Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Rhodium/Copper-Cocatalyzed Annulation of Benzylamine with Diazo Compounds: Accesses to Fused Isoquinolines

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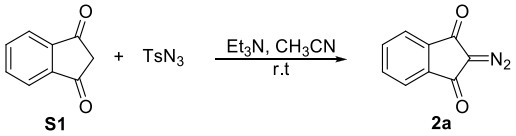
General information

Commercially available solvents were used as received. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 spectrometer. Chemical shifts are reported in δ units relative to $CDCl_3$ [^{1}H δ = 7.26, ^{13}C δ = 77.00], CD_2Cl_2 [^{1}H δ = 5.32, ^{13}C δ = 53.30]. Abbreviations used in the description of resonances are: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). High resolution mass spectra were recorded using the electrospray ionization (ESI) method. Benzylamines and other chemicals in the experimental section were purchased from commercial sources unless otherwise noted.

General procedures

Preparation of 2-diazo-1H-indene-1,3(2H)-dione



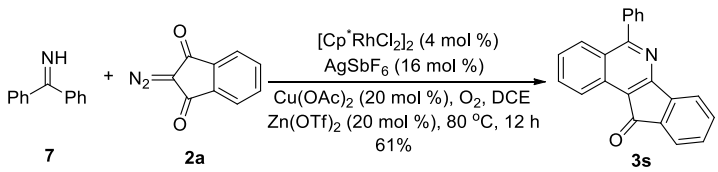
To a solution of 1*H*-indene-1,3(2*H*)-dione **S1** (2.92 g, 20 mmol) and TsN_3 (5.91 g, 30 mmol) in CH_3CN (30 ml) at 0 °C was added Et_3N (4.0 g, 40 mmol) dropwise. The reaction mixture was allowed to warm to room temperature and stirred for 10 h. Afterwards, the reaction mixture was pre-adsorbed onto silica gel under reduced pressure and purified by flash column chromatography to afford the pure product **2a** (2.7 g, 81%) as a yellow solid.

Typical procedure for the annulation of benzylamines with diazo compounds

A dried Schlenk tube equipped with a stir bar was loaded with benzylamine (0.2 mmol), diazo compound (0.22 mmol), $[Cp^*RhCl_2]_2$ (4 mol %, 0.0050 g), $AgSbF_6$ (16 mol %, 0.0110 g), $Zn(OTf)_2$ (20 mol %, 0.0150 g), $Cu(OAc)_2$ (20 mol %, 0.0072 g) and DCE (3 mL). The reaction mixture was then stirred at 80 °C under a balloon pressure of O_2 for 12 h. After cooled down to room temperature, the solvent was evaporated under vacuum, and the residue was purified by flash column chromatography on silica gel to afford the pure product.

Mechanistic studies

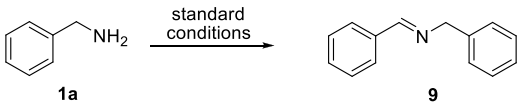
The annulation of benzophenone imine with diazo compound 2a



Benzophenone imine **7** (0.0362 g, 0.2 mmol), diazo compound **2a** (0.0379 g, 0.22 mmol), $[Cp^*RhCl_2]_2$ (4 mol %, 0.0050 g), $AgSbF_6$ (16 mol %, 0.0110 g), $Zn(OTf)_2$ (20 mol %, 0.0150 g) and $Cu(OAc)_2$ (20 mol %, 0.0072 g) were added to a dried Schlenk tube which equipped with a stir bar, then DCE (3 ml) was added. The mixture was stirred at 80 °C under a balloon pressure of O_2 for 12 h. After cooled down to room temperature, the solvent was evaporated in vacuum, and the residue was purified

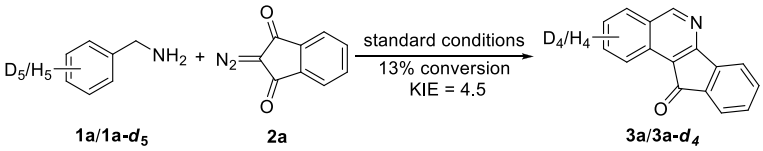
through flash column chromatography on silica gel to afford the pure product **3s** in 61% yield.

The oxidation of benzylamine 1a via Rh/Cu catalysis

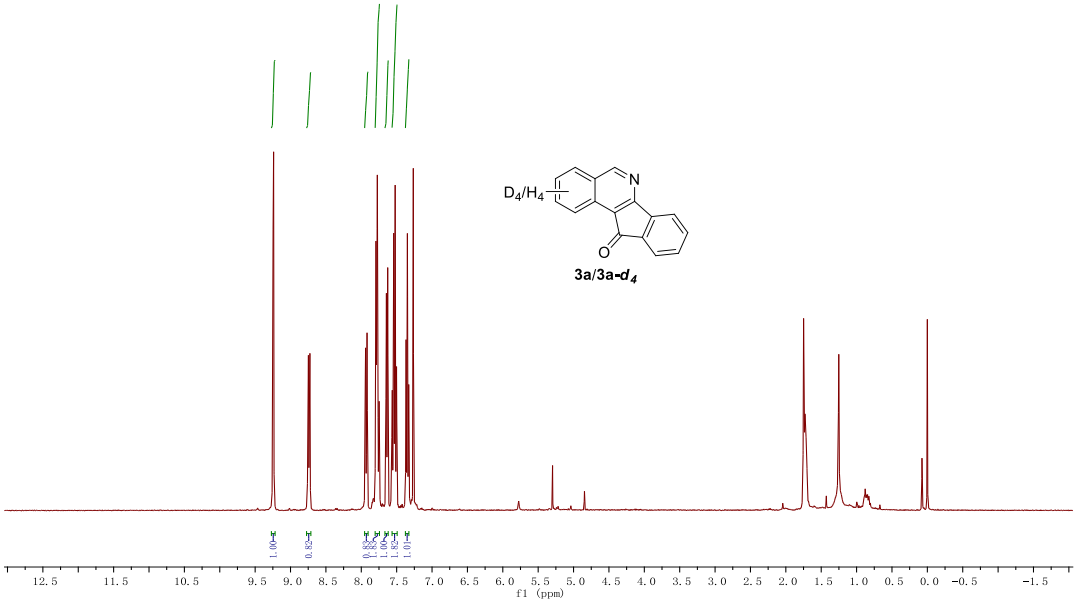


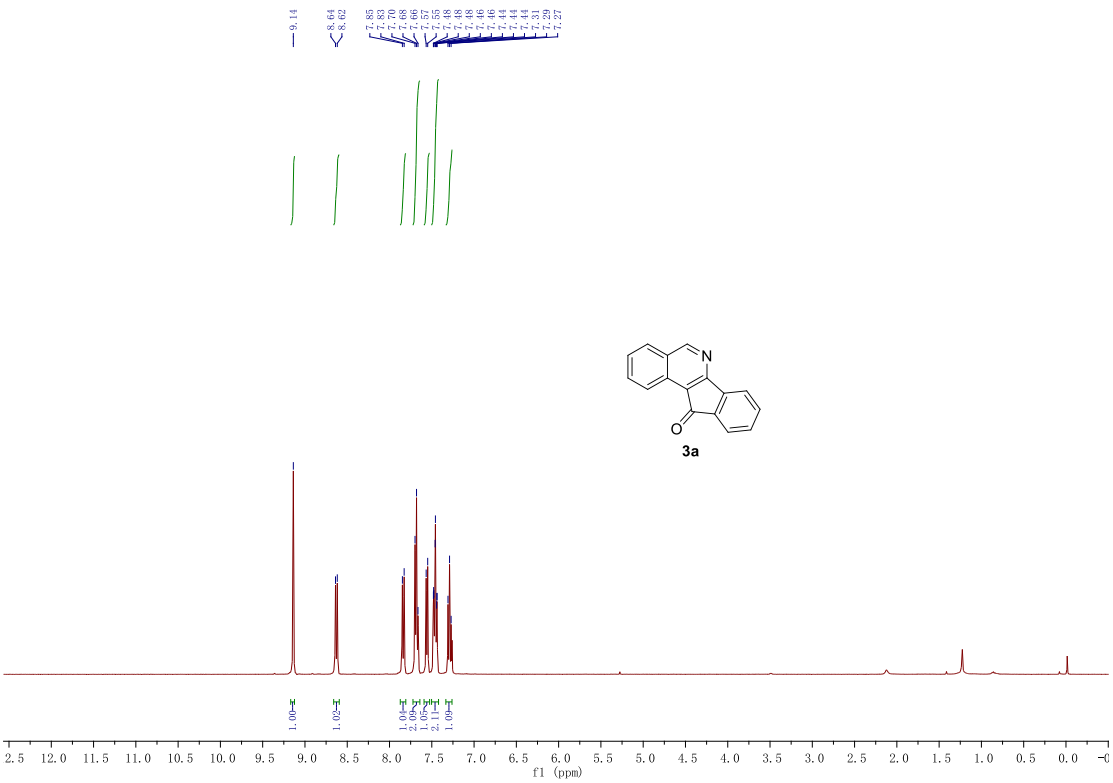
Benzylamine **1a** was added into a dried Schlenk tube under the standard conditions without the diazo compound. The reaction mixture was stirred at 80 °C under a balboon pressure of O_2 for 12 h, then the product *N*-benzylidene-1-phenylmethanamine **9** was detected by GC-MS.

KIE experiment

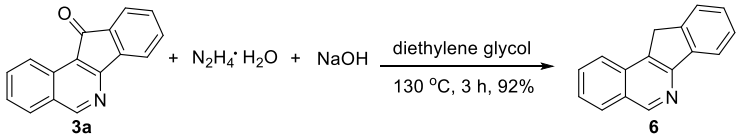


Benzylamine **1a** (0.0216 g, 0.2 mmol) and benzylamine-d_5 **1a-*d*$_5$** (0.0226g, 0.2 mmol) were added to a dried Schlenk tube, along with diazo compound **2a** (0.0379 g, 0.22 mmol), $[Cp^*RhCl_2]_2$ (4 mol%, 0.0050 g), $AgSbF_6$ (16 mol %, 0.0110 g), $Zn(OTf)_2$ (20 mol %, 0.0150 g), $Cu(OAc)_2$ (20 mol %, 0.0072 g) and DCE (3 mL). The mixture was stirred at 80 °C under a balloon pressure of O_2 for 1.5 h (13% conversion). The crude product was purified by flash column chromatography on silica gel. Then the product was analyzed by ^{1}H NMR to obtain a KIE value of 4.5.



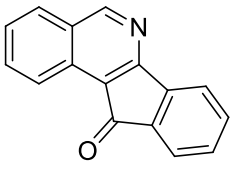


The reduction of product 3a



To a round-bottom flask, 11*H*-indeno[1,2-*c*]isoquinolin-11-one **3a** (0.0461 g, 0.2 mmol), NaOH (0.0160 g, 0.4 mmol) and diethylene glycol (5 ml) were added. To this mixture was added N_2H_4•H_2O (64%, 1 mL) dropwise. The reaction mixture was stirred at 130 °C for 3 h. After cooled down to rt, saturated aq NH_4Cl was added and the mixture was extracted by EtOAc for three times. The organic layers were collected, washed with aqueous NaCl, dried over anhydrous sodium sulfate, and concentrated by rotary evaporation under reduced pressure. The crude product was purified on silica gel column using petroleum ether and ethyl acetate (50/1) as the eluent to give the desired product **6** in 92% yield.

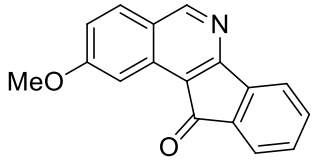
Product Characterization



3a

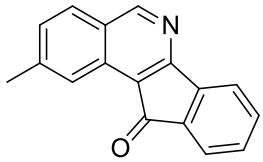
11*H*-Indeno[1,2-*c*]isoquinolin-11-one **3a** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 93% yield (43.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.70 (d, *J* =

8.4 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 1H), 7.75 (t, *J* = 7.0 Hz, 2H), 7.63 (d, *J* = 7.2 Hz, 1H), 7.55 – 7.51 (m, 2H), 7.36 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.7, 162.0, 158.0, 143.5, 134.6, 134.3, 133.2, 132.1, 130.2, 128.8, 128.5, 127.3, 123.5, 123.2, 120.3, 119.4. HRMS (ESI)**:** calcd for $C_{16}H_{10}NO$ ($[M+H]^+$) 232.0762, found 232.0762.



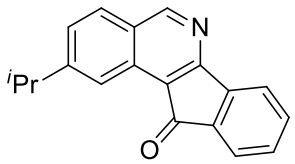
3b

2-Methoxy-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3b** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 89% yield (46.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (s, 1H), 8.03 (s, 1H), 7.89 – 7.75 (m, 2H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.15 (d, *J* = 9.0 Hz, 1H), 4.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 163.6, 162.8, 156.6, 143.5, 134.7, 134.6, 134.5, 130.2, 130.2, 125.0, 123.3, 121.0, 120.4, 118.6, 100.5, 55.7. HRMS (ESI)**:** calcd for $C_{17}H_{12}NO_2$ ($[M+H]^+$) 262.0868, found 262.0869.



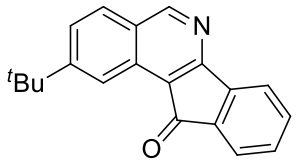
3c

2-Methyl-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3c** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 90% yield (44.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (s, 1H), 8.43 (s, 1H), 7.75 (t, *J* = 7.8 Hz, 2H), 7.63 (d, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 2.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.8, 162.1, 157.4, 144.4, 143.5, 134.5, 134.4, 132.4, 130.0, 129.6, 128.2, 127.4, 123.3, 122.0, 120.2, 118.8, 22.3. HRMS (ESI)**:** calcd for $C_{17}H_{12}NO$ ($[M+H]^+$) 246.0919, found 246.0917.



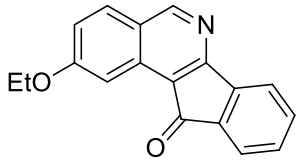
3d

2-Methyl-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3d** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 82% yield (44.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (s, 1H), 8.54 (s, 1H), 7.83 (d, *J* = 8.6 Hz, 1H), 7.74 (d, *J* = 7.3 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.54 – 7.46 (m, 1H), 7.43 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.32 (t, *J* = 8 Hz, 1H), 3.14 – 3.08 (m, 1H), 1.35 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 162.2, 157.5, 155.1, 143.6, 134.6, 134.5, 132.8, 130.2, 128.6, 127.9, 127.4, 123.5, 120.4, 119.6, 119.3, 34.8, 23.5. HRMS (ESI)**:** calcd for $C_{19}H_{16}NO$ ($[M+H]^+$) 274.1232, found 274.1232.



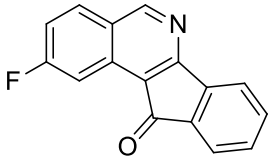
3e

2-*tert*-Butyl-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3e** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 20/1, v/v) as a yellow solid in 83% yield (47.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.71 (s, 1H), 7.85 (d, *J* = 8.8 Hz, 1H), 7.76 (d, *J* = 7.3 Hz, 1H), 7.64 – 7.60 (m, 2H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 1H), 1.44 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.2, 162.2, 157.3, 157.2, 143.6, 134.6, 134.5, 132.8, 130.2, 128.1, 127.5, 126.6, 123.4, 120.4, 119.6, 118.3, 35.7, 30.8. HRMS (ESI)**:** calcd for $C_{20}H_{18}NO$ ($[M+H]^+$) 288.1388, found 288.1390.



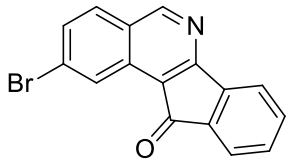
3f

2-Ethoxy-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3f** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 10/1, v/v) as a yellow solid in 79% yield (43.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (s, 1H), 7.92 (d, *J* = 2.2 Hz, 1H), 7.73 (d, *J* = 9.0 Hz, 2H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.06 (dd, *J* = 9.0, 2.4 Hz, 1H), 4.21 (q, *J* = 7.0 Hz, 2H), 1.50 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 163.1, 162.7, 156.5, 143.5, 134.7, 134.7, 134.5, 130.2, 130.2, 124.9, 123.3, 121.3, 120.5, 118.6, 101.1, 64.2, 14.5. HRMS (ESI)**:** calcd for $C_{18}H_{14}NO_2$ ($[M+H]^+$) 276.1025, found 276.1028.



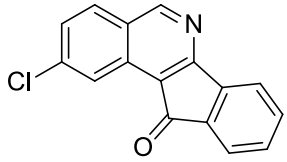
3g

2-Fluoro-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3g** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 87% yield (43.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.37 (d, *J* = 9.7 Hz, 1H), 8.06 – 7.94 (m, 1H), 7.82 (d, *J* = 7.1 Hz, 1H), 7.68 (d, *J* = 6.8 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.41 (dd, *J* = 9.9, 4.7 Hz, 1H), 7.34 (dd, *J* = 8.7, 2.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.3, 165.5 (d, *J* = 256 Hz), 162.8, 157.5, 143.1, 134.7, 134.4, 133.8 (d, *J* = 5 Hz), 131.6 (d, *J* = 11 Hz), 130.5, 126.2, 123.6, 120.6, 118.2 (d, *J* = 26 Hz), 107.3, 107.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.13. HRMS (ESI)**:** calcd for $C_{16}H_9FNO$ ($[M+H]^+$) 250.0668, found 250.0668.



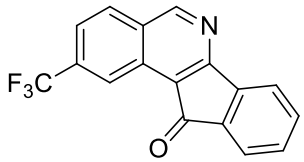
3h

2-Bromo-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3h** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 50/1, v/v) as a yellow solid in 79% yield (49 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.92 (s, 1H), 7.83 – 7.80 (m, 2H), 7.75 – 7.62 (m, 2H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.42 (t, *J* = 7.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.1, 162.7, 157.8, 143.1, 134.8, 134.3, 132.8, 131.2, 130.6, 129.8, 129.2, 127.2, 125.7, 123.7, 120.7, 118.2. HRMS (ESI)**:** calcd for $C_{16}H_9BrNO$ ($[M+H]^+$) 309.9868, found 309.9868, 311.9848.



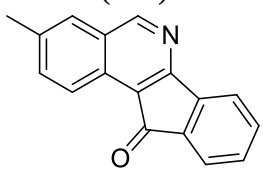
3i

2-Chloro-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3i** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 20/1, v/v) as a yellow solid in 83% yield (43.9 mg). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 9.25 (s, 1H), 8.69 (s, 1H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.79 (d, *J* = 7.3 Hz, 1H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 193.0, 162.8, 157.9, 143.2, 140.0, 134.7, 134.3, 132.5, 130.5, 130.1, 128.5, 127.1, 123.4, 122.1, 120.6, 118.3. HRMS (ESI)**:** calcd for $C_{16}H_9ClNO$ ($[M+H]^+$) 266.0373, found 266.0372.



3j

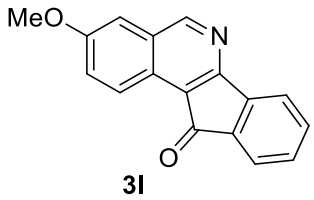
2-(Trifluoromethyl)-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3j** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 73% yield (43 mg). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 9.36 (s, 1H), 9.01 (s, 1H), 8.13 (d, *J* = 8.6 Hz, 1H), 7.78 (m, 2H), 7.67 (d, *J* = 7.3 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, CD_2Cl_2) δ 192.8, 162.9, 158.2, 143.1, 134.9, 134.2, 134.1 (q, *J* = 32 Hz), 131.1, 130.7, 129.7, 129.4, 123.5 (q, *J* = 271 Hz), 123.6, 122.9 (q, *J* = 3 Hz), 120.9 (q, *J* = 5 Hz), 120.7, 119.5. HRMS (ESI)**:** calcd for $C_{17}H_9F_3NO$ ($[M+H]^+$) 300.0636, found 300.0638.



3k

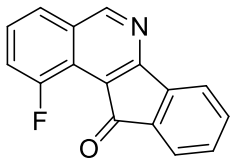
3-Methyl-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3k** was purified

via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 78% yield (38 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (s, 1H), 8.59 (d, *J* = 8.2 Hz, 1H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.69 – 7.63 (m, 2H), 7.61 – 7.51 (m, 2H), 7.37 (t, *J* = 7.4 Hz, 1H), 2.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.9, 161.3, 157.2, 143.7, 137.5, 135.6, 134.6, 134.4, 130.4, 129.9, 129.2, 127.2, 123.4, 123.0, 120.2, 119.5, 21.7. HRMS (ESI)**:** calcd for $C_{17}H_{12}NO$ ($[M+H]^+$) 246.0919, found 246.0916.



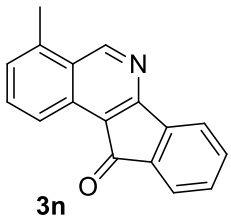
3l

3-Methoxy-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3l** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 10/1, v/v) as a yellow solid in 83% yield (43.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 7.78 (d, *J* = 7.3 Hz, 1H), 7.63 (d, *J* = 7.2 Hz, 1H), 7.52 – 7.41 (m, 3H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.06 (d, *J* = 7.3 Hz, 1H), 4.05 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 162.8, 158.0, 155.7, 142.8, 134.3, 134.1, 130.6, 130.3, 127.9, 125.5, 123.5, 121.1, 120.7, 119.9, 111.5, 55.8. HRMS (ESI)**:** calcd for $C_{17}H_{12}NO_2$ ($[M+H]^+$) 262.0868, found 262.0870.



3m

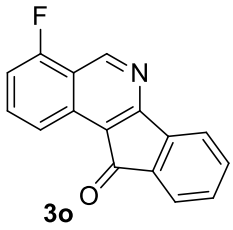
1-Fluoro-11H-indeno[1,2-*c*]isoquinolin-11-one **3m** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 71% yield (35.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.26 (d, *J* = 1.6 Hz, 1H), 7.78 (d, *J* = 7.3 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.56 – 7.48 (m, 2H), 7.47 – 7.41 (m, 1H), 7.38 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 163.3, 158.2, 157.5 (d, *J* = 261 Hz), 142.7, 134.6, 133.8, 130.7, 130.5 (d, *J* = 7 Hz), 127.7 (d, *J* = 7 Hz), 124.9 (d, *J* = 4 Hz), 123.8, 122.3 (d, *J* = 21 Hz), 120.3, 118.9, 117.9 (d, *J* = 21 Hz). HRMS (ESI)**:** calcd for $C_{16}H_9FNO$ ($[M+H]^+$) 250.0668, found 250.0668.



