Supporting Information

For

Halogen cation-promoted and solvent-regulated electrophilic cyclization for the regioselective synthesis of 3-haloquinolines and 3-halospirocyclohexadienones

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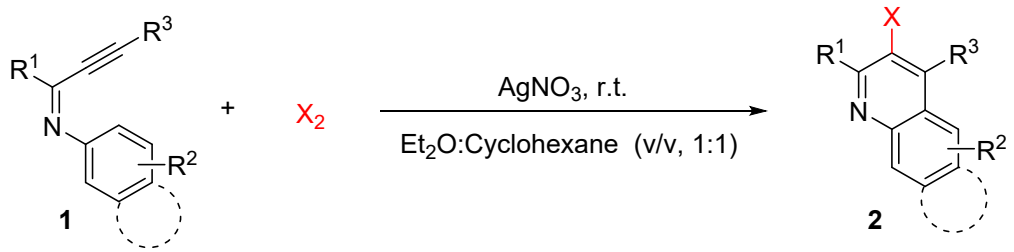
1. General information

All reactions were carried out in oven-dried glassware sealed with rubber septa under nitrogen condition. All solvents were distilled under nitrogen atmosphere prior to use. Purification of products was conducted by flash chromatography on silica gel (200-300 mesh). NMR spectra were measured on a Bruker magnetic resonance spectrometer (^{1}H at 500 MHz, ^{13}C at 126 MHz). Chemical shifts are reported in ppm using tetramethylsilane as internal standard (s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet). MS data were obtained on an Agilent 5975C inert 350 EI mass spectrometer (GC-MS). HRMS data were obtained on a VG ZAB-HS mass spectrometer, Brucker Apex IV FTMS spectrometer. Absorption spectra were obtained on a HITACHI U-2910 spectrometer. Fluorescence spectra were collected on a Horiba Jobin Yvon-Edison Fluoromax-4 fluorescence spectrometer. X-Ray single-crystal diffraction data were collected on an Agilent Technologies Gemini single-crystal diffractometer. Compounds described in the literature were characterized by the comparison of ^{1}H and/or ^{13}C NMR spectra to the previously reported data.

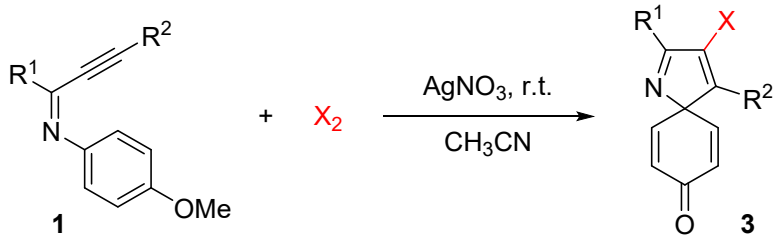
2. General procedure for the reaction

General Procedure A: Synthesis of 3-haloquinolines **2**



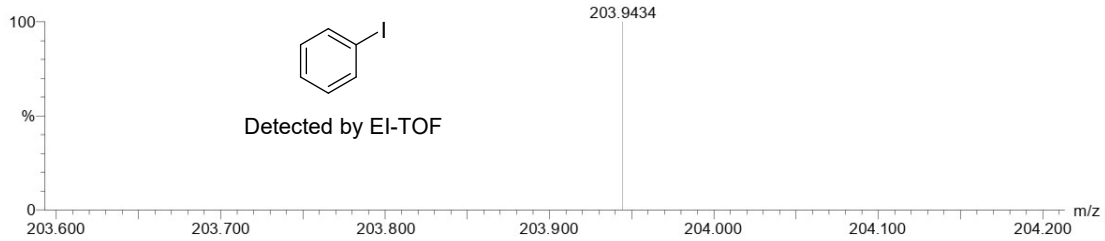
Under nitrogen atmosphere, a solution of alkynyl imine **1** (0.2 mmol), halogen (0.3 mol), $AgNO_3$ (0.3 mmol) and solvent Et_2O : Cyclohexane (v/v = 1:1, 2 mL) were added to a test tube. The mixture was stirred at room temperature for 5-10 min, then diluted with the saturated solution of sodium thiosulfate (10 mL) and extracted with EtOAc (3×5 mL). The combined organic layer was dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by column chromatography to afford the pure product **2**.

General Procedure B: Synthesis of 3-halospirocyclohexadienones **3**

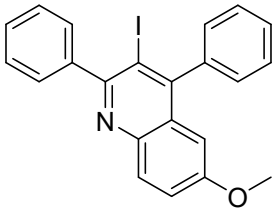


Under nitrogen atmosphere, a solution of alkynyl imine **1** (0.2 mmol), halogen (0.3 mol), $AgNO_3$ (0.3 mmol) and solvent Et_2O : Cyclohexane (v/v = 1:1, 2 mL) were added to a test tube. The mixture was stirred at room temperature for 5-10 min, then diluted with the saturated solution of sodium thiosulfate (10 mL) and extracted with EtOAc (3×5 mL). The combined organic layer was dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by column chromatography to afford the pure product **3**.

3. The detection of iodine cation



4. Characterization data



2a

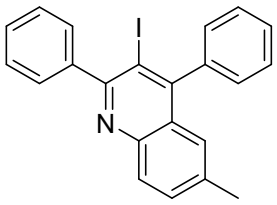
3-iodo-6-methoxy-2,4-diphenylquinoline (2a)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 8/1) to give **2a** 66 mg (76% yield) as a pale yellow solid (Mp 137-138 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 9.0 Hz, 1H), 7.56 (dd, *J* = 8.0, 1.0 Hz, 2H), 7.52–7.34 (m, 6H), 7.30 (dd, *J* = 9.0, 3.0 Hz, 1H), 7.25–7.20 (m, 2H), 6.56 (d, *J* = 3.0 Hz, 1H), 3.62 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.5, 158.3, 153.2, 143.8, 143.1, 142.4, 130.9, 129.4, 129.1, 128.8, 128.5, 128.4, 128.0, 122.5, 104.9, 99.1, 55.4;

HRMS (EI-TOF) calcd for $C_{22}H_{16}INO$ 437.0277, found 437.0273.



2b

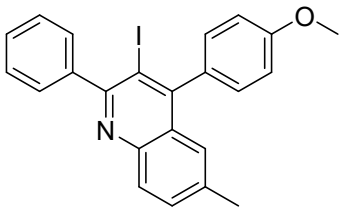
3-iodo-6-methyl-2,4-diphenylquinoline (2b)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 10/1) to give **2b** 61 mg (72% yield) as a yellow solid (Mp 83-84 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 9.0 Hz, 1H), 7.64 (d, *J* = 7.0 Hz, 2H), 7.59–7.52 (m, 4H), 7.50–7.43 (m, 3H), 7.28 (d, *J* = 7.0 Hz, 2H), 7.14 (s, 1H), 2.40 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 161.0, 154.0, 145.5, 143.8, 142.4, 137.4, 132.4, 129.4, 129.2, 129.1, 128.7, 128.5, 128.4, 128.0, 127.4, 125.6, 98.6, 21.8;

HRMS (EI-TOF) calcd for $C_{22}H_{16}IN$ 421.0327, found 421.0325.



2c

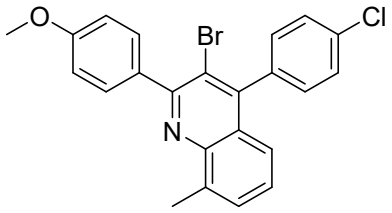
3-iodo-4-(4-methoxyphenyl)-6-methyl-2-phenylquinoline (2c)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 8/1) to give **2c** 64 mg (71% yield) as a yellow solid (Mp 96-97 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, *J* = 9.0 Hz, 1H), 7.66–7.59 (m, 2H), 7.52 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.49–7.38 (m, 3H), 7.20 (t, *J* = 7.0 Hz, 3H), 7.06 (d, *J* = 9.0 Hz, 2H), 3.88 (s, 3H), 2.39 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 161.0, 159.6, 153.9, 145.6, 144.0, 137.3, 134.7, 132.4, 130.5, 129.4, 129.2, 128.5, 128.0, 127.8, 125.7, 114.1, 99.6, 55.4, 21.9;

HRMS (EI-TOF) calcd for $C_{23}H_{18}INO$ 451.0433, found 451.0431.



2d

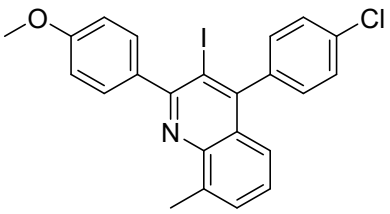
3-bromo-4-(4-chlorophenyl)-2-(4-methoxyphenyl)-8-methylquinoline (2d)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 8/1) to give **2d** 65 mg (74% yield) as a yellow solid (Mp 67-68 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.0 Hz, 2H), 7.56 (d, *J* = 6.0 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.32 (q, *J* = 9.0 Hz, 2H), 7.26–7.21 (m, 2H), 7.07 (d, *J* = 9.0 Hz, 2H), 3.91 (s, 3H), 2.81 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.6, 155.9, 149.8, 145.5, 139.8, 137.7, 134.7, 131.4, 130.8, 130.6, 129.9, 128.4, 128.0, 127.2, 124.6, 118.5, 113.9, 55.3, 18.1;

HRMS (EI-TOF) calcd for $C_{23}H_{17}BrClNO$ 437.0182, found 437.0185.



2e

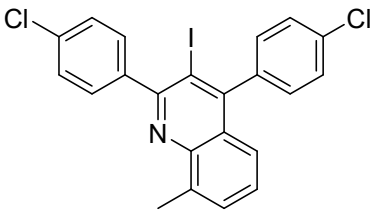
4-(4-chlorophenyl)-3-iodo-2-(4-methoxyphenyl)-8-methylquinoline (2e)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 8/1) to give **2e** 77 mg (79% yield) as a yellow solid (Mp 82-83 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.51–7.45 (m, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 4.0 Hz, 2H), 7.10 (d, *J* = 9.0 Hz, 2H), 6.99 (d, *J* = 9.0 Hz, 2H), 3.83 (s, 3H), 2.71 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.5, 157.8, 153.8, 145.0, 141.3, 136.5, 134.0, 133.5, 130.3, 129.4, 129.1, 126.9, 126.8, 126.0, 124.0, 112.9, 97.5, 54.3, 17.0;

HRMS (EI-TOF) calcd for $C_{23}H_{17}ClINO$ 485.0043, found 485.0041.



2f

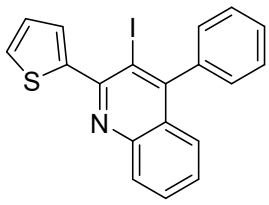
2,4-bis(4-chlorophenyl)-3-iodo-8-methylquinoline (2f)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 10/1) to give **2f** 64 mg (65% yield) as a yellow solid (Mp 85-86 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 7.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.34–7.28 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 3H), 2.80 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.9, 153.7, 146.0, 142.1, 140.9, 137.8, 134.7, 134.6, 131.3, 130.6, 130.4, 129.0, 128.0, 127.4, 127.3, 124.5, 97.6, 18.0;

HRMS (EI-TOF) calcd for $C_{22}H_{14}Cl_2IN$ 488.9548, found 488.9546.



2g

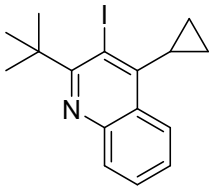
3-iodo-4-phenyl-2-(thiophen-2-yl)quinoline (2g)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 10/1) to give **2g** 58 mg (70% yield) as an amorphous solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 3.0 Hz, 1H), 7.71 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.59–7.53 (m, 3H), 7.51 (d, *J* = 5.0 Hz, 1H), 7.36 (dd, *J* = 13.0, 7.0 Hz, 2H), 7.30–7.26 (m, 2H), 7.15 (dd, *J* = 5.0, 4.0 Hz, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.5, 154.5, 146.8, 145.2, 142.5, 130.3, 130.1, 129.2, 129.1, 128.7, 128.5, 128.1, 127.4, 127.3, 126.9, 126.8, 97.3;

HRMS (EI-TOF) calcd for $C_{19}H_{12}INS$ 412.9735, found 412.9731.



2h

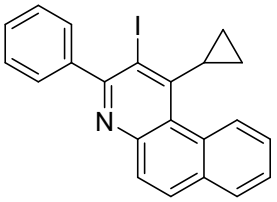
2-(*tert*-butyl)-4-cyclopropyl-3-iodoquinoline (2h)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 10/1) to give **2h** 48 mg (68% yield) as an amorphous solid;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42 (d, *J* = 9.0 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 2.11–2.01 (m, 1H), 1.72 (s, 9H), 1.49–1.43 (m, 2H), 0.77 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.2, 152.7, 145.5, 129.7, 128.9, 128.1, 125.8, 124.1, 99.4, 41.3, 30.1, 21.1, 12.9, 8.7;

HRMS (EI-TOF) calcd for $C_{16}H_{18}IN$ 351.0484, found 351.0487.



2i

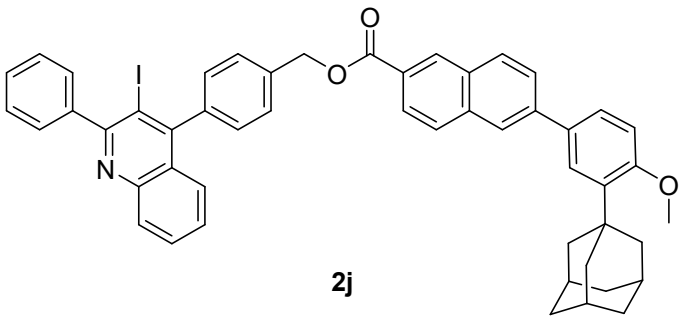
1-cyclopropyl-2-iodo-3-phenylbenzo[*f*]quinoline (2i)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 10/1) to give **2i** 53 mg (63% yield) as a yellow solid (Mp 103-104 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.29 (d, *J* = 7.0 Hz, 1H), 8.40 (d, *J* = 9.0 Hz, 1H), 7.86 (d, *J* = 7.0 Hz, 1H), 7.79 (d, *J* = 9.0 Hz, 1H), 7.72 (d, *J* = 7.0 Hz, 2H), 7.68–7.59 (m, 2H), 7.50 (dd, *J* = 15.0, 7.0 Hz, 3H), 2.22–2.07 (m, 1H), 1.49 (m, 2H), 0.88 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.6, 152.0, 145.3, 144.2, 133.3, 131.6, 130.0, 128.4, 128.3, 127.7, 127.6, 127.5, 127.0, 126.6, 125.2, 121.9, 102.3, 20.0, 12.1;

HRMS (EI-TOF) calcd for $C_{22}H_{16}IN$ 421.0327, found 421.0325.



2j

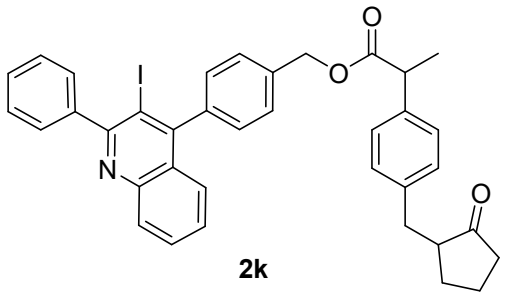
4-(3-iodo-2-phenylquinolin-4-yl)benzyl 6-(3-((3r,5r,7r)-adamantan-1-yl)-4-methoxyphenyl)-2-naphthoate (2j)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 3/1) to give **2j** 91 mg (55% yield) as a white solid (Mp 112-113 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (s, 1H), 8.21 (t, *J* = 8.0 Hz, 2H), 8.05 (d, *J* = 10.0 Hz, 2H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.81–7.72 (m, 3H), 7.69 (d, *J* = 7.0 Hz, 2H), 7.65 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 7.0 Hz, 2H), 7.51–7.43 (m, 3H), 7.40 (d, *J* = 7.0 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 5.62 (s, 2H), 3.94 (s, 3H), 2.22 (s, 6H), 2.14 (s, 3H), 1.84 (s, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.7, 161.9, 159.0, 154.4, 146.9, 143.6, 142.0, 141.6, 139.1, 136.6, 136.1, 132.5, 131.3, 131.1, 130.2, 129.8, 129.5, 129.4, 129.3, 128.7, 128.4, 128.3, 128.0, 127.4, 127.3, 126.8, 126.7, 126.6, 126.0, 125.8, 125.7, 124.8, 112.2, 98.4, 66.4, 55.2, 40.6, 37.2, 29.7, 29.1;

HRMS (EI-TOF) calcd for $C_{50}H_{42}INO_3$ 831.2209, found 831.2205.



2k

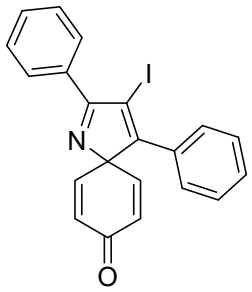
4-(3-iodo-2-phenylquinolin-4-yl)benzyl 2-(4-((2-oxocyclopentyl)methyl)phenyl)propanoate (2k)

Following the General Procedure A, and target product was purified by flash chromatography (PE/EA = 2/1) to give **2k** 64 mg (48% yield) as a white solid (Mp 90-91 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 7.0 Hz, 2H), 7.55–7.47 (m, 3H), 7.45 (t, *J* = 7.0 Hz, 3H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.28 (t, *J* = 7.0 Hz, 4H), 7.16 (d, *J* = 8.0 Hz, 2H), 5.32–5.23 (m, 2H), 3.86 (q, *J* = 7.0 Hz, 1H), 3.15 (dd, *J* = 14.0, 4.0 Hz, 1H), 2.53 (dd, *J* = 14.0, 10.0 Hz, 1H), 2.39–2.28 (m, 2H), 2.15–2.06 (m, 2H), 1.94 (m, 1H), 1.71 (m, 1H), 1.59 (d, *J* = 7.0 Hz, 3H), 1.57–1.50 (m, 1H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 174.4, 161.9, 154.3, 146.9, 143.6, 141.7, 139.0, 138.2, 136.5, 130.2, 129.5, 129.4, 129.3, 129.2, 128.7, 128.0, 127.9, 127.6, 127.4, 127.3, 126.7, 98.4, 66.0, 51.0, 45.2, 38.2, 35.2, 29.2, 20.5, 18.5;

HRMS (EI-TOF) calcd for $C_{37}H_{32}INO_3$ 665.1427, found 665.1429.



3a

3-iodo-2,4-diphenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3a)

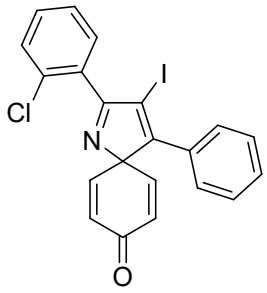
Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3a** 58 mg (68% yield) as a pale yellow solid (Mp 125-126 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.0 Hz, 2H), 7.56–7.49 (m, 3H), 7.38 (d, *J* = 3.0 Hz, 3H), 7.31 (dd, *J* = 6.0, 3.0 Hz, 2H), 6.45 (d, *J* = 10.0 Hz, 2H), 6.37 (d, *J* = 10.0 Hz, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.2, 177.0, 170.0, 142.6, 133.2, 133.0, 131.7,

131.0, 129.6, 129.2, 128.7, 128.3, 127.7, 93.7, 83.0;

HRMS (EI-TOF) calcd for $C_{21}H_{14}INO$ 423.0120, found 423.0123.



3b

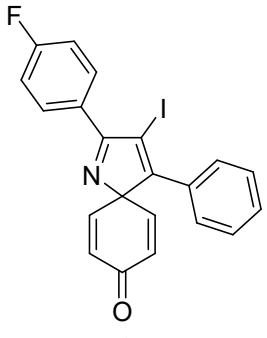
2-(2-chlorophenyl)-3-iodo-4-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3b)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3b** 57 mg (62% yield) as a pale yellow solid (Mp 106-107 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.40–7.37 (m, 3H), 7.31 (dd, *J* = 7.0, 3.0 Hz, 2H), 6.46 (d, *J* = 10.0 Hz, 2H), 6.35 (d, *J* = 10.0 Hz, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.0, 175.8, 170.5, 142.2, 134.7, 134.4, 133.0, 131.8, 131.0, 129.8, 129.6, 129.4, 128.7, 127.6, 127.4, 92.9, 83.1;

HRMS (EI-TOF) calcd for $C_{21}H_{13}ClINO$ 456.9730, found 456.9732.



3c

2-(4-fluorophenyl)-3-iodo-4-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3c)

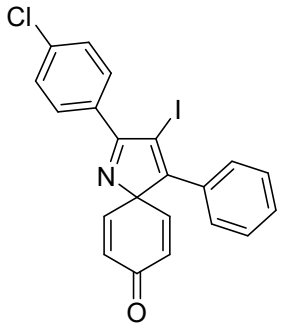
Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3c** 62 mg (70% yield) as a pale yellow solid (Mp 114-115 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01–7.95 (m, 2H), 7.41–7.35 (m, 3H), 7.33–7.28 (m, 2H), 7.19 (t, *J* = 9.0 Hz, 2H), 6.45 (d, *J* = 10.0 Hz, 2H), 6.36 (d, *J* = 10.0 Hz, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.1, 175.8, 170.3, 164.4 (d, J_{C-F} = 253.0 Hz), 142.5, 133.1, 131.7, 131.5 (d, J_{C-F} = 9.0 Hz), 129.7, 129.2 (d, J_{C-F} = 4.0 Hz), 128.7, 127.6, 115.5 (d, J_{C-F} = 21.0 Hz), 93.3, 83.0;

^{19}F NMR (471 MHz, $CDCl_3$) δ -112.8;

HRMS (EI-TOF) calcd for $C_{21}H_{13}FINO$ 441.0026, found 441.0025.



3d

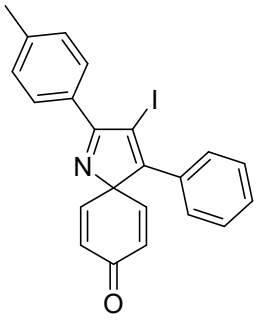
2-(4-chlorophenyl)-3-iodo-4-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3d)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3d** 65 mg (71% yield) as a pale yellow solid (Mp 117-118 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 9.0 Hz, 2 H), 7.48 (d, *J* = 9.0 Hz, 2 H), 7.41-7.35 (m, 3 H), 7.33-7.28 (m, 2 H), 6.45 (d, *J* = 10.0 Hz, 2H), 6.35 (d, *J* = 10.0 Hz, 2 H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.0, 175.9, 170.5, 142.3, 137.3, 133.1, 131.7, 131.4, 130.7, 129.7, 128.7, 128.6, 127.6, 93.1, 83.1;

HRMS (EI-TOF) calcd for $C_{21}H_{13}ClINO$ 456.9730, found 456.9732.



3e

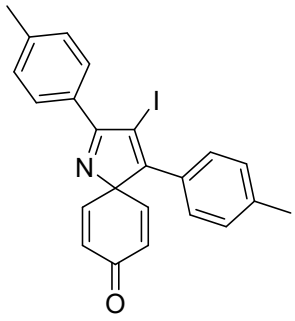
3-iodo-4-phenyl-2-(*p*-tolyl)-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3e)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3e** 67 mg (77% yield) as a pale yellow solid (Mp 120-121 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 2H), 7.40–7.34 (m, 3H), 7.30 (t, *J* = 8.0 Hz, 4H), 6.43 (d, *J* = 10.0 Hz, 2H), 6.36 (d, *J* = 10.0 Hz, 2H), 2.43 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.2, 176.7, 169.8, 142.8, 141.3, 133.3, 131.6, 130.2, 129.6, 129.2, 129.0, 128.6, 127.7, 93.9, 82.9, 21.6;

HRMS (EI-TOF) calcd for $C_{22}H_{16}INO$ 437.0277, found 437.0279.



3f

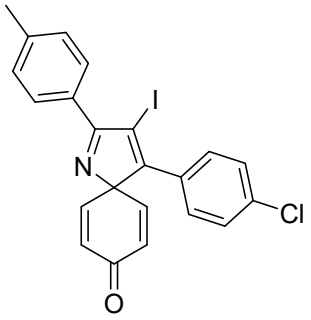
3-iodo-2,4-di-*p*-tolyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3f)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3f** 68 mg (75% yield) as a pale yellow solid (Mp 116-117 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 6.43 (d, *J* = 10.0 Hz, 2H), 6.35 (d, *J* = 10.0 Hz, 2H), 2.42 (s, 3H), 2.35 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.3, 176.8, 169.7, 143.1, 141.2, 139.7, 131.5, 130.3, 129.4, 129.2, 129.0, 127.6, 93.4, 82.8, 21.6, 21.5;

HRMS (EI-TOF) calcd for $C_{23}H_{18}INO$ 451.0433, found 451.0434.



3g

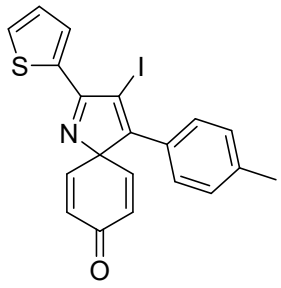
4-(4-chlorophenyl)-3-iodo-2-(*p*-tolyl)-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3g)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3g** 65 mg (69% yield) as a pale yellow solid (Mp 105-106 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 9.0 Hz, 2H), 6.45 (d, *J* = 10.0 Hz, 2H), 6.35 (d, *J* = 10.0 Hz, 2H), 2.44 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.0, 176.7, 168.5, 142.5, 141.5, 135.7, 131.7, 131.6, 130.0, 129.3, 129.2, 129.1, 129.0, 94.4, 82.8, 21.6;

HRMS (EI-TOF) calcd for $C_{22}H_{15}ClINO$ 470.9887, found 470.9885.



3h

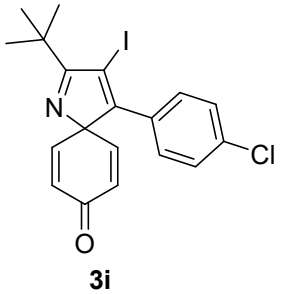
3-iodo-2-(thiophen-2-yl)-4-(*p*-tolyl)-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3h)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3h** 68 mg (77% yield) as a yellow solid (Mp 94-95 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.0 Hz, 2H), 7.62 (d, *J* = 4.0 Hz, 1H), 7.50 (d, *J* = 5.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.10 (t, *J* = 4.0 Hz, 1H), 6.57 (d, *J* = 10.0 Hz, 2H), 6.39 (d, *J* = 10.0 Hz, 2H), 2.43 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.4, 177.9, 160.1, 144.6, 141.1, 133.7, 131.5, 130.4, 129.9, 129.2, 128.9, 128.8, 127.5, 89.9, 81.8, 21.6;

HRMS (EI-TOF) calcd for $C_{20}H_{14}INOS$ 442.9841, found 442.9844.



3i

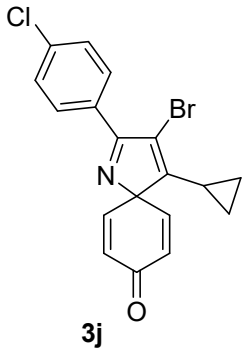
2-(*tert*-butyl)-4-(4-chlorophenyl)-3-iodo-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3i)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3i** 56 mg (64% yield) as a pale yellow solid (Mp 72-73 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.39 (d, *J* = 10.0 Hz, 2H), 6.18 (d, *J* = 10.0 Hz, 2H), 1.54 (s, 9H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.0, 183.5, 169.1, 142.8, 135.4, 131.9, 131.7, 129.3, 128.9, 91.5, 81.4, 37.1, 28.2;

HRMS (EI-TOF) calcd for $C_{19}H_{17}ClINO$ 437.0043, found 437.0045.



3j

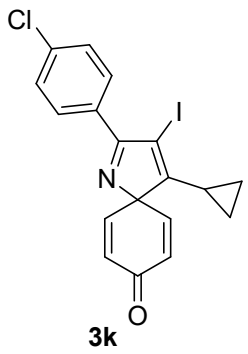
3-bromo-2-(4-chlorophenyl)-4-cyclopropyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3j)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3j** 43 mg (57% yield) as a white solid (Mp 88-89 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 6.53 (d, *J* = 10.0 Hz, 2H), 6.25 (d, *J* = 10.0 Hz, 2H), 1.70 (m, 1H), 1.23–1.16 (m, 2H), 1.00–0.93 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.3, 174.3, 165.7, 143.4, 137.3, 131.5, 130.7, 130.3, 128.6, 115.0, 80.0, 11.8, 7.3;

HRMS (EI-TOF) calcd for $C_{18}H_{13}BrClNO$ 372.9869, found 372.9866.



