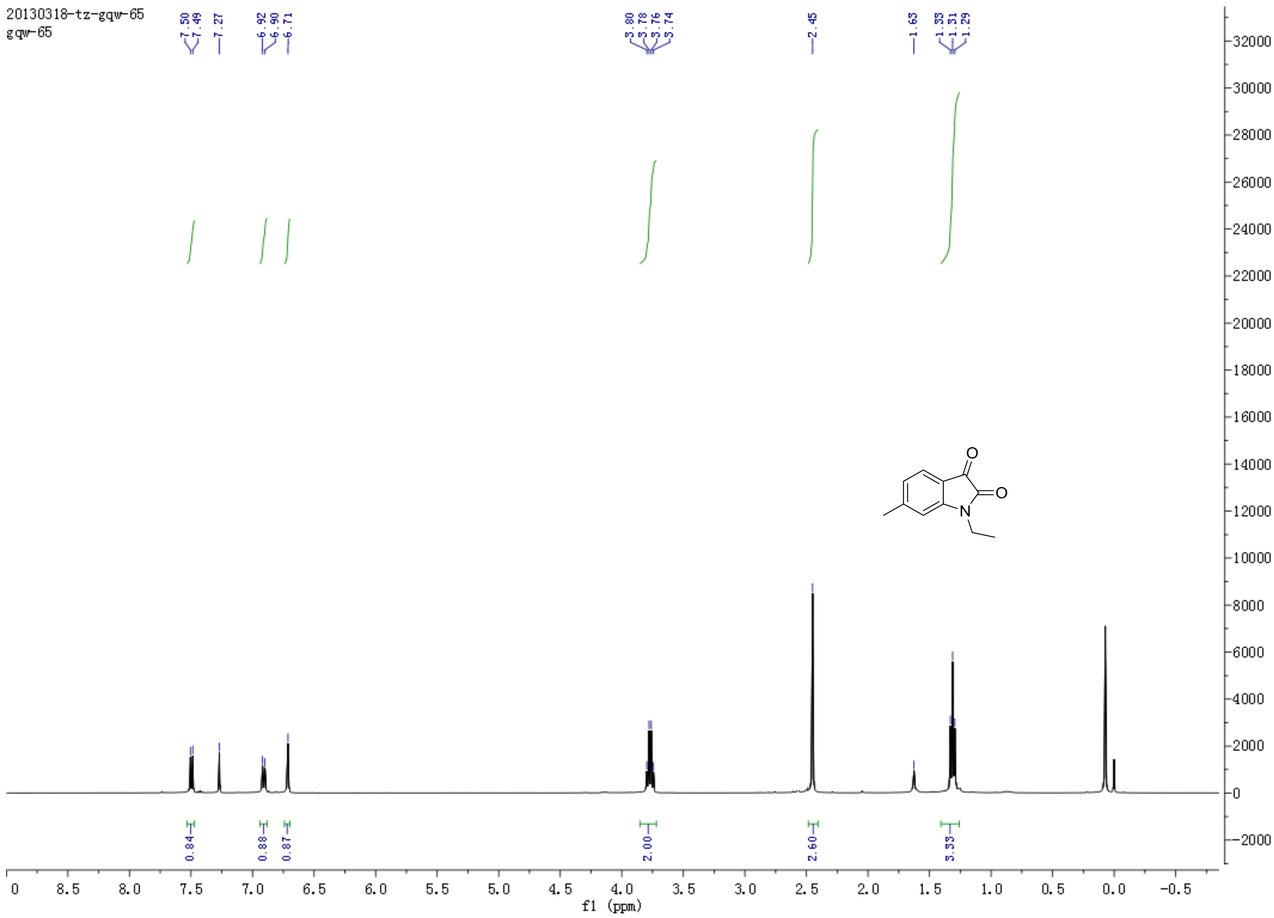

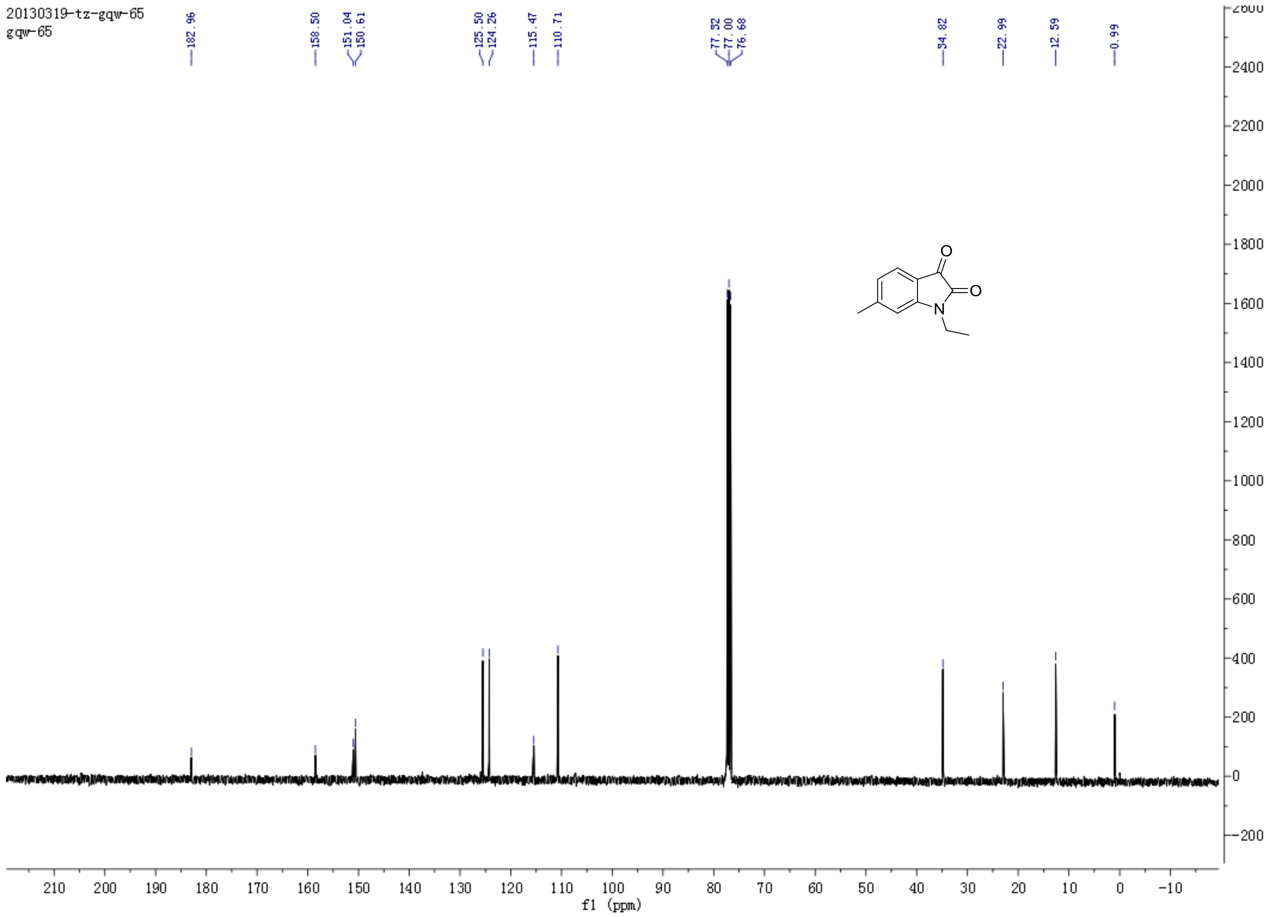

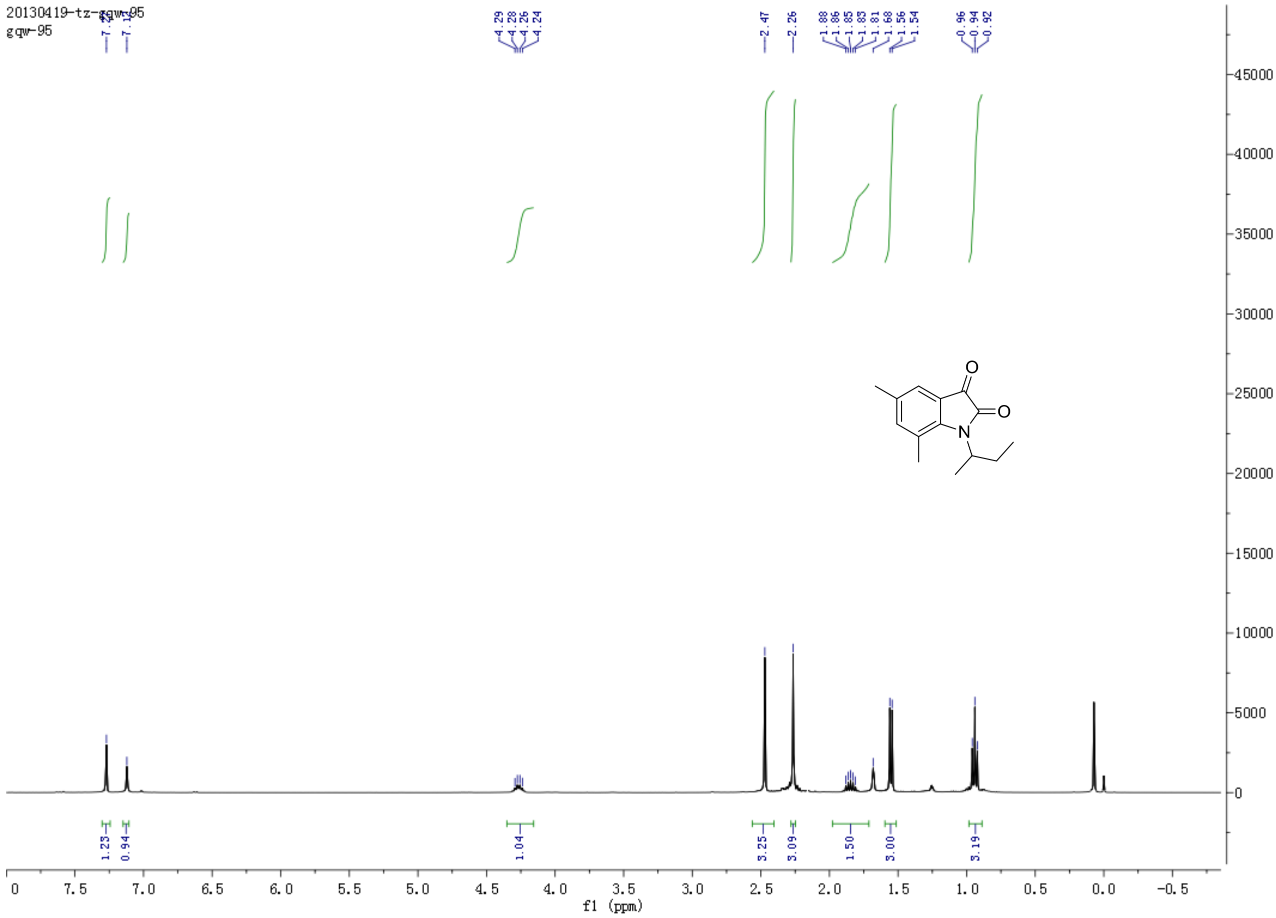
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1.81