3n

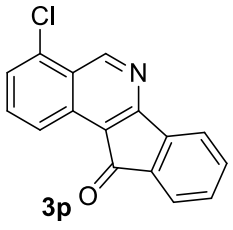
4-Methyl-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3n** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 73% yield (35.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.37 (s, 1H), 8.55 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 7.3 Hz, 1H), 7.60 – 7.55 (m, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 1H), 7.24 (d, *J* = 6.9 Hz, 1H), 2.71 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.8, 161.6, 154.6, 143.4, 136.3, 134.6, 134.5, 133.2, 132.7, 130.2,

128.3, 128.0, 123.5, 121.5, 120.3, 119.5, 18.7. HRMS (ESI)**:** calcd for $C_{17}H_{12}NO$ ($[M+H]^+$) 246.0919, found 246.0919.



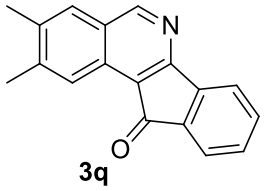
3o

4-Fluoro-11*H*-indeno[1,2-*c*]isoquinolin-11-one was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) afforded **3o** as a yellow solid (40.3 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.49 (s, 1H), 8.46 (d, *J* = 8.3 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.69 – 7.64 (m, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.3 Hz, 1H), 7.16 – 7.06 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.2, 162.8, 159.6 (d, *J* = 257 Hz), 151.9 (d, *J* = 5 Hz), 143.2, 134.8, 134.2, 133.9 (d, *J* = 8 Hz), 133.2, 130.6, 123.6, 120.7, 119.3 (d, *J* = 4 Hz), 118.7 (d, *J* = 2 Hz), 111.2 (d, *J* = 19 Hz), 105.0. HRMS (ESI)**:** calcd for $C_{16}H_9FNO$ ($[M+H]^+$) 250.0668, found 250.0668.



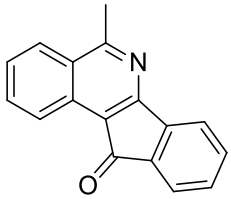
3p

4-Chloro-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3p** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 73% yield (38.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (s, 1H), 8.69 (d, *J* = 8.3 Hz, 1H), 7.81 (d, *J* = 7.3 Hz, 1H), 7.67 – 7.63 (m, 2H), 7.58 – 7.49 (m, 2H), 7.37 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.3, 162.8, 155.3, 143.1, 134.9, 134.5, 133.8, 133.5, 133.3, 130.6, 127.7, 126.1, 123.7, 122.4, 120.8, 119.0. HRMS (ESI)**:** calcd for $C_{16}H_9ClNO$ ($[M+H]^+$) 266.0373, found 266.0371.



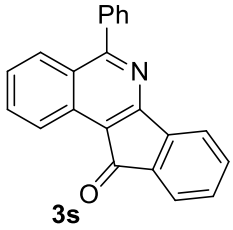
3q

2,3-Dimethyl-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3q** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 87% yield (45.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.33 (s, 1H), 7.68 (d, *J* = 7.3 Hz, 1H), 7.56 (d, *J* = 7.2 Hz, 1H), 7.53 (s, 1H), 7.50 – 7.42 (m, 1H), 7.29 (t, *J* = 7.4 Hz, 1H), 2.39 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 161.3, 156.6, 144.7, 143.8, 137.6, 134.5, 134.5, 131.1, 129.9, 128.2, 127.6, 123.3, 122.6, 120.1, 118.8, 20.8, 20.2. HRMS (ESI)**:** calcd for $C_{18}H_{14}NO$ ($[M+H]^+$) 260.1075, found 260.1079.



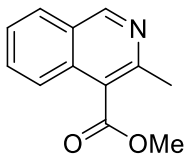
3r

5-Methyl-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3r** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 30/1, v/v) as a yellow solid in 75% yield (36.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.2 Hz, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 7.88 – 7.75 (m, 2H), 7.68 (d, *J* = 7.0 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.55 (d, *J* = 7.4 Hz, 1H), 7.39 (t, *J* = 7.4 Hz, 1H), 3.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 166.1, 161.3, 143.6, 134.7, 134.3, 132.6, 132.3, 130.1, 127.4, 127.1, 126.4, 123.9, 123.3, 120.2, 118.2, 23.4. HRMS (ESI)**:** calcd for $C_{17}H_{12}NO$ ($[M+H]^+$) 246.0919, found 246.0918.



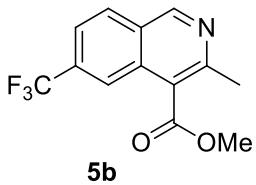
3s

5-Phenyl-11*H*-indeno[1,2-*c*]isoquinolin-11-one **3s** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 50/1, v/v) as a yellow solid in 78% yield (47.8 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 8.6 Hz, 1H), 7.86 (d, *J* = 7.3 Hz, 1H), 7.78 – 7.74 (m, 3H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.59 – 7.57 (m, 3H), 7.53 – 7.42 (m, 2H), 7.35 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.0, 166.7, 161.3, 143.5, 139.0, 134.8, 134.5, 133.5, 132.7, 130.2, 130.2, 129.5, 128.7, 128.4, 127.1, 126.9, 123.6, 123.4, 120.7, 118.4. HRMS (ESI)**:** calcd for $C_{22}H_{14}NO$ ($[M+H]^+$) 308.1075, found 308.1075.



5a 79%

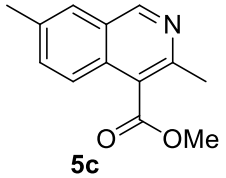
Methyl 3-methylisoquinoline-4-carboxylate **5a** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 60/1, v/v) as a white solid in 79% yield (31.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.73 – 7.69 (m, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 4.05 (s, 3H), 2.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 153.4, 149.7, 133.2, 131.5, 127.9, 126.8, 126.4, 123.7, 122.9, 52.5, 23.0. HRMS (ESI)**:** calcd for $C_{12}H_{12}NO_2$ ($[M+H]^+$) 202.0868, found 202.0867.



5b

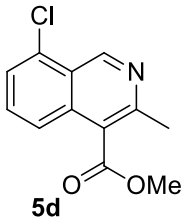
Methyl 3-methyl-6-(trifluoromethyl)isoquinoline-4-carboxylate **5b** was purified via silica gel column chromatography (petroleum ether/ethyl acetate =

60/1, v/v) as a white solid 70% yield (37.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.29 (s, 1H), 8.19 (s, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.74 (d, *J* = 8.5 Hz, 1H), 4.08 (s, 3H), 2.77 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 153.5, 151.7, 132.9 (q, *J* = 33 Hz), 132.5, 129.1, 127.0, 123.6 (q, *J* = 271 Hz), 123.3, 122.6 (q, *J* = 3 Hz), 121.7 (q, *J* = 5 Hz), 52.7, 23.3. HRMS (ESI)**:** calcd for $C_{13}H_{11}F_3NO_2$ ($[M+H]^+$) 270.0740, found 270.0742.



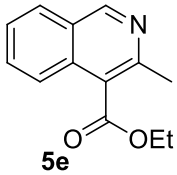
5c

Methyl 3,7-dimethylisoquinoline-4-carboxylate **5c** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 60/1, v/v) as a white solid in 71% yield (30.5 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (s, 1H), 7.77 (d, *J* = 8.6 Hz, 1H), 7.72 (s, 1H), 7.55 (d, *J* = 8.6 Hz, 1H), 4.05 (s, 3H), 2.72 (s, 3H), 2.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 152.8, 148.8, 136.8, 133.7, 131.5, 126.6, 126.6, 123.5, 122.7, 52.4, 22.9, 21.5. HRMS (ESI)**:** calcd for $C_{13}H_{14}NO_2$ ($[M+H]^+$) 216.1025 found 216.1027.



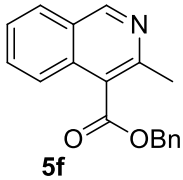
5d

Methyl 8-chloro-3-methylisoquinoline-4-carboxylate **5d** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 60/1, v/v) as a white solid in 61% yield (28.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.64 (s, 1H), 7.92 – 7.65 (m, 1H), 7.67 – 7.44 (m, 2H), 4.06 (s, 3H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 150.6, 150.3, 149.7, 134.7, 132.9, 131.3, 127.2, 123.5, 122.8, 52.6, 23.0. HRMS (ESI)**:** calcd for $C_{12}H_{11}ClNO_2$ ($[M+H]^+$) 236.0478, found 236.0478.



5e

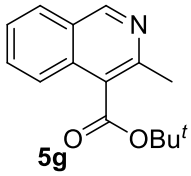
Ethyl 3-methylisoquinoline-4-carboxylate **5e** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 60/1, v/v) as a white solid in 73% yield (31.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 8.5 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 4.54 (q, *J* = 7.1 Hz, 2H), 2.74 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 153.3, 149.5, 133.2, 131.4, 127.9, 126.8, 126.4, 123.6, 123.2, 61.6, 22.9, 14.3. HRMS (ESI)**:** calcd for $C_{13}H_{14}NO_2$ ($[M+H]^+$) 216.1025, found 216.1025.



5f

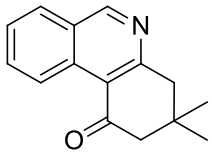
Benzyl 3-methylisoquinoline-4-carboxylate **5f** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 50/1, v/v) as a white solid

in 51% yield (29.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.53 – 7.46 (m, 2H), 7.45 – 7.34 (m, 3H), 5.52 (s, 2H), 2.70 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 153.5, 149.6, 135.2, 133.2, 131.5, 128.7, 128.7, 128.6, 127.9, 126.8, 126.4, 123.6, 122.8, 67.5, 23.0. HRMS (ESI)**:** calcd for $C_{18}H_{16}NO_2$ ($[M+H]^+$) 278.1181, found 278.1183.



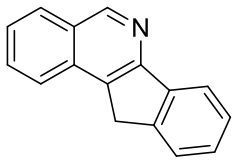
5g

tert-Butyl 3-methylisoquinoline-4-carboxylate **5g** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 50/1, v/v) as a white solid in 63% yield (30.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 8.5 Hz, 1H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 2.74 (s, 3H), 1.69 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 152.7, 148.5, 133.0, 131.1, 127.7, 126.6, 126.4, 124.5, 123.4, 82.8, 28.2, 22.6. HRMS (ESI)**:** calcd for $C_{15}H_{18}NO_2$ ($[M+H]^+$) 244.1338, found 244.1339.



5h

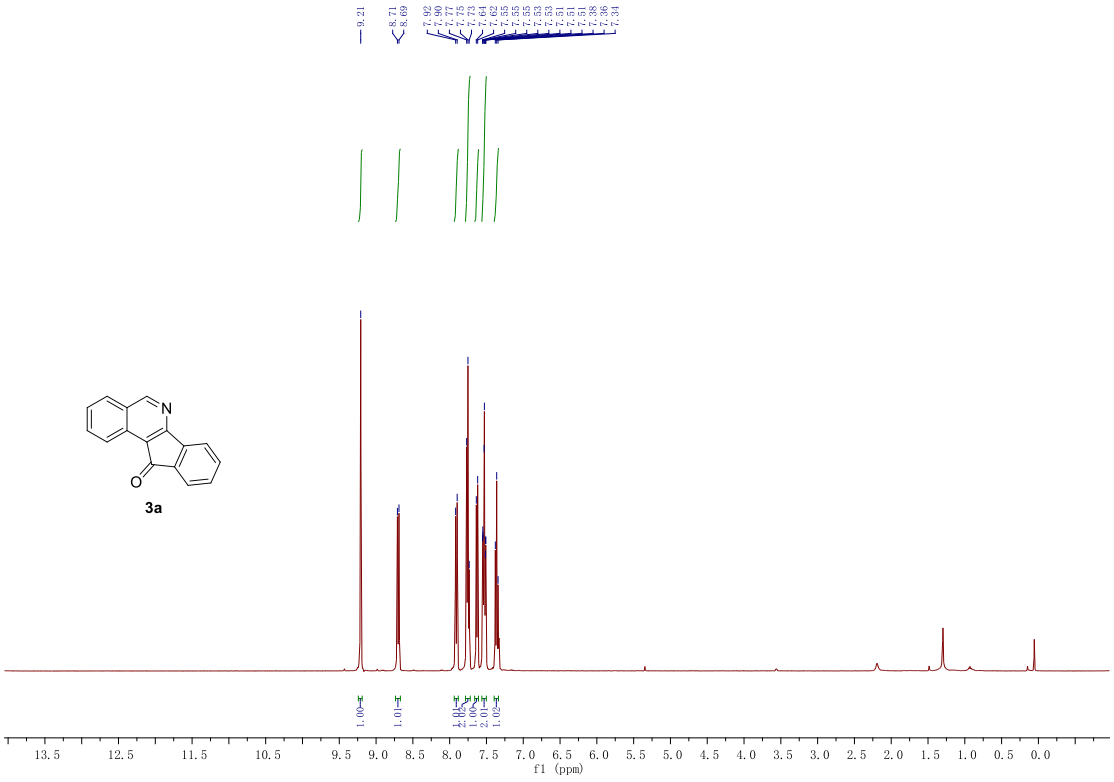
3,3-Dimethyl-3,4-dihydrophenanthridin-1(2H)-one **5h** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 50/1, v/v) as a white solid in 63% yield (30.7 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.39 (d, *J* = 8.7 Hz, 1H), 9.28 (s, 1H), 7.95 (d, *J* = 8.1 Hz, 1H), 7.82 (t, *J* = 7.8 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 3.22 (s, 2H), 2.65 (s, 2H), 1.16 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.1, 159.6, 157.3, 133.5, 133.2, 128.2, 127.7, 127.1, 125.7, 119.7, 54.1, 47.7, 32.8, 28.1. HRMS (ESI)**:** calcd for $C_{15}H_{16}NO$ ($[M+H]^+$) 226.1232, found 226.1235.

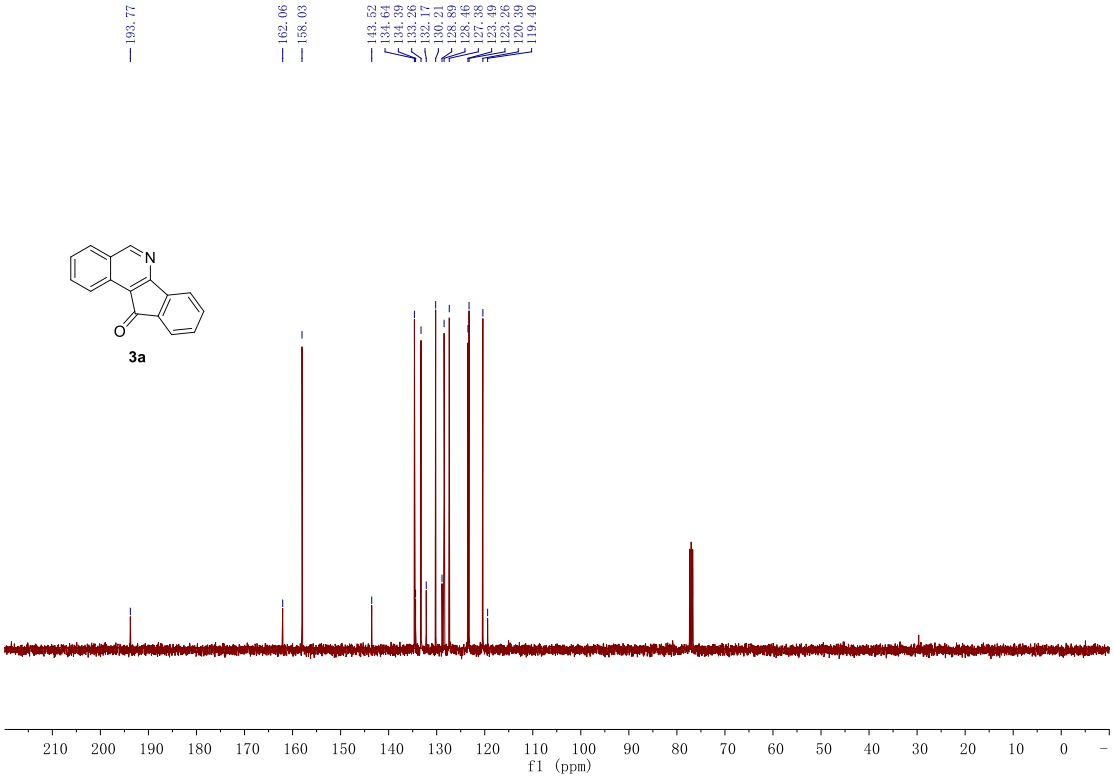


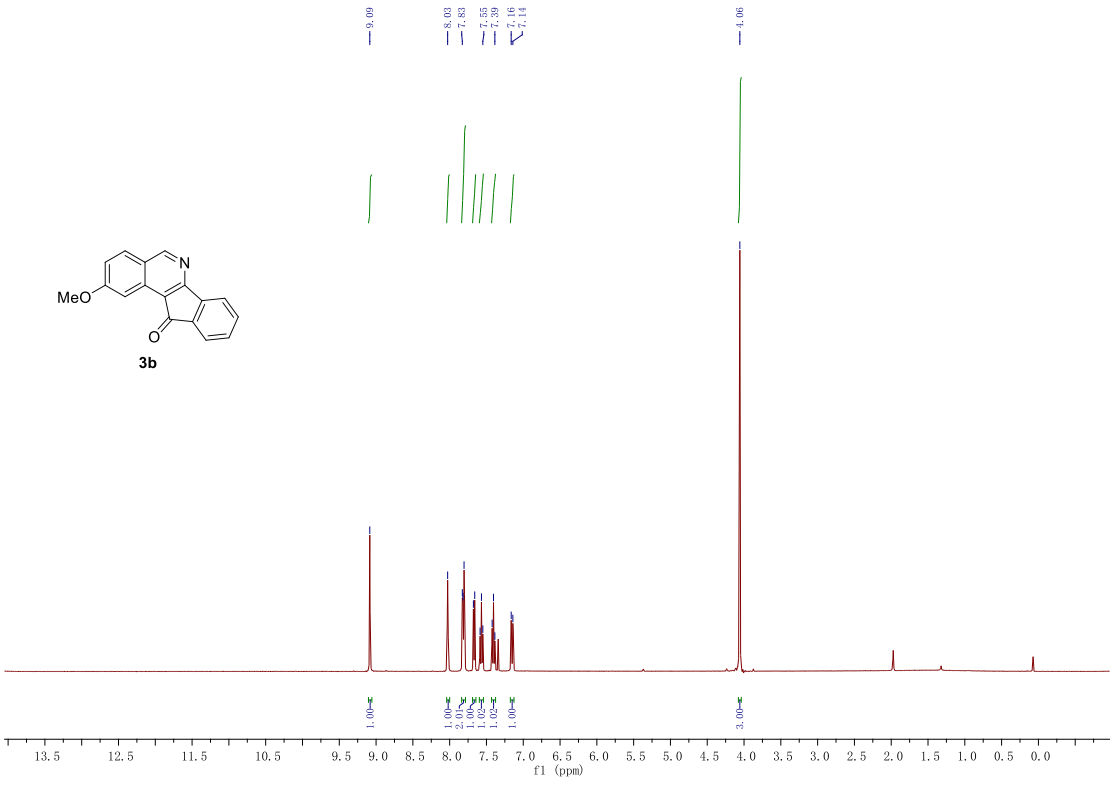
6

*11*H-Indeno[1,2-*c*]isoquinoline **6** was purified via silica gel column chromatography (petroleum ether/ethyl acetate = 50/1, v/v) as a white solid in 92% yield (40.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.11 (d, *J* = 7.5 Hz, 1H), 8.00 – 7.89 (m, 1H), 7.84 (dd, *J* = 8.2, 4.5 Hz, 1H), 7.72 – 7.61 (m, 1H), 7.57 – 7.55 (m, 1H), 7.52 – 7.42 (m, 2H), 7.36 (td, *J* = 7.4, 1.2 Hz, 1H), 4.02 – 3.93 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.9, 152.5, 142.8, 142.0, 133.5, 131.1, 130.7, 128.8, 127.5, 127.5, 127.2, 126.2, 124.9, 123.1, 120.2, 33.1. HRMS (ESI)**:** calcd for $C_{16}H_{12}N$ ($[M+H]^+$) 218.0970, found 218.0973.