3k

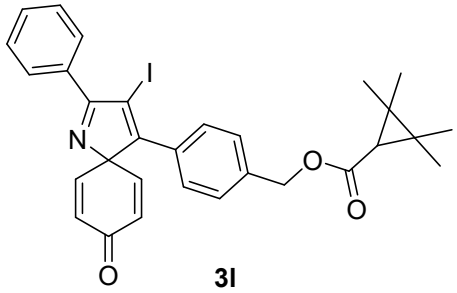
2-(4-chlorophenyl)-4-cyclopropyl-3-iodo-1-azaspiro[4.5]deca-1,3,6,9-tetraen-8-one (3k)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 5/1) to give **3k** 56 mg (66% yield) as a pale yellow solid (Mp 96-97 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (d, *J* = 9.0 Hz, 2H), 7.45 (d, *J* = 9.0 Hz, 2H), 6.51 (d, *J* = 10.0 Hz, 2H), 6.23 (d, *J* = 10.0 Hz, 2H), 1.77 (m, 1H), 1.11 (m, 2H), 0.97 (m, 2H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.3, 175.9, 171.4, 143.3, 137.0, 131.5, 131.3, 130.5, 128.5, 90.3, 81.4, 14.5, 7.6;

HRMS (EI-TOF) calcd for $C_{18}H_{13}ClINO$ 420.9730, found 420.9731.



3l

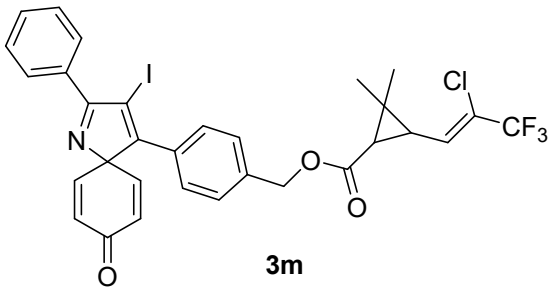
4-(3-iodo-8-oxo-2-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-4-yl)benzyl 2,2,3,3-tetramethylcyclopropane-1-carboxylate (3l)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 2/1) to give **3l** 63 mg (55% yield) as a pale yellow solid (Mp 91-92 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.0 Hz, 2H), 7.55 (m, 3H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 6.48 (d, *J* = 10.0 Hz, 2H), 6.39 (d, *J* = 10.0 Hz, 2H), 5.10 (s, 2H), 1.30 (s, 1H), 1.28 (s, 6H), 1.22 (s, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.1, 177.0, 171.9, 169.5, 142.6, 138.2, 133.0, 132.7, 131.7, 130.9, 129.2, 128.3, 128.1, 127.8, 93.8, 83.0, 64.9, 35.6, 30.6, 23.6, 16.6;

HRMS (EI-TOF) calcd for $C_{30}H_{28}INO_3$ 577.1114, found 577.1118.



3m

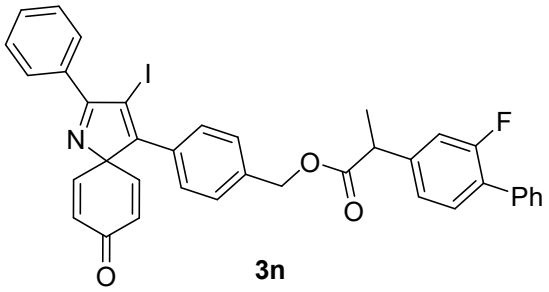
4-(3-iodo-8-oxo-2-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-4-yl)benzyl (*Z*)-3-(2-chloro-3,3,3-trifluoroprop-1-en-1-yl)-2,2-dimethylcyclopropane-1-carboxylate (3m)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 2/1) to give **3m** 70 mg (52% yield) as a white solid (Mp 83-84 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.0 Hz, 2H), 7.59–7.52 (m, 3H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 9.0 Hz, 1H), 6.48 (d, *J* = 10.0 Hz, 2H), 6.39 (d, *J* = 10.0 Hz, 2H), 5.18–5.10 (m, 2H), 2.22 (t, *J* = 9.0 Hz, 1H), 2.09 (d, *J* = 8.0 Hz, 1H), 1.33 (d, *J* = 5.0 Hz, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.1, 177.0, 170.0, 169.4, 142.6, 137.2, 133.1, 132.9, 131.7, 131.0, 130.0 (q, $J_{C\text{-}F}$ = 5.0 Hz), 129.2, 128.3, 128.3, 127.9, 121.5, 119.4, 93.9, 83.0, 65.8, 32.9, 31.0, 28.4, 14.9;

HRMS (EI-TOF) calcd for $C_{31}H_{24}ClF_3INO_3$ 677.0441, found 677.0438.



3n

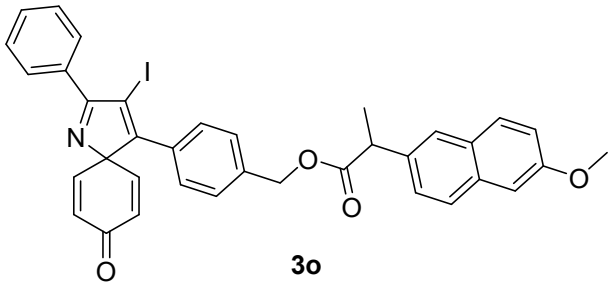
4-(3-iodo-8-oxo-2-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-4-yl)benzyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (3n)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 2/1) to give **3n** 90 mg (66% yield) as a pale yellow solid (Mp 108-109 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00–7.92 (m, 2H), 7.60–7.52 (m, 5H), 7.47 (t, J = 8.0 Hz, 2H), 7.41 (m, 2H), 7.35–7.29 (m, 4H), 7.22–7.13 (m, 2H), 6.47 (d, J = 10.0 Hz, 2H), 6.37 (d, J = 10.0 Hz, 2H), 5.17 (q, J = 13.0 Hz, 2H), 3.87 (q, J = 7.0 Hz, 1H), 1.60 (d, J = 7.0 Hz, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.1, 177.0, 173.7, 169.4, 159.7 (d, $J_{C\text{-}F}$ = 248.0 Hz), 142.6, 141.6 (d, $J_{C\text{-}F}$ = 8.0 Hz), 137.3, 135.5, 133.0, 132.9, 131.7, 131.0, 130.9 (d, $J_{C\text{-}F}$ = 4.0 Hz), 129.2, 129.0 (d, $J_{C\text{-}F}$ = 4.0 Hz), 128.5, 128.3, 127.9, 127.8, 127.7, 123.6 (d, $J_{C\text{-}F}$ = 5.0 Hz), 115.3 (d, $J_{C\text{-}F}$ = 23.0 Hz), 93.9, 83.0, 65.9, 45.0, 18.3;

HRMS (EI-TOF) calcd for $C_{37}H_{27}FINO_3$ 679.1020, found 679.1025.



3o

4-(3-iodo-8-oxo-2-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-4-yl)benzyl 2-(6-methoxynaphthalen-2-yl)propanoate (3o)

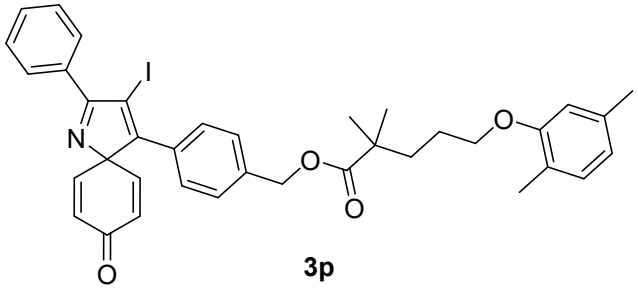
Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 2/1) to give **3o** 80 mg (60% yield) as a pale yellow solid

(Mp 102-103 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.0 Hz, 2H), 7.75–7.68 (m, 3H), 7.55 (m, 3H), 7.43 (d, *J* = 9.0 Hz, 1H), 7.28–7.22 (m, 4H), 7.20–7.12 (m, 2H), 6.47 (d, *J* = 8.0 Hz, 2H), 6.36 (d, *J* = 10.0 Hz, 2H), 5.15 (q, *J* = 13.0 Hz, 2H), 4.01–3.95 (m, 1H), 3.94 (s, 3H), 1.64 (d, *J* = 7.0 Hz, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.1, 177.0, 174.4, 169.4, 157.7, 142.6, 137.6, 135.4, 133.8, 133.0, 132.8, 131.7, 131.0, 129.3, 129.2, 128.9, 128.3, 127.8, 127.7, 127.2, 126.3, 126.1, 119.0, 105.6, 93.8, 82.9, 65.7, 55.4, 45.4, 18.5;

HRMS (EI-TOF) calcd for $C_{36}H_{28}INO_4$ 665.1063, found 665.1061.



3p

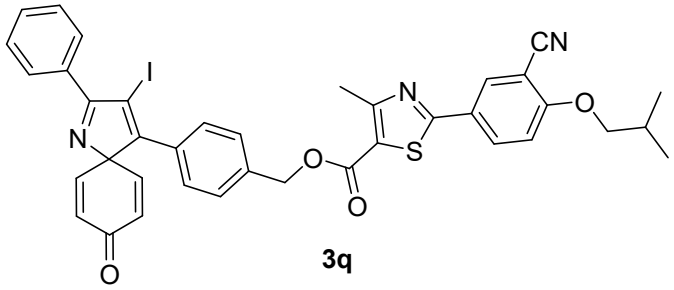
4-(3-iodo-8-oxo-2-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-4-yl)benzyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (3p)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 2/1) to give **3p** 59 mg (43% yield) as a pale yellow solid (Mp 86-87 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00–7.91 (m, 2H), 7.56 (m, 3H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 7.0 Hz, 1H), 6.68 (d, *J* = 7.0 Hz, 1H), 6.62 (s, 1H), 6.48 (d, *J* = 10.0 Hz, 2H), 6.38 (d, *J* = 10.0 Hz, 2H), 5.15 (s, 2H), 3.92 (t, *J* = 6.0 Hz, 2H), 2.32 (s, 3H), 2.17 (s, 3H), 1.76 (m, 4H), 1.29 (s, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.1, 177.5, 177.0, 169.4, 156.9, 142.6, 137.9, 136.5, 133.0, 132.8, 131.7, 131.0, 130.3, 129.2, 128.3, 127.8, 127.7, 123.6, 120.7, 111.9, 93.8, 83.0, 67.8, 65.4, 42.2, 37.2, 25.2, 21.5, 15.8;

HRMS (EI-TOF) calcd for $C_{37}H_{36}INO_4$ 685.1689, found 685.1687.



3q

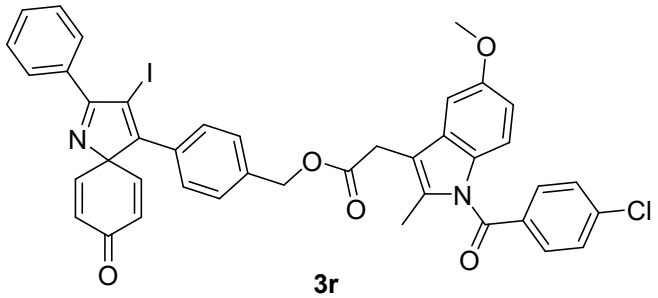
4-(3-iodo-8-oxo-2-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-4-yl)benzyl 2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazole-5-carboxylate (3q)

Following the General Procedure B, and target product was purified by flash chromatography (PE/EA = 1/1) to give **3q** 63 mg (42% yield) as a white solid (Mp 117-118 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 2.0 Hz, 1H), 8.12 (dd, *J* = 9.0, 2.0 Hz, 1H), 7.96 (d, *J* = 7.0 Hz, 2H), 7.59–7.50 (m, 3H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 9.0 Hz, 1H), 6.49 (d, *J* = 10.0 Hz, 2H), 6.40 (d, *J* = 10.0 Hz, 2H), 5.37 (s, 2H), 3.92 (d, *J* = 7.0 Hz, 2H), 2.81 (s, 3H), 2.22 (m, 1H), 1.11 (d, *J* = 7.0 Hz, 6H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.2, 177.0, 169.3, 167.6, 162.6, 162.0, 161.7, 142.6, 137.1, 133.2, 132.9, 132.6, 132.2, 131.7, 131.0, 129.2, 128.3, 128.1, 128.0, 125.9, 121.1, 115.4, 112.7, 103.0, 94.0, 83.0, 75.7, 66.1, 28.2, 19.1, 17.6;

HRMS (EI-TOF) calcd for $C_{38}H_{30}IN_3O_4S$ 751.1002, found 751.1006.



3r

4-(3-iodo-8-oxo-2-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraen-4-yl)benzyl 2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetate (3r)

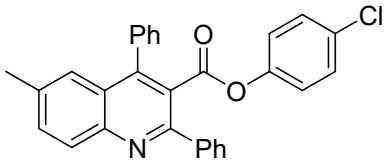
Following the General Procedure B, and target product was purified by flash

chromatography (PE/EA = 1/1) to give **3r** 59 mg (37% yield) as a pale yellow solid (Mp 102-103 °C);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.0 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.48–7.41 (m, 3H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.23 (q, *J* = 8.0 Hz, 4H), 6.89 (d, *J* = 2.0 Hz, 1H), 6.80 (d, *J* = 9.0 Hz, 1H), 6.59 (dd, *J* = 9.0, 2.0 Hz, 1H), 6.38 (d, *J* = 10.0 Hz, 2H), 6.29 (d, *J* = 10.0 Hz, 2H), 5.07 (s, 2H), 3.71 (s, 3H), 3.67 (s, 2H), 2.30 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 185.1, 177.0, 170.6, 169.3, 168.3, 156.1, 142.6, 139.3, 137.3, 136.1, 133.9, 133.1, 132.9, 131.7, 131.2, 131.0, 130.8, 130.6, 129.2, 129.1, 128.3, 128.1, 127.9, 115.0, 112.4, 111.8, 101.3, 94.0, 83.0, 66.1, 55.8, 30.4, 13.4;

HRMS (EI-TOF) calcd for $C_{41}H_{30}ClIN_2O_5$ 792.0888, found 792.0884.



4

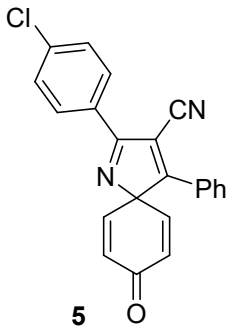
4-chlorophenyl 6-methyl-2,4-diphenylquinoline-3-carboxylate (4)

Pale yellow oil (PE/EA = 5/1), 59 mg, 66% yield;

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 9.0 Hz, 2H), 7.59 (q, *J* = 8.0 Hz, 6H), 7.44 (t, *J* = 9.0 Hz, 2H), 7.36 (t, *J* = 7.0 Hz, 1H), 7.01 (d, *J* = 9.0 Hz, 2H), 6.51 (d, *J* = 10.0 Hz, 2H), 6.40 (d, *J* = 10.0 Hz, 2H), 2.35 (s, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 161.5, 149.3, 143.2, 139.2, 133.6, 132.0, 131.3, 130.9, 130.8, 130.0, 129.8, 128.8, 128.7, 127.7, 127.6, 127.5, 127.1, 126.5, 125.3, 124.8, 120.3, 21.6;

HRMS (EI-TOF) calcd for $C_{29}H_{20}ClNO_2$ 449.1183, found 449.1185.



5

2-(4-chlorophenyl)-8-oxo-4-phenyl-1-azaspiro[4.5]deca-1,3,6,9-tetraene-3-carbonitrile (5)

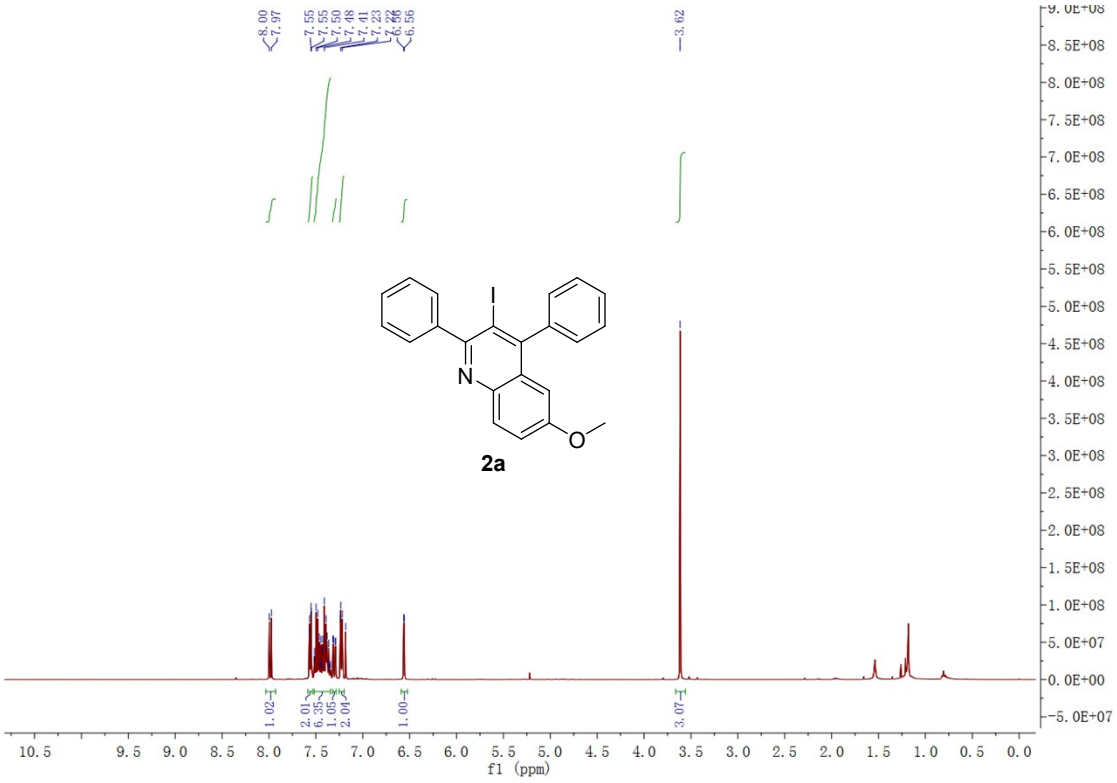
White solid (PE/EA = 2/1), 51 mg, 71% yield;

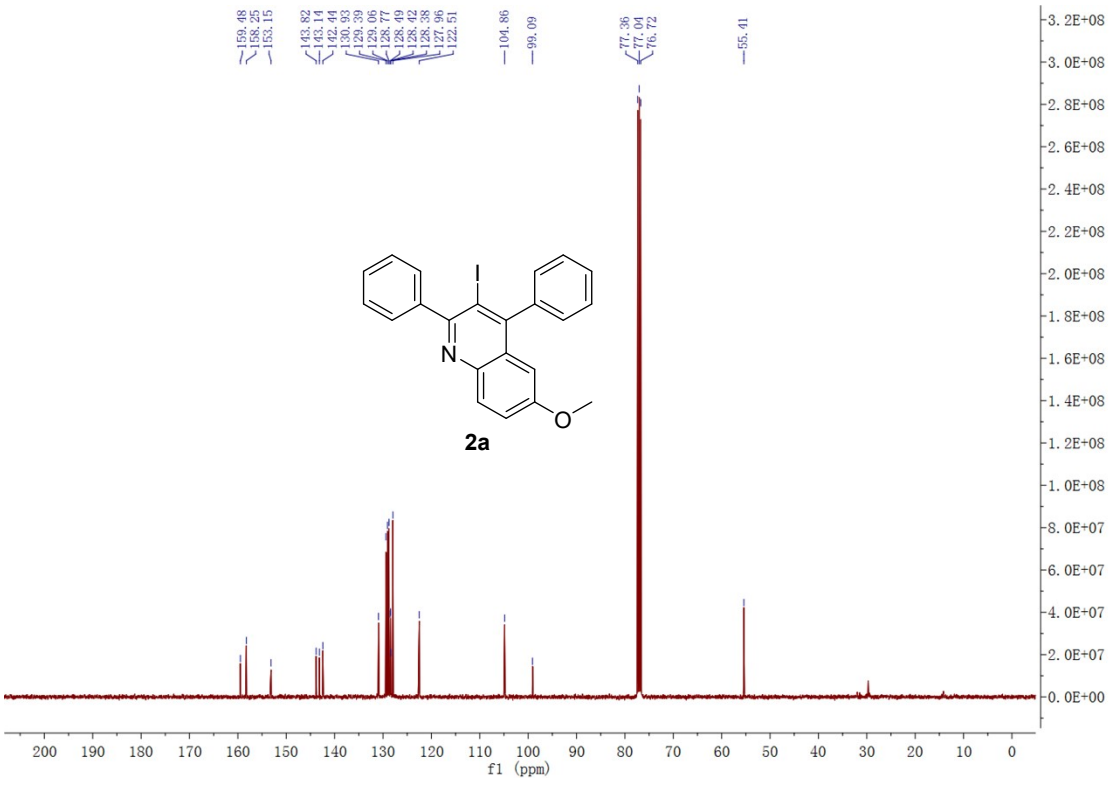
^{1}H NMR (500 MHz, $CDCl_3$): = 7.94 (d, *J* = 7.0 Hz, 2 H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.54 (m, 3 H), 7.43 (d, *J* = 8.0 Hz, 2 H), 6.48 (d, *J* = 10.0 Hz, 2H), 6.36 (d, *J* = 10.0 Hz, 2 H);

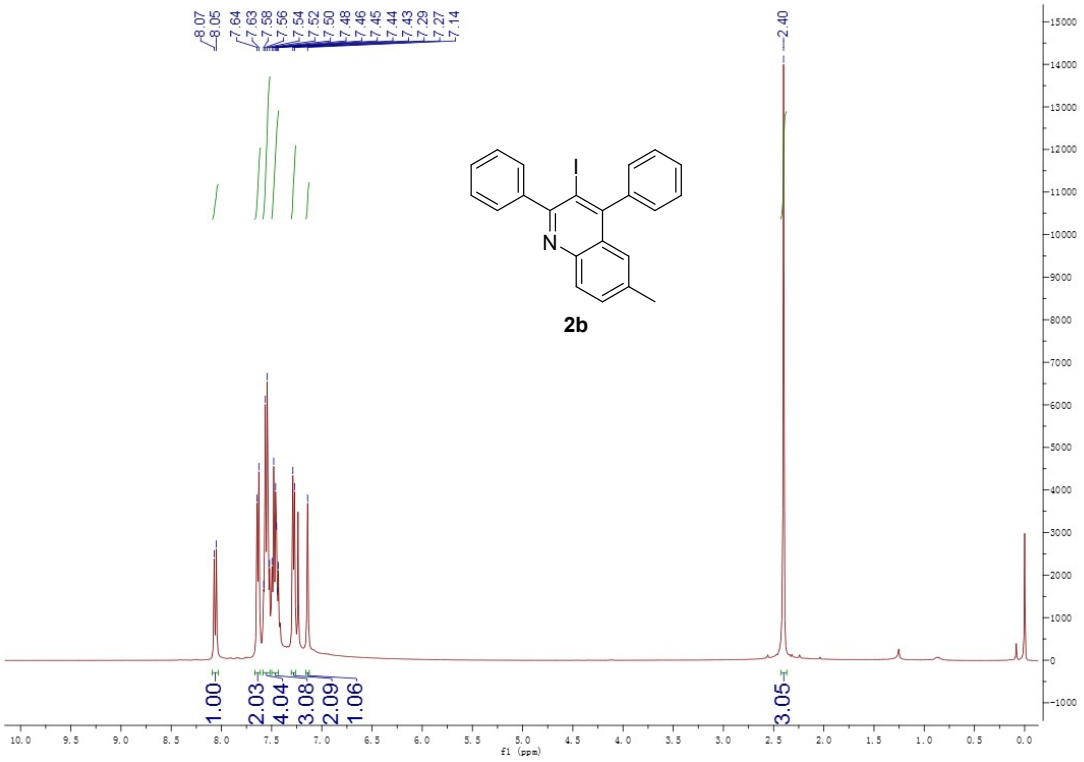
^{13}C NMR (126 MHz, $CDCl_3$): = 184.6, 176.6, 167.9, 141.8, 137.9, 132.5, 132.0, 131.2, 129.2, 128.6, 128.4, 127.0, 118.0, 113.4, 83.2;

HRMS (EI-TOF) calcd for $C_{22}H_{13}ClN_2O$: 356.0716; found: 356.0719.