1.68
1.56
1.54
0.96
0.94
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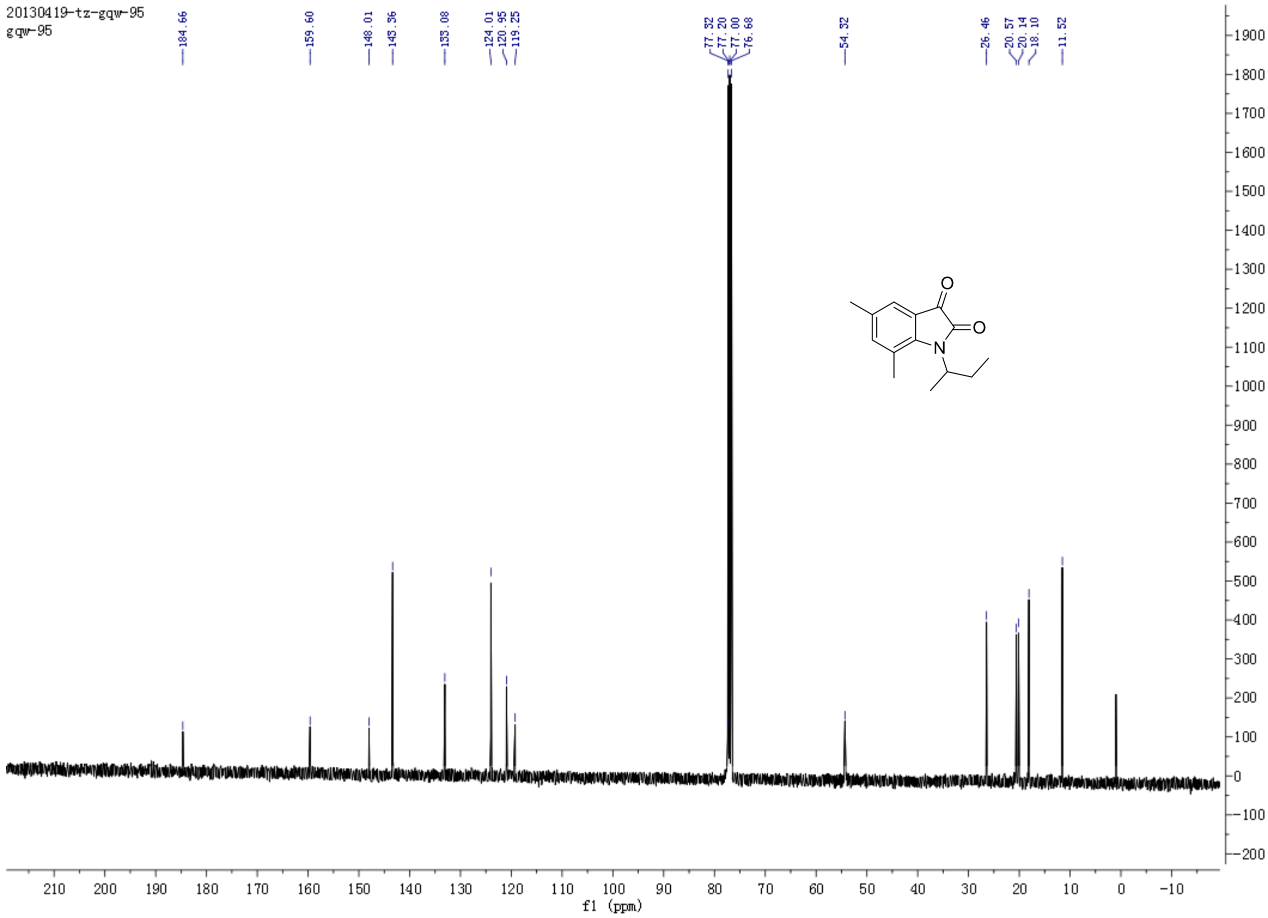
f1 (ppm)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26.46
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11.52
O
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N
f1 (ppm)