Copies of ^{1}H NMR and ^{13}C NMR Spectra



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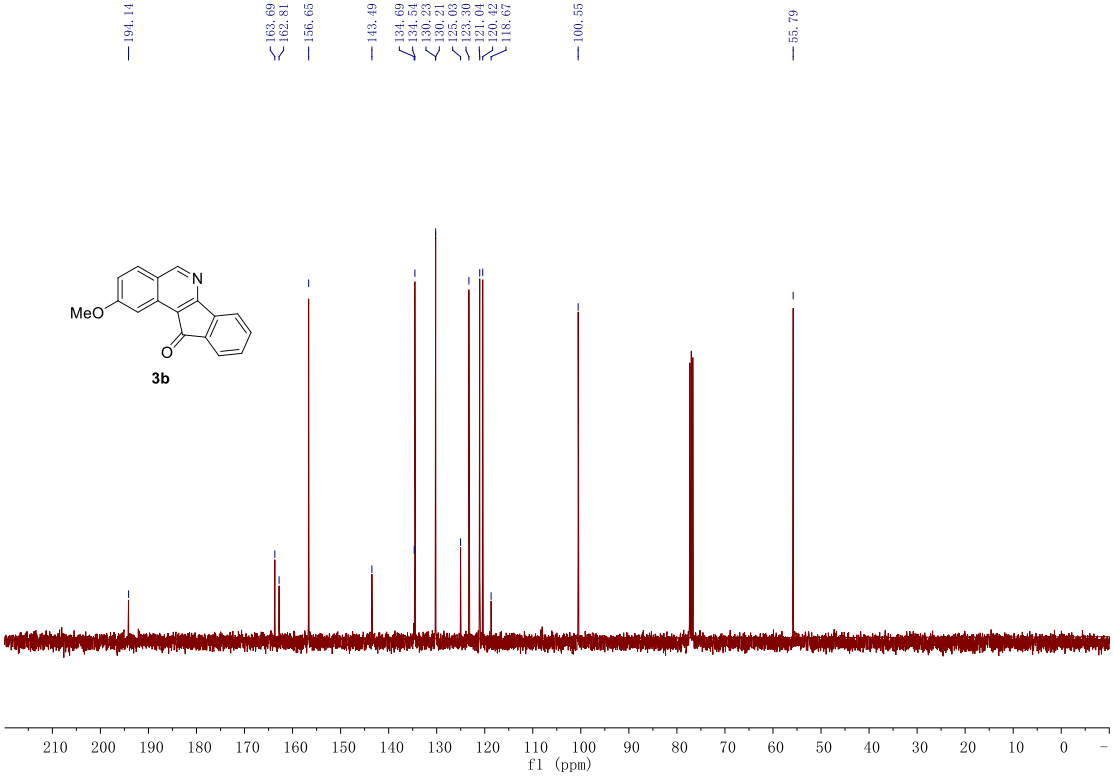
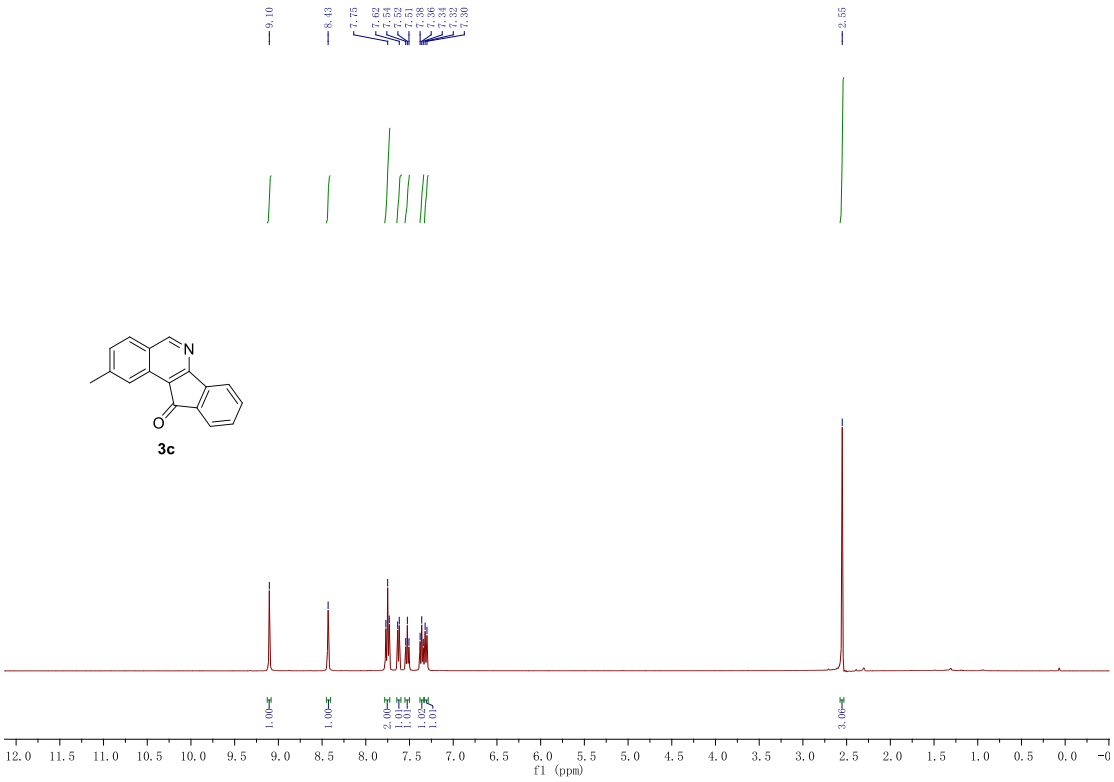
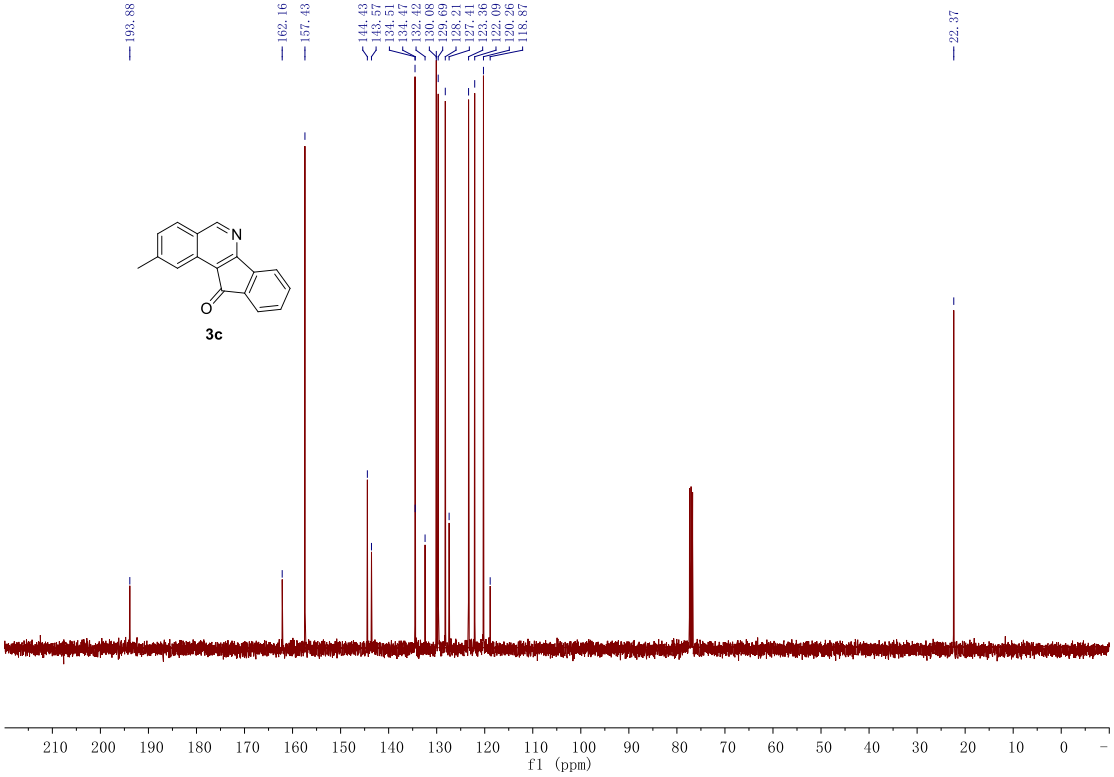
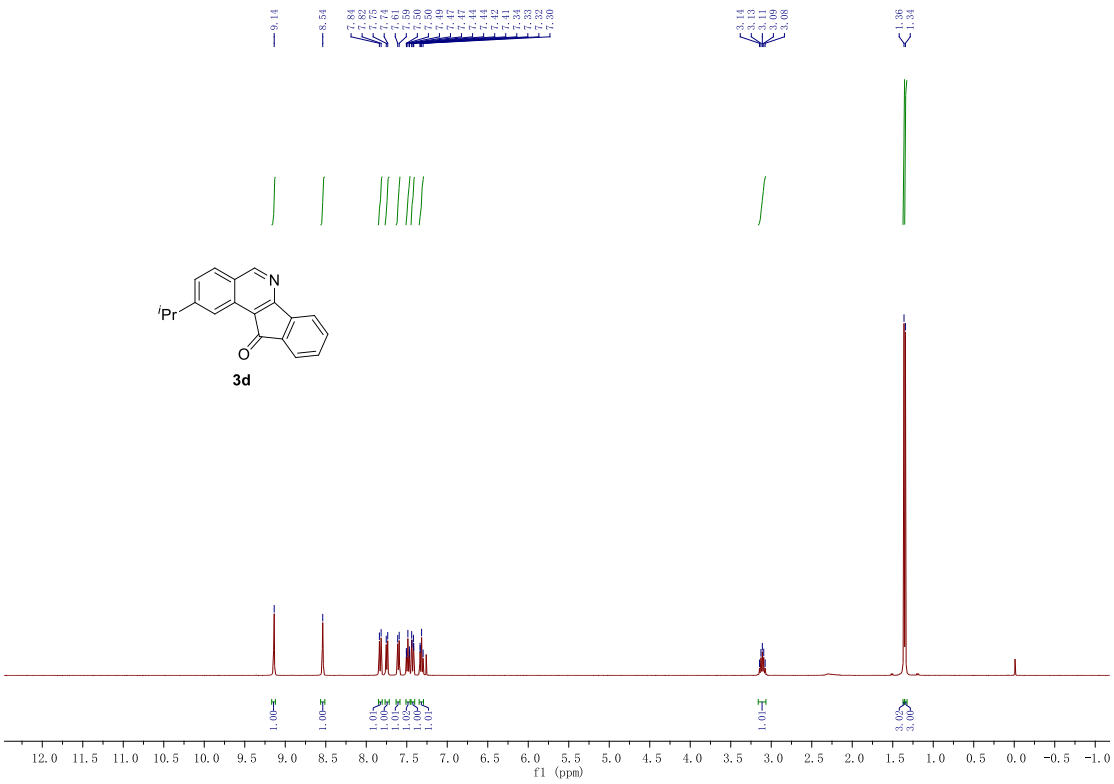
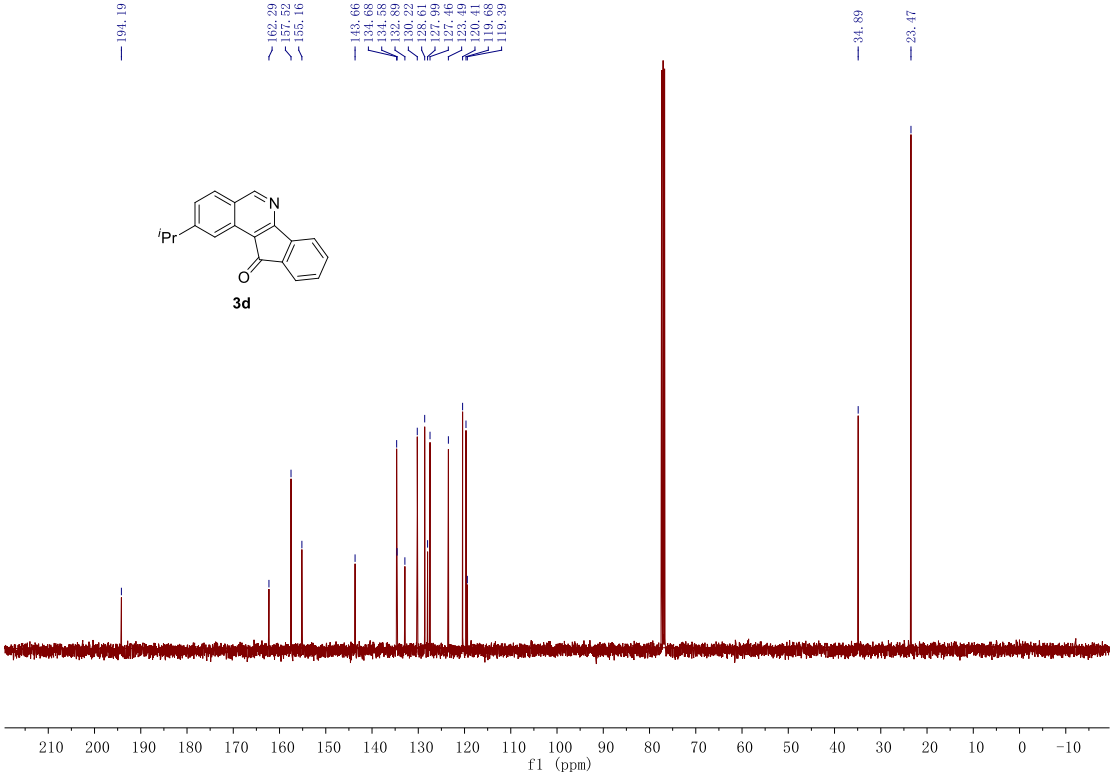
8.03
7.83
7.55
7.39
7.16
7.14
4.06
MeO
N
O
3b
1.00
2.01
1.00
1.02
1.02
1.00
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

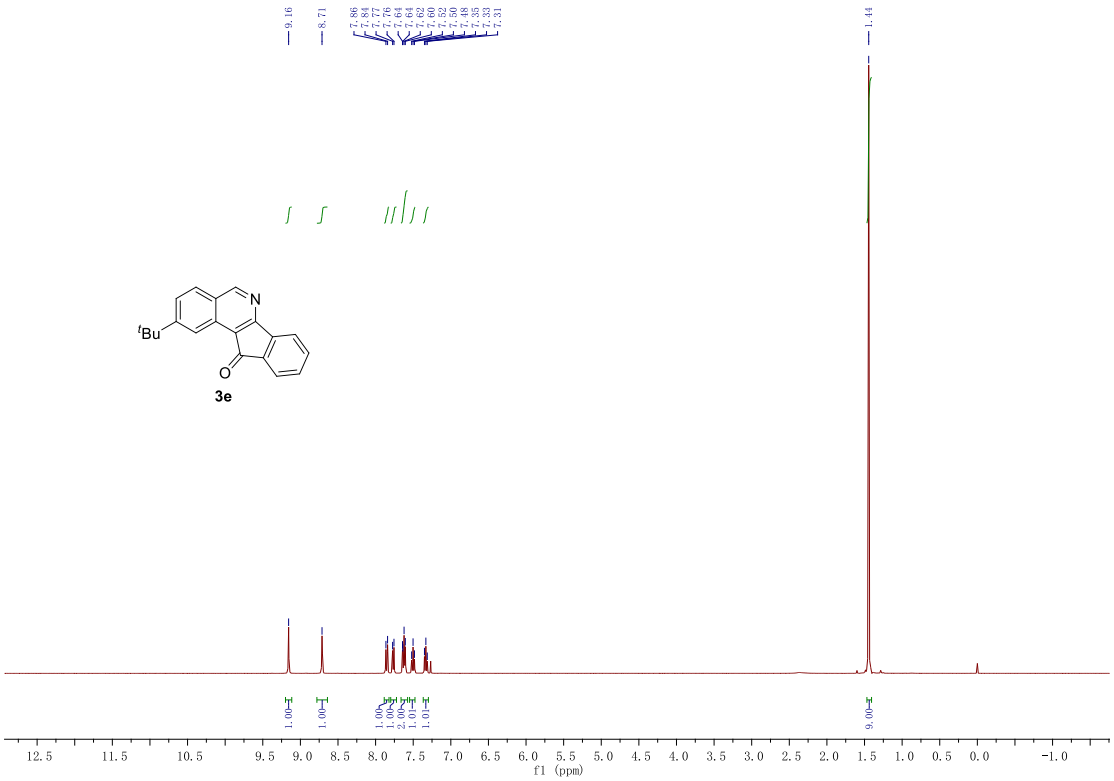

194.14
163.69
162.81
156.65
143.49
134.69
134.54
130.23
130.21
125.03
123.30
121.04
120.42
118.67
100.55
55.79
MeO
N
O
3b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

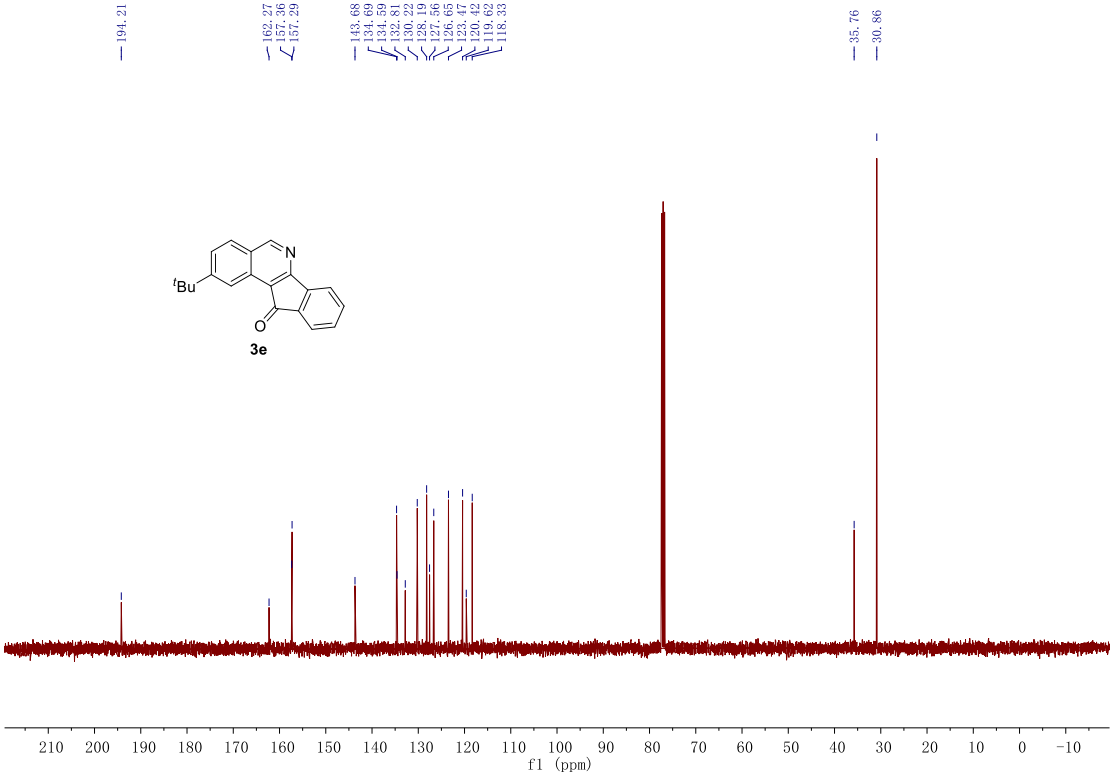

9.10
8.43
7.75
7.62
7.54
7.52
7.51
7.38
7.36
7.34
7.32
7.30
2.55
N
O
3c
1.00
1.00
2.00
1.01
1.01
1.02
1.07
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


193.88
162.16
157.43
144.43
143.57
134.51
134.47
132.42
130.08
129.69
128.21
127.41
123.36
122.09
120.26
118.87
22.37
N
O
3c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.14
8.54
7.84
7.82
7.75
7.74
7.61
7.59
7.50
7.49
7.47
7.47
7.44
7.42
7.41
7.34
7.33
7.32
7.30
3.14
3.13
3.11
3.09
3.08
1.36
1.34
iPr
N
O
3d
f1 (ppm)


194.19
162.29
157.52
155.16
143.66
134.68
134.38
132.89
130.22
128.61
127.99
127.46
123.49
120.41
119.68
119.39
34.89
23.47
iPr
N
O
3d
f1 (ppm)