5. The ^{1}H and ^{13}C NMR spectra of compounds



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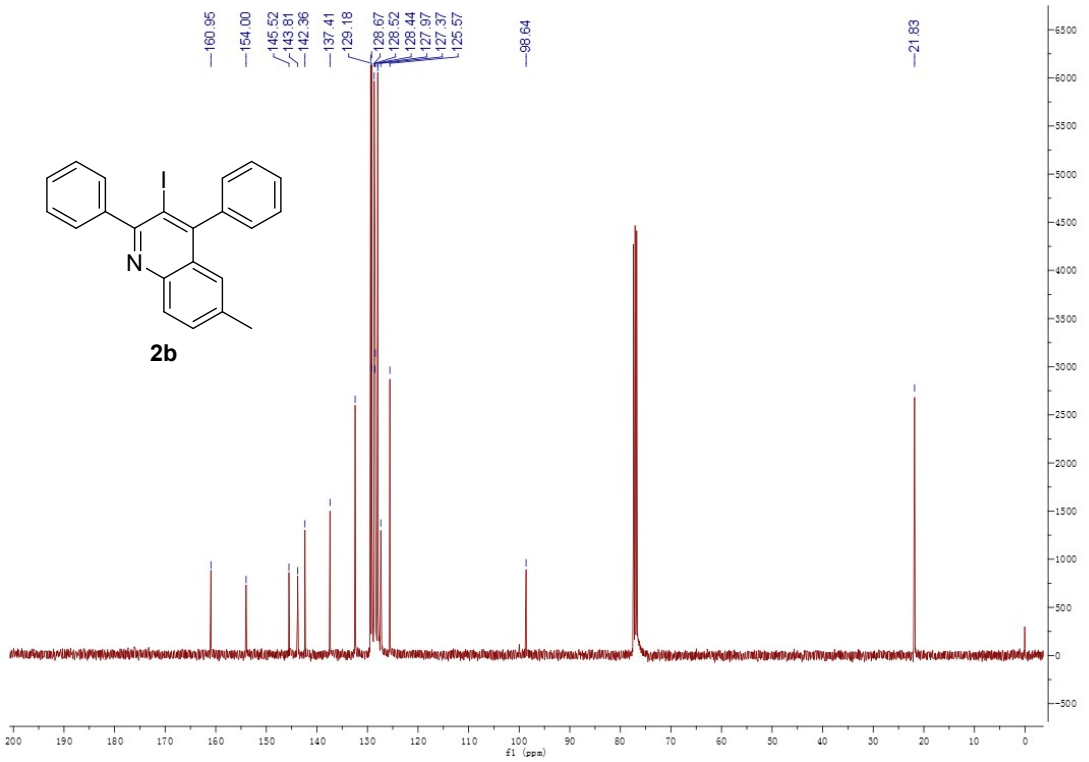
7.54
7.52
7.50
7.48
7.46
7.45
7.44
7.43
7.29
7.27
7.14
2.40
I
N
1.00
2.03
4.04
3.08
2.09
1.06
3.05
f1 (ppm)

2b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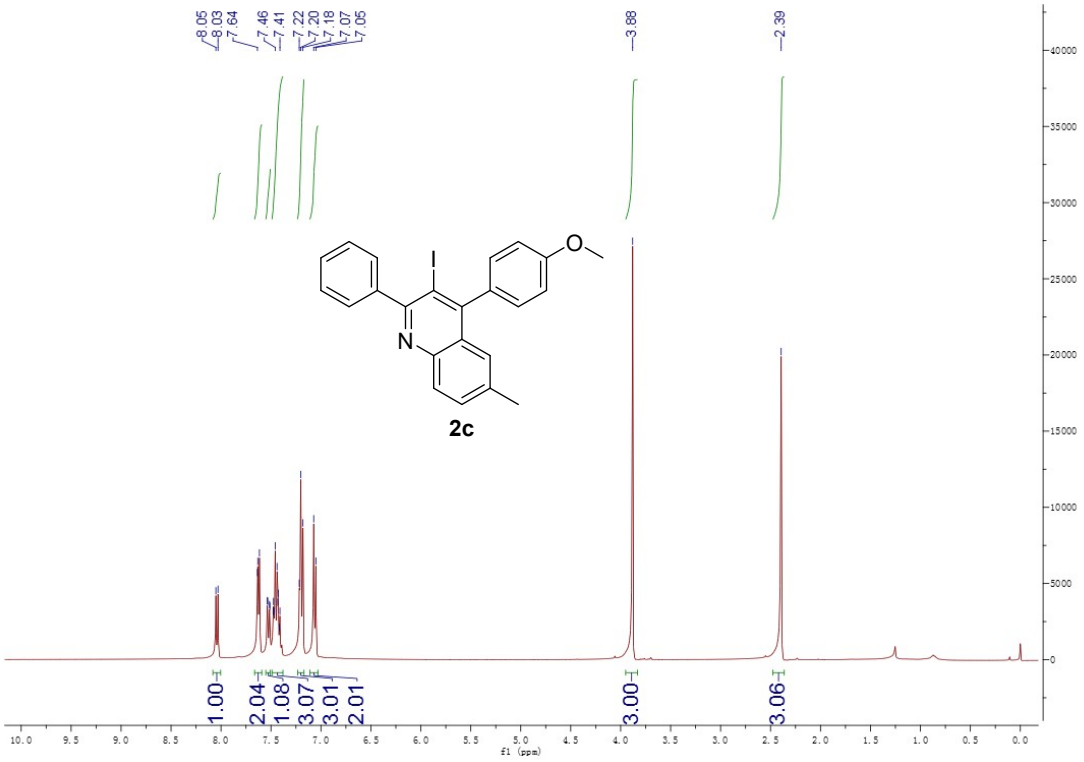
21.83
I
N
f1 (ppm)

2b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7.05
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3.00
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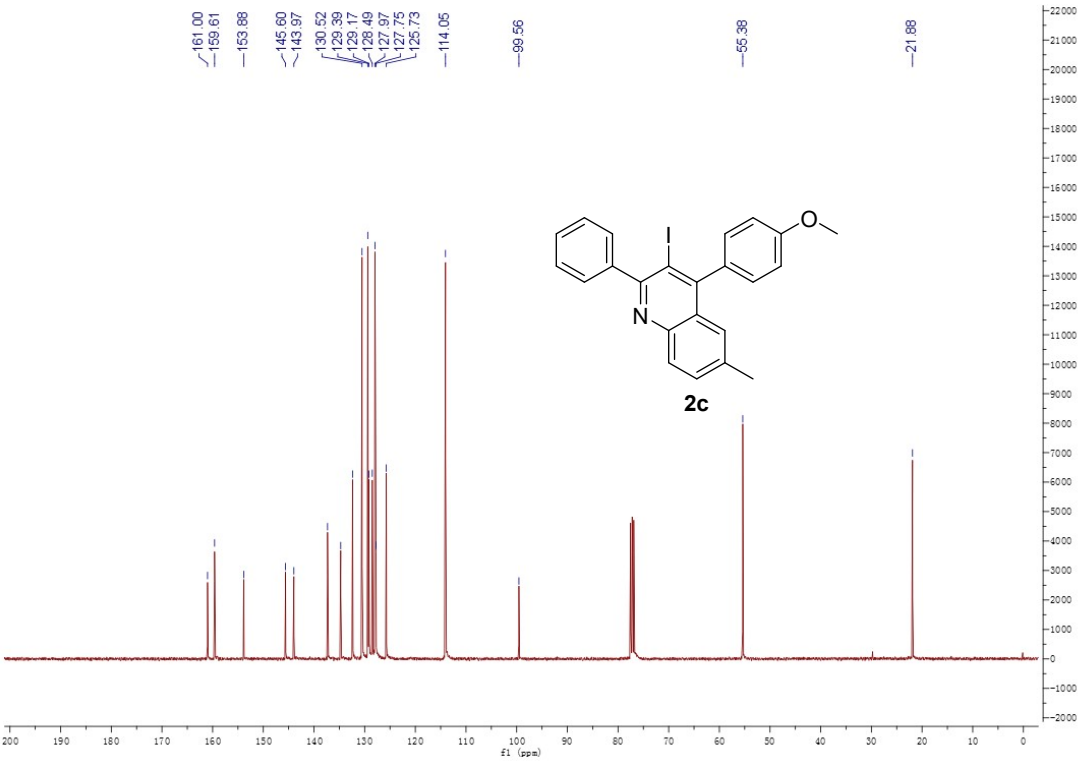
f1 (ppm)

2c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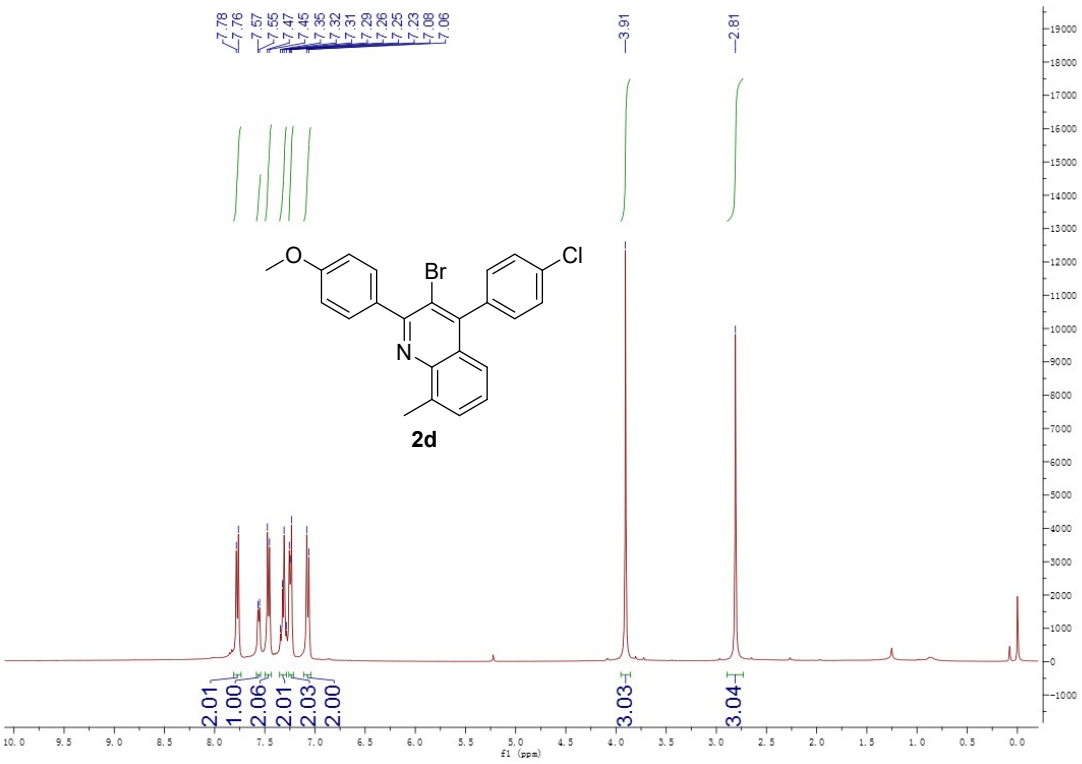
55.38
21.88
I
O
N
f1 (ppm)

2c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7.25
7.23
7.08
7.06
3.91
2.81
O
Br
Cl
N
2d
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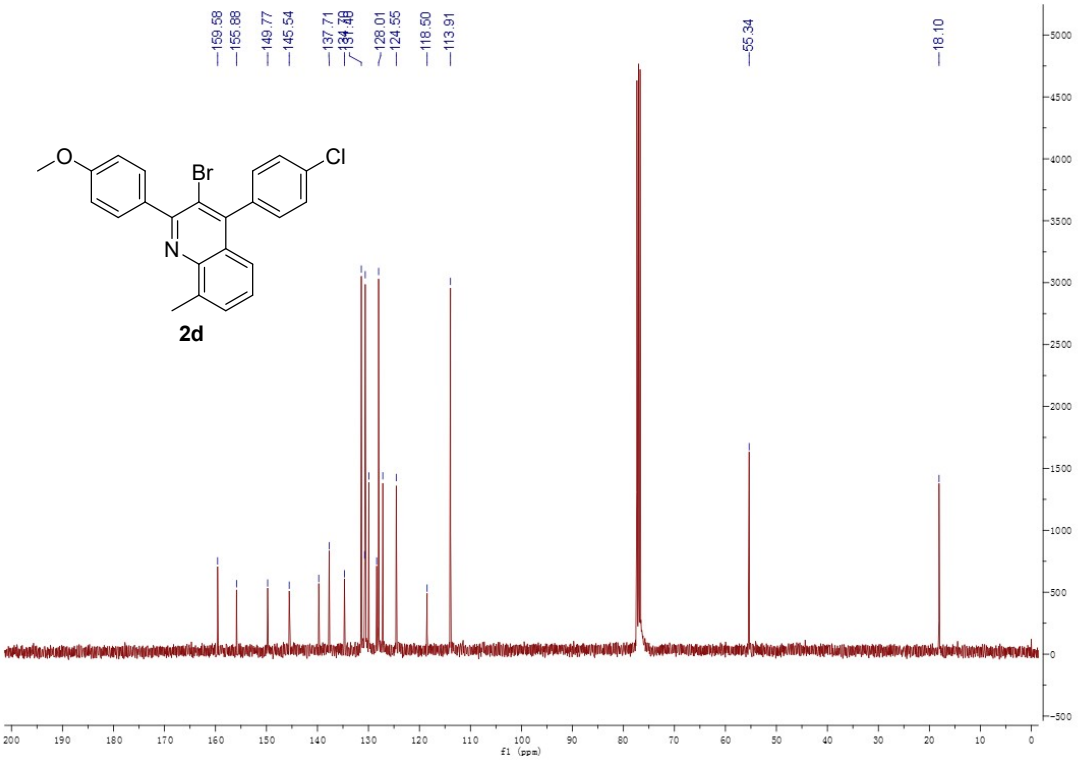
2.06
2.01
2.03
2.00
3.03
3.04
f1 (ppm)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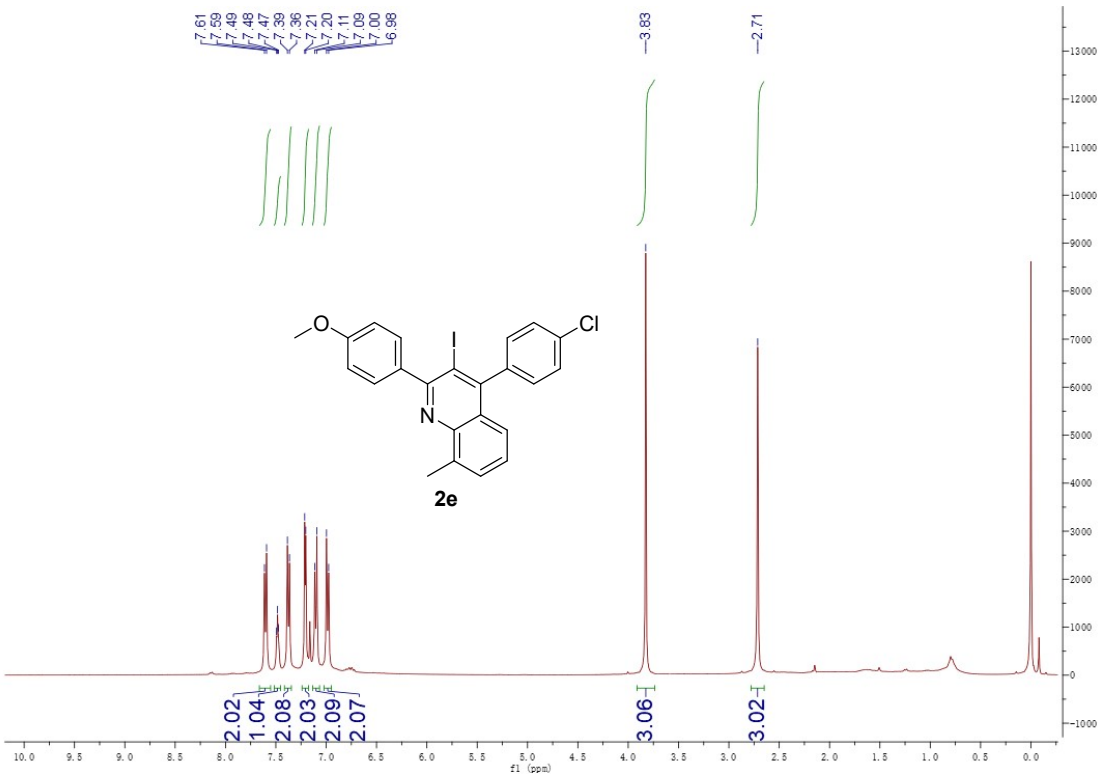
Br
Cl
N
2d
f1 (ppm)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7.21
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7.11
7.09
7.00
6.98
3.83
2.71
O
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Cl
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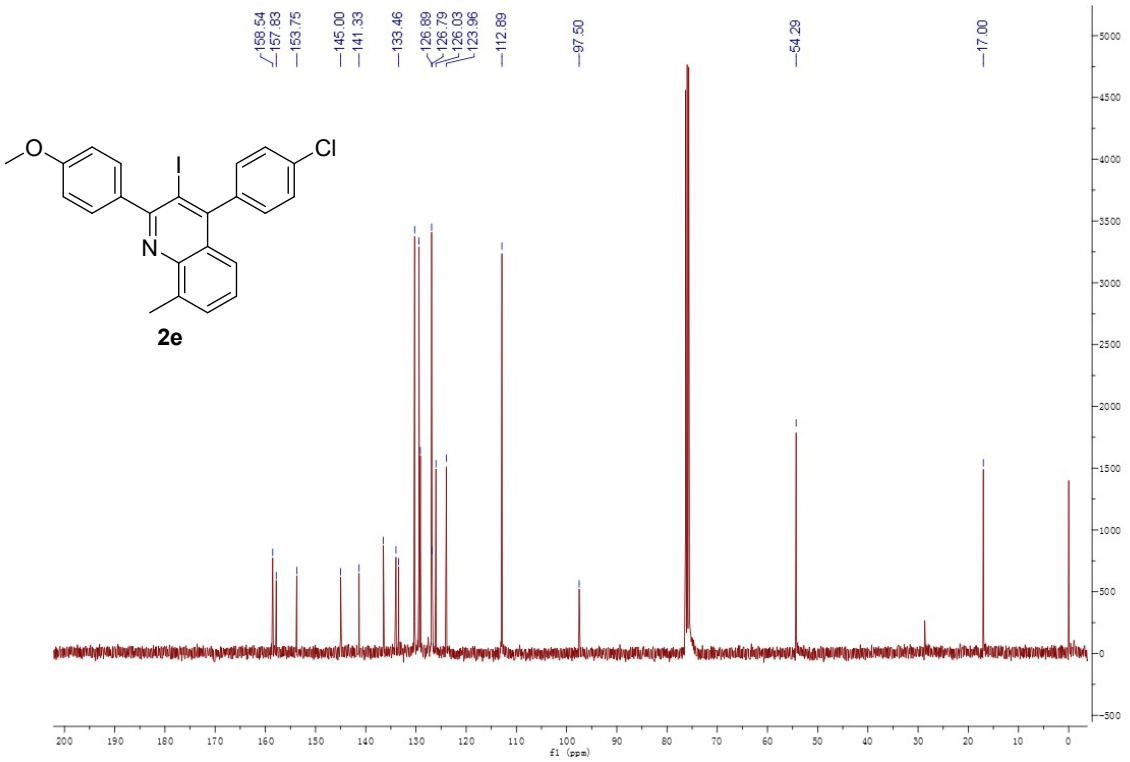
3.02
f1 (ppm)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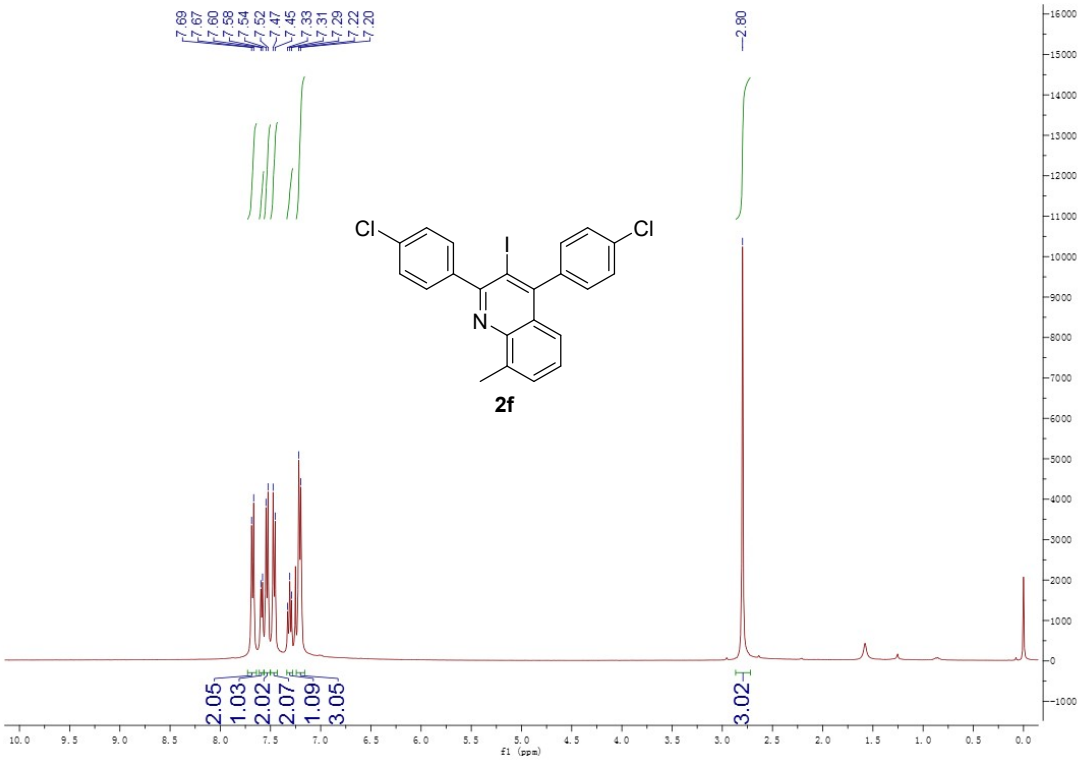
17.00
O
I
Cl
N
2e
f1 (ppm)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7.45
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7.29
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Cl
N
2f
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1.03
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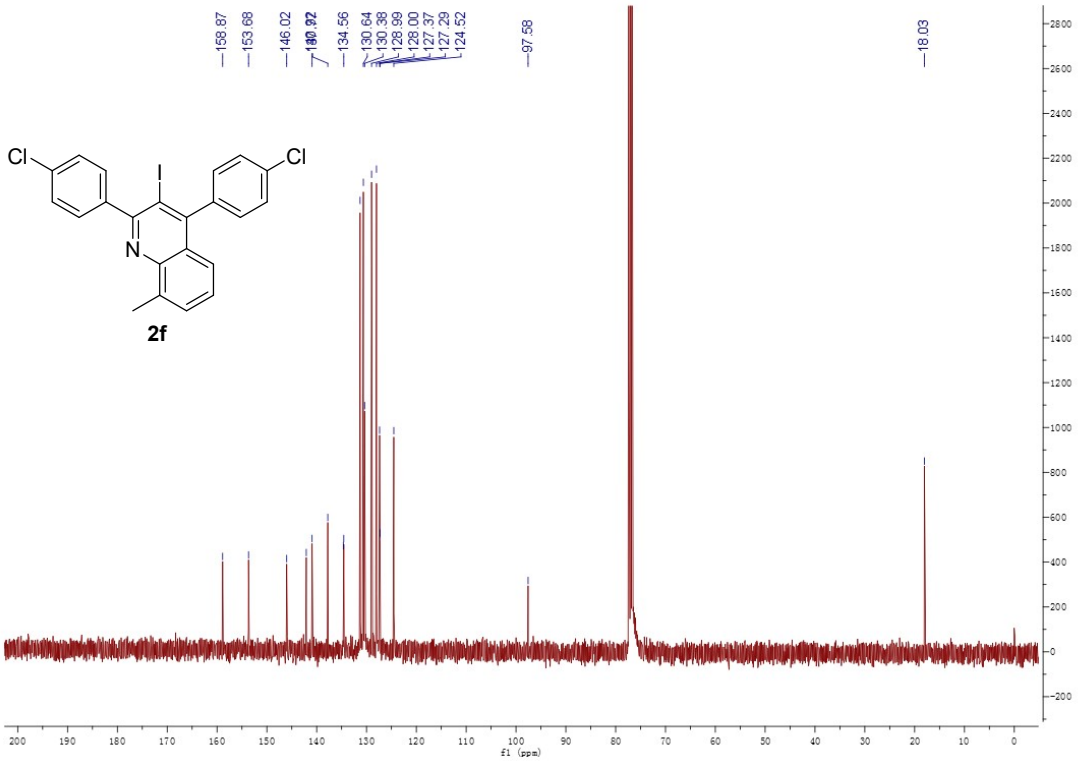
2.07
1.09
3.05
3.02
f1 (ppm)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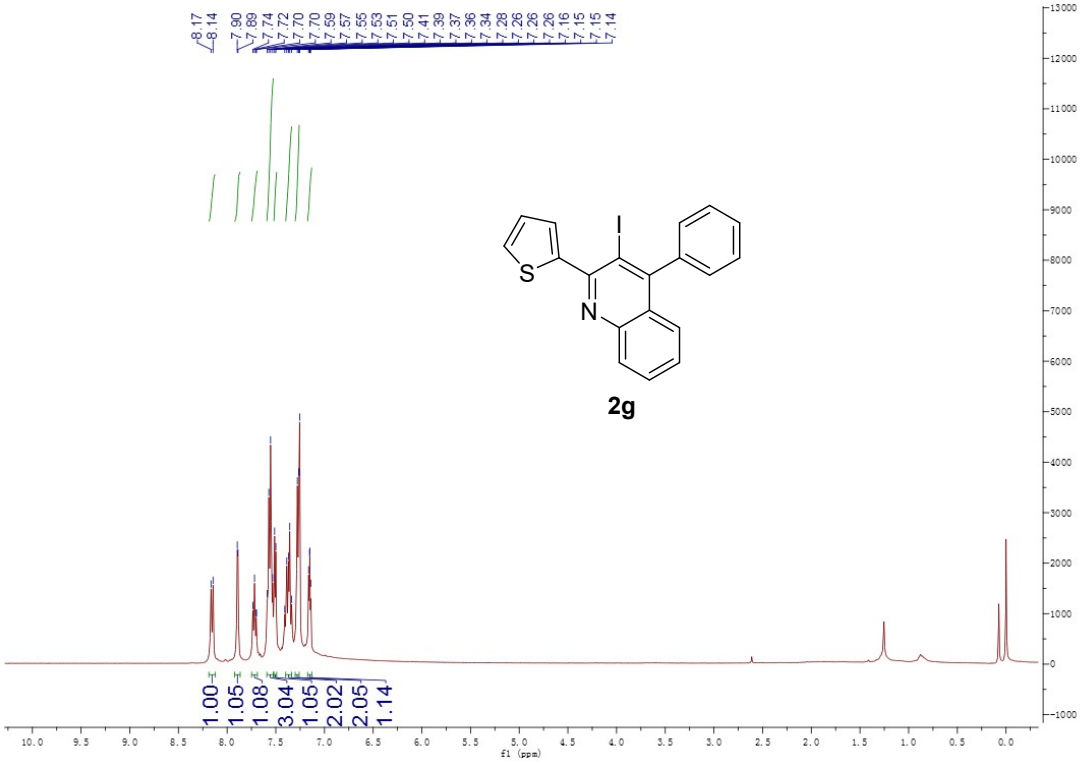
Cl
I
Cl
N
2f
f1 (ppm)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7.50
7.41
7.39
7.37
7.36
7.34
7.28
7.26
7.26
7.16
7.15
7.15
7.14
I
S
N
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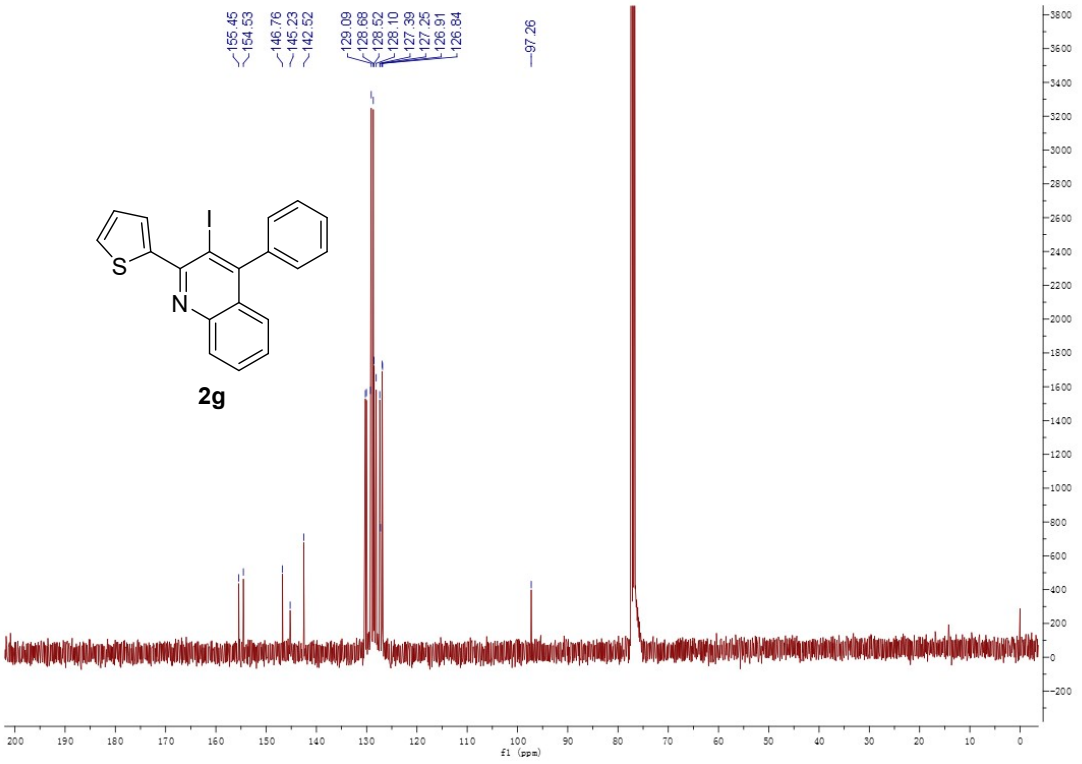
1.05
2.02
2.05
1.14
f1 (ppm)

2g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145.23
142.52
129.09
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128.52
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127.25
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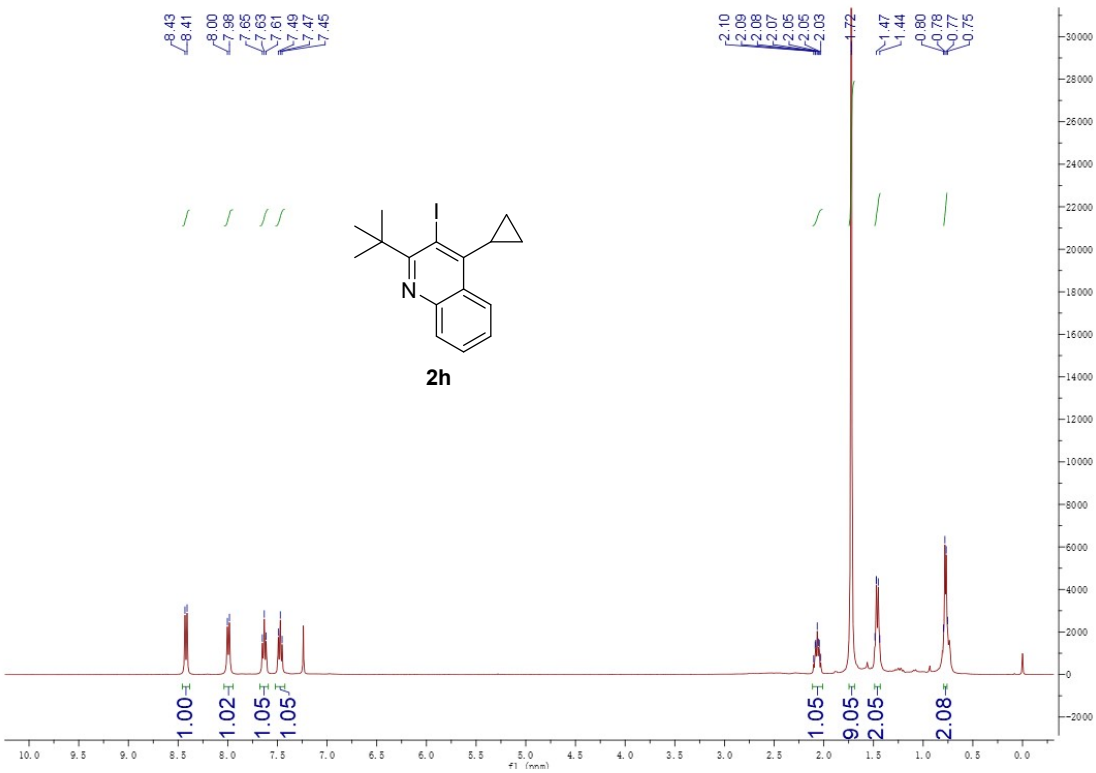
126.84
97.26
I
S
N
f1 (ppm)