9.16
8.71
7.86
7.84
7.77
7.76
7.64
7.62
7.60
7.52
7.50
7.48
7.35
7.33
7.31
1.44
tBu
N
O
3e
1.00
1.00
1.00
1.08
2.00
1.01
1.01
9.00
12.5
11.5
10.5
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
-1.0
f1 (ppm)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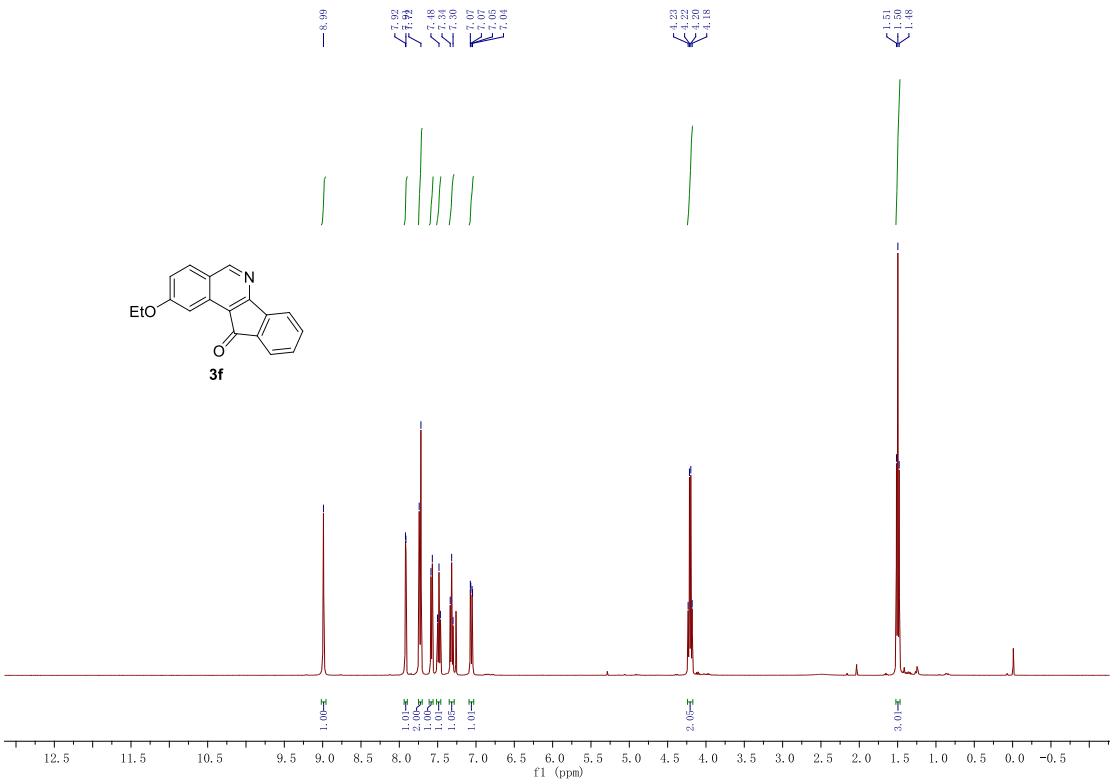
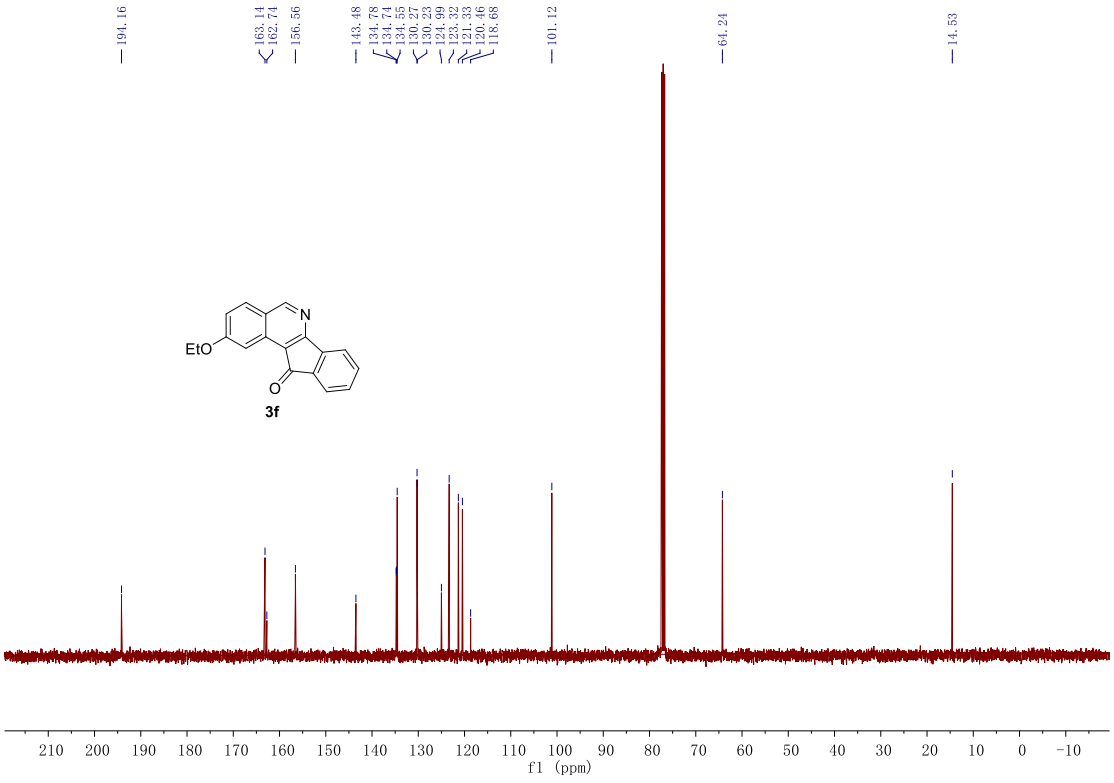
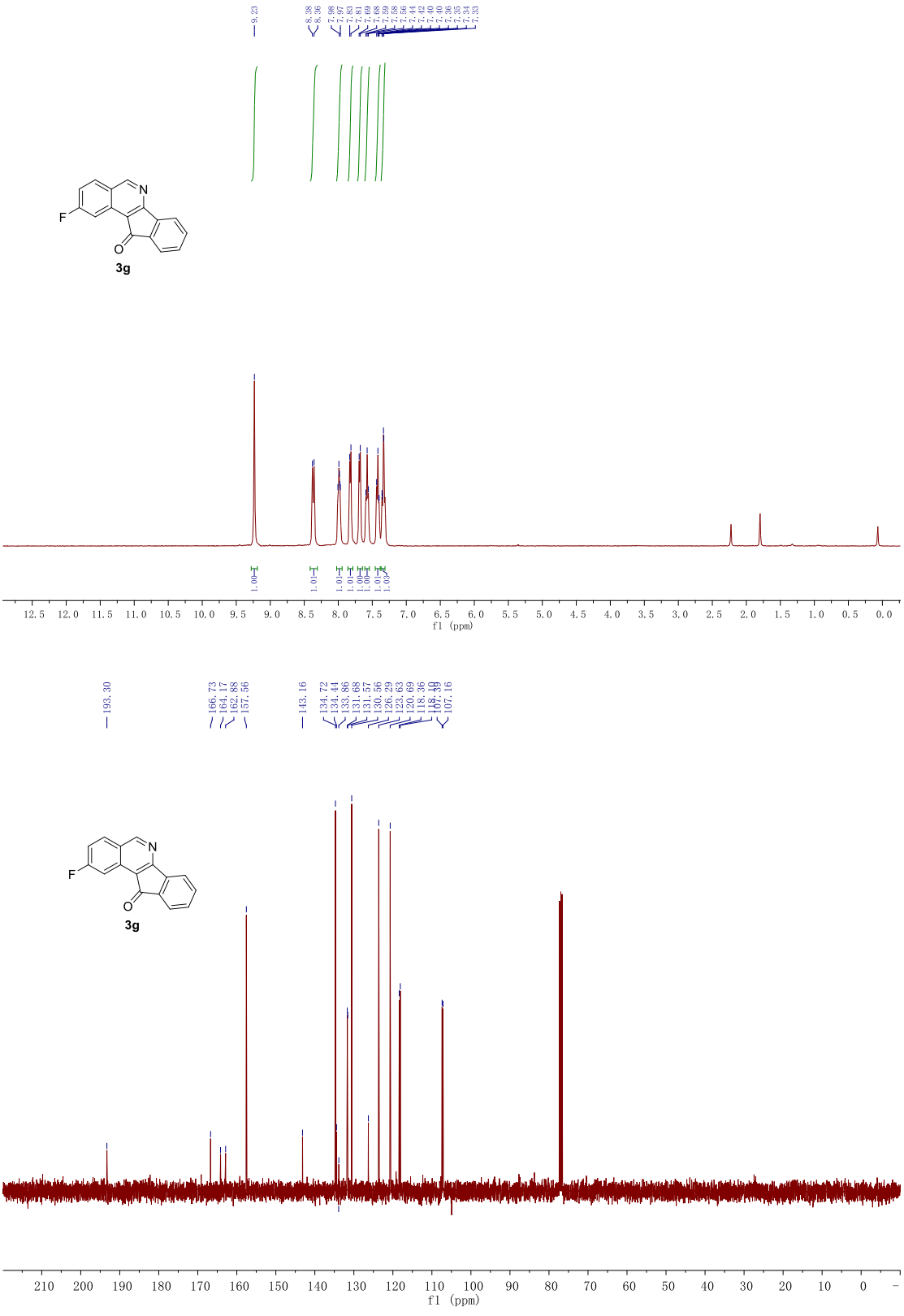
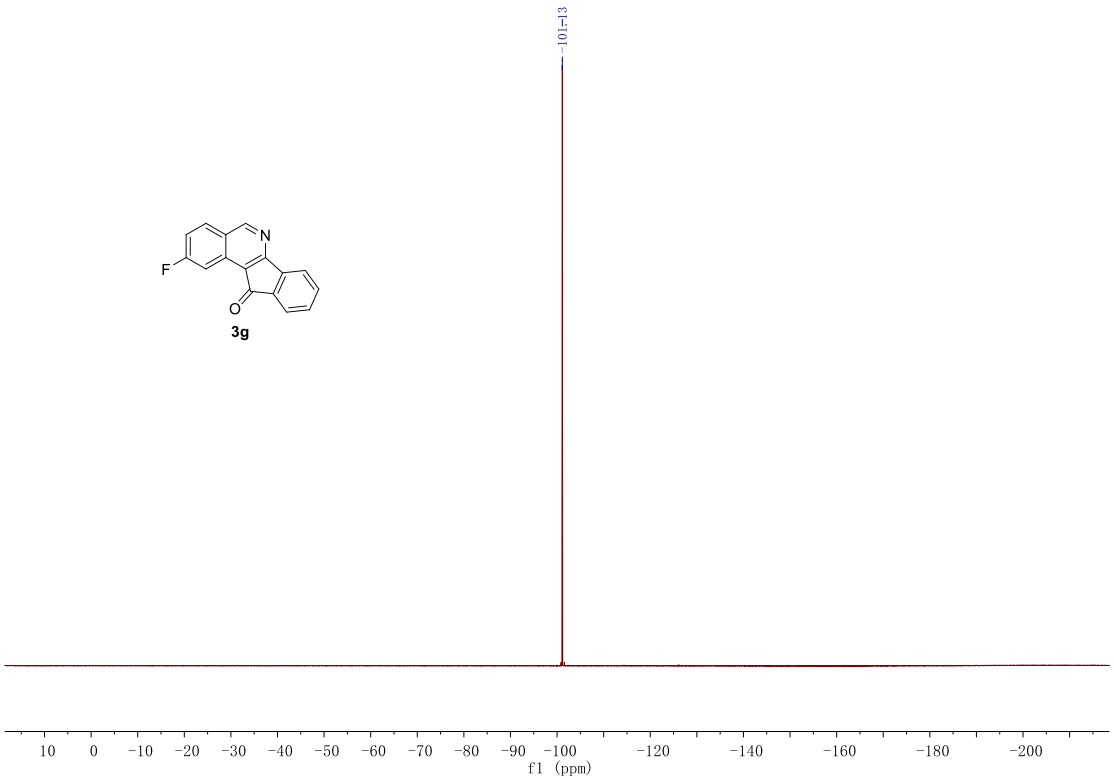
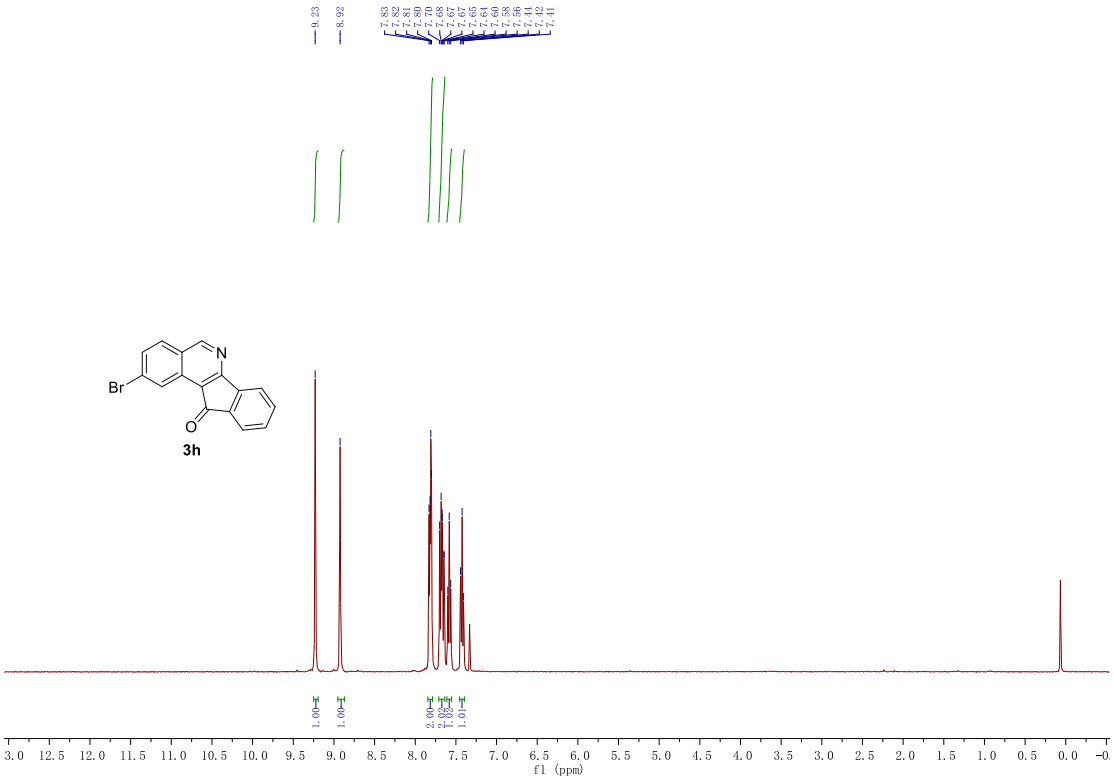
162.27
157.36
157.29
143.68
134.69
134.59
132.81
130.22
128.19
127.56
126.65
123.47
120.42
119.62
118.33
35.76
30.86
tBu
N
O
3e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

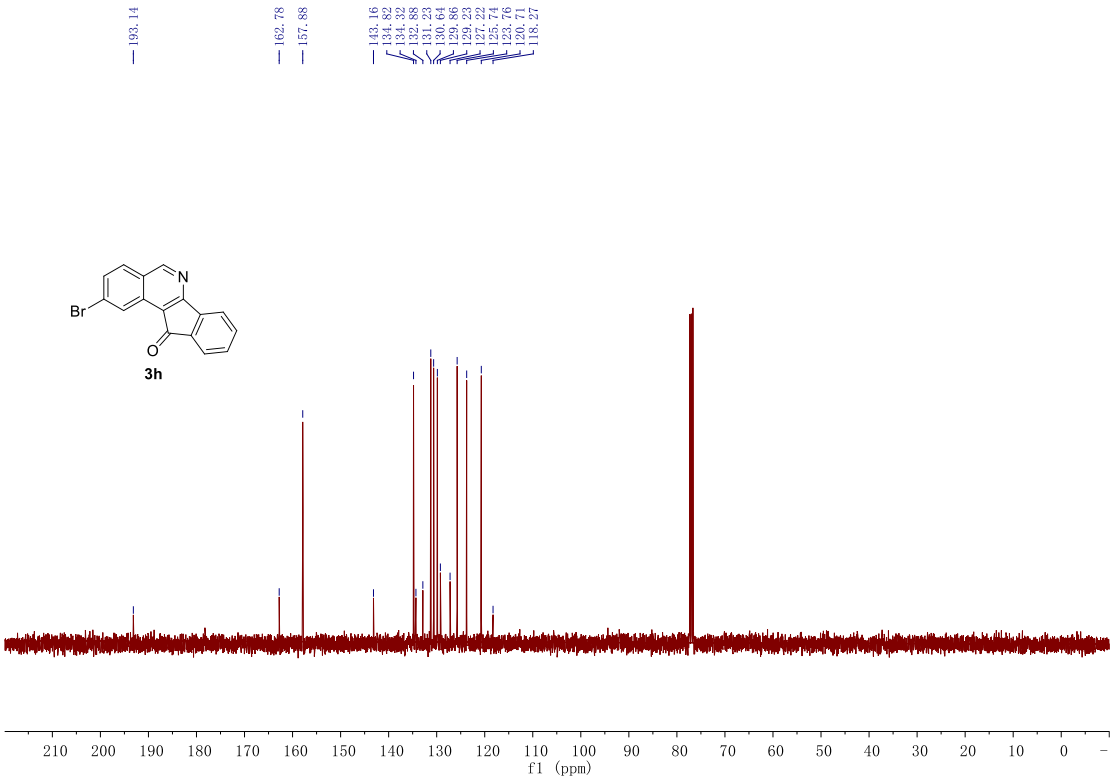

8.99
7.92
7.91
7.48
7.34
7.30
7.07
7.05
7.04
4.23
4.22
4.20
4.18
1.51
1.50
1.48
EtO
N
O
3f
1.00
1.01
2.06
1.00
1.01
1.05
1.01
2.05
3.01
f1 (ppm)

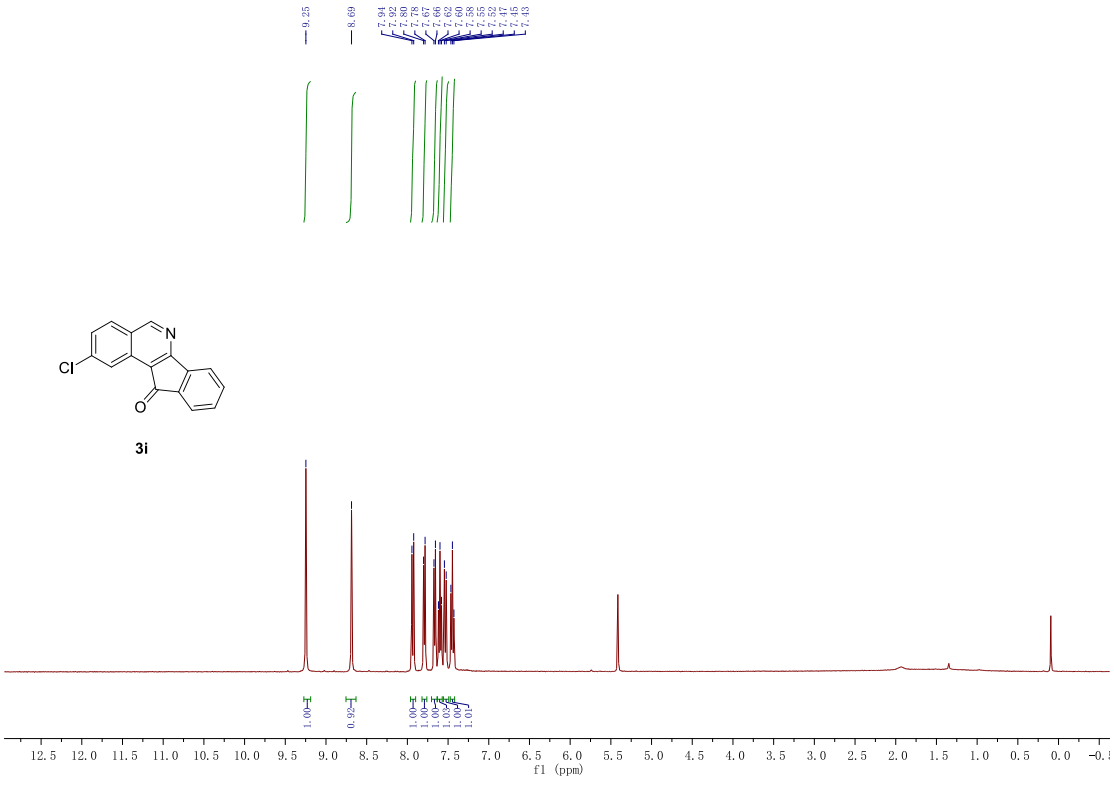

194.16
163.14
162.74
156.56
143.48
134.78
134.74
134.55
130.27
130.23
124.99
123.32
121.33
120.46
118.68
101.12
64.24
14.53
EtO
N
O
3f
f1 (ppm)

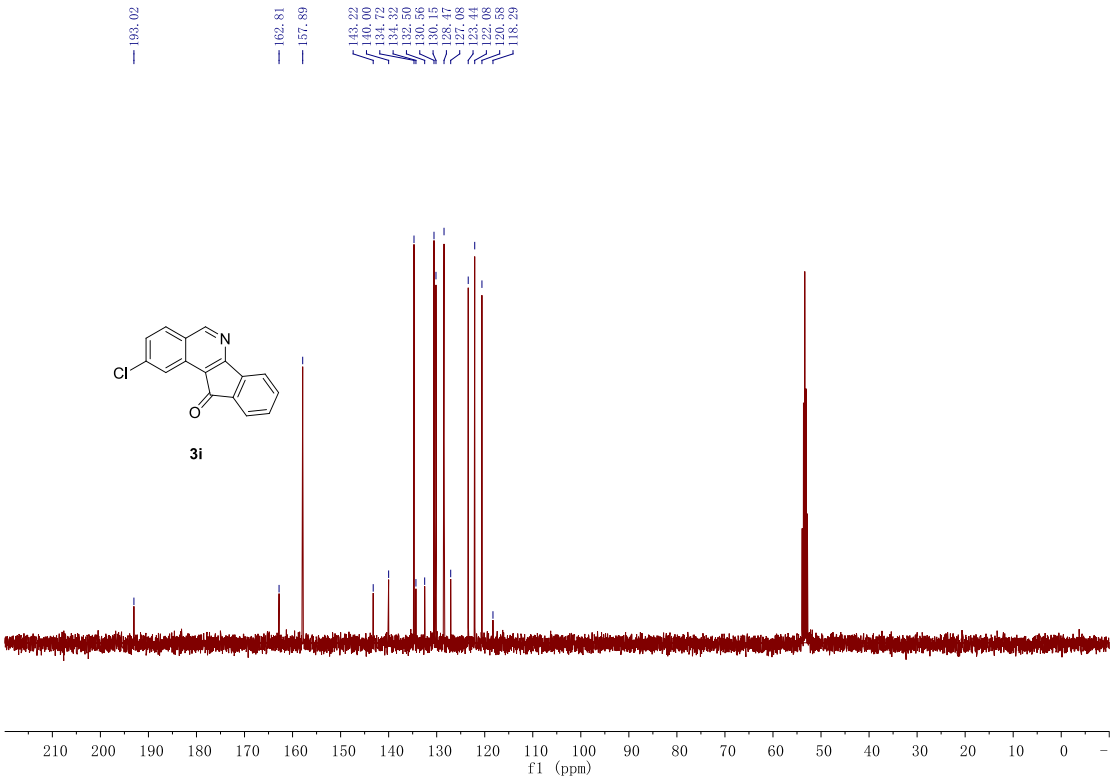

9.23
8.38
8.36
7.98
7.97
7.83
7.81
7.69
7.68
7.59
7.58
7.56
7.44
7.42
7.40
7.40
7.36
7.35
7.34
7.33
F
N
O
3g
1.00
1.01
1.01
1.01
1.00
1.00
1.01
1.05
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
193.30
166.73
164.17
162.88
157.56
143.16
134.72
134.44
133.86
131.68
131.57
130.56
126.29
123.63
120.69
118.36
114.39
114.10
107.16
F
N
O
3g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

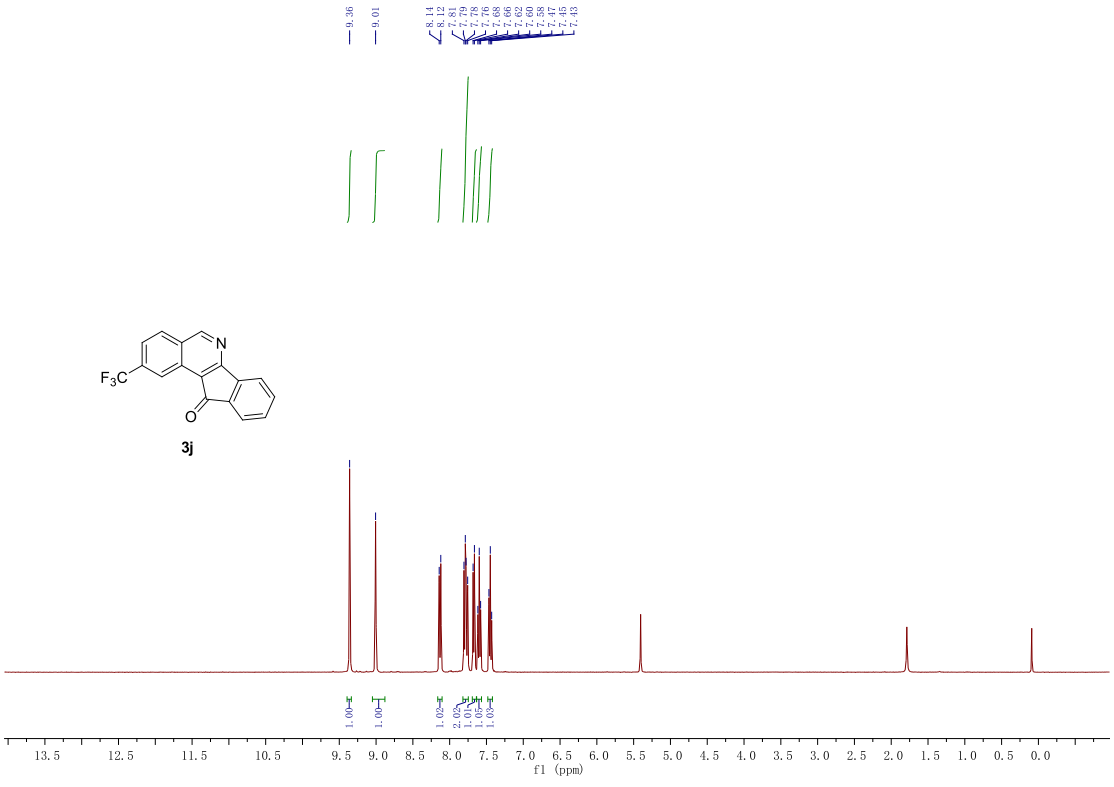

-101.13
F
N
O
3g
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

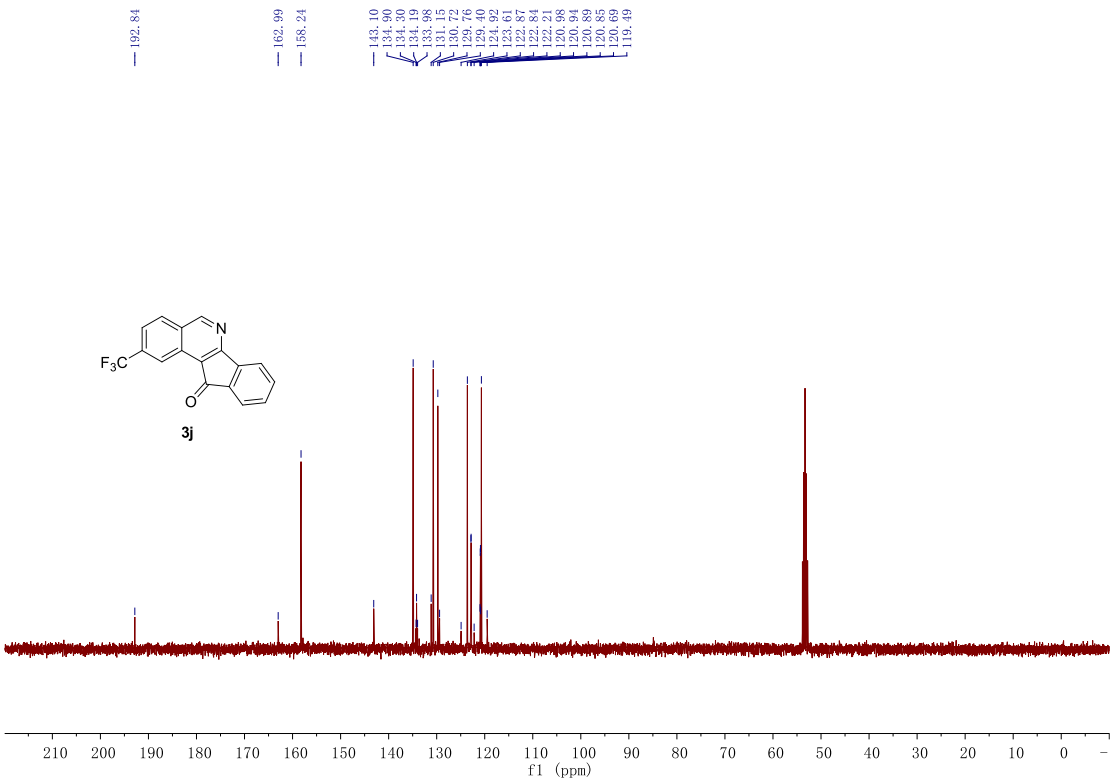

9.23
8.92
7.83
7.82
7.81
7.80
7.70
7.68
7.67
7.67
7.65
7.64
7.60
7.58
7.56
7.44
7.42
7.41
Br
N
O
3h
1.00
1.00
2.00
2.02
2.01
1.01
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


193.14
162.78
157.88
143.16
134.82
134.32
132.88
131.23
130.64
129.86
129.23
127.22
125.74
123.76
120.71
118.27
Br
N
O
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.25
8.69
7.94
7.92
7.80
7.78
7.67
7.66
7.62
7.60
7.58
7.55
7.52
7.47
7.45
7.43
Cl
N
O
3i
1.00
0.92
1.00
1.00
1.02
1.04
1.01
12.5 12.0 11.5 11.0 10.5 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)


193.02
162.81
157.89
143.22
140.00
134.72
134.32
132.50
130.56
130.15
128.47
127.08
123.44
122.08
120.58
118.29
Cl
N
O
3i
f1 (ppm)


9.36
9.01
8.14
8.12
7.81
7.79
7.78
7.76
7.68
7.66
7.62
7.60
7.58
7.47
7.45
7.43
F3C
N
O
3j
1.00
1.00
1.02
2.02
1.01
1.05
1.05
f1 (ppm)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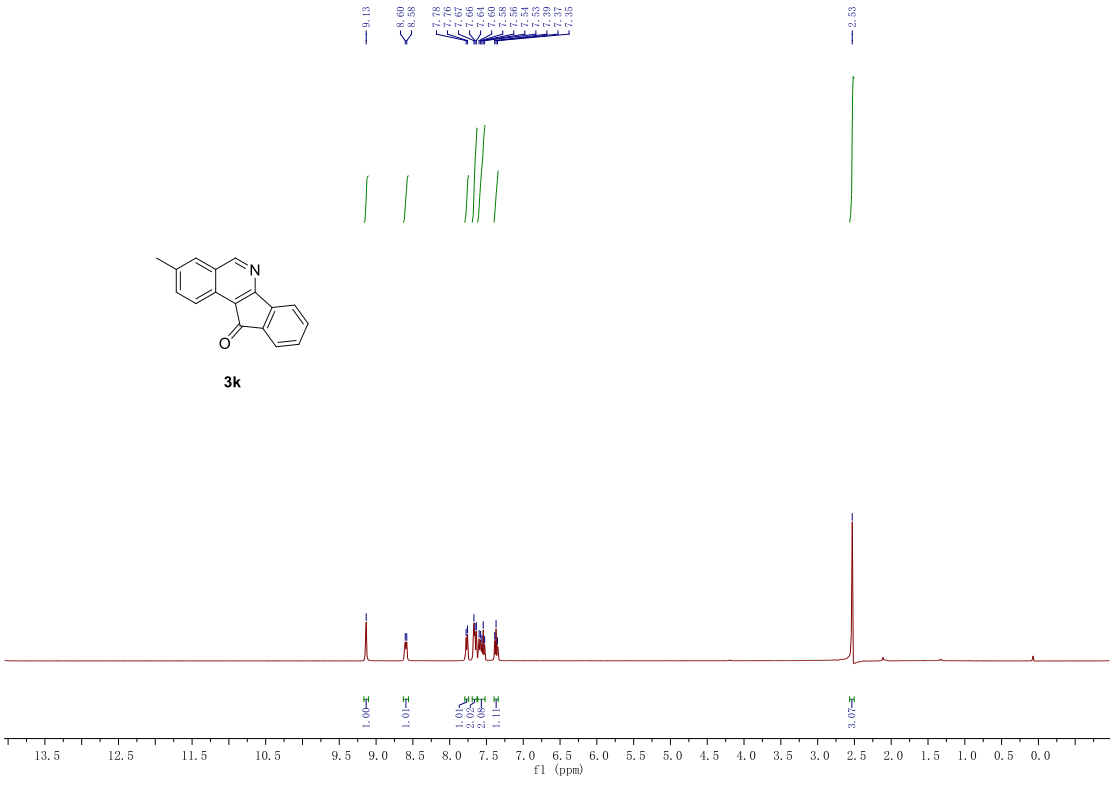
143.10
134.90
134.30
134.19
133.98
131.15
130.72
129.76
129.40
124.92
123.61
122.87
122.84
122.21
120.98
120.94
120.89
120.85
120.69
119.49
F3C
N
O
3j
f1 (ppm)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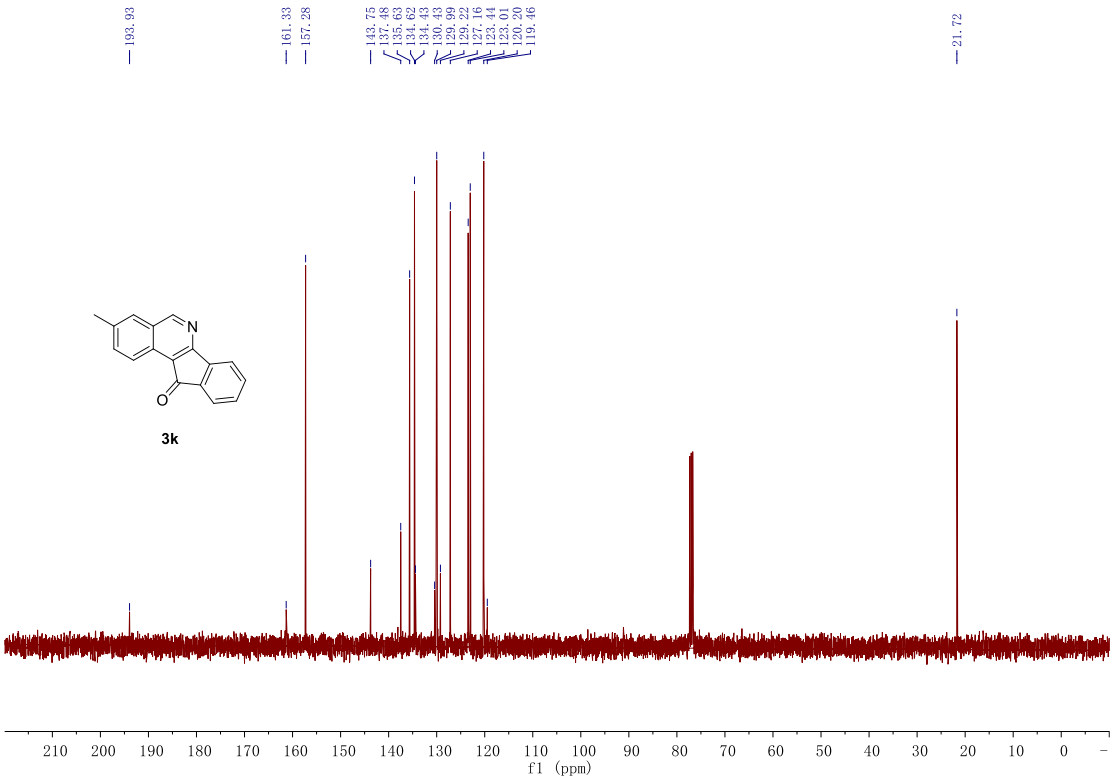
8.60
8.58
7.78
7.76
7.67
7.66
7.64
7.60
7.58
7.56
7.54
7.53
7.39
7.37
7.35
2.53
N
O
3k
1.00
1.01
1.01
2.02
2.09
1.11
3.07
f1 (ppm)


193.93
161.33
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143.75
137.48
135.63
134.62
134.43
130.43
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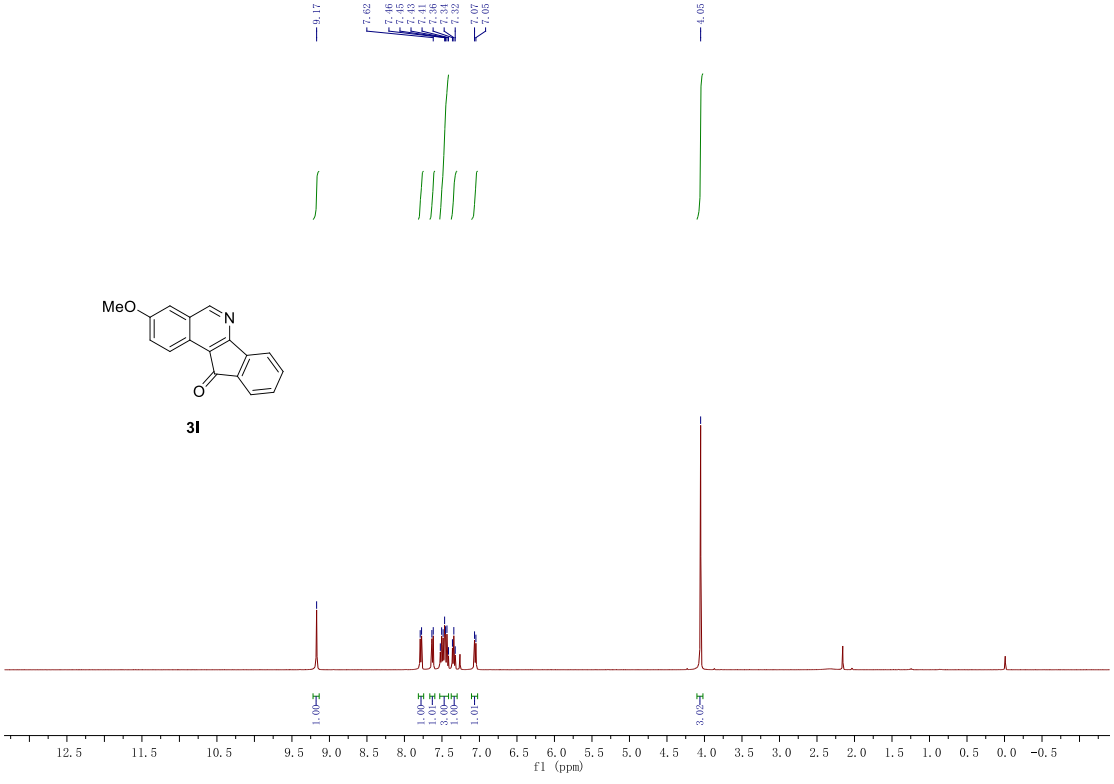
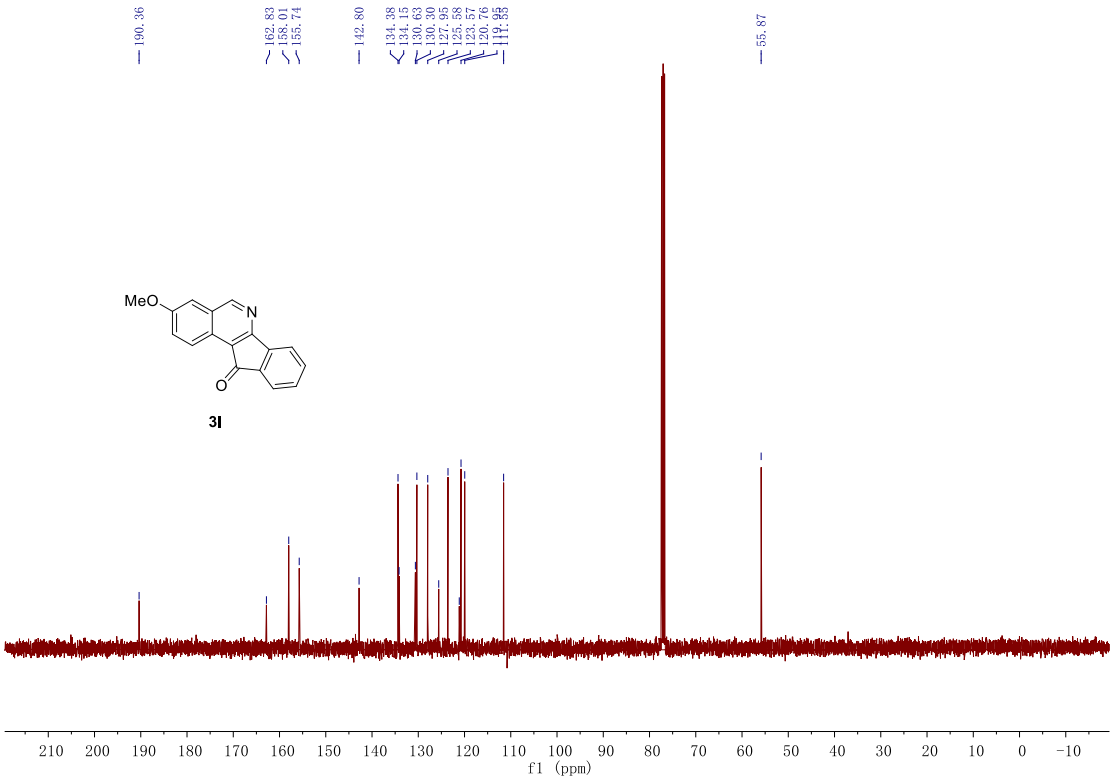
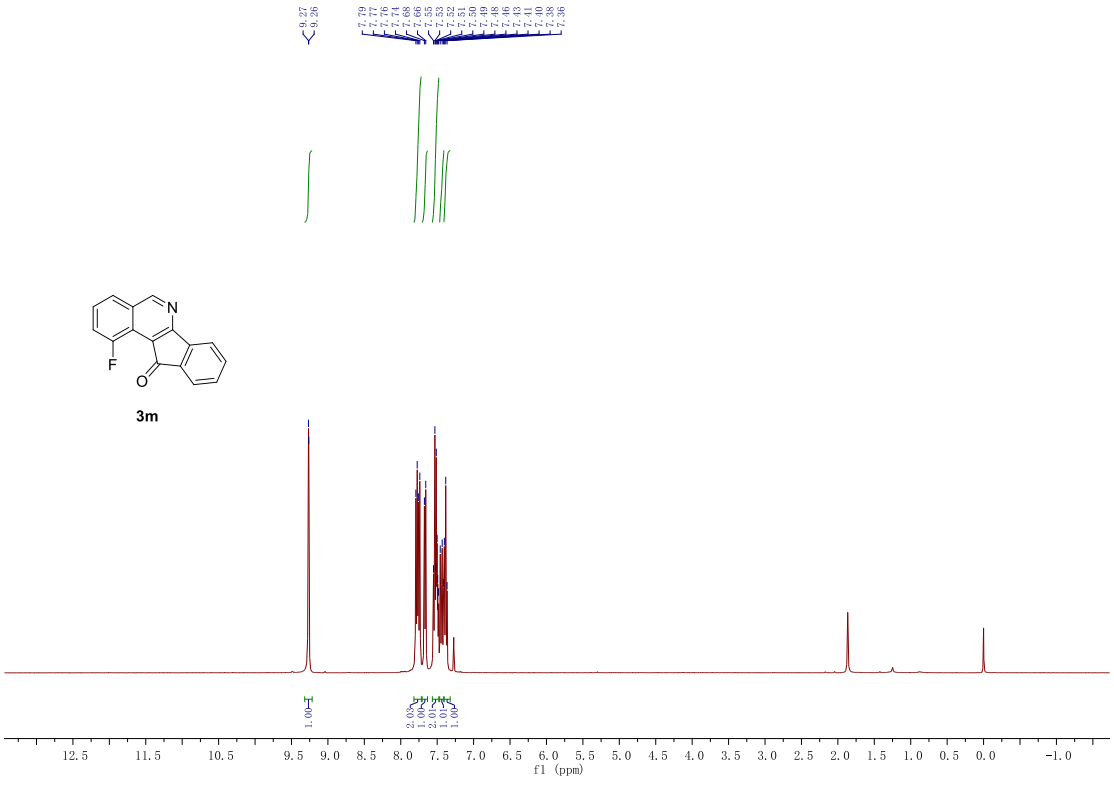
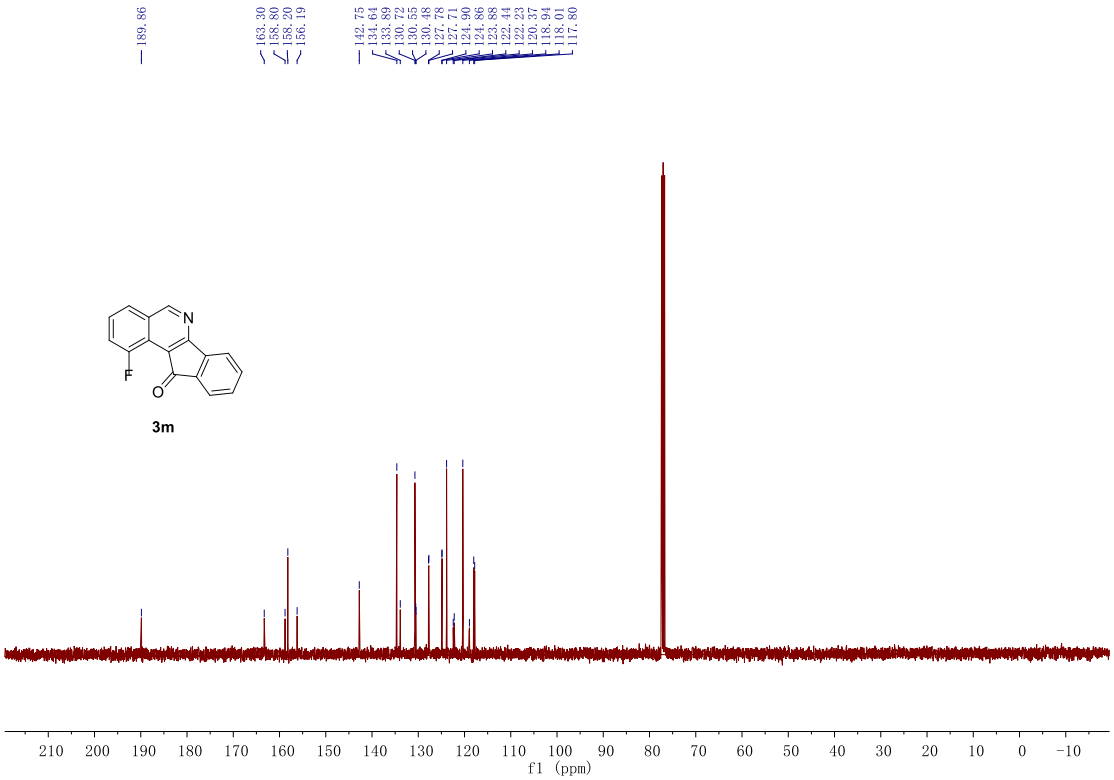
127.16
123.44
123.01
120.20
119.46
21.72
N
O
3k
f1 (ppm)


9.17
7.62
7.46
7.45
7.43
7.41
7.36
7.34
7.32
7.07
7.05
4.05
MeO
N
O
3l
1.00
1.00
1.01
3.00
1.00
1.01
3.02
f1 (ppm)


190.36
162.83
158.01
155.74
142.80
134.38
134.15
130.63
130.30
127.95
125.58
123.57
120.76
111.93
55.87
MeO
N
O
3l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


9.27
9.26
7.79
7.77
7.76
7.74
7.68
7.66
7.55
7.53
7.52
7.51
7.50
7.49
7.48
7.46
7.43
7.41
7.40
7.38
7.36
N
F
O
3m
1.00
2.08
1.96
2.01
1.01
1.00
12.5 11.5 10.5 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 -1.0
f1 (ppm)