2g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2.05
2.05
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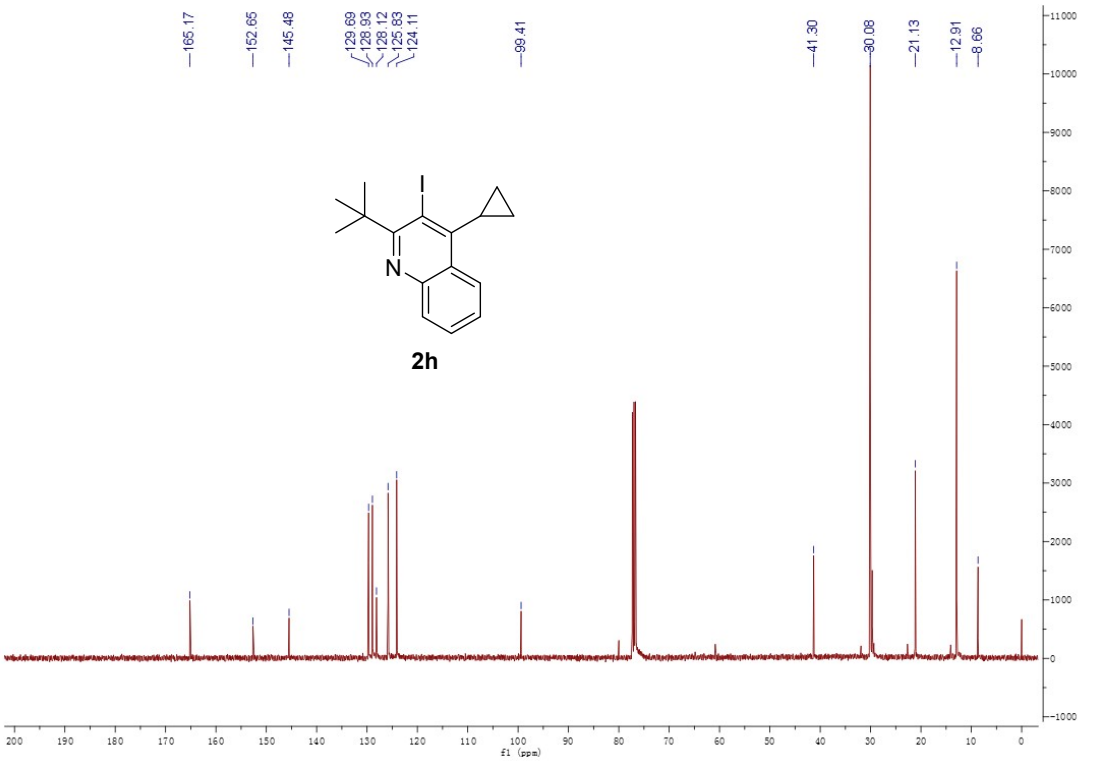
f1 (ppm)

2h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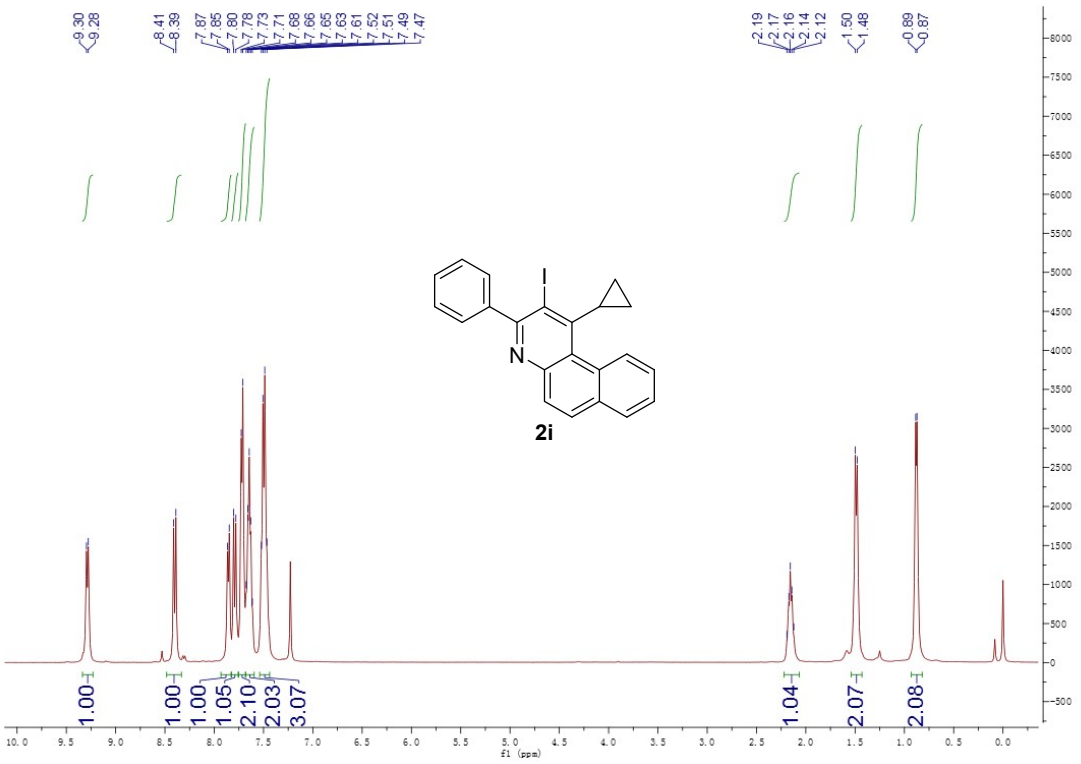
30.08
21.13
12.91
8.66
I
N
f1 (ppm)

2h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7.65
7.63
7.61
7.52
7.51
7.49
7.47
2.19
2.17
2.16
2.14
2.12
1.50
1.48
0.89
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1.04
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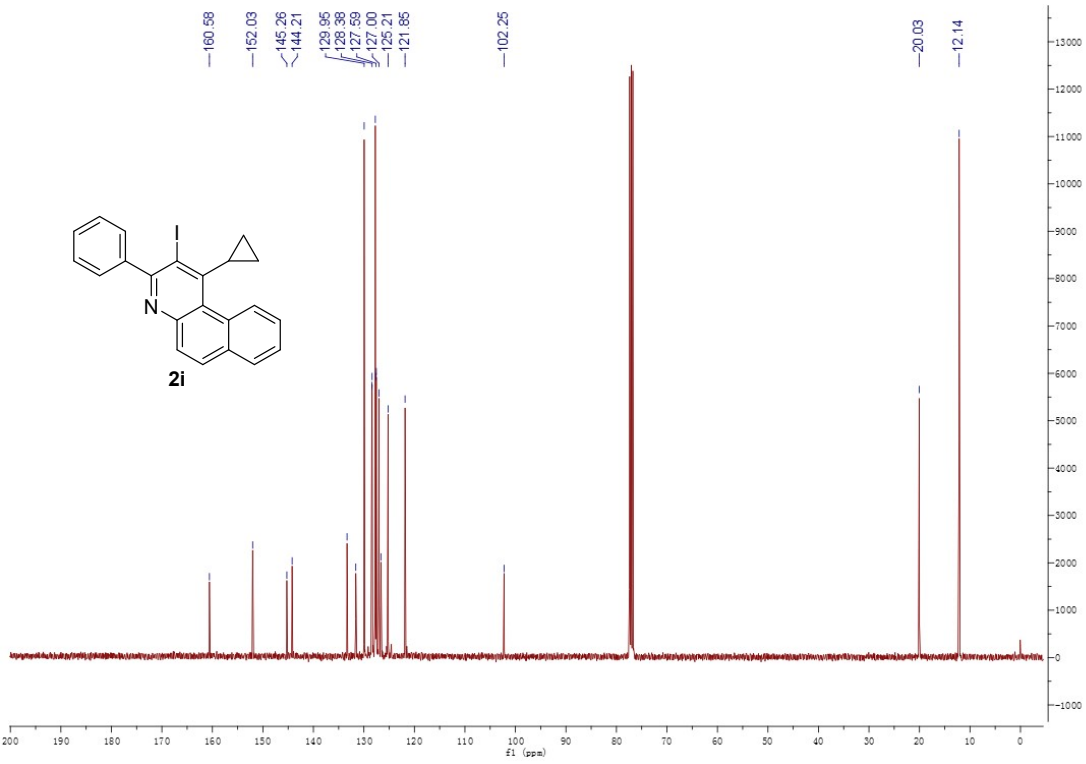
2i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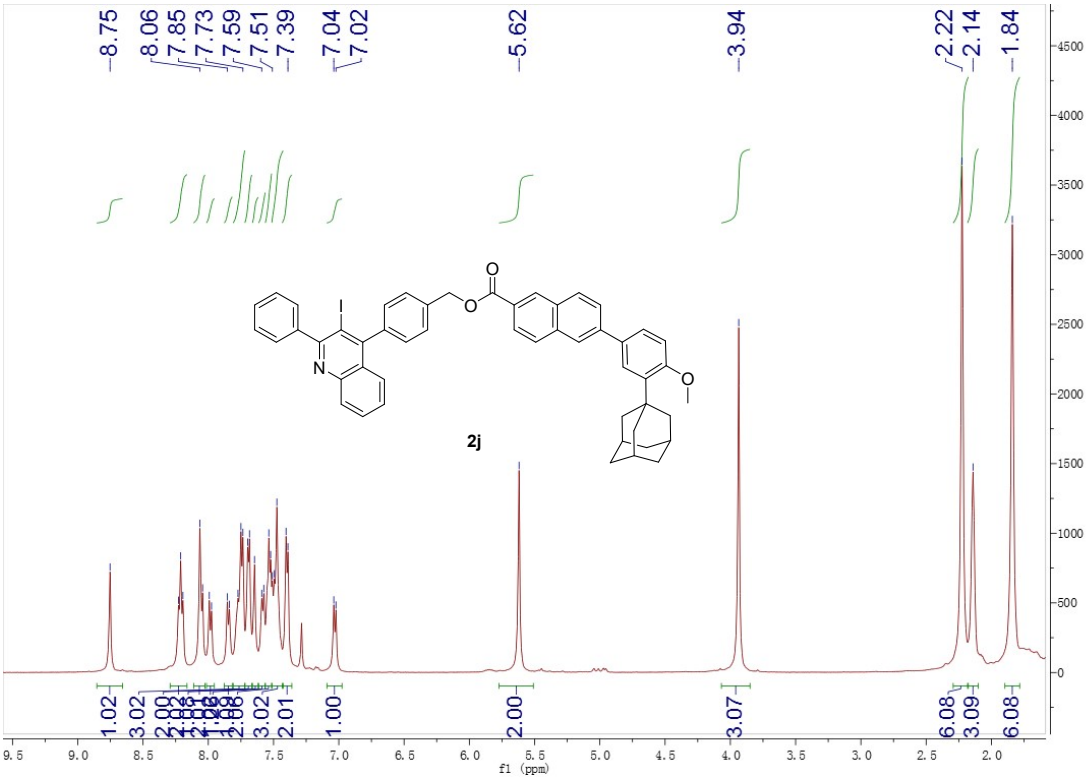
f1 (ppm)

2i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2.00
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3.09
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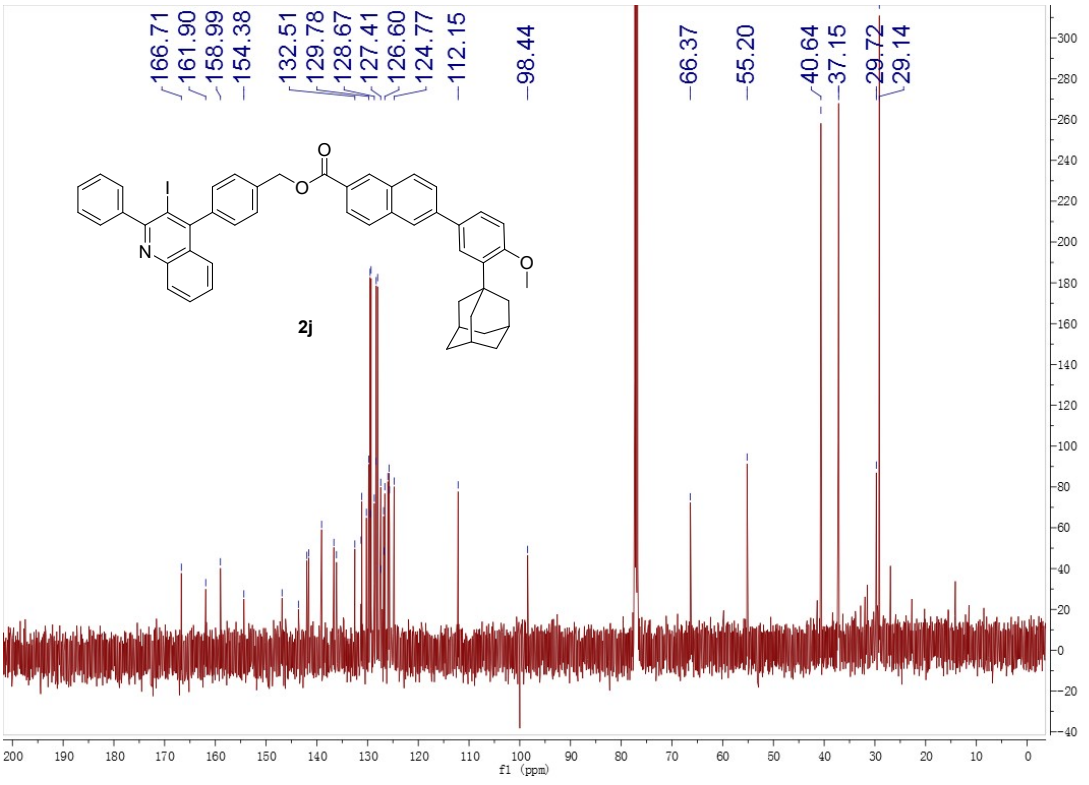
2j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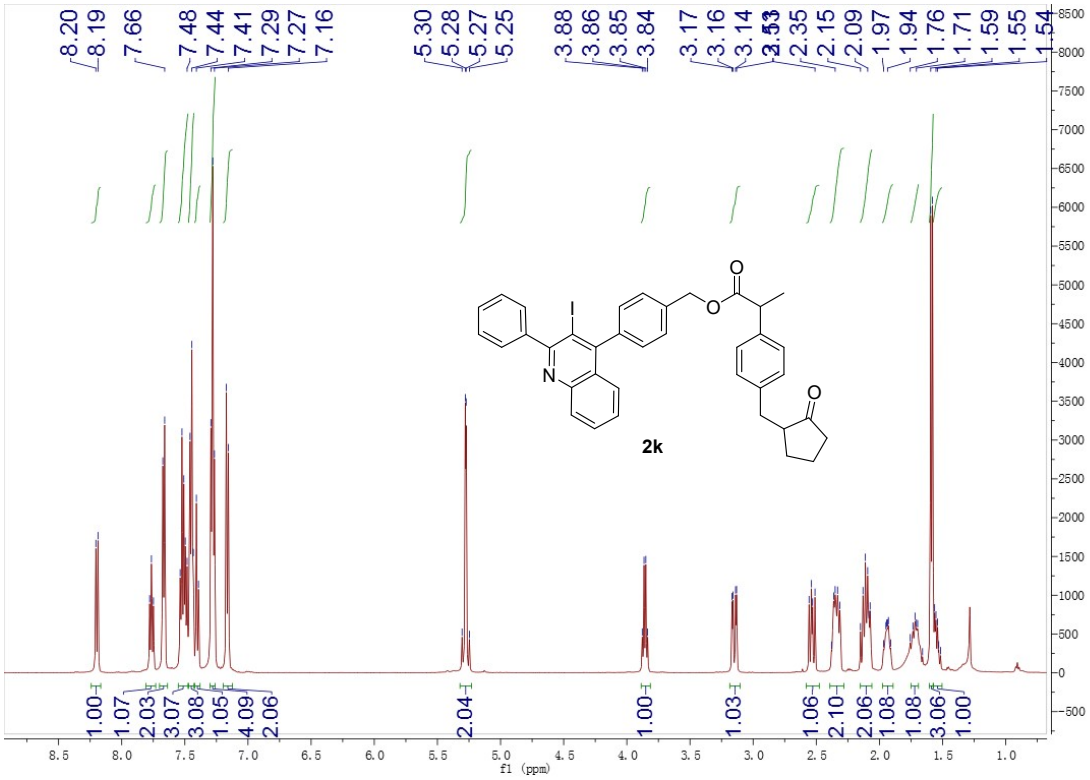
29.72
29.14
f1 (ppm)

2j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3.84
3.17
3.16
3.14
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2.15
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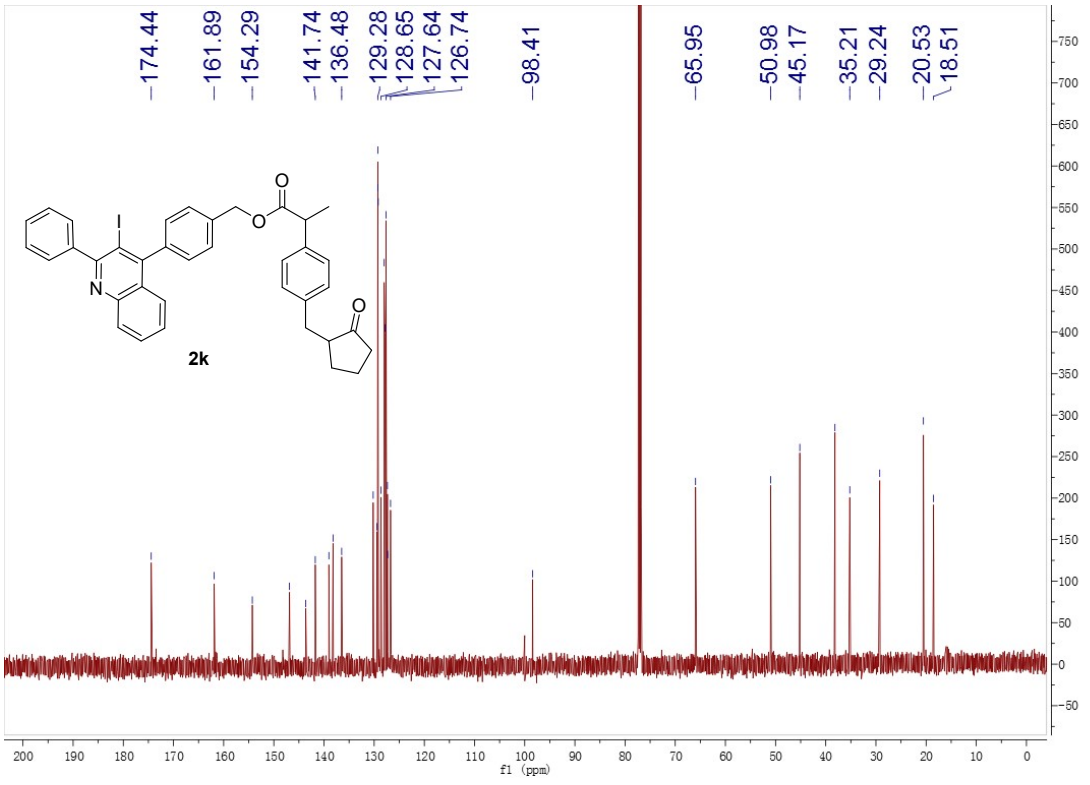
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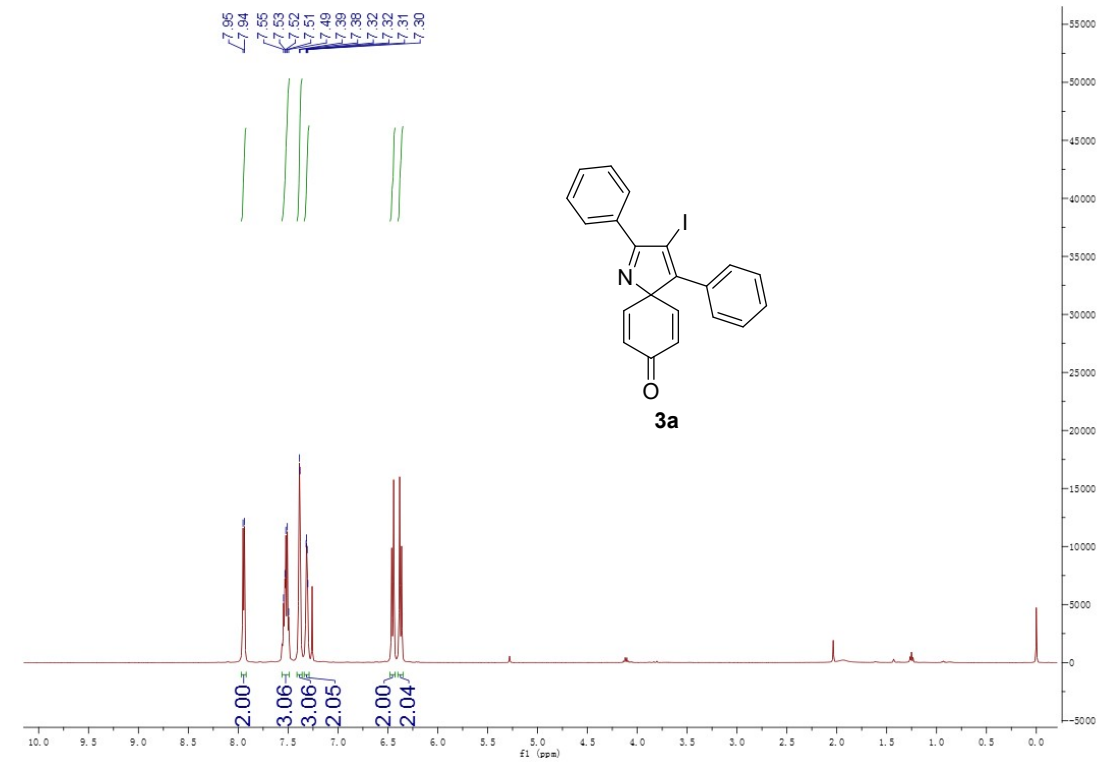
f1 (ppm)
2k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N
O
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2.00
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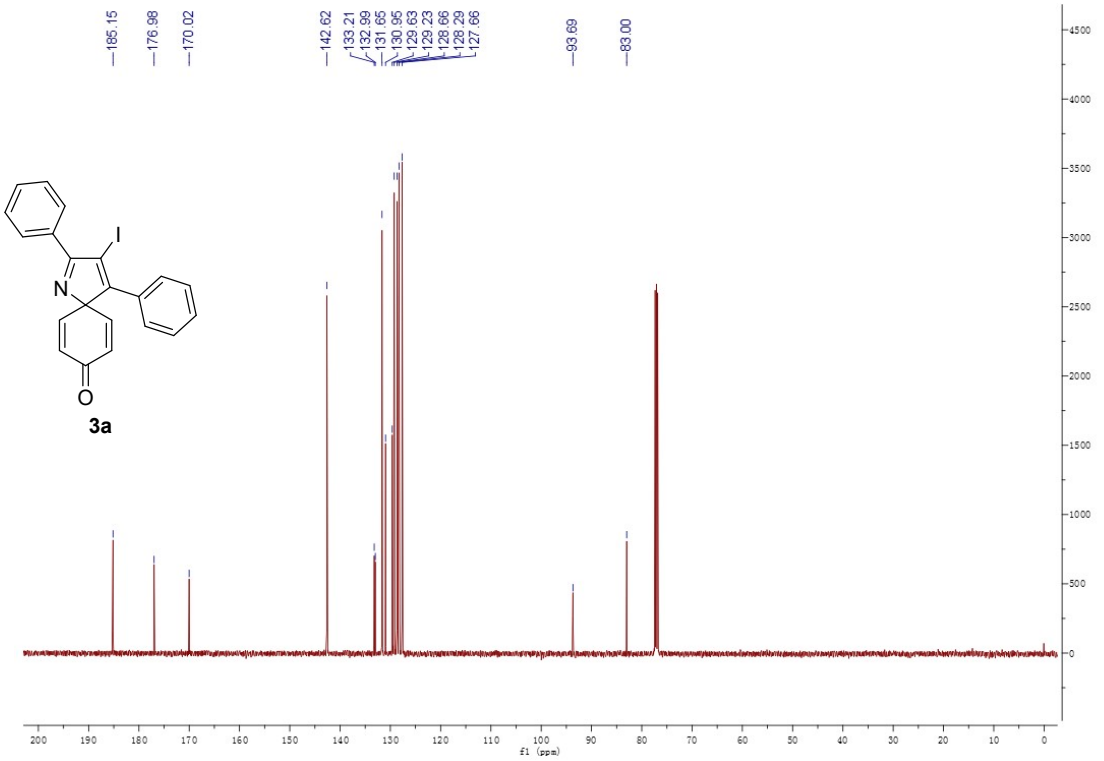
f1 (ppm)

3a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83.00
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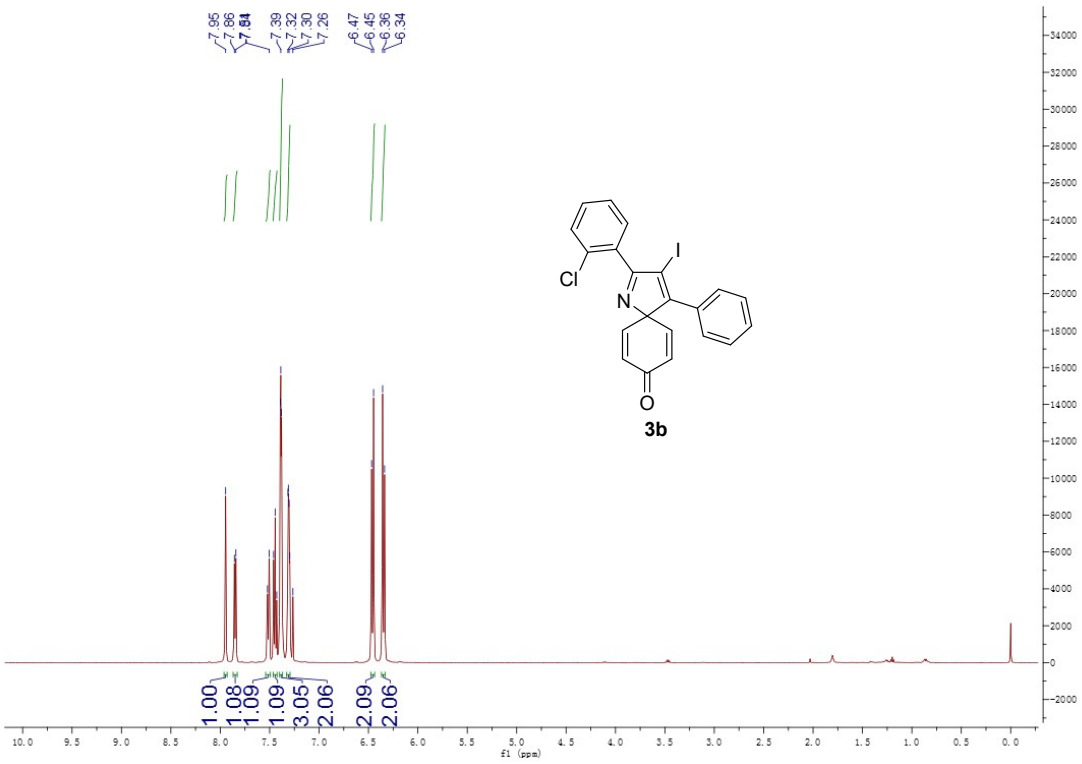
O
f1 (ppm)

3a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O
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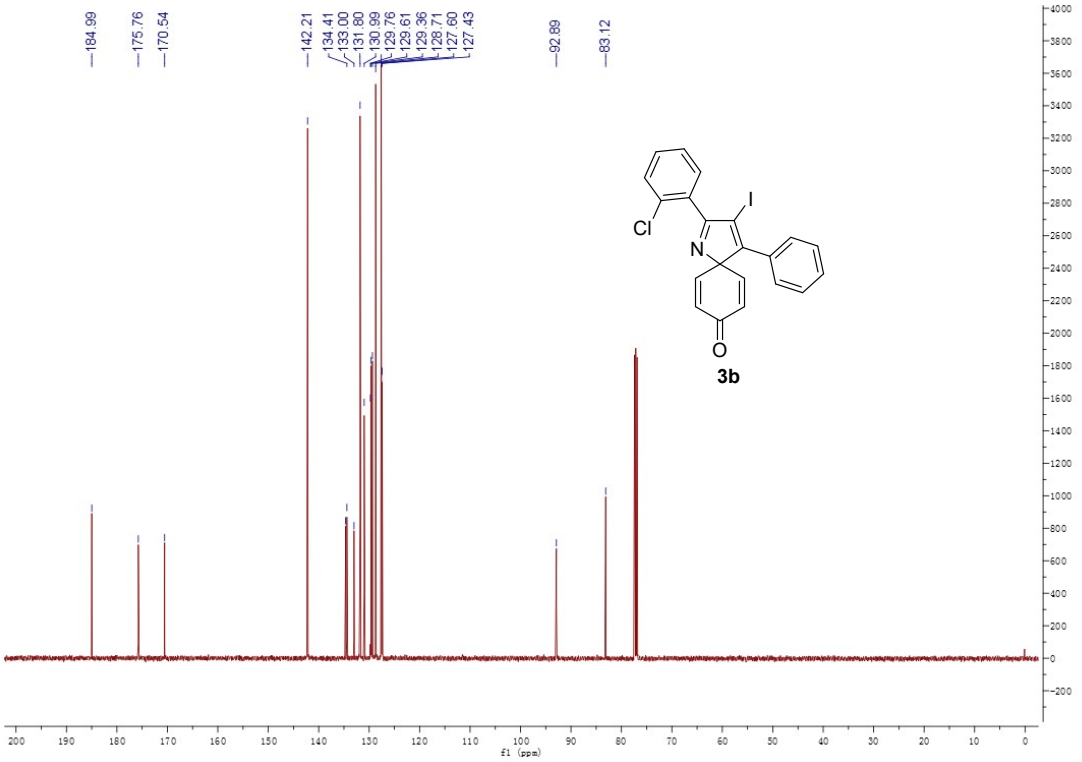
2.06
2.09
2.06
f1 (ppm)

3b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129.36
128.71
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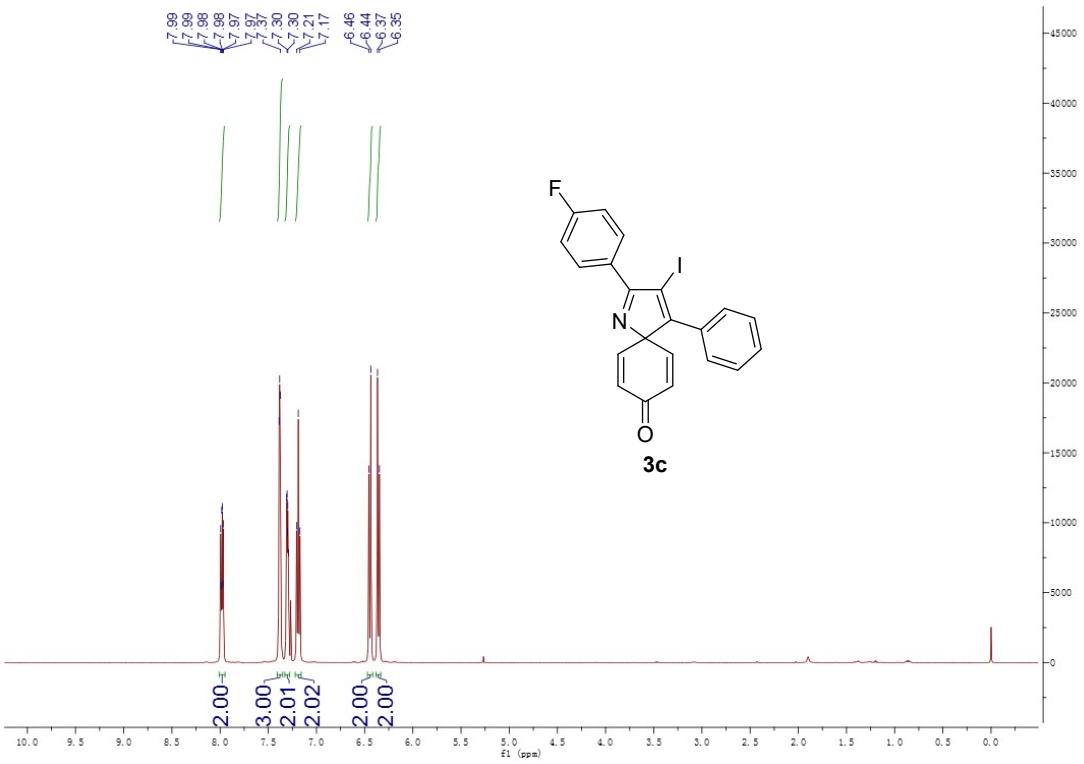
127.43
92.89
83.12
Cl
I
N
O
f1 (ppm)

3b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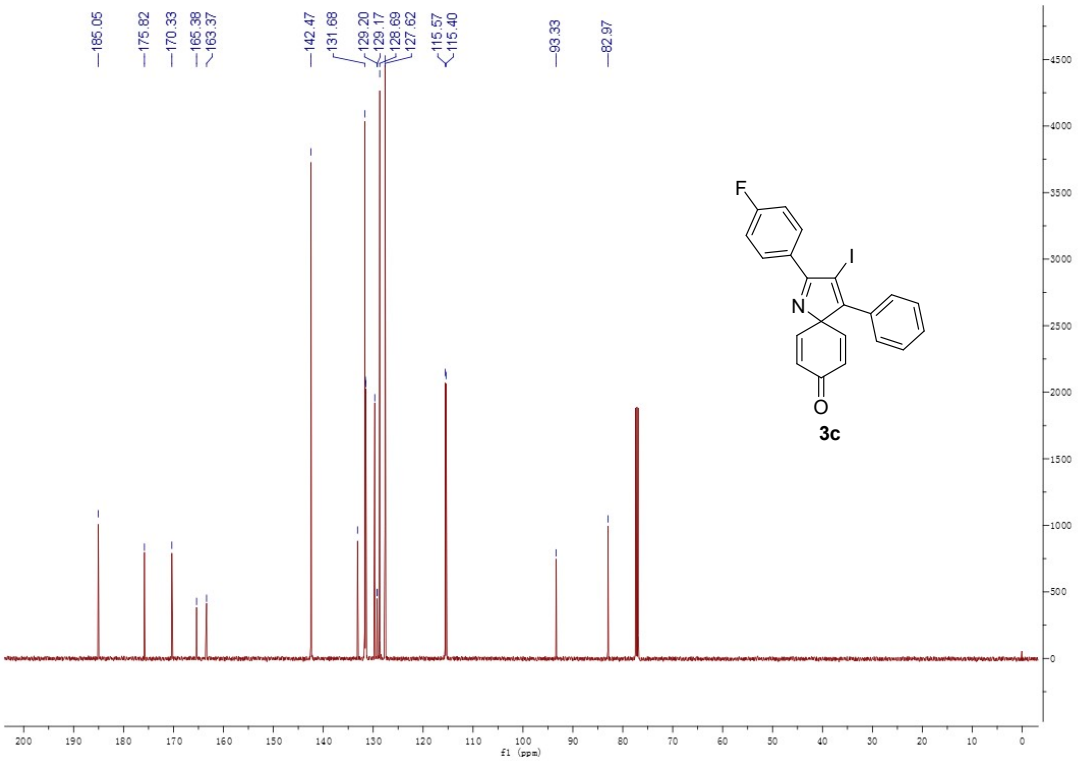
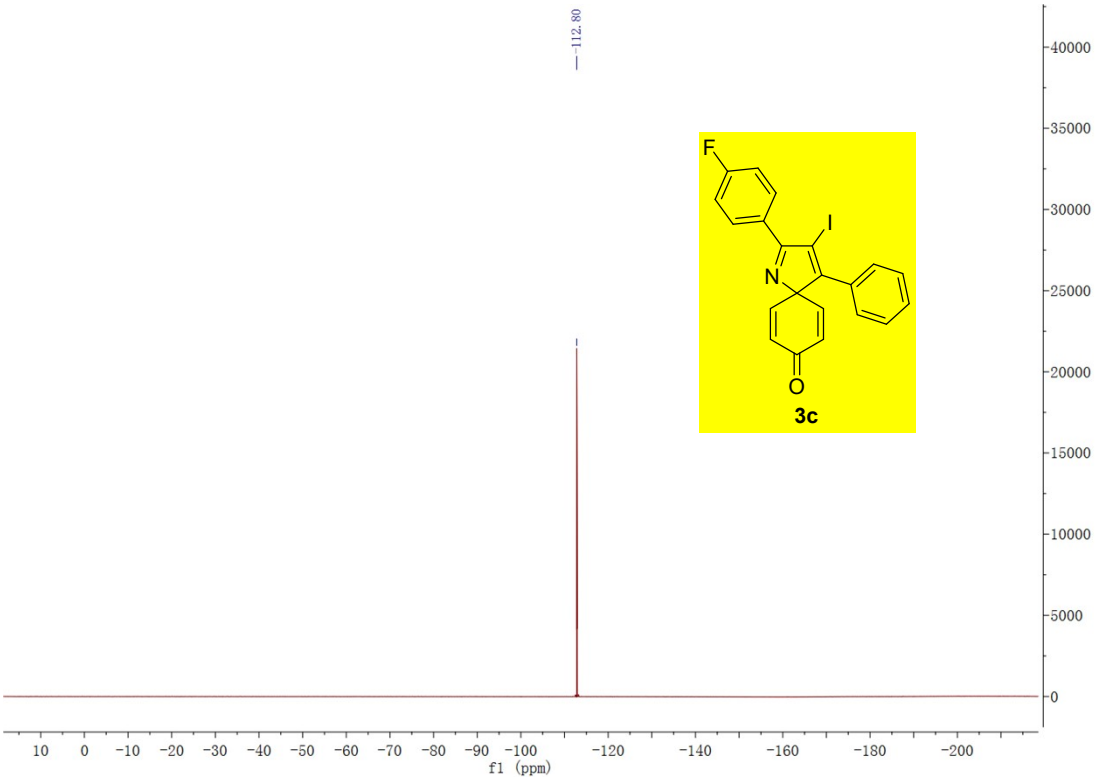
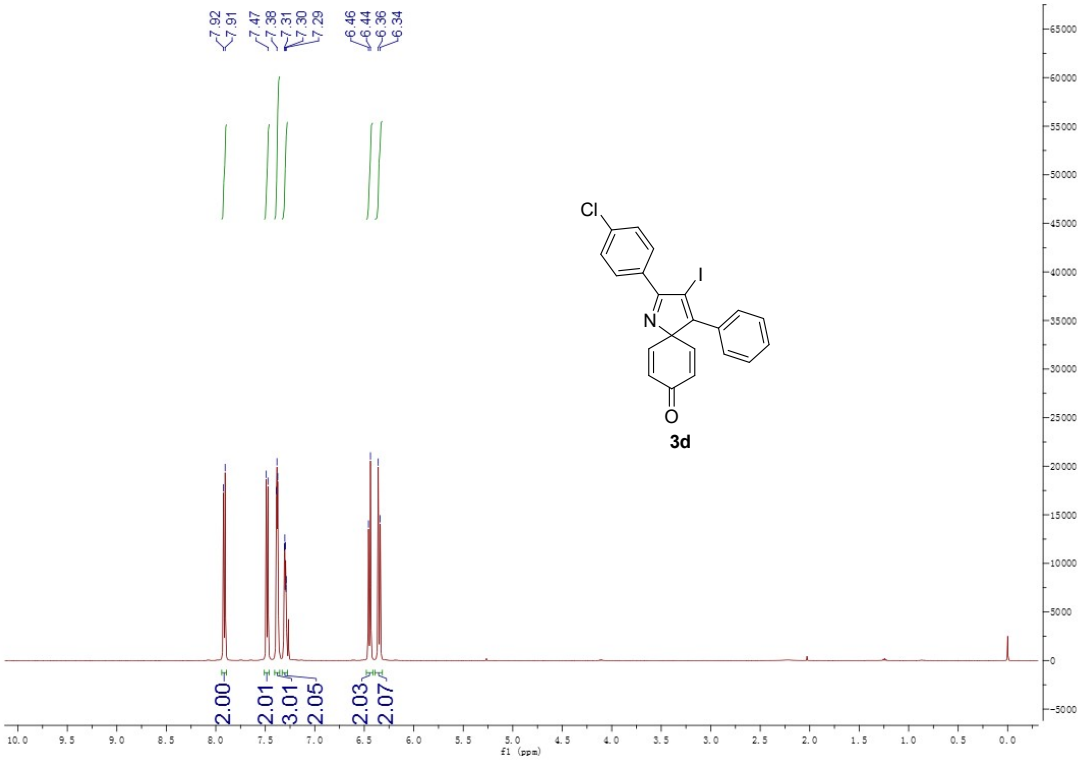
7.99
7.98
7.98
7.97
7.97
7.30
7.30
7.21
7.17
6.46
6.44
6.37
6.35
F
I
N
O
2.00
3.00
2.01
2.02
2.00
2.00
f1 (ppm)

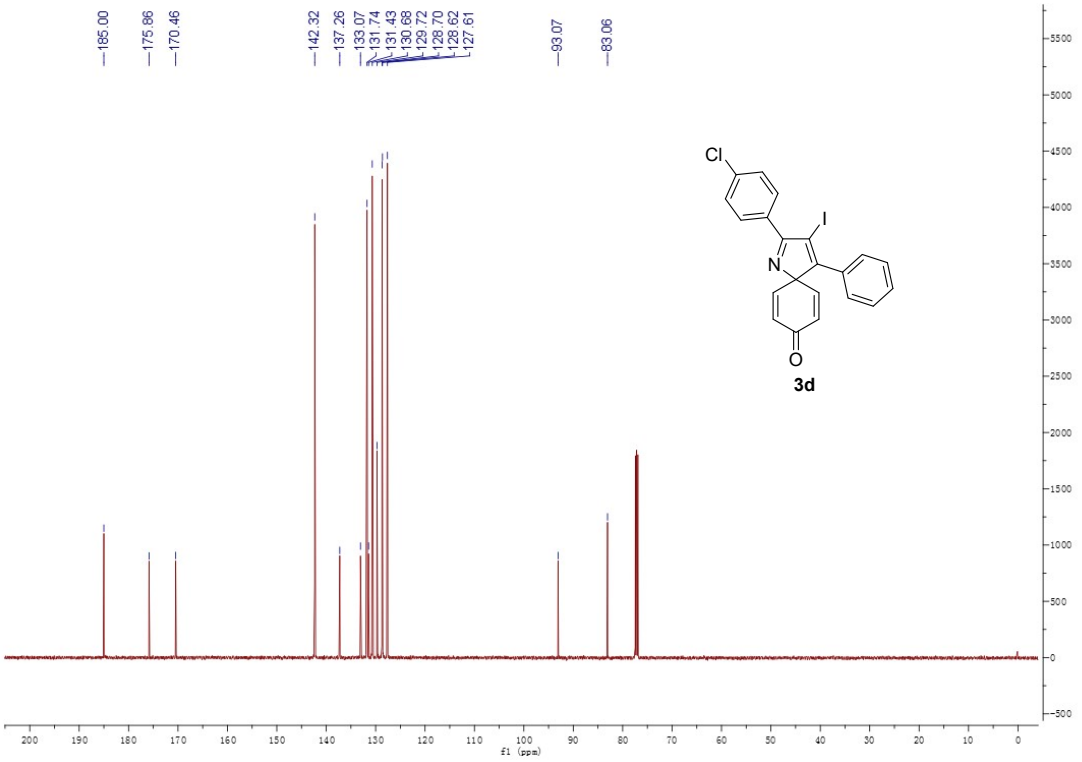
3c


185.05
175.82
170.33
165.38
163.37
142.47
131.68
129.20
129.17
128.69
127.62
115.57
115.40
93.33
82.97
F
I
N
O
f1 (ppm)

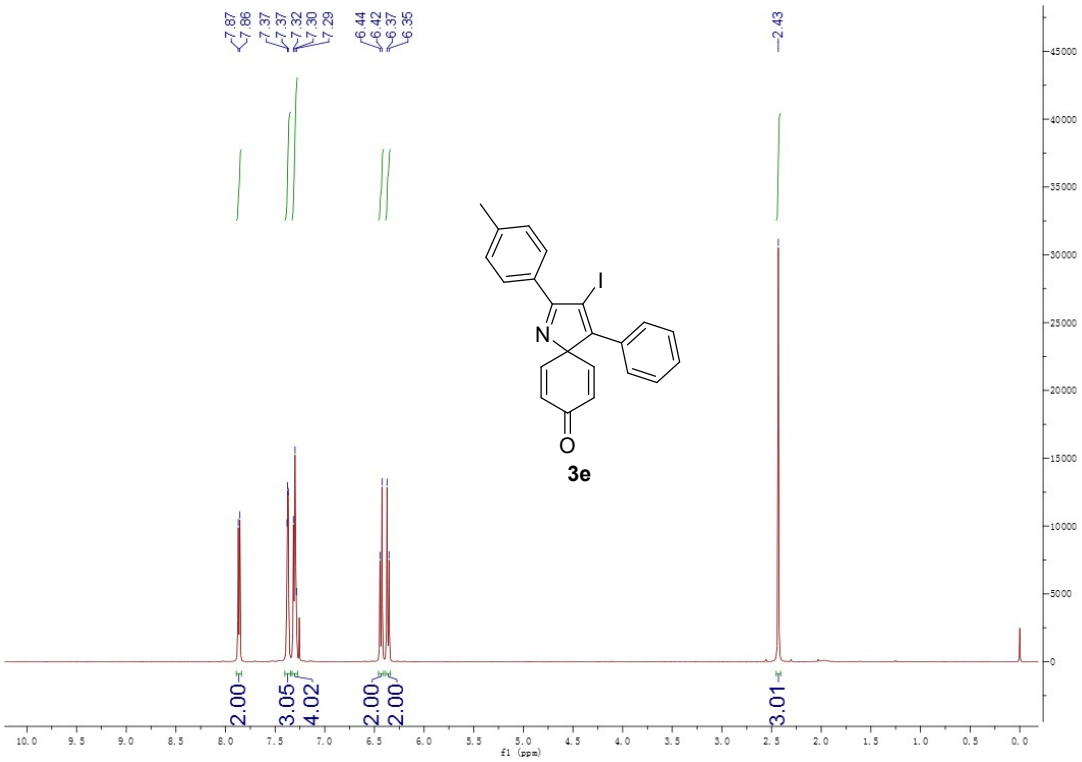
3c


-112.80
F
I
N
O
3c
f1 (ppm)

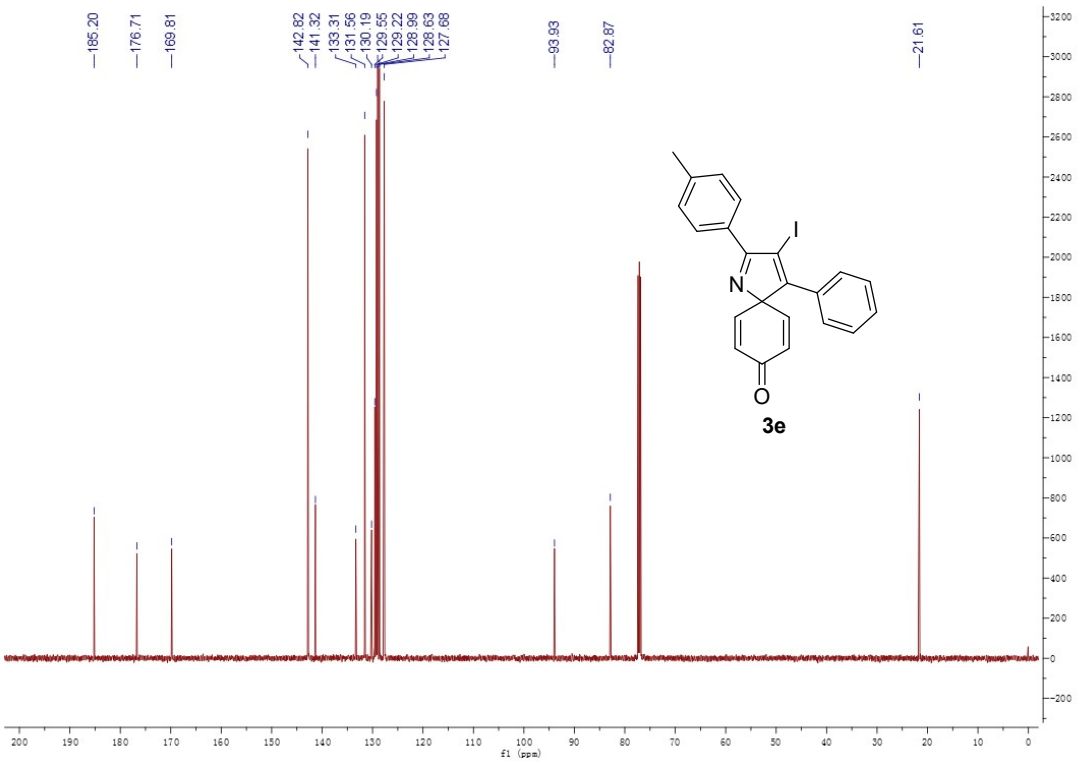

7.92
7.91
7.47
7.38
7.31
7.30
7.29
6.46
6.44
6.36
6.34
Cl
I
N
O
3d
2.00
2.01
3.01
2.05
2.03
2.07
f1 (ppm)


185.00
175.86
170.46
142.32
137.26
133.07
131.74
131.43
130.68
129.72
128.70
128.62
127.61
93.07
83.06
Cl
I
N
O
f1 (ppm)

3d


7.87
7.86
7.37
7.37
7.32
7.30
7.29
6.44
6.42
6.37
6.35
2.43
I
N
O
2.00
3.05
4.02
2.00
2.00
3.01
f1 (ppm)

3e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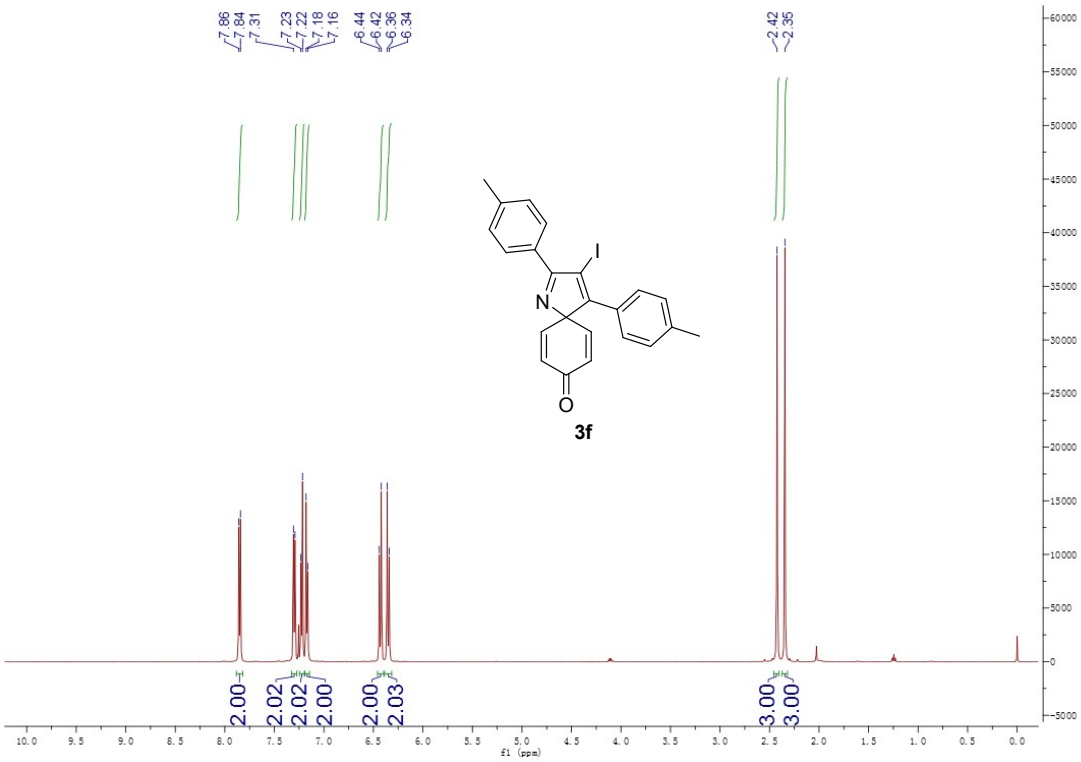
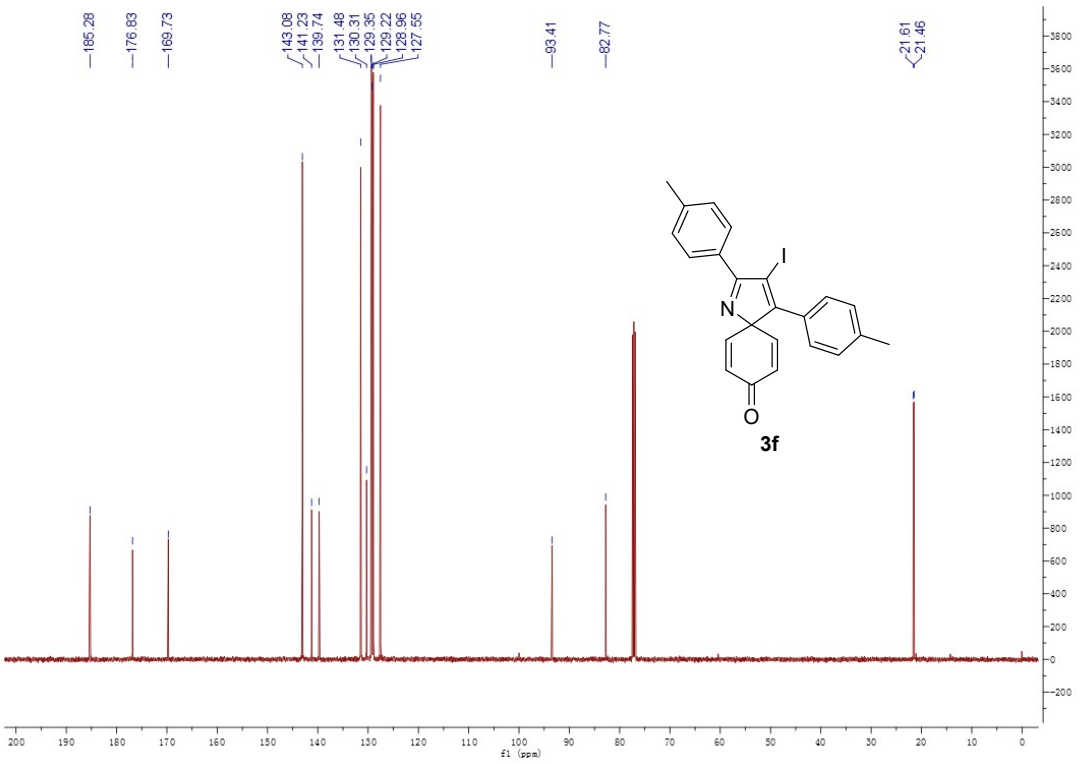
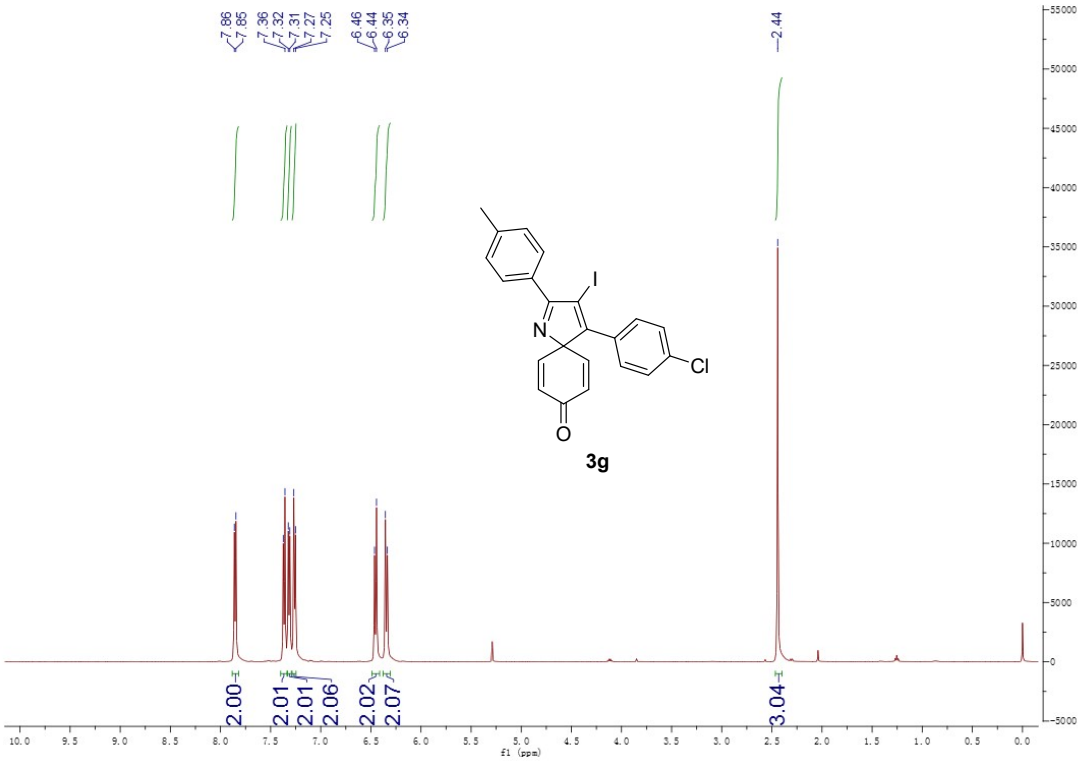
176.71
169.81
142.82
141.32
133.31
131.56
130.19
129.55
129.22
128.99
128.63
127.68
93.93
82.87
21.61
I
N
O
f1 (ppm)