189.86
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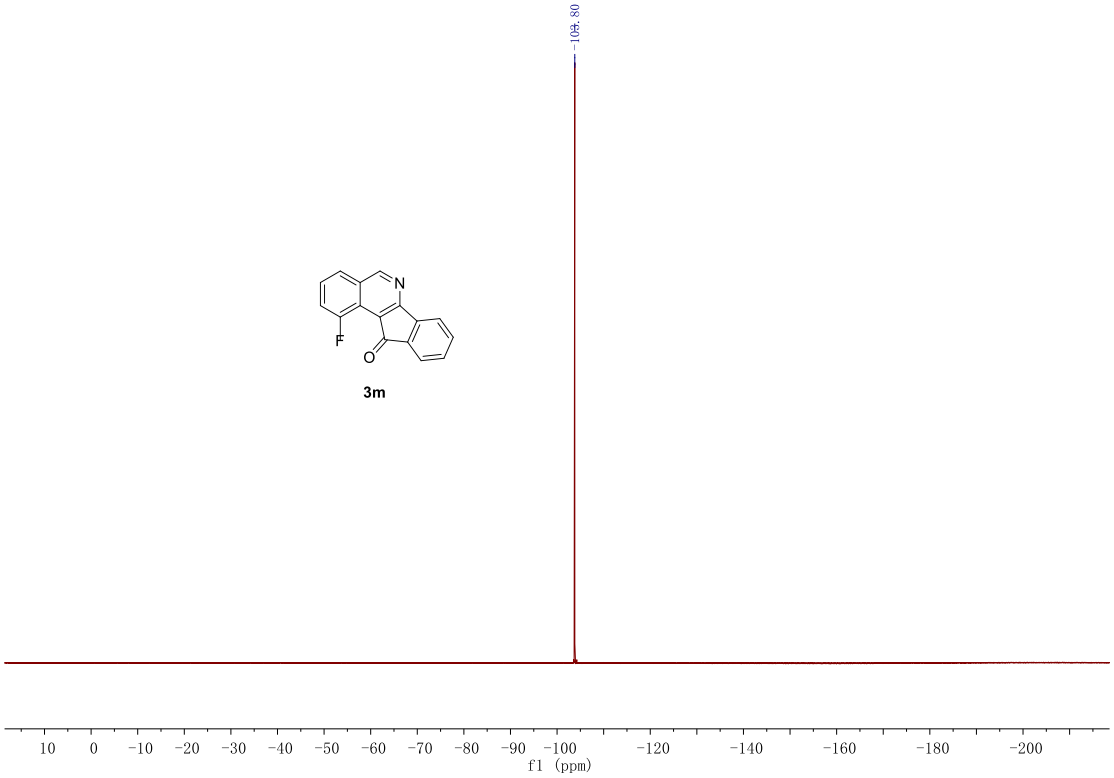
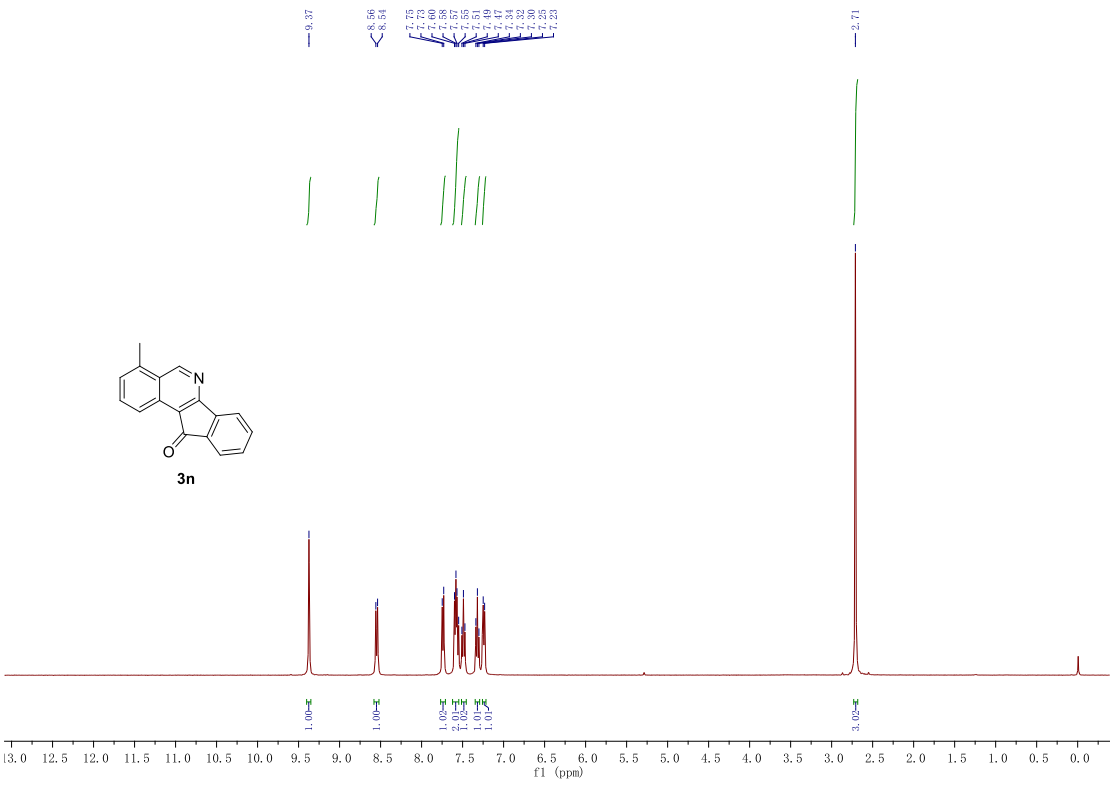
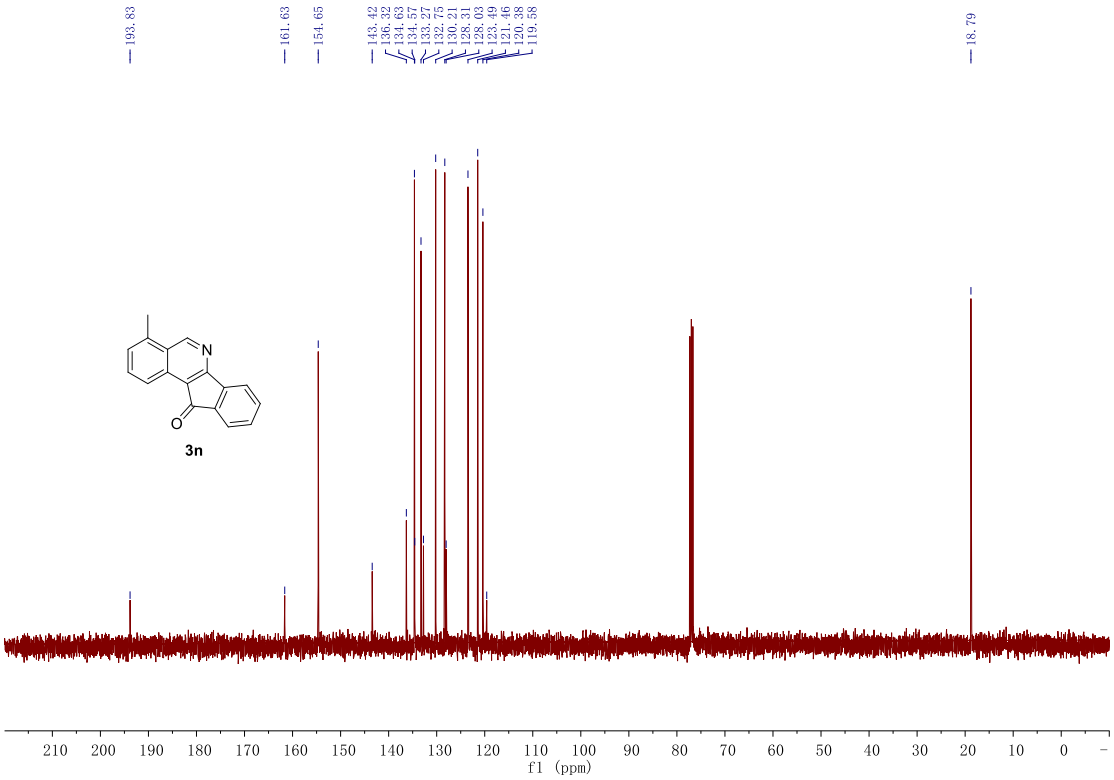
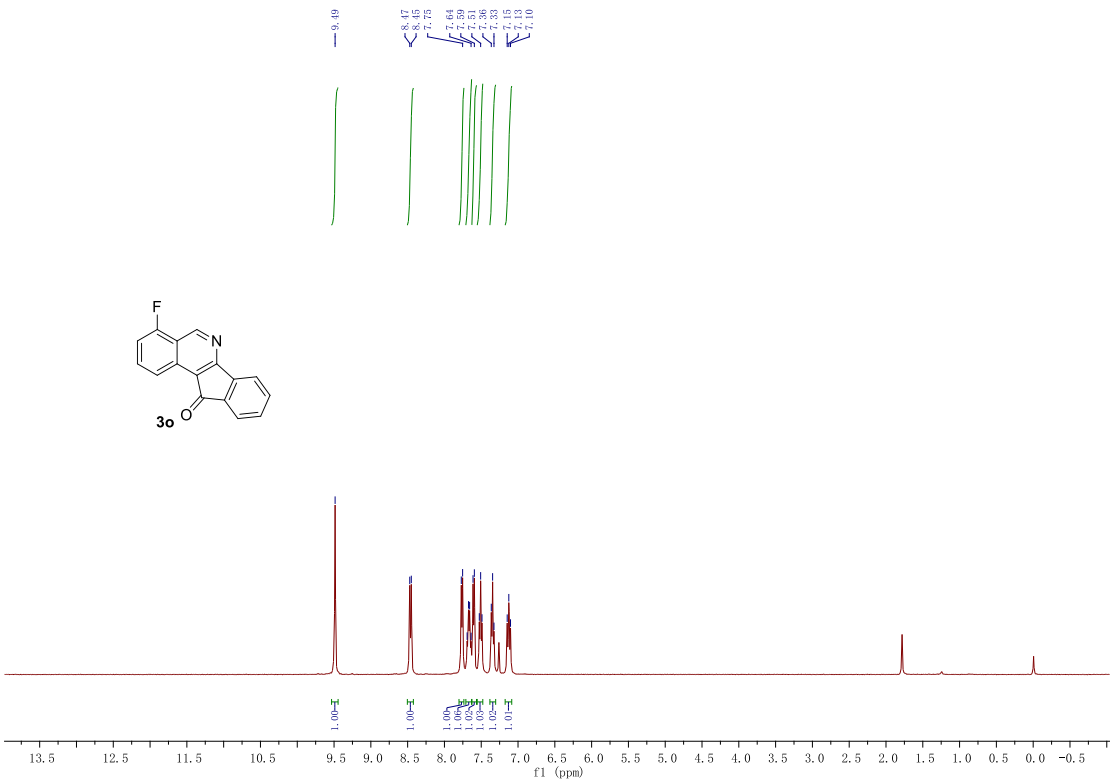
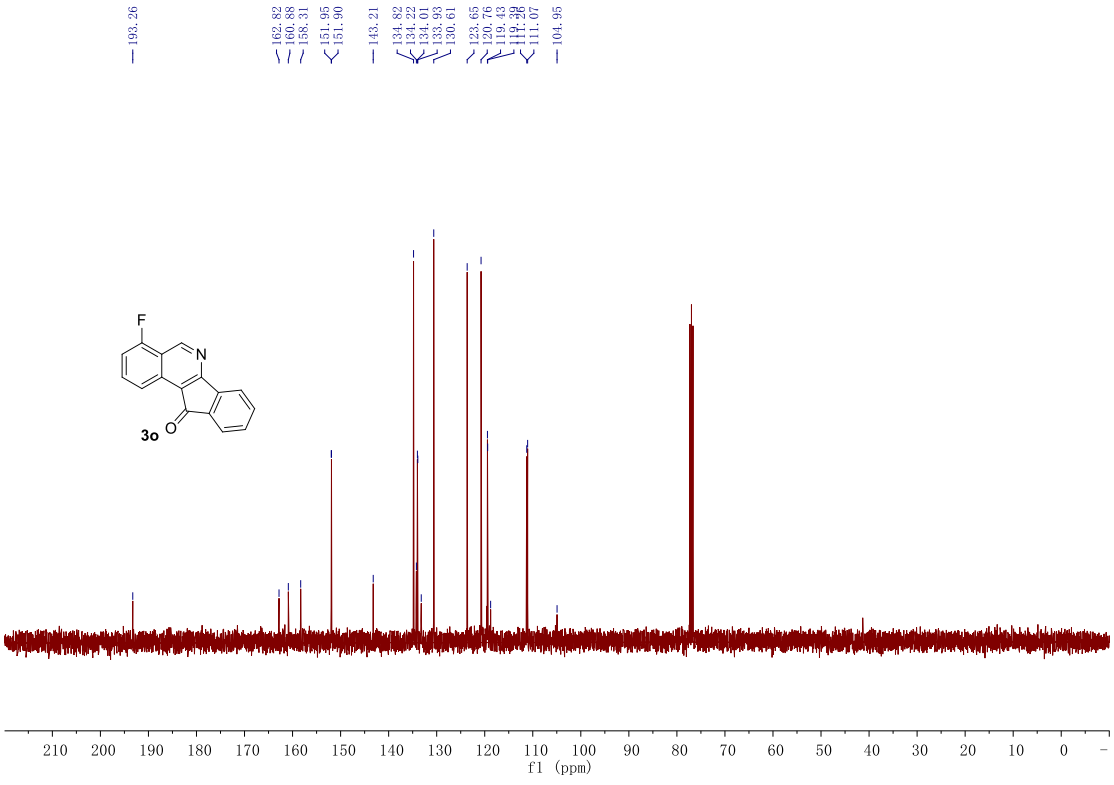
158.80
158.20
156.19
142.75
134.64
133.89
130.72
130.55
130.48
127.78
127.71
124.90
124.86
123.88
122.44
122.23
120.37
118.94
118.01
117.80
N
F
O
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

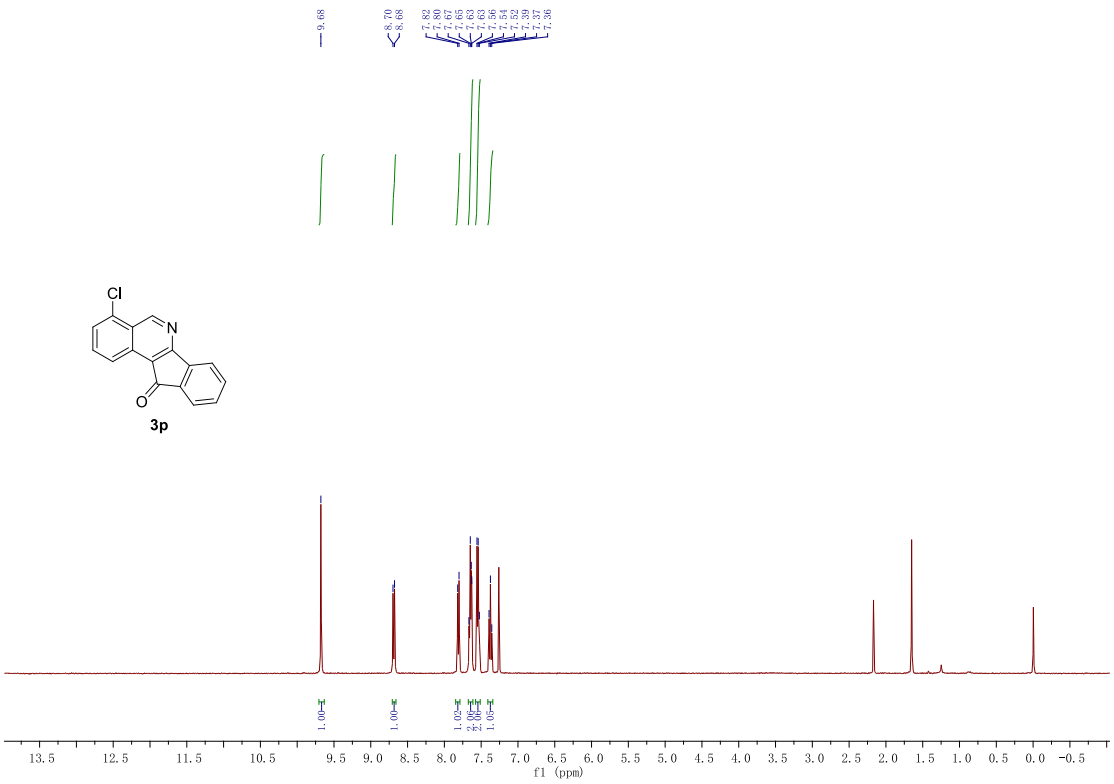

-109.80
N
F
O
3m
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

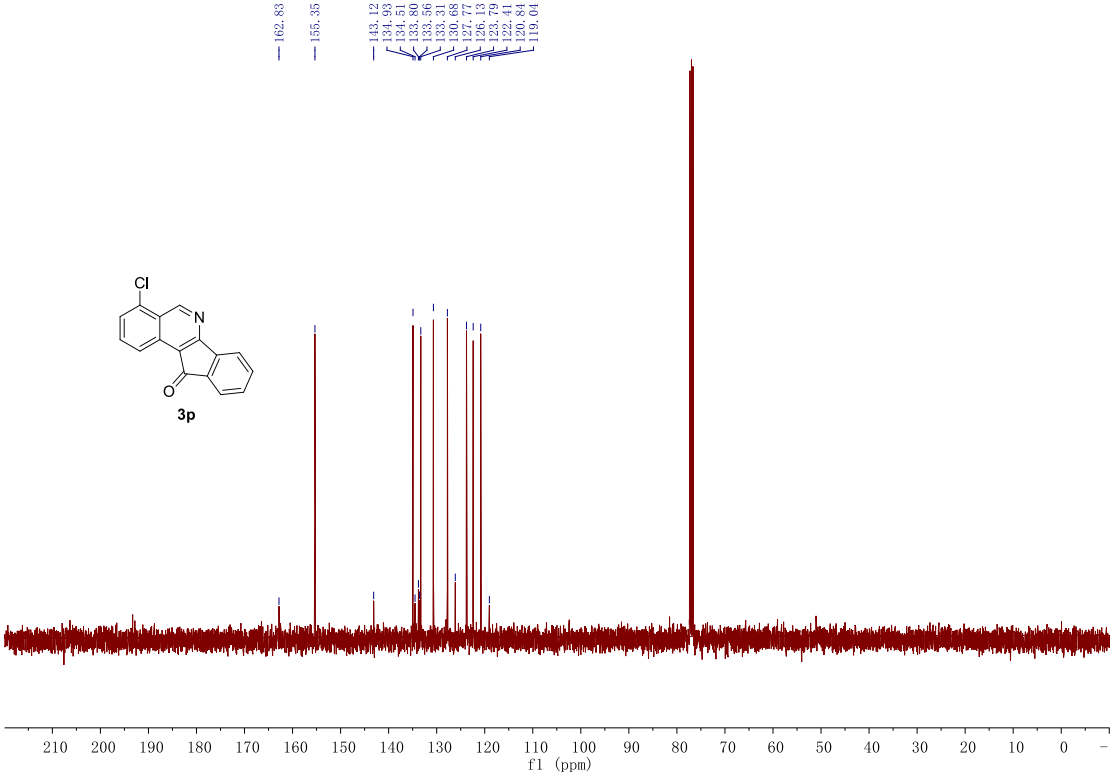

9.37
8.56
8.54
7.75
7.73
7.60
7.58
7.57
7.55
7.51
7.49
7.47
7.34
7.32
7.30
7.25
7.23
2.71
1.00
1.00
1.02
2.01
1.03
1.01
3.02
f1 (ppm)
3n

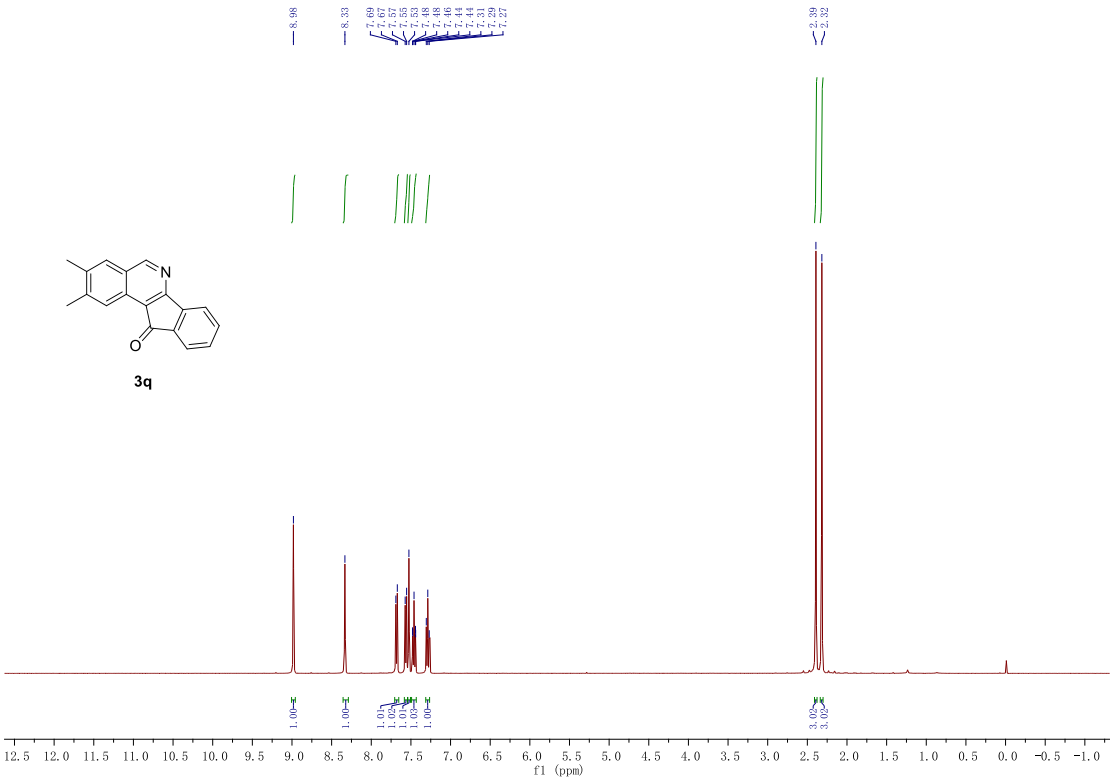

193.83
161.63
154.65
143.42
136.32
134.63
134.57
133.27
132.75
130.21
128.31
128.03
123.49
121.46
120.38
119.58
18.79
f1 (ppm)
3n