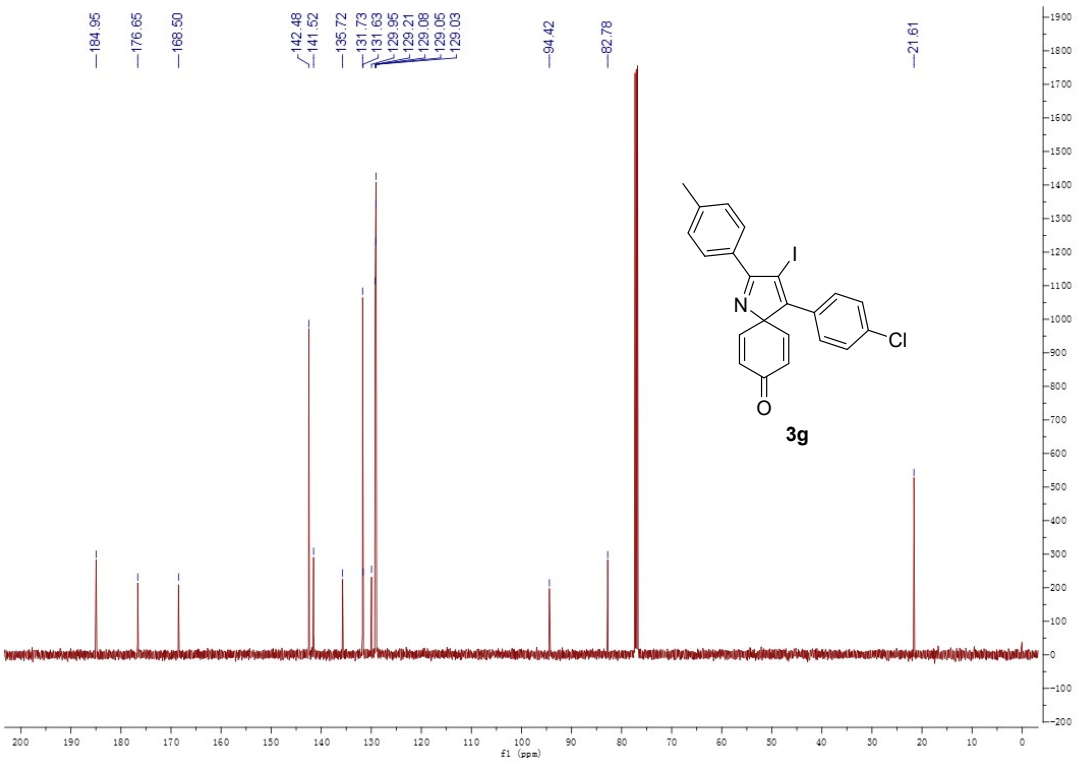
3e


7.86
7.84
7.31
7.23
7.22
7.18
7.16
6.44
6.42
6.36
6.34
2.42
2.35
I
N
O
2.00
2.02
2.02
2.00
2.00
2.03
3.00
3.00
f1 (ppm)

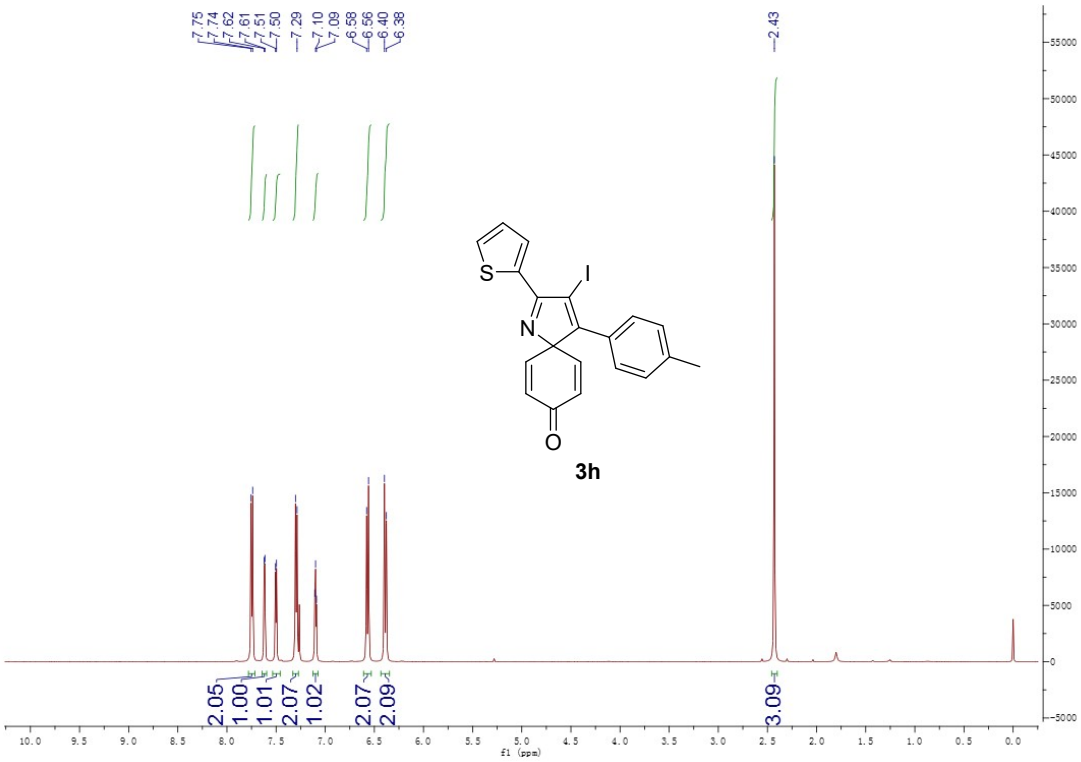
3f


185.28
176.83
169.73
143.08
141.23
139.74
131.48
130.31
129.35
129.22
128.96
127.55
93.41
82.77
21.61
21.46
I
N
O
3f
f1 (ppm)

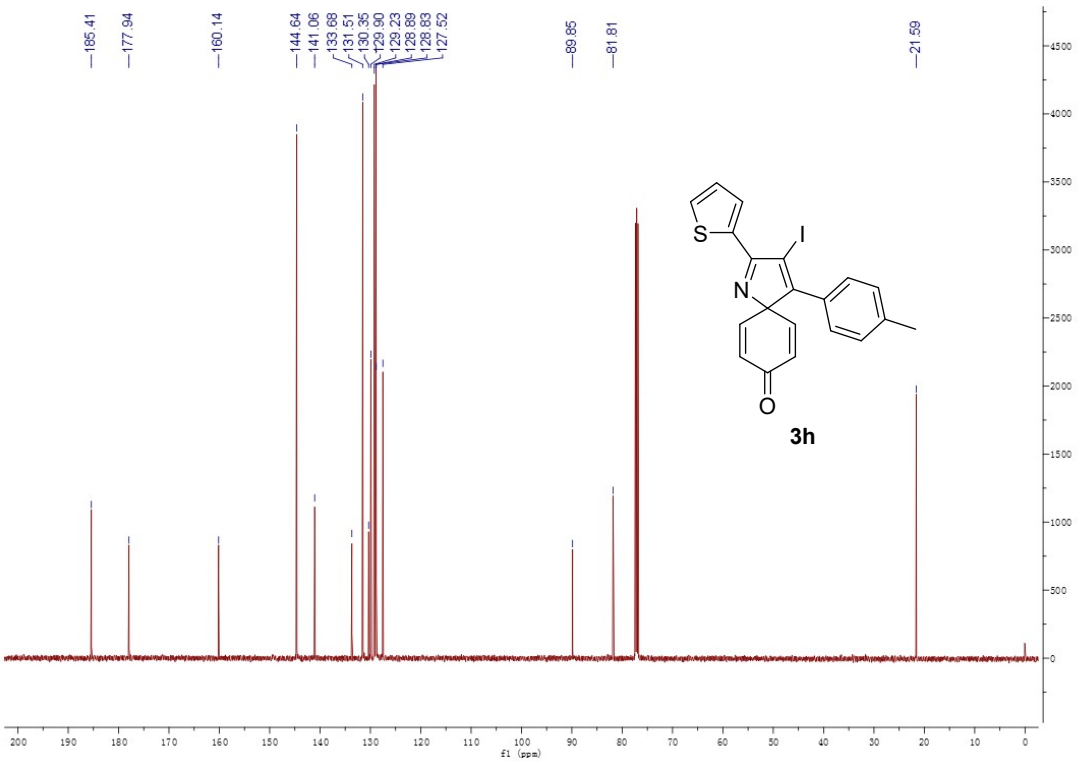

7.86
7.85
7.36
7.32
7.31
7.27
7.25
6.46
6.44
6.35
6.34
2.44
I
N
Cl
O
3g
2.00
2.01
2.01
2.06
2.02
2.07
3.04
f1 (ppm)


184.95
176.65
168.50
142.48
141.52
135.72
131.73
131.63
129.95
129.21
129.08
129.05
129.03
94.42
82.78
21.61
I
N
Cl
O
f1 (ppm)

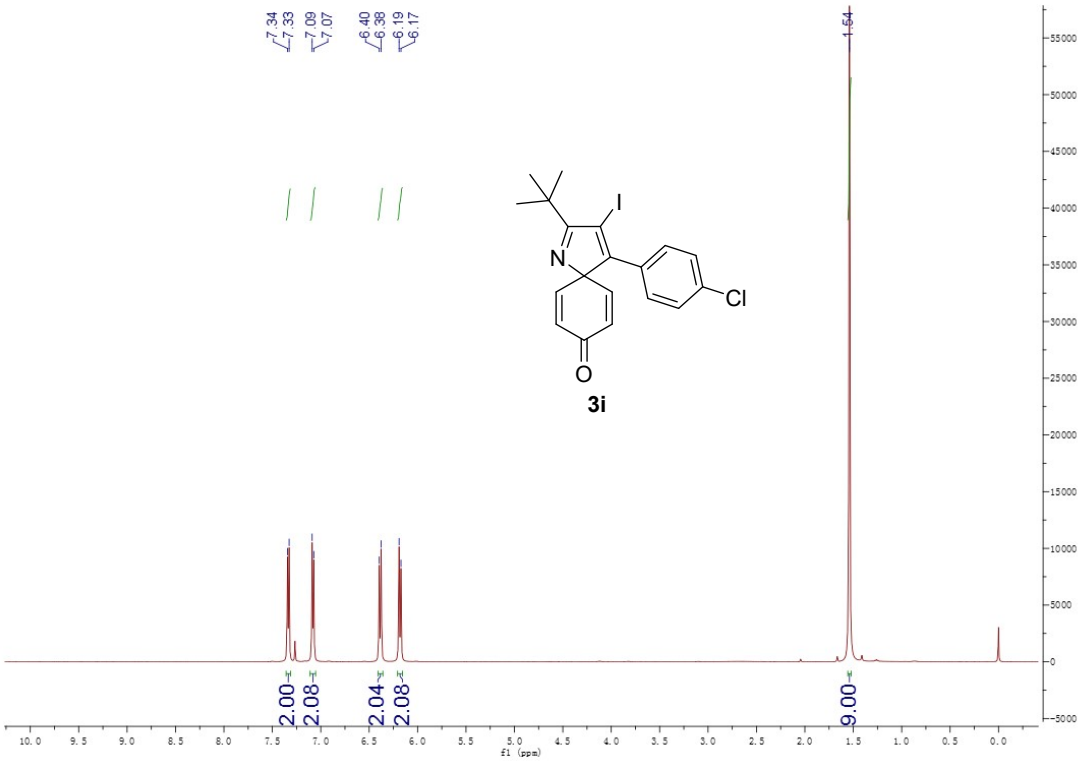
3g


7.75
7.74
7.62
7.61
7.51
7.50
7.29
7.10
7.09
6.58
6.56
6.40
6.38
2.43
S
I
N
O
2.05
1.00
1.01
2.07
1.02
2.07
2.09
3.09
f1 (ppm)

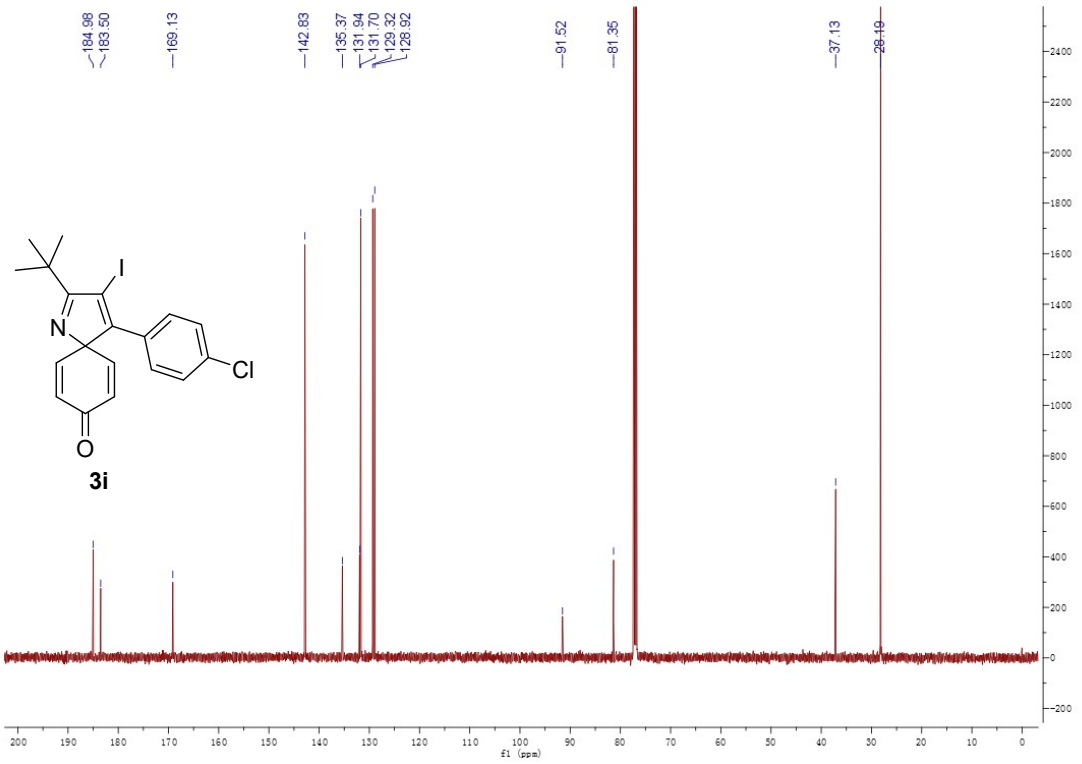
3h


185.41
177.94
160.14
144.64
141.06
133.68
131.51
130.35
129.90
129.23
128.89
128.83
127.52
89.85
81.81
21.59
S
I
N
O
f1 (ppm)

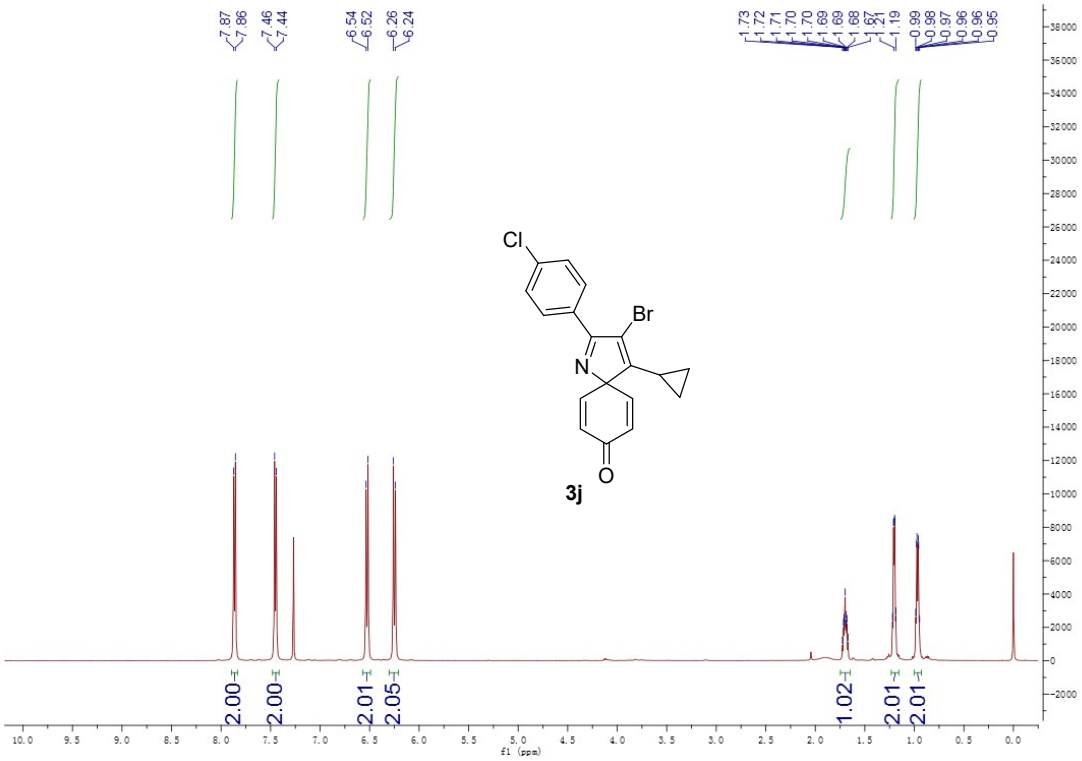
3h


7.34
7.33
7.09
7.07
6.40
6.38
6.19
6.17
1.54
I
N
Cl
O
2.00
2.08
2.04
2.08
9.00
f1 (ppm)

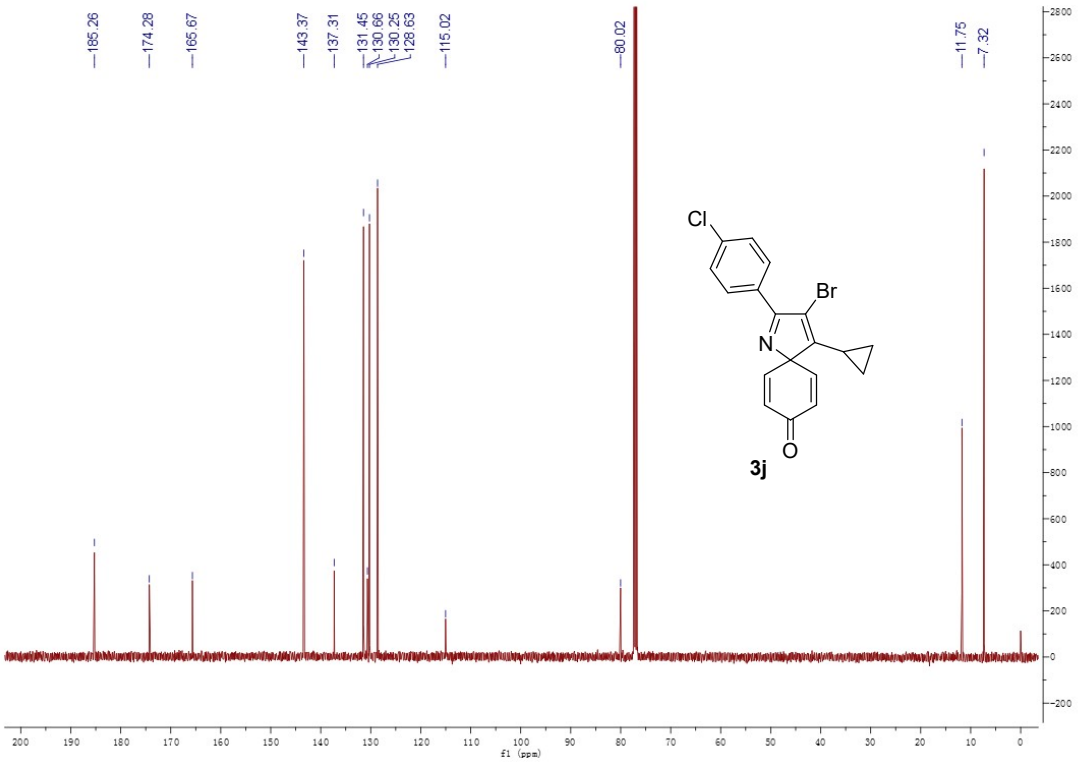
3i

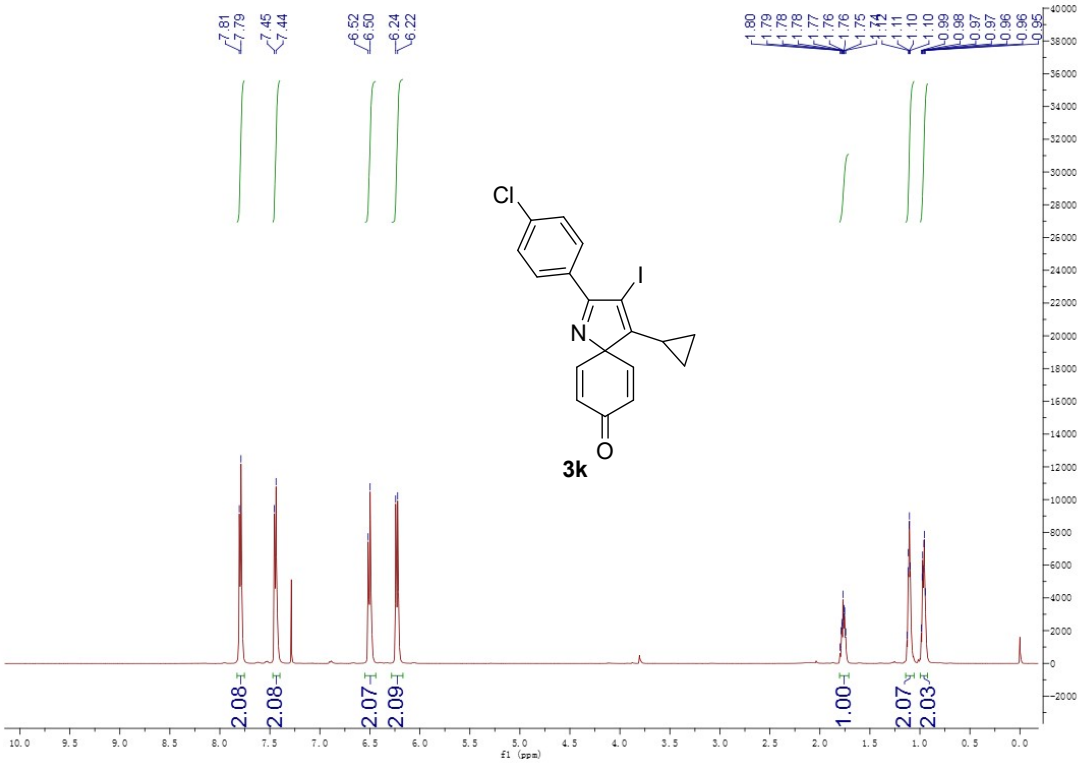

184.98
183.50
169.13
142.83
135.37
131.94
131.70
129.32
128.92
91.52
81.35
37.13
28.19
I
N
Cl
O
f1 (ppm)

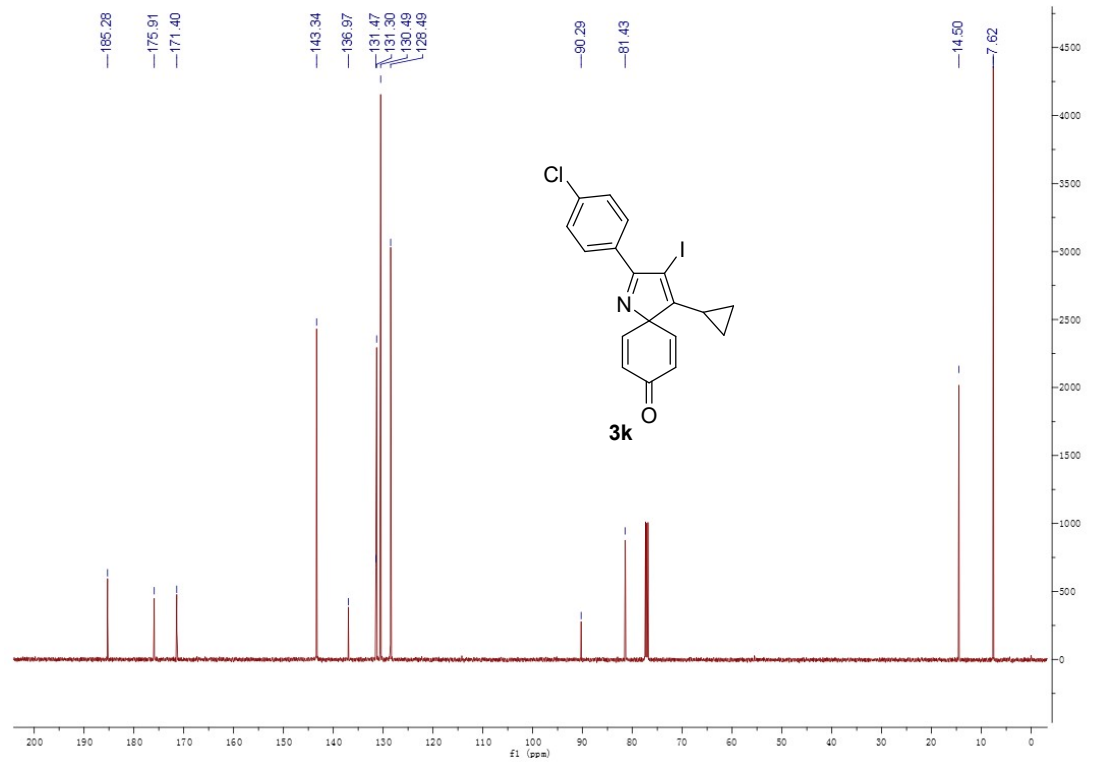
3i

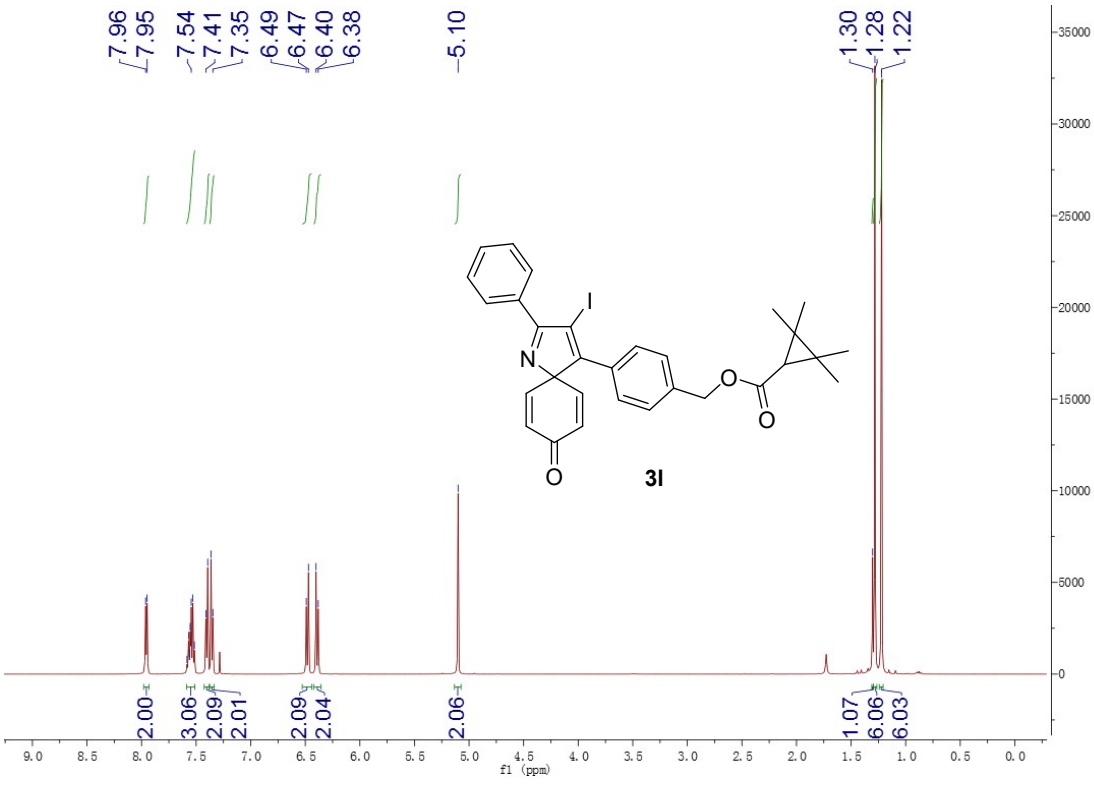

7.87
7.86
7.46
7.44
6.54
6.52
6.26
6.24
1.73
1.72
1.71
1.70
1.70
1.69
1.69
1.68
1.67
1.19
0.99
0.98
0.97
0.96
0.96
0.95
Cl
Br
N
O
2.00
2.00
2.01
2.05
1.02
2.01
2.01
f1 (ppm)

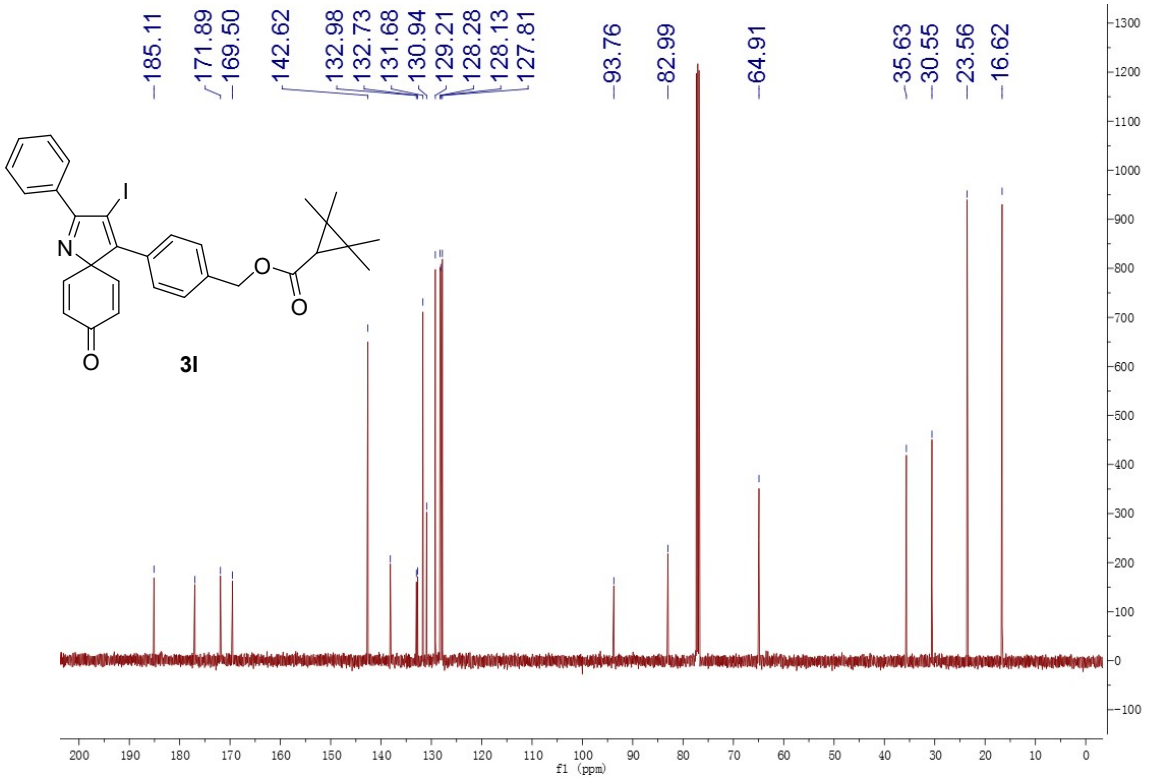
3j

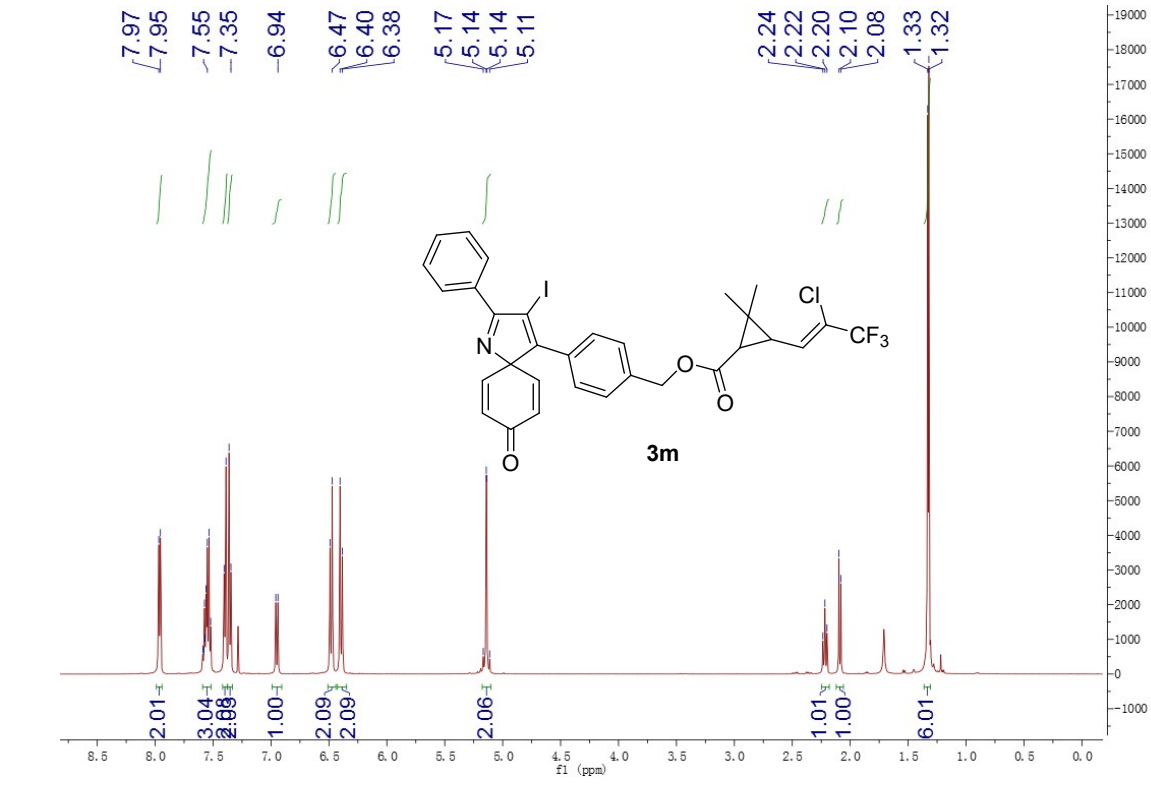

185.26
174.28
165.67
143.37
137.31
131.45
130.66
130.25
128.63
115.02
80.02
11.75
7.32
Cl
Br
N
O
3j
f1 (ppm)

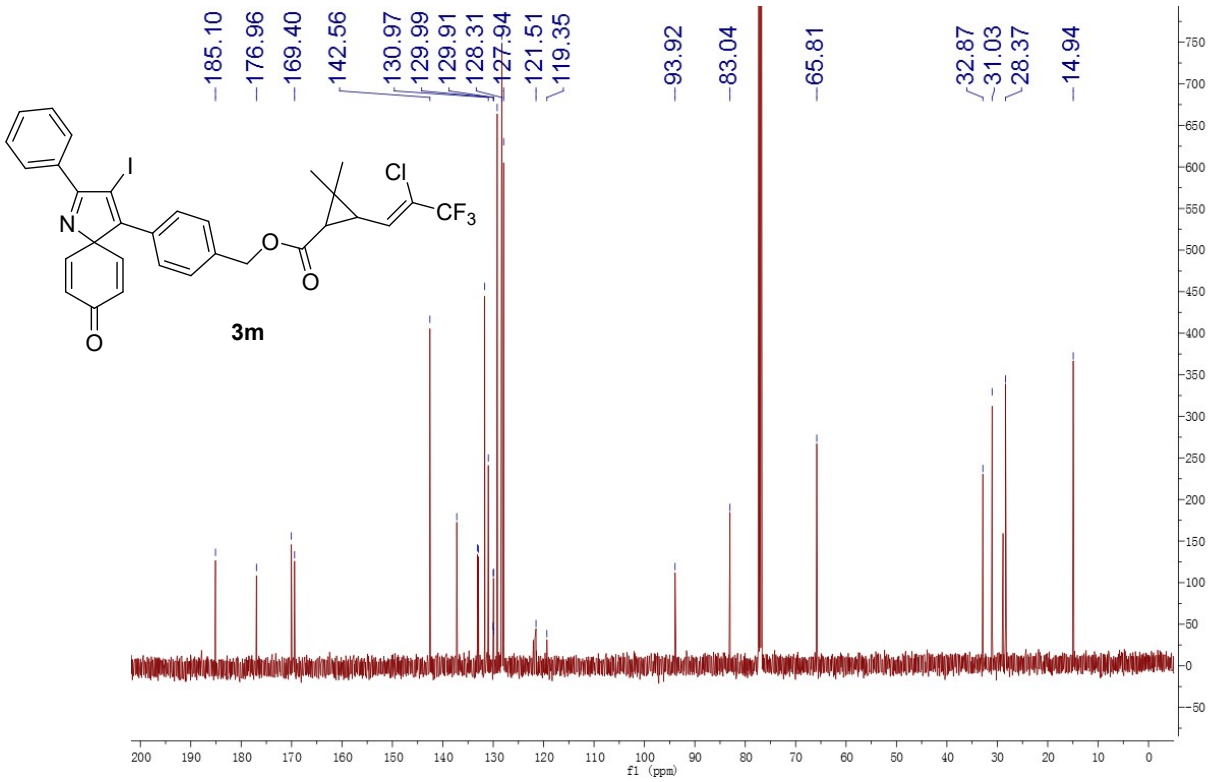

7.81
7.79
7.45
7.44
6.52
6.50
6.24
6.22
1.80
1.79
1.78
1.78
1.77
1.76
1.76
1.75
1.74
1.11
1.10
1.10
0.99
0.98
0.97
0.97
0.96
0.96
0.95
Cl
I
N
O
3k
2.08
2.08
2.07
2.09
1.00
2.07
2.03
f1 (ppm)


185.28
175.91
171.40
143.34
136.97
131.47
131.30
130.49
128.49
90.29
81.43
14.50
7.62
Cl
I
N
O
3k
f1 (ppm)


7.96
7.95
7.54
7.41
7.35
6.49
6.47
6.40
6.38
5.10
1.30
1.28
1.22
I
N
O
O
O
3l
2.00
3.06
2.09
2.01
2.09
2.04
2.06
1.07
6.06
6.03
f1 (ppm)


185.11
171.89
169.50
142.62
132.98
132.73
131.68
130.94
129.21
128.28
128.13
127.81
93.76
82.99
64.91
35.63
30.55
23.56
16.62
I
N
O
O
O
3l
f1 (ppm)


7.97
7.95
7.55
7.35
6.94
6.47
6.40
6.38
5.17
5.14
5.14
5.11
2.24
2.22
2.20
2.10
2.08
1.33
1.32
I
N
O
O
O
Cl
CF3
3m
2.01
3.04
1.00
2.09
2.09
2.06
1.01
1.00
6.01
f1 (ppm)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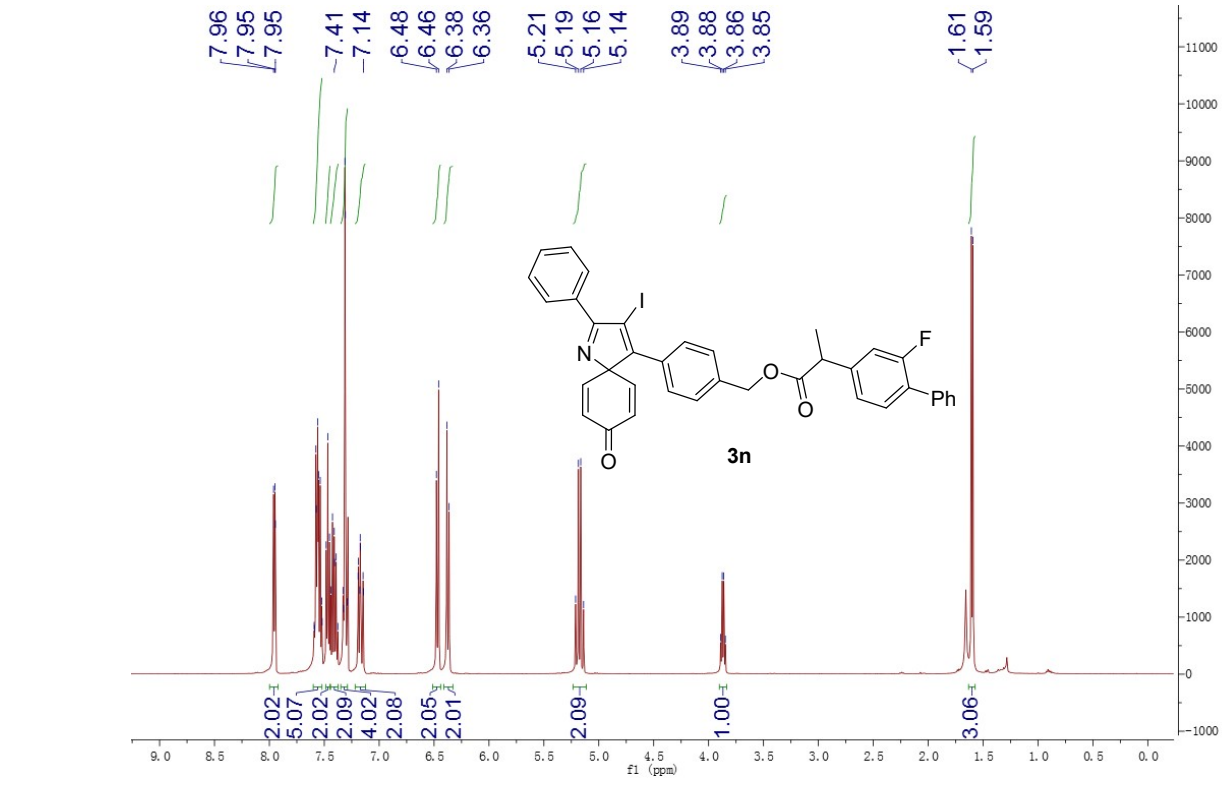
176.96
169.40
142.56
130.97
129.99
129.91
128.31
127.94
121.51
119.35
93.92
83.04
65.81
32.87
31.03
28.37
14.94
I
N
O
Cl
CF3
O
O
O
3m
f1 (ppm)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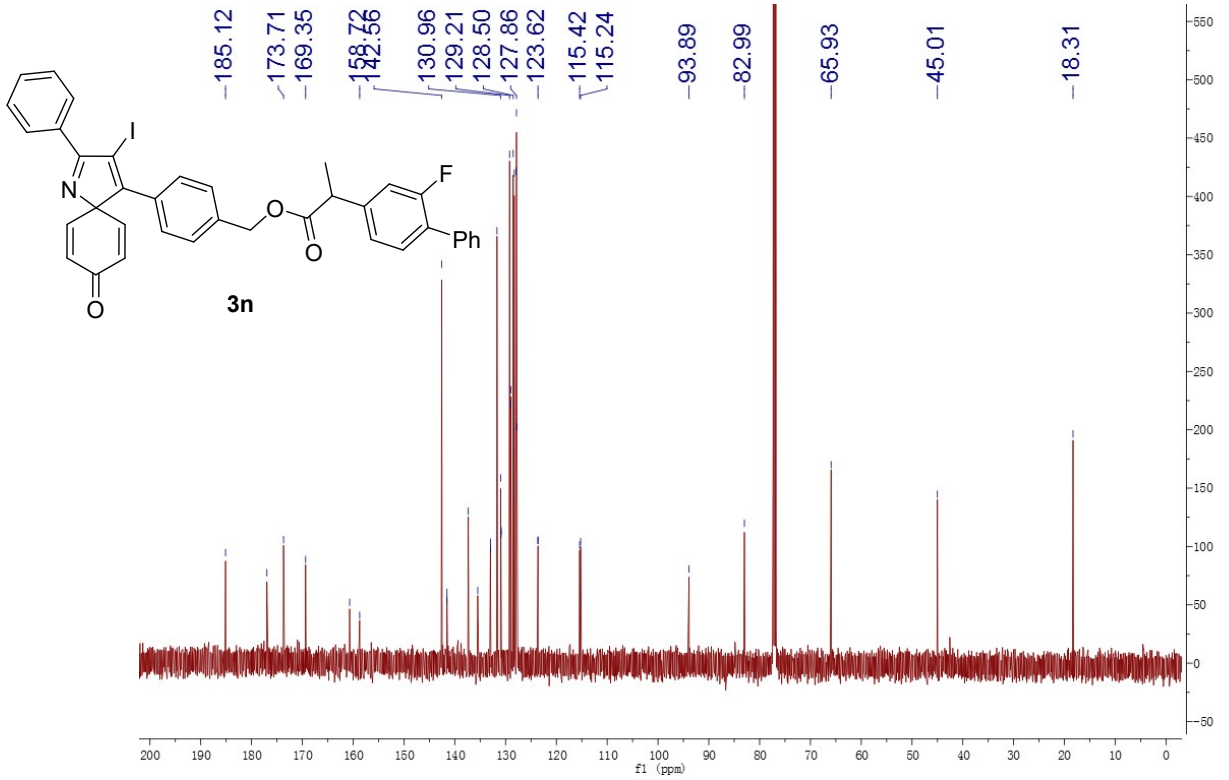
7.95
7.95
7.41
7.14
6.48
6.46
6.38
6.36
5.21
5.19
5.16
5.14
3.89
3.88
3.86
3.85
1.61
1.59
I
N
O
O
O
F
Ph
O
3n
2.02
5.07
2.02
2.09
4.02
2.08
2.05
2.01
2.09
1.00
3.06
f1 (ppm)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158.72
142.56
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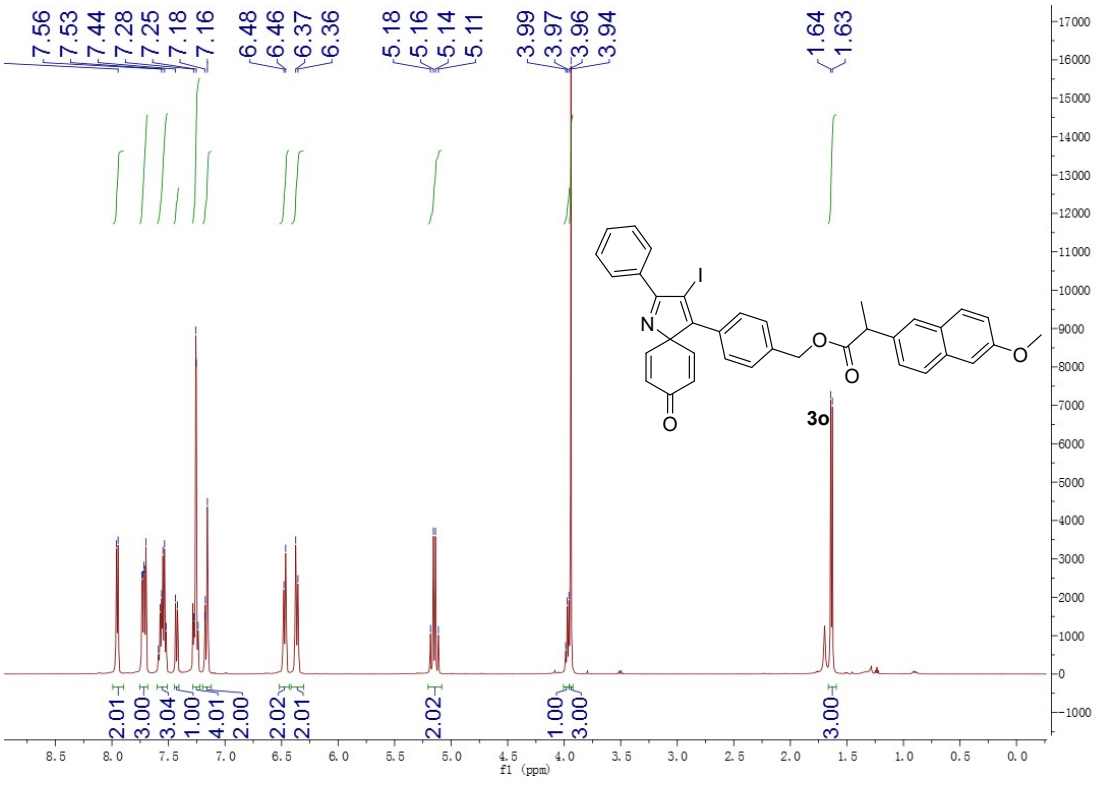
129.21
128.50
127.86
123.62
115.42
115.24
93.89
82.99
65.93
45.01
18.31
I
N
O
O
O
F
Ph
O
3n
f1 (ppm)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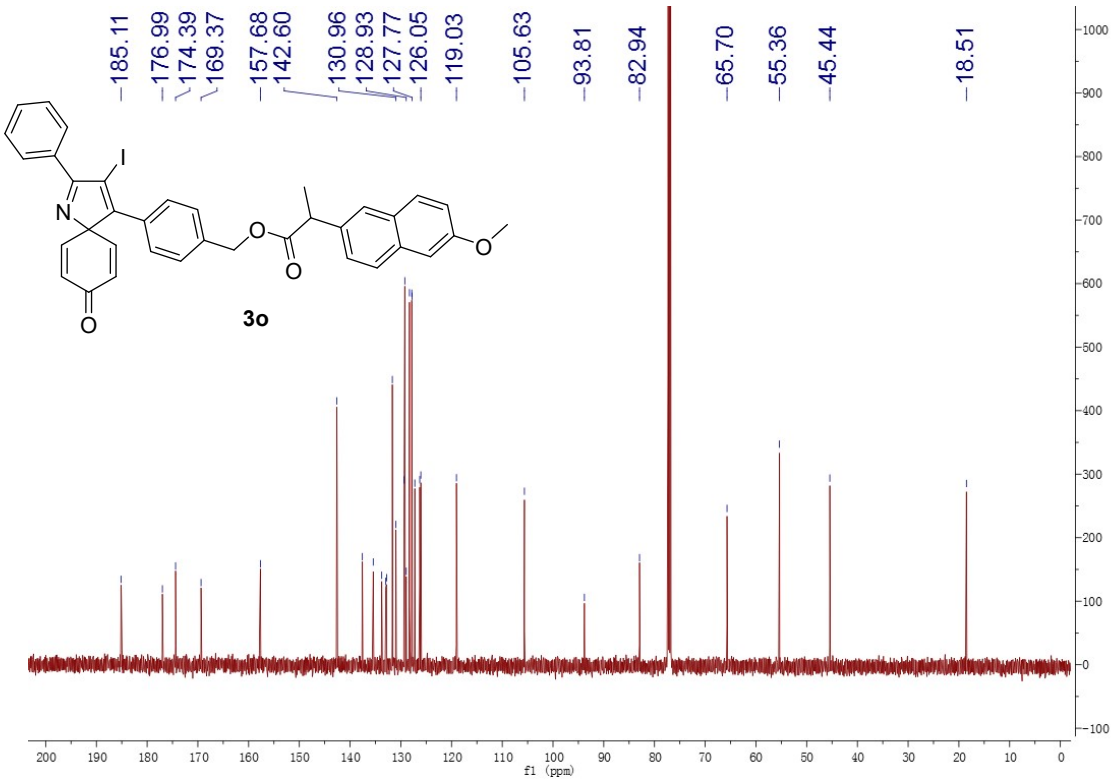
7.18
7.16
6.48
6.46
6.37
6.36
5.18
5.16
5.14
5.11
3.99
3.97
3.96
3.94
1.64
1.63
2.01
3.00
3.04
1.00
4.01
2.00
2.02
2.01
2.02
1.00
3.00
3.00
I
N
O
O
O
O
3o
f1 (ppm)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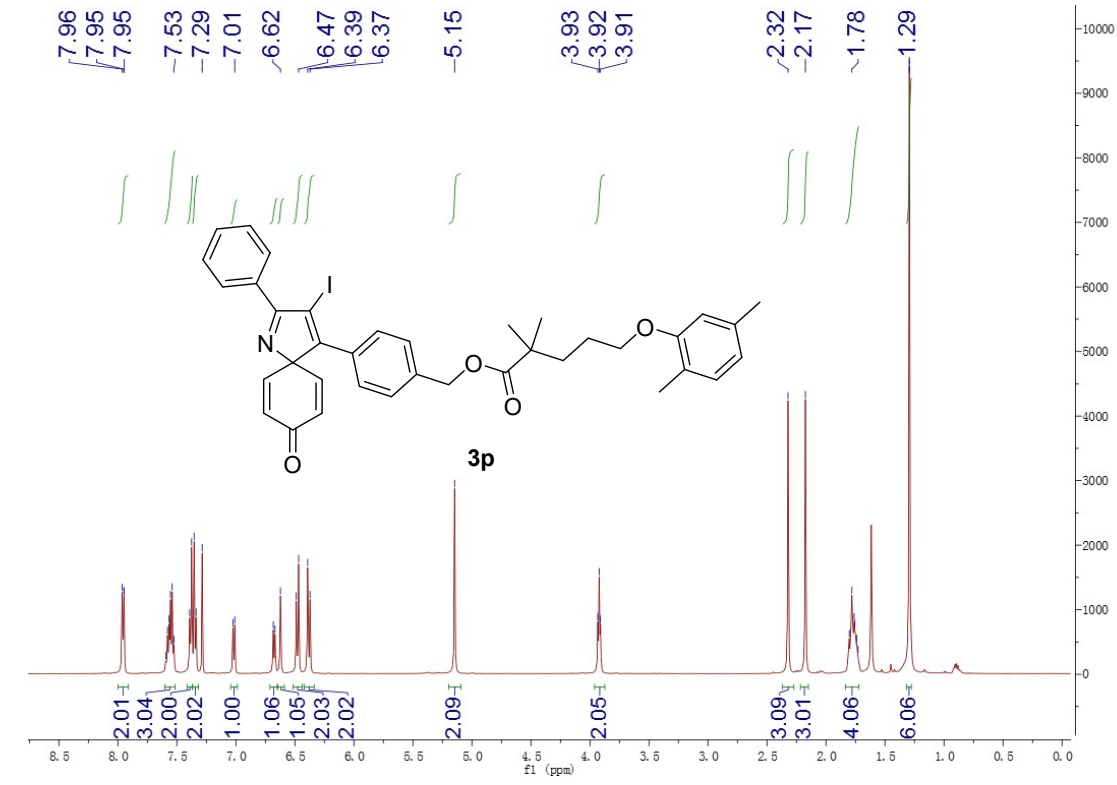
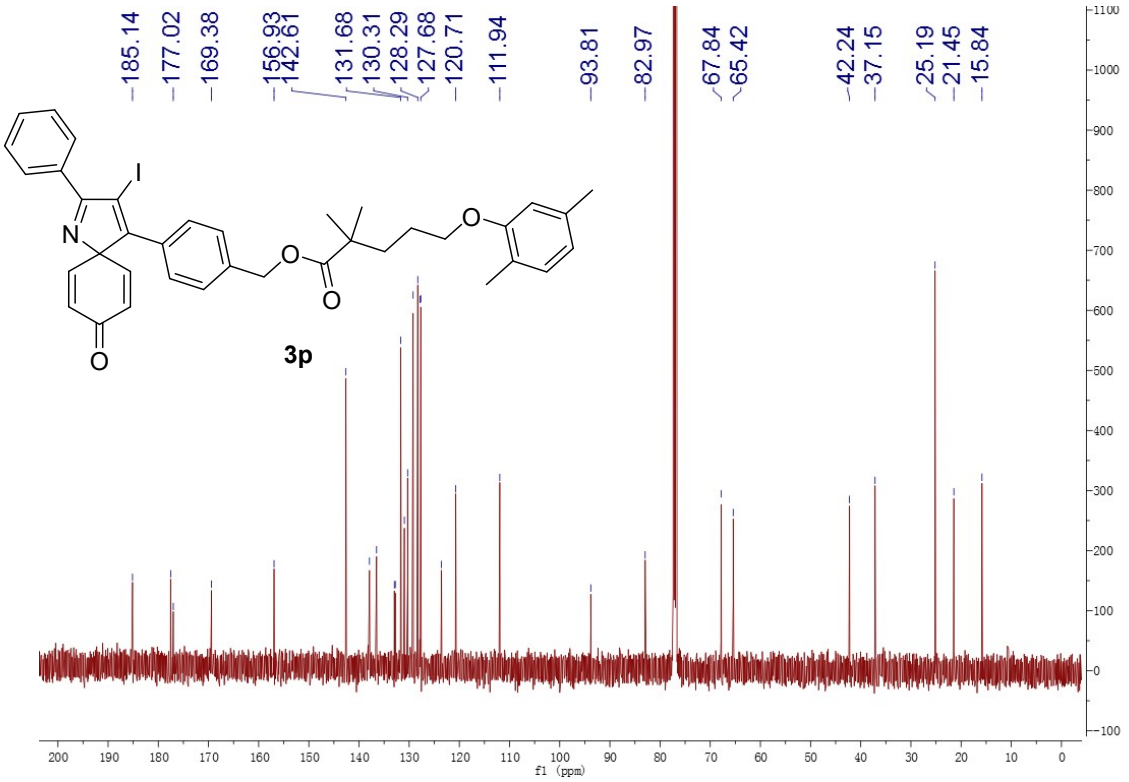
130.96
128.93
127.77
126.05
119.03
105.63
93.81
82.94
65.70
55.36
45.44
18.51
I
N
O
O
O
O
3o
f1 (ppm)