9.49
8.47
8.45
7.75
7.64
7.59
7.51
7.36
7.33
7.15
7.13
7.10
F
N
O
3o
1.00
1.00
1.00
1.06
1.05
1.00
1.02
1.01
13.5 12.5 11.5 10.5 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 -0.5
f1 (ppm)

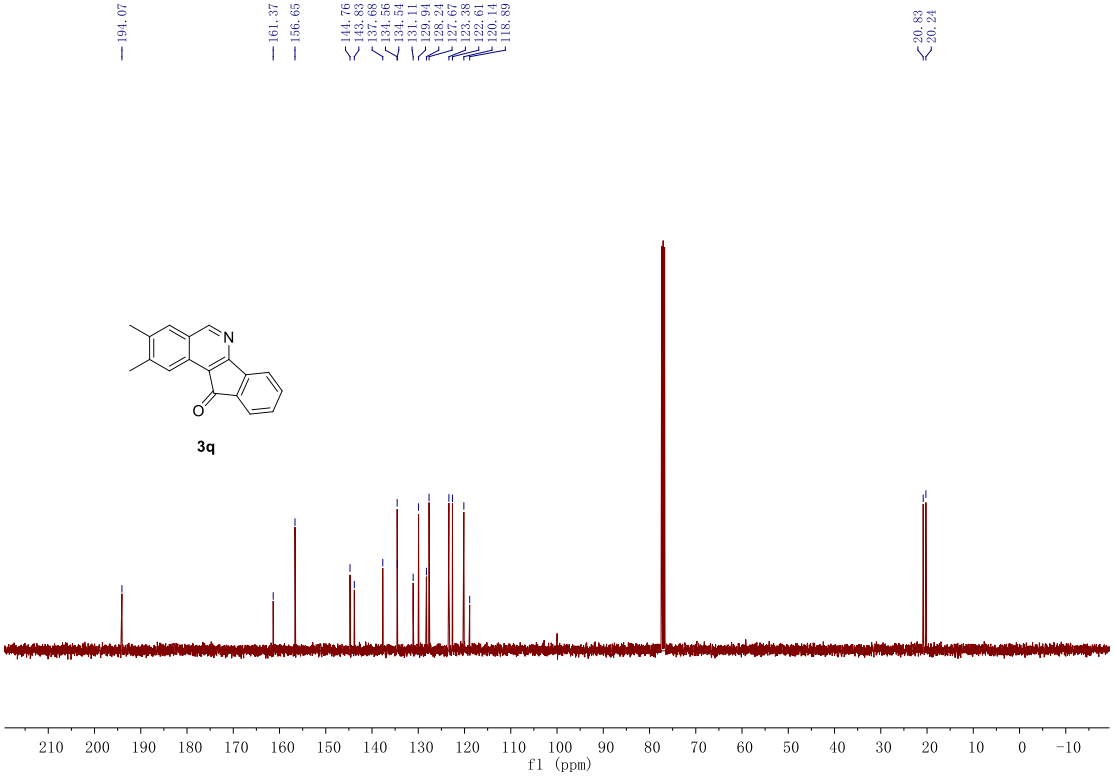

193.26
162.82
160.88
158.31
151.95
151.90
143.21
134.82
134.22
134.01
133.93
130.61
123.65
120.76
119.43
111.26
111.07
104.95
F
N
O
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -
f1 (ppm)


9.68
8.70
8.68
7.82
7.80
7.67
7.65
7.63
7.56
7.54
7.52
7.39
7.37
7.36
Cl
N
O
3p
1.00
1.00
1.02
2.05
1.05
1.05
13.5
12.5
11.5
10.5
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
-0.5
f1 (ppm)

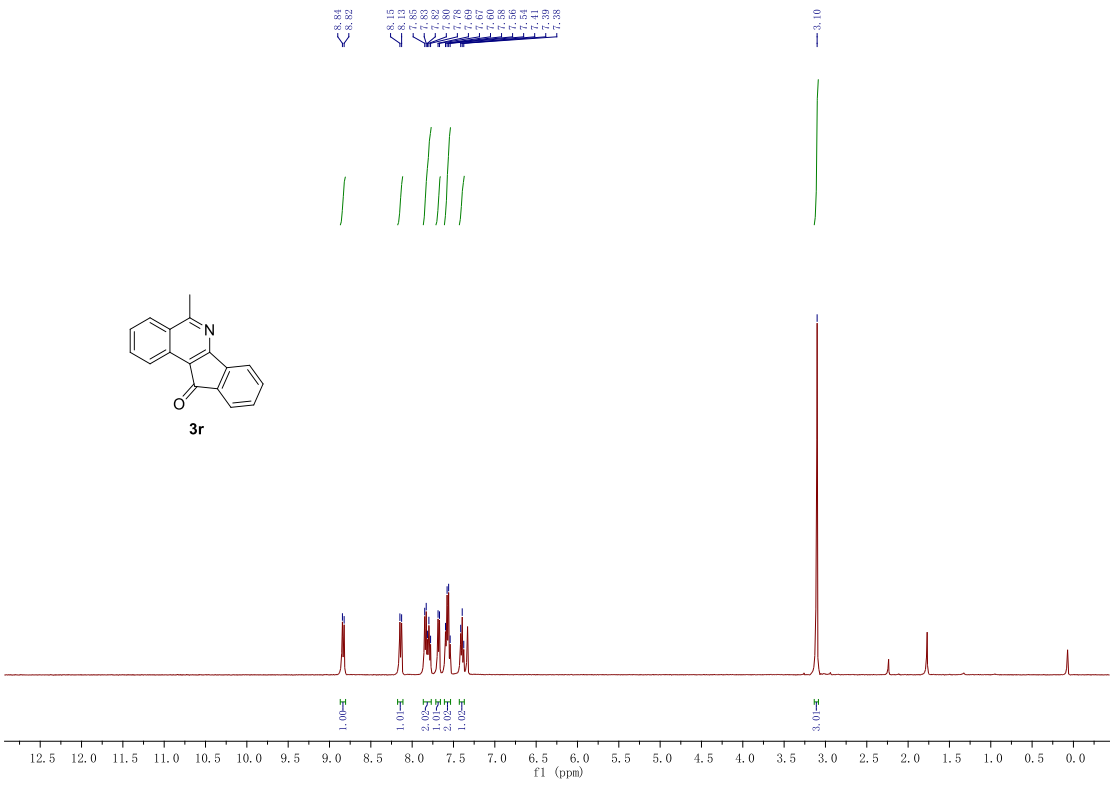

162.83
155.35
143.12
134.93
134.51
133.80
133.56
133.31
130.68
127.77
126.13
123.79
122.41
120.84
119.04
Cl
N
O
3p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

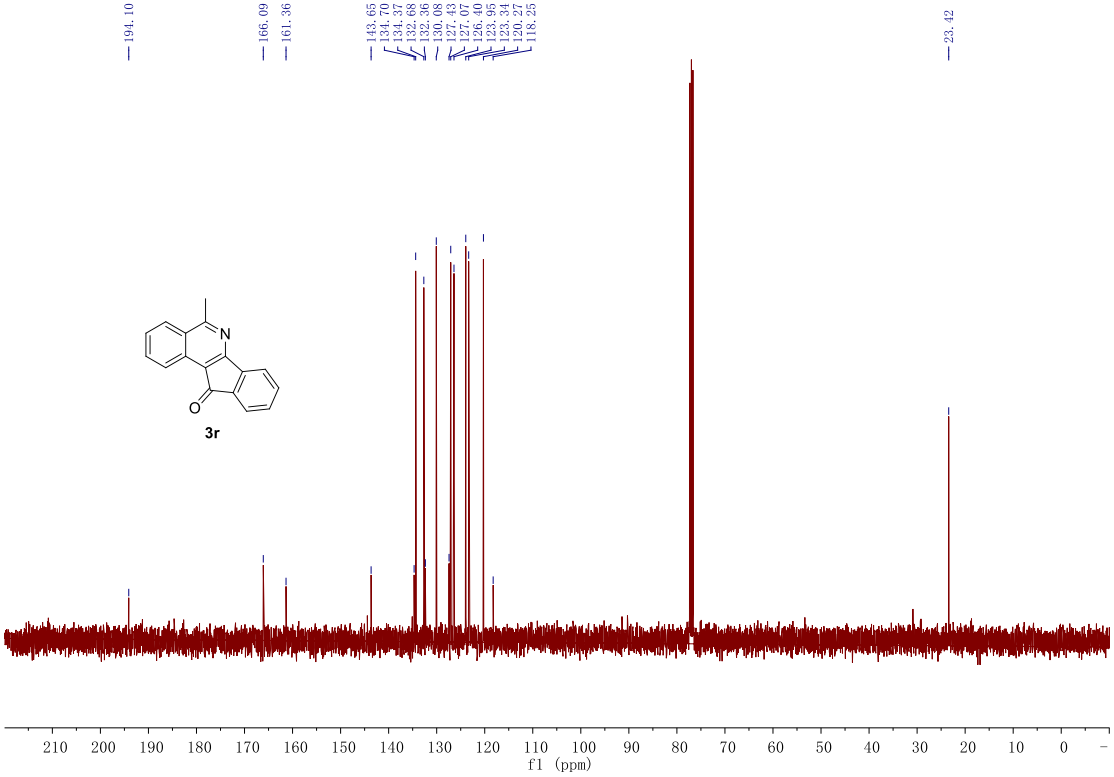

8.98
8.33
7.69
7.67
7.57
7.55
7.53
7.48
7.46
7.44
7.31
7.29
7.27
2.39
2.32
1.00
1.00
1.01
1.02
1.01
1.05
1.00
3.02
3.02
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

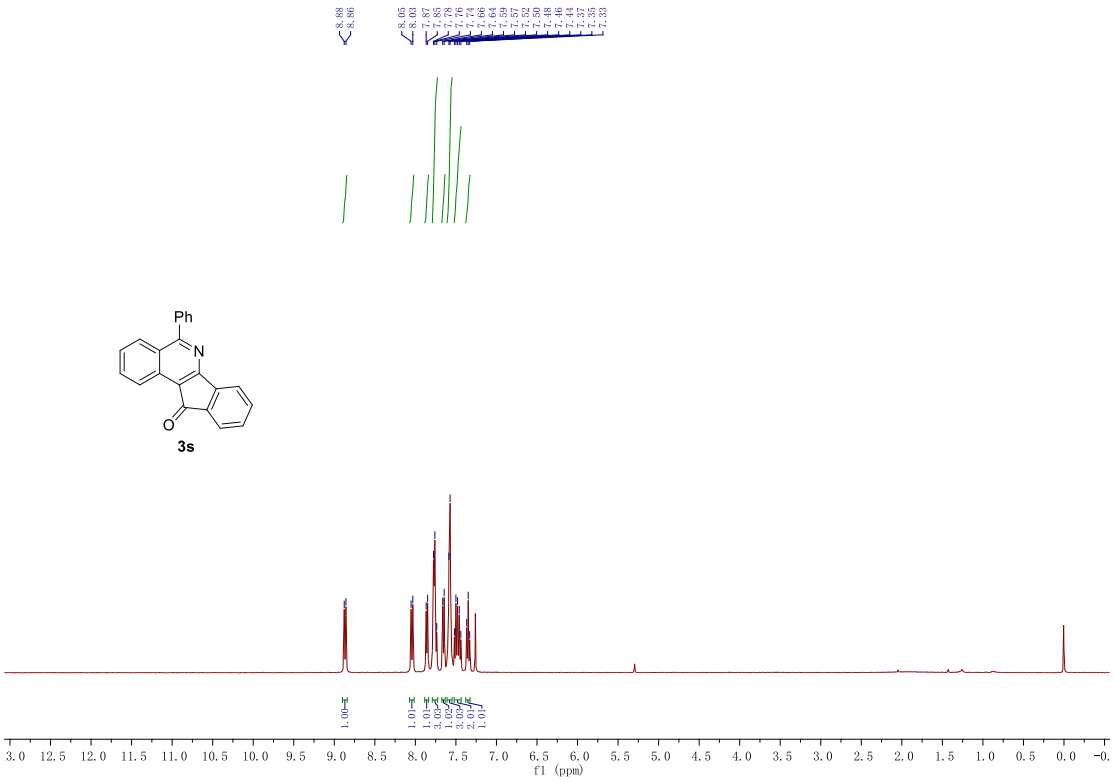
3q

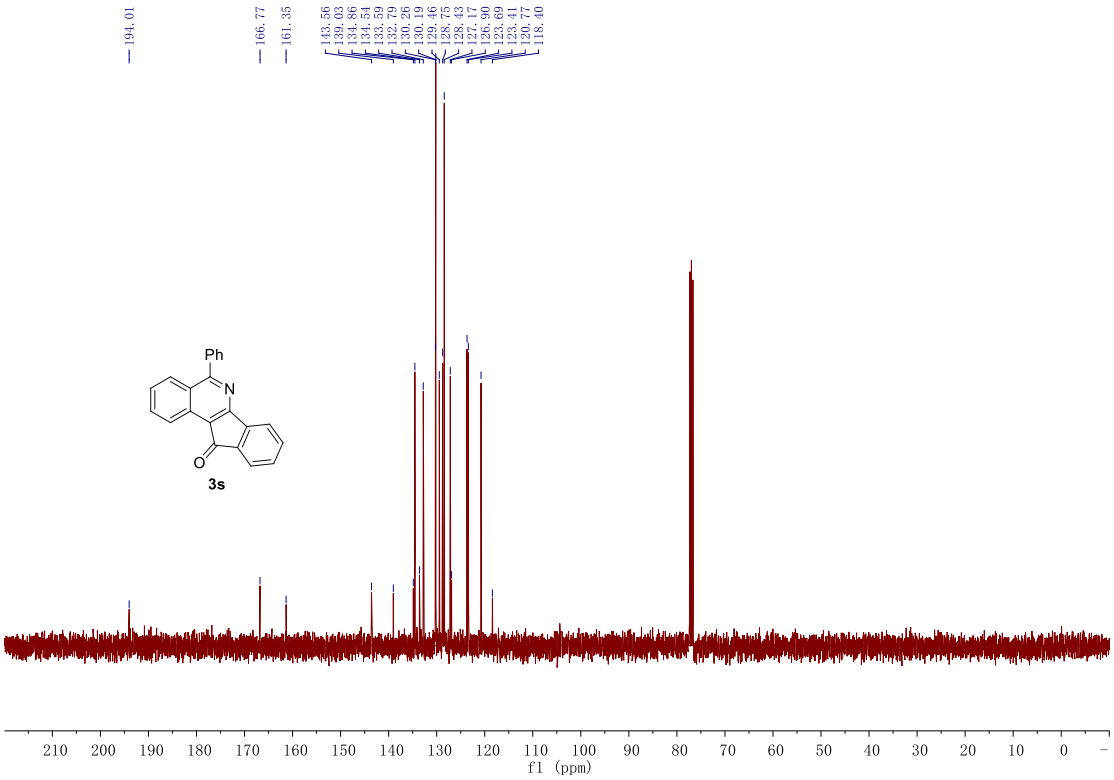

194.07
161.37
156.65
144.76
143.83
137.68
134.56
134.54
131.11
129.94
128.24
127.67
123.38
122.61
120.14
118.89
20.83
20.24
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3q


8.84
8.82
8.15
8.13
7.85
7.83
7.82
7.80
7.78
7.69
7.67
7.60
7.58
7.56
7.54
7.41
7.39
7.38
3.10
1.00
1.01
2.02
2.03
2.00
1.02
3.01
12.5 12.0 11.5 11.0 10.5 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)
N
O
3r


194.10
166.09
161.36
143.65
134.70
134.37
132.68
132.36
130.08
127.43
127.07
126.40
123.95
123.34
120.27
118.25
23.42
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
N
O
3r