7.96
7.95
7.95
7.53
7.29
7.01
6.62
6.47
6.39
6.37
5.15
3.93
3.92
3.91
2.32
2.17
1.78
1.29
I
N
O
O
O
O
3p
2.01
3.04
2.00
2.02
1.00
1.06
1.05
2.03
2.02
2.09
2.05
3.09
3.01
4.06
6.06
f1 (ppm)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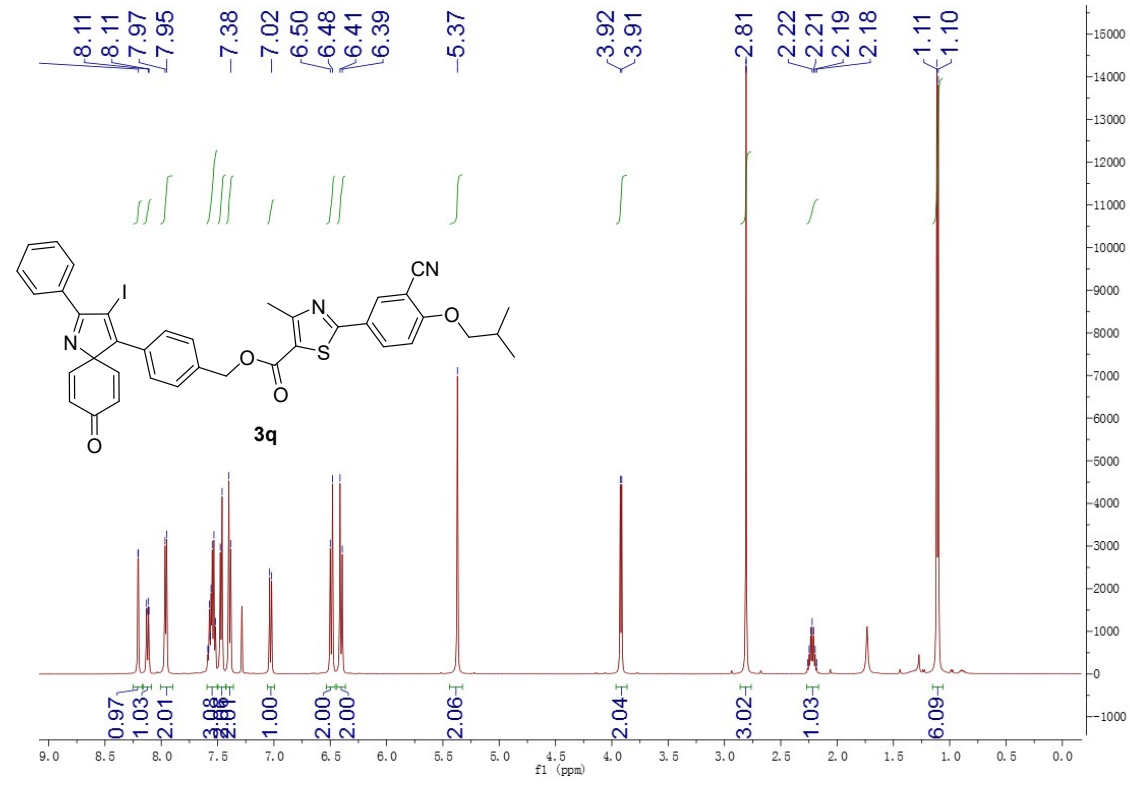
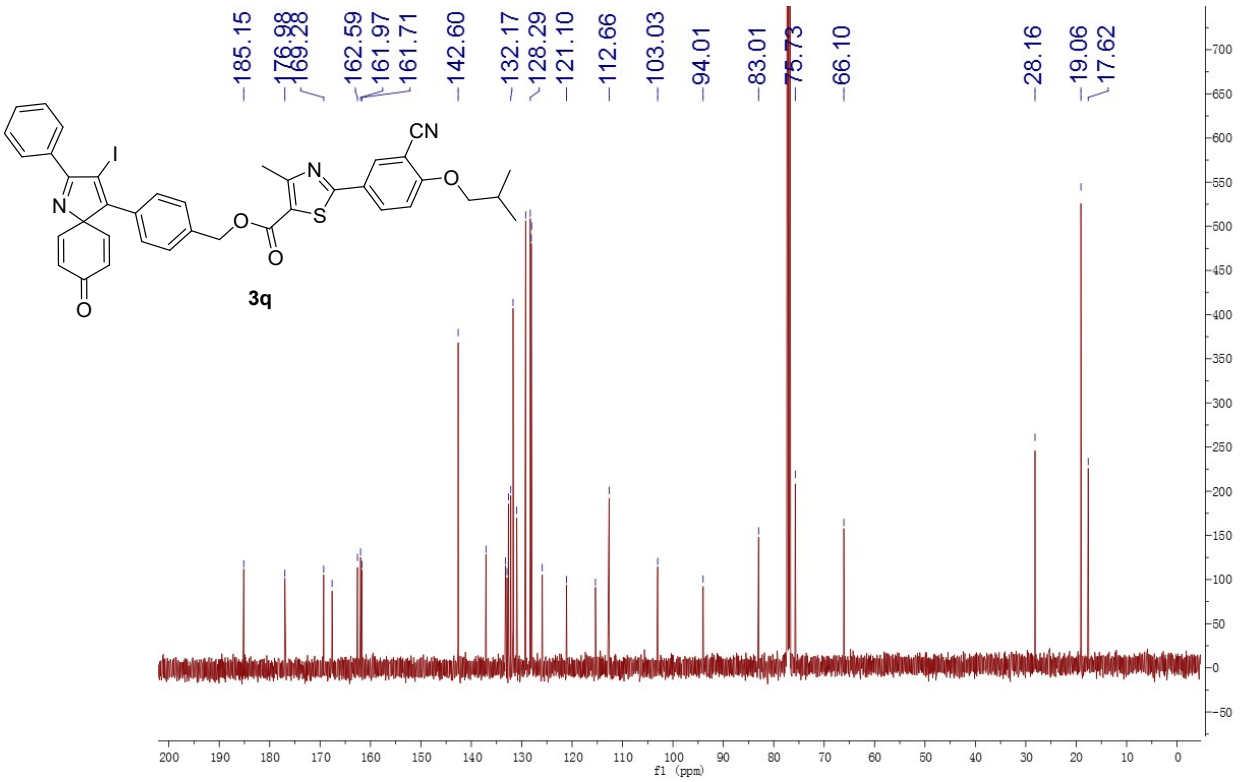
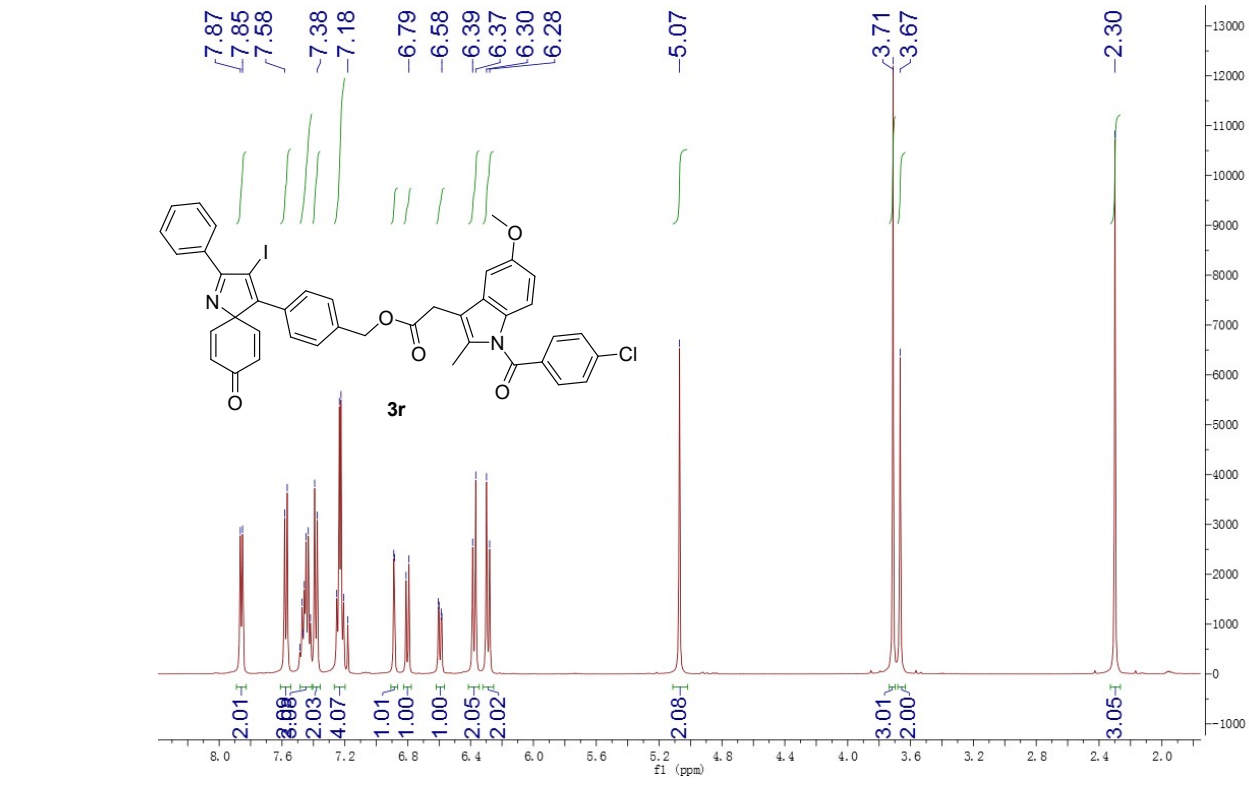
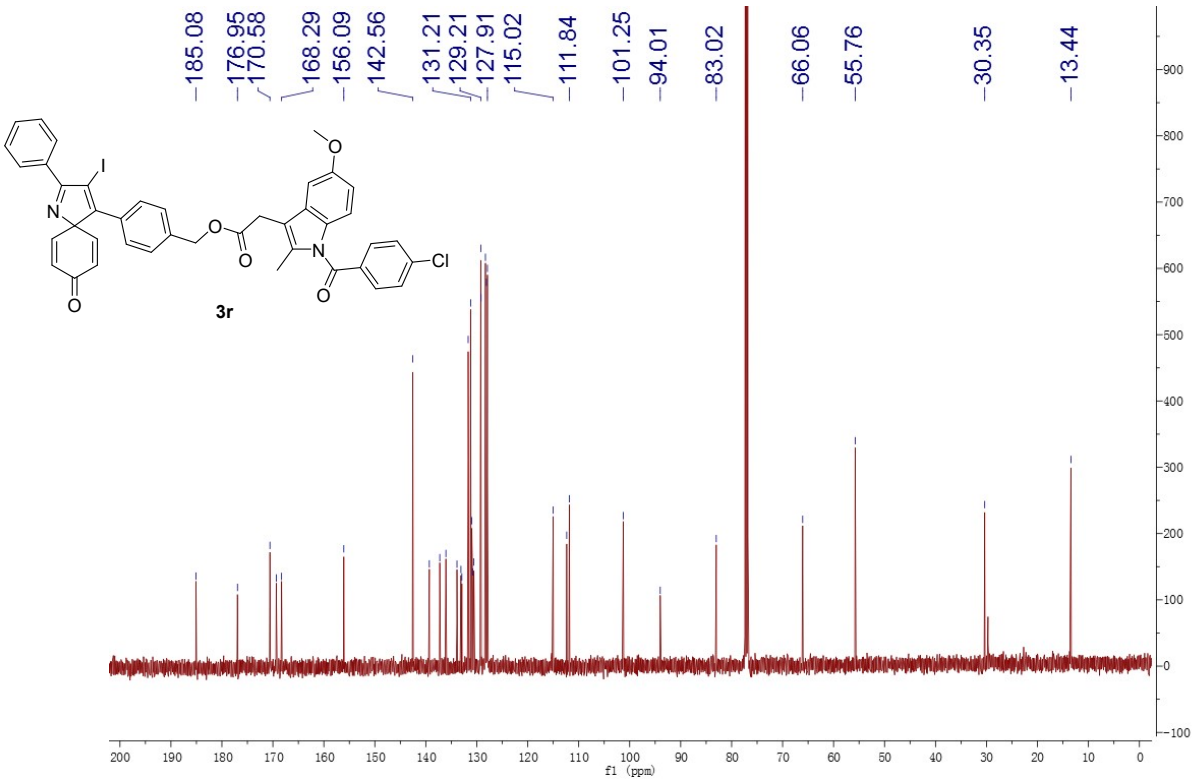
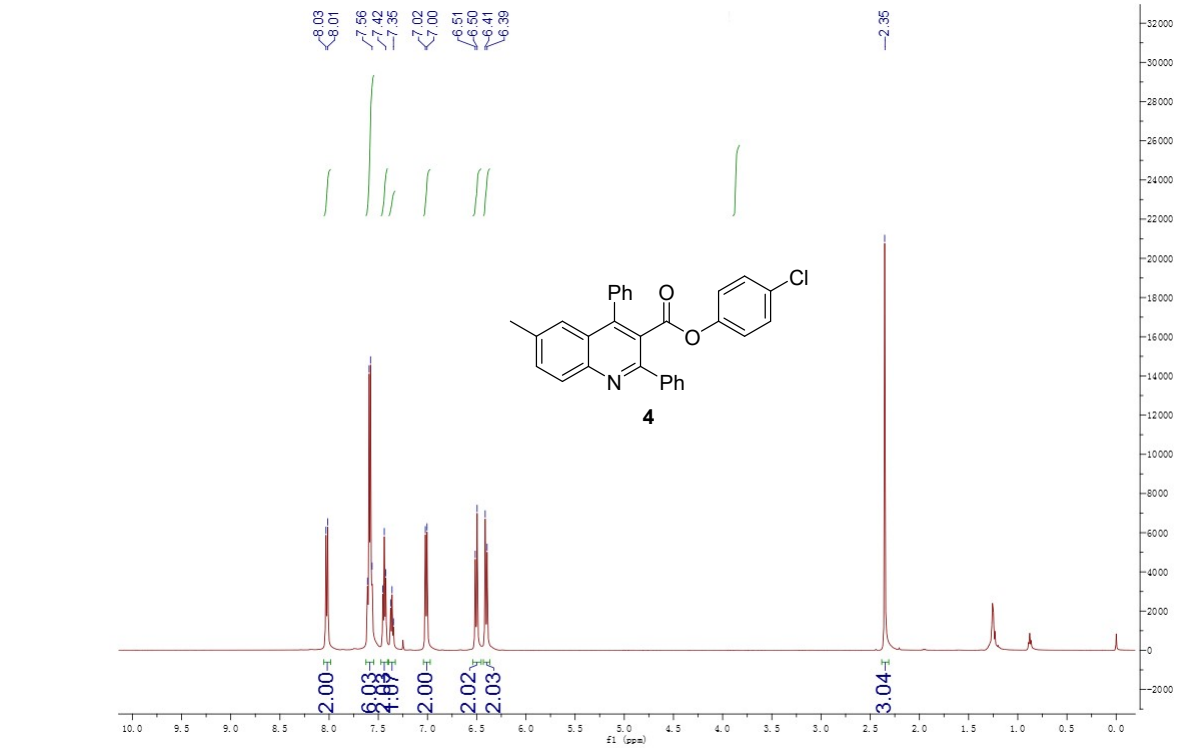
177.02
169.38
156.93
142.61
131.68
130.31
128.29
127.68
120.71
111.94
93.81
82.97
67.84
65.42
42.24
37.15
25.19
21.45
15.84
I
N
O
O
O
O
3p
f1 (ppm)

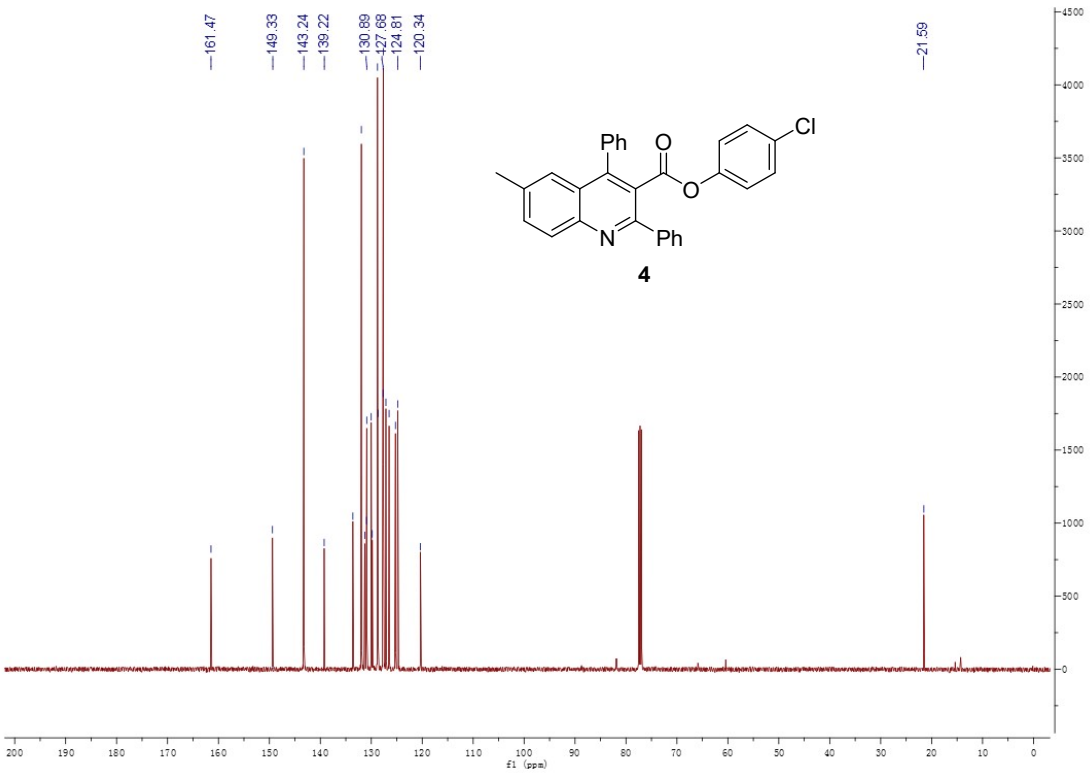

8.11
8.11
7.97
7.95
7.38
7.02
6.50
6.48
6.41
6.39
5.37
3.92
3.91
2.81
2.22
2.21
2.19
2.18
1.11
1.10
CN
I
N
S
O
O
O
O
3q
0.97
1.03
2.01
1.00
2.00
2.00
2.06
2.04
3.02
1.03
6.09
f1 (ppm)

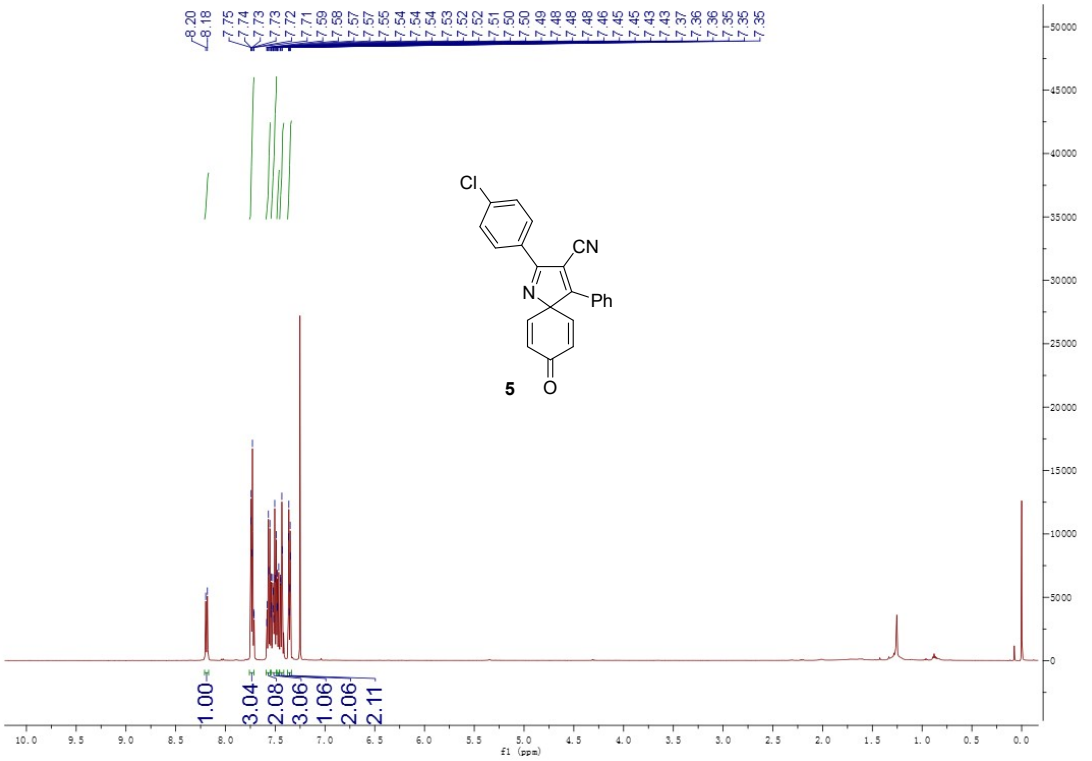

185.15
176.98
169.28
162.59
161.97
161.71
142.60
132.17
128.29
121.10
112.66
103.03
94.01
83.01
75.73
66.10
28.16
19.06
17.62
CN
I
N
S
O
O
O
O
3q
f1 (ppm)

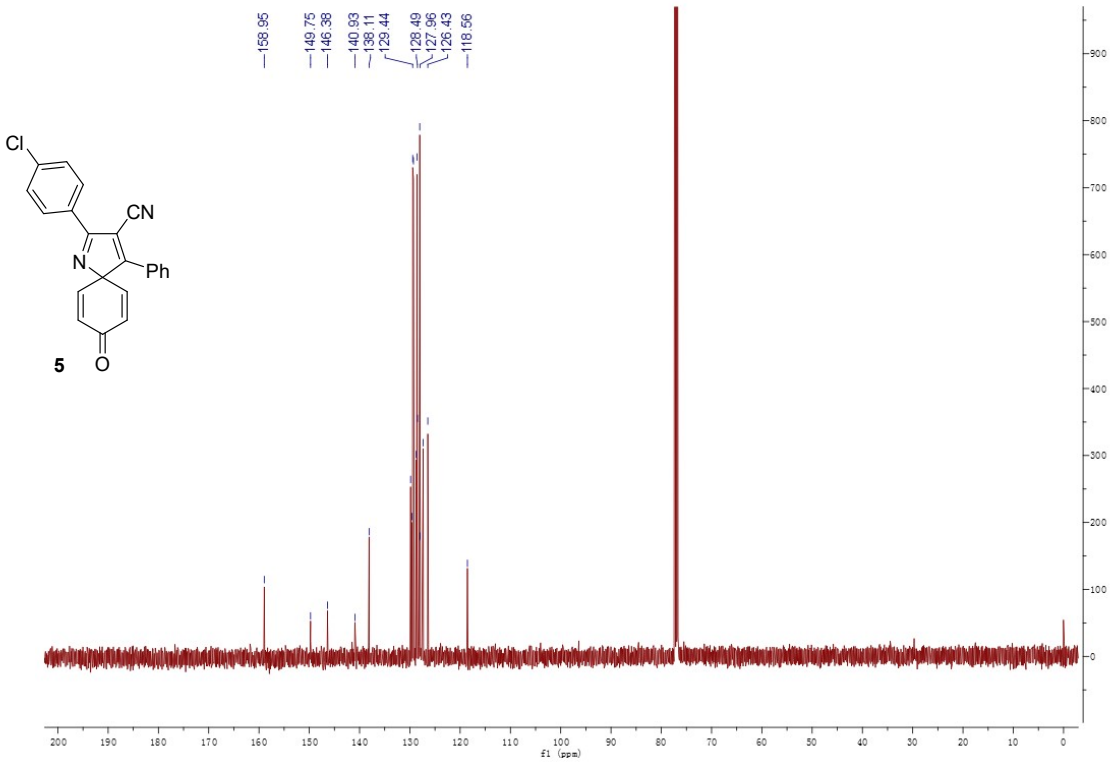

7.87
7.85
7.58
7.38
7.18
6.79
6.58
6.39
6.37
6.30
6.28
5.07
3.71
3.67
2.30
I
N
O
O
O
O
N
Cl
O
3r
2.01
2.03
4.07
1.01
1.00
1.00
2.05
2.02
2.08
3.01
2.00
3.05
f1 (ppm)


185.08
176.95
170.58
168.29
156.09
142.56
131.21
129.21
127.91
115.02
111.84
101.25
94.01
83.02
66.06
55.76
30.35
13.44
I
N
O
O
O
O
N
Cl
O
3r
f1 (ppm)


8.03
8.01
7.56
7.42
7.35
7.02
7.00
6.51
6.50
6.41
6.39
2.35
Ph
O
Cl
O
N
Ph
4
2.00
6.03
4.07
2.00
2.02
2.03
3.04
f1 (ppm)


161.47
149.33
143.24
139.22
130.89
127.68
124.81
120.34
21.59
Ph
O
Cl
O
N
Ph
4
f1 (ppm)


8.20
8.18
7.75
7.74
7.73
7.73
7.72
7.71
7.59
7.58
7.57
7.57
7.55
7.54
7.54
7.54
7.53
7.52
7.52
7.51
7.50
7.50
7.49
7.48
7.48
7.48
7.46
7.45
7.45
7.43
7.43
7.37
7.36
7.36
7.35
7.35
7.35
Cl
CN
N
Ph
O
5
1.00
3.04
2.08
3.06
1.06
2.06
2.11
f1 (ppm)


158.95
149.75
146.38
140.93
138.11
129.44
128.49
127.96
126.43
118.56
Cl
CN
N
Ph
O
5
f1 (ppm)