8.88
8.86
8.05
8.03
7.87
7.85
7.78
7.76
7.74
7.66
7.64
7.59
7.57
7.52
7.50
7.48
7.46
7.44
7.37
7.35
7.33
Ph
N
O
3s
1.00
1.01
1.01
3.02
3.05
3.05
2.01
1.01
3.0 12.5 12.0 11.5 11.0 10.5 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 -0.
f1 (ppm)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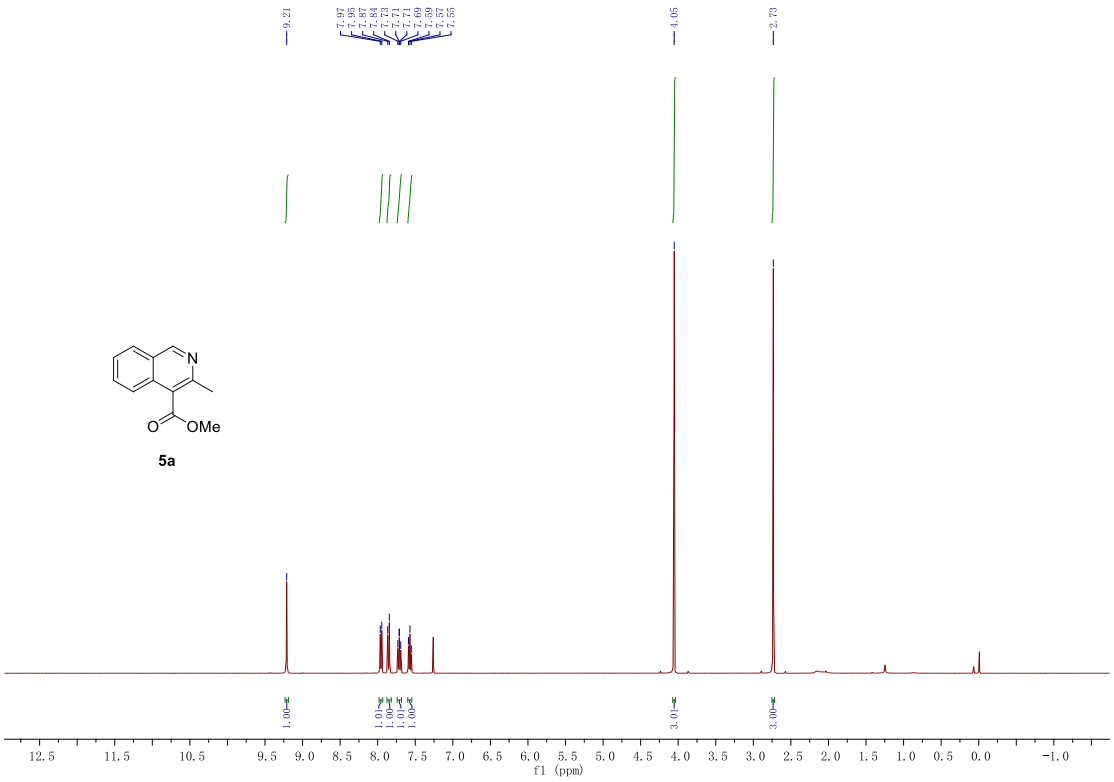
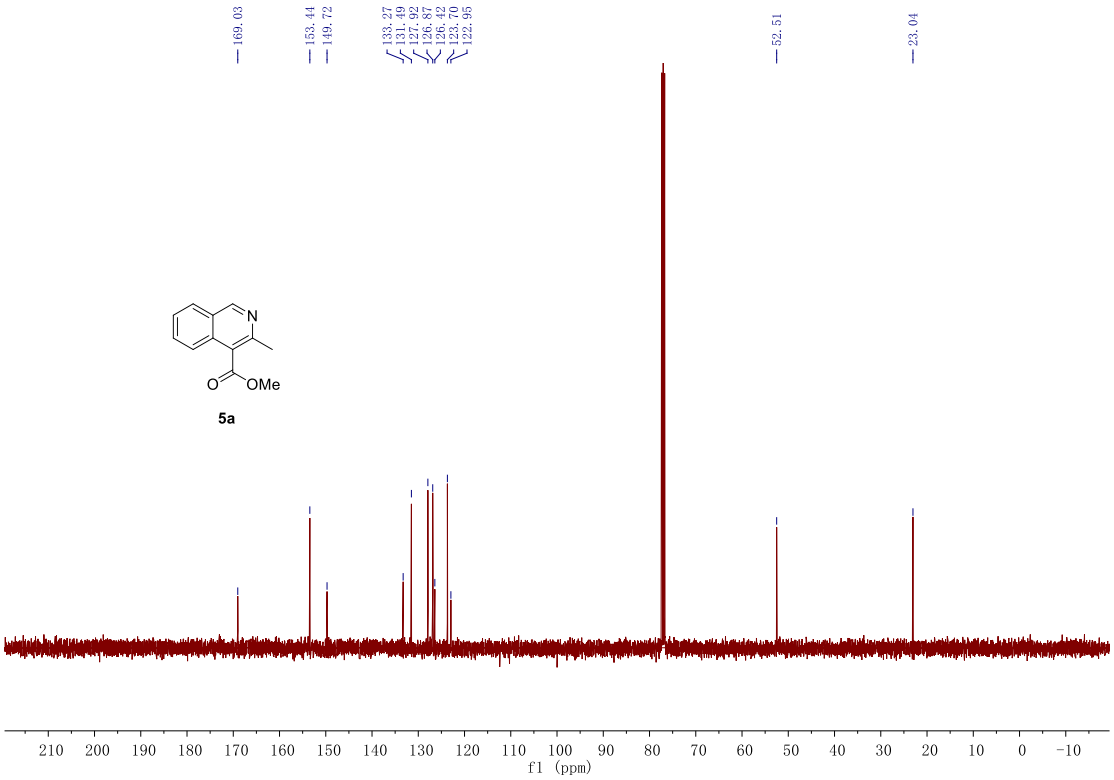
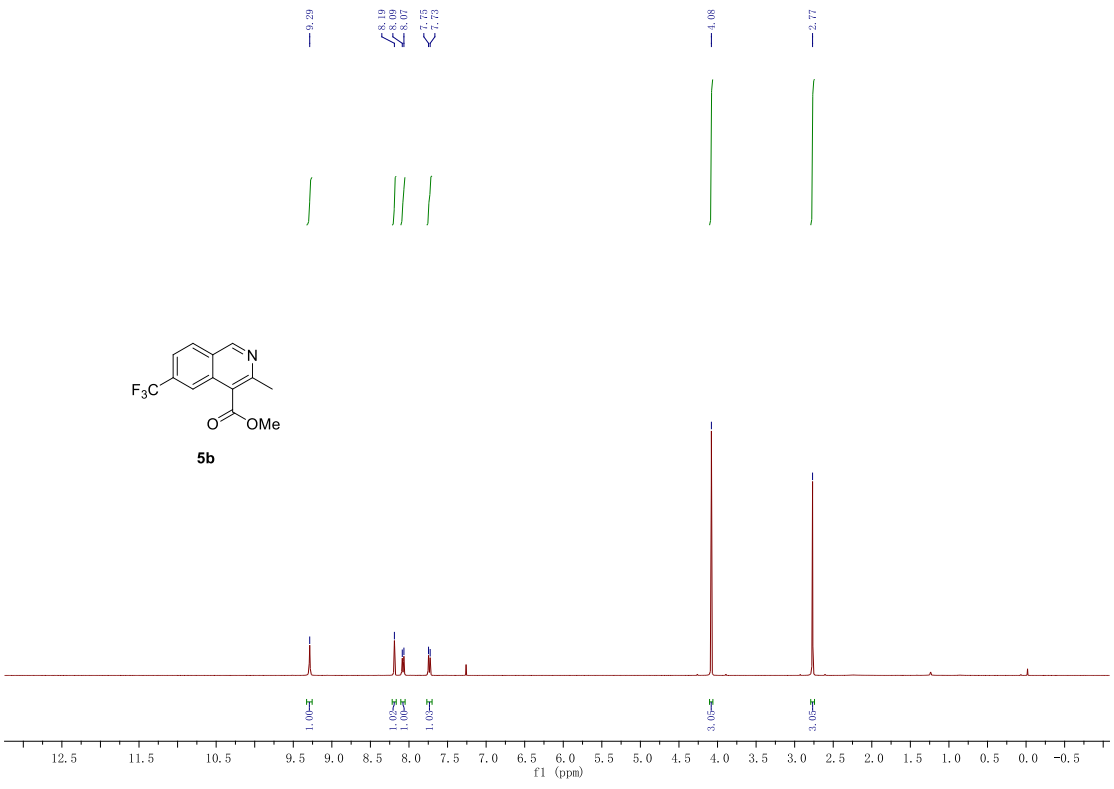
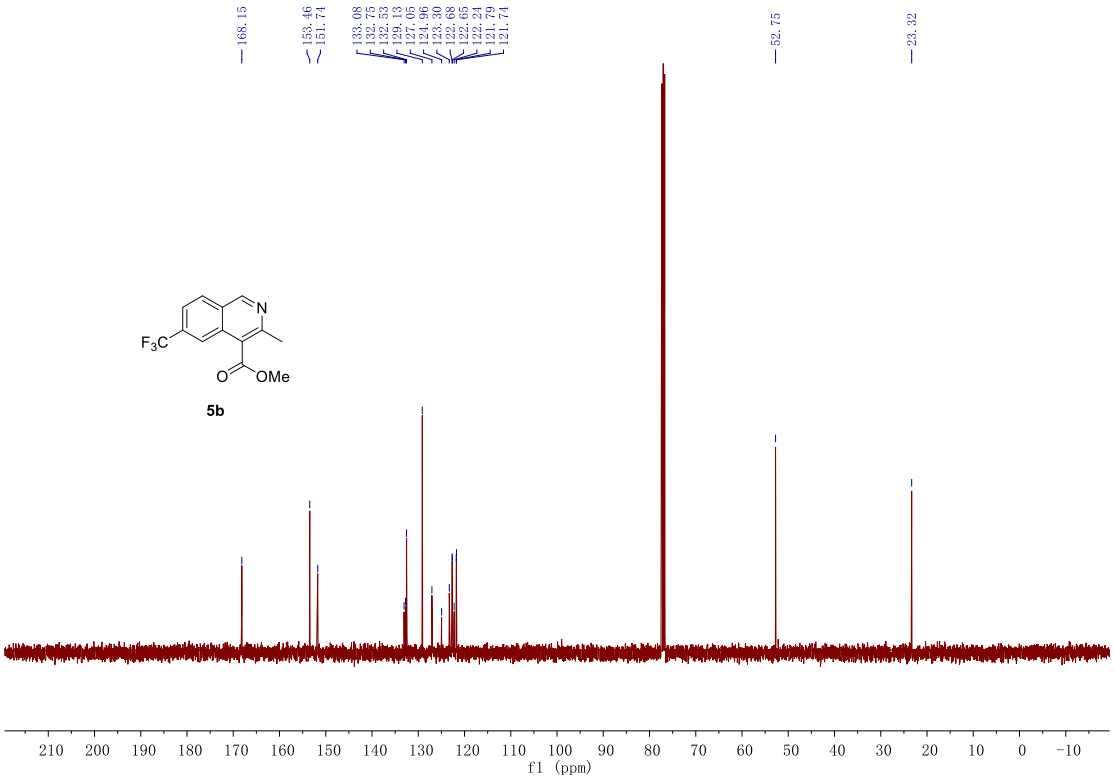
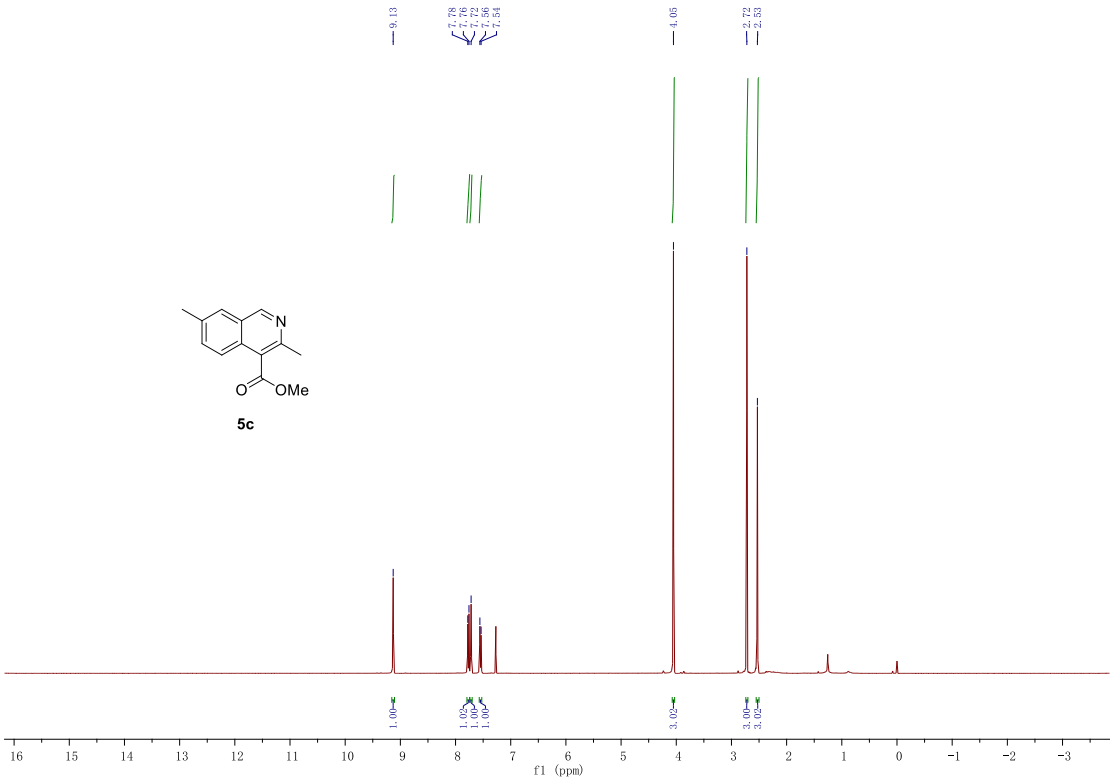
166.77
161.35
143.56
139.03
134.86
134.54
133.59
132.79
130.26
130.19
129.46
128.75
128.43
127.17
126.90
123.69
123.41
120.77
118.40
Ph
N
O
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -
f1 (ppm)

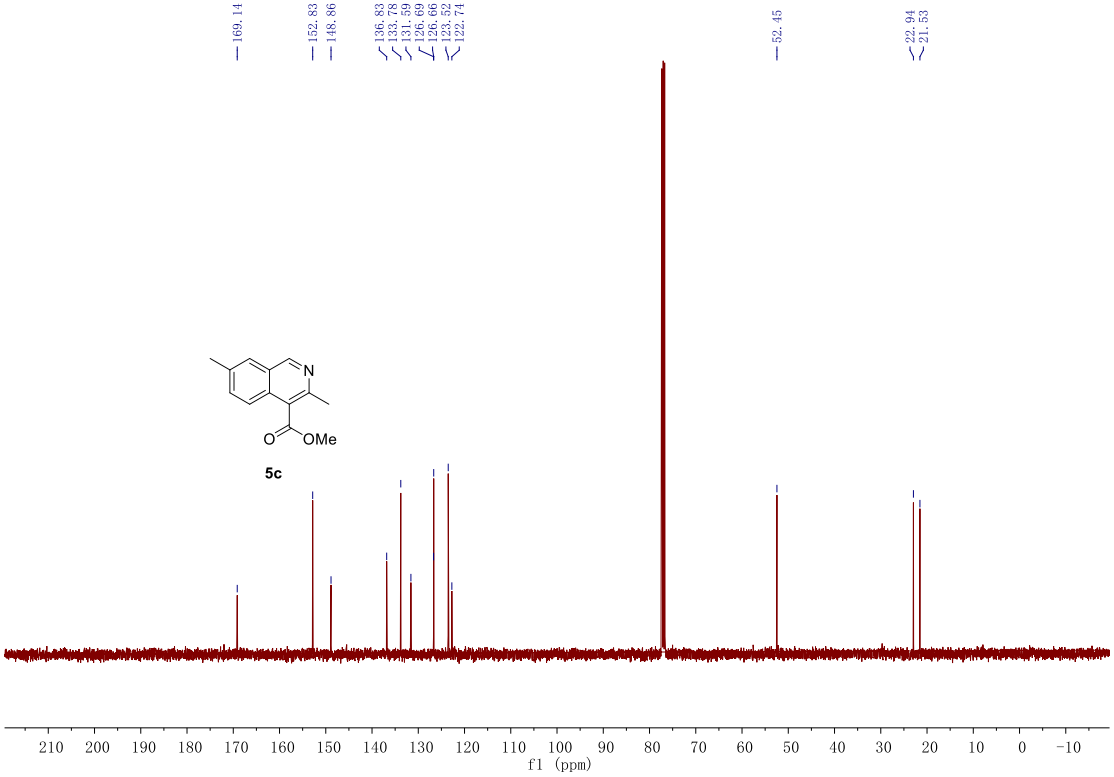

9.21
7.97
7.95
7.87
7.84
7.73
7.71
7.71
7.69
7.57
7.55
4.05
2.73
N
O
OMe
5a
1.00
1.01
1.00
1.01
1.00
3.01
3.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)

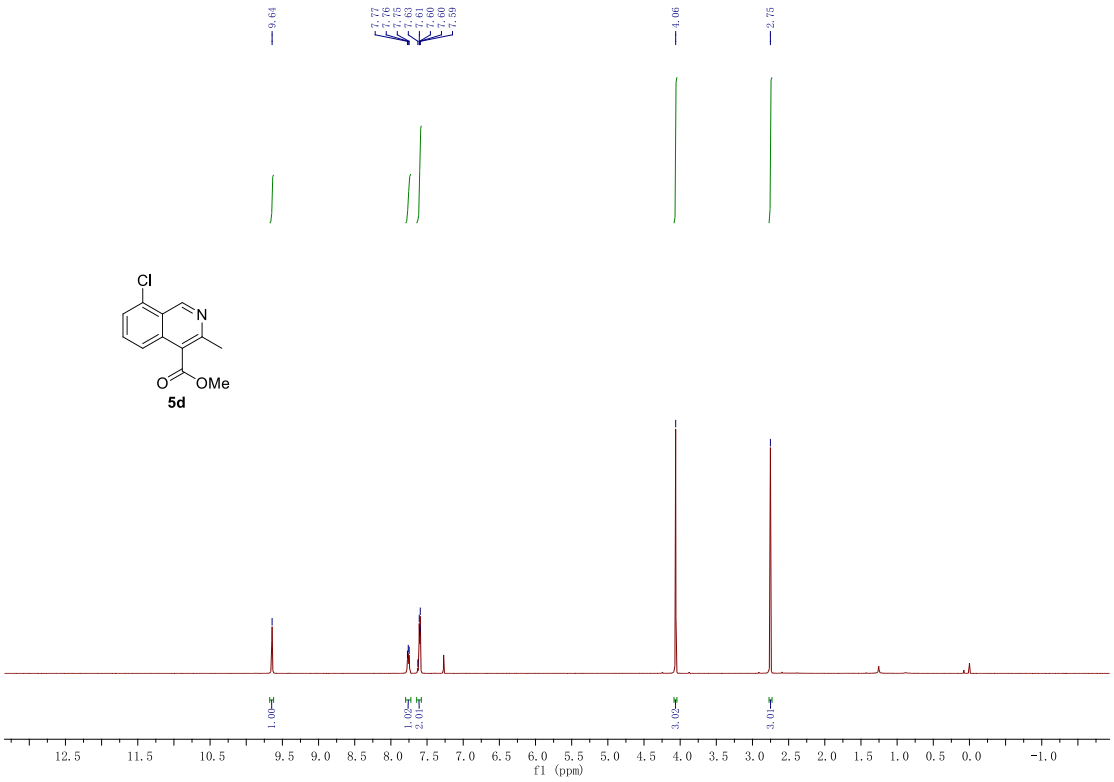

169.03
153.44
149.72
133.27
131.49
127.92
126.87
126.42
123.70
122.95
52.51
23.04
N
O
OMe
5a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

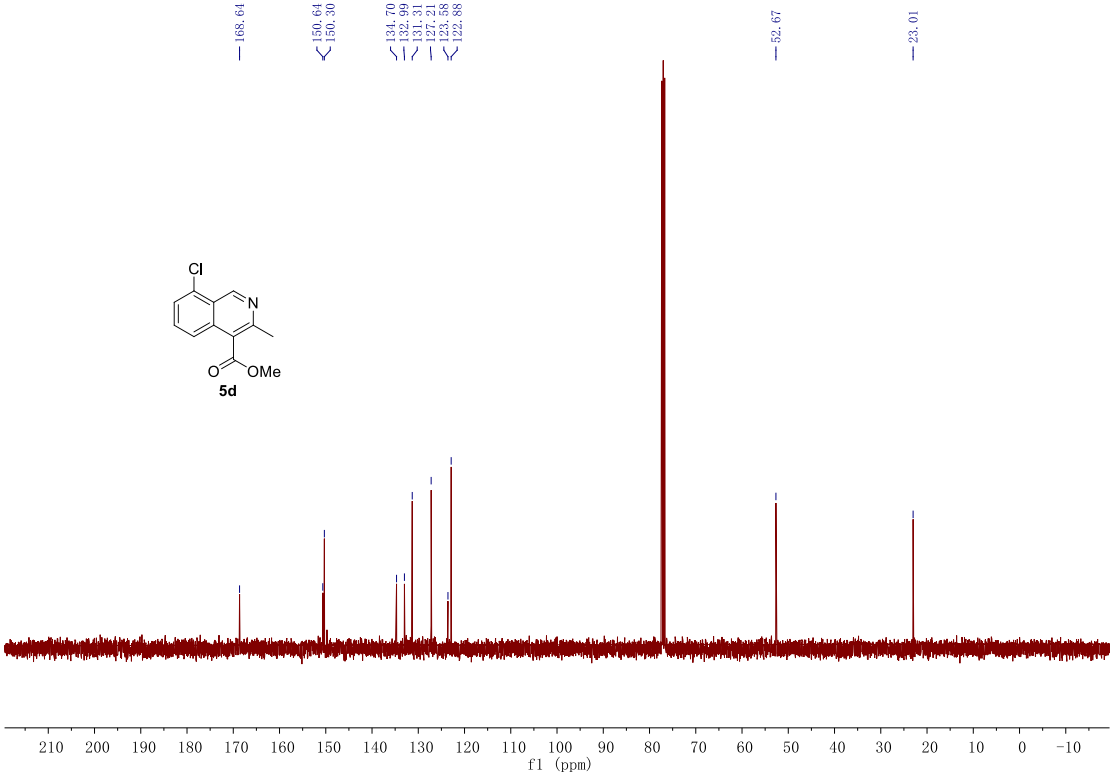

9.29
8.19
8.09
8.07
7.75
7.73
4.08
2.77
N
F3C
O
OMe
5b
1.00
1.02
1.00
1.03
3.05
3.05
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

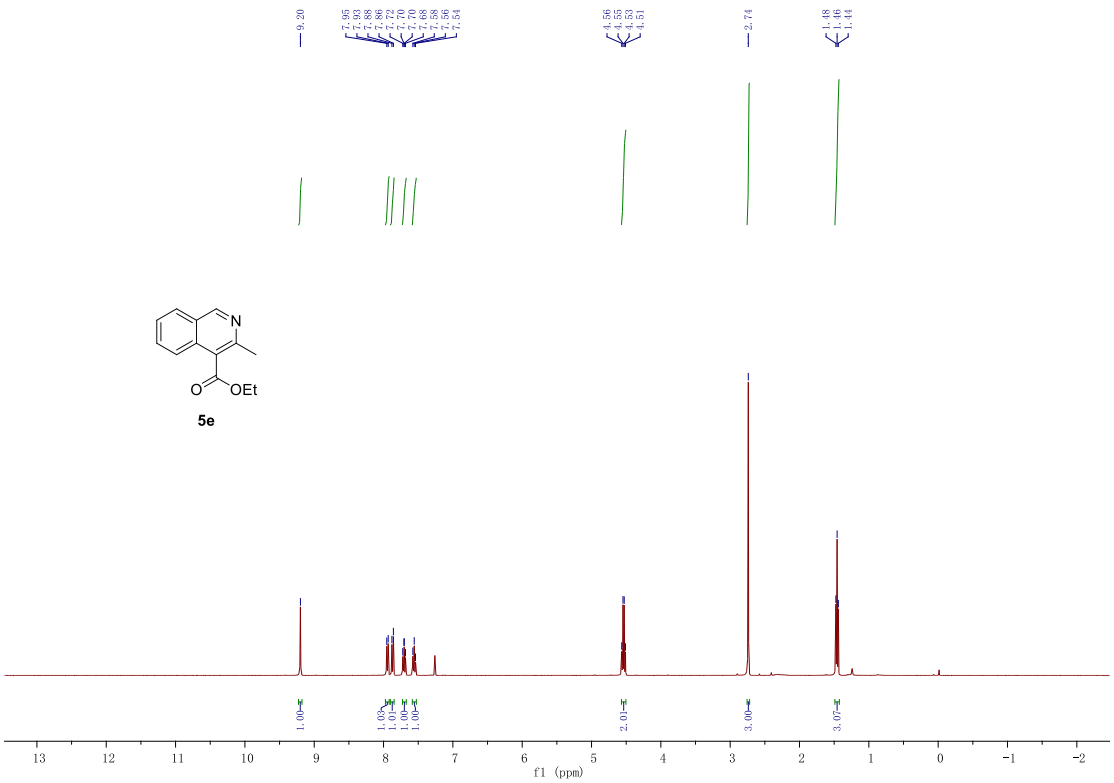

168.15
153.46
151.74
133.08
132.75
132.53
129.13
127.05
124.96
123.30
122.68
122.65
122.24
121.79
121.74
82.75
23.32
N
F3C
O
OMe
5b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

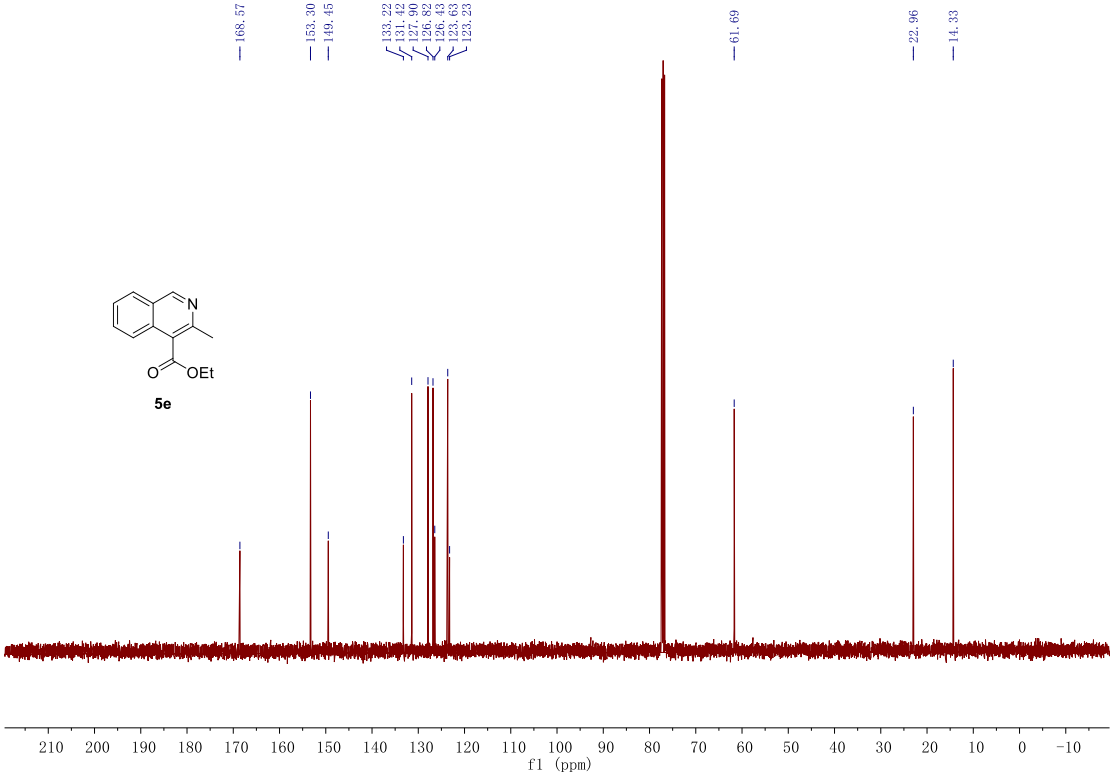

9.13
7.78
7.76
7.72
7.56
7.54
4.05
2.72
2.53
N
O
OMe
5c
1.00
1.02
1.00
1.00
3.02
3.00
3.02
f1 (ppm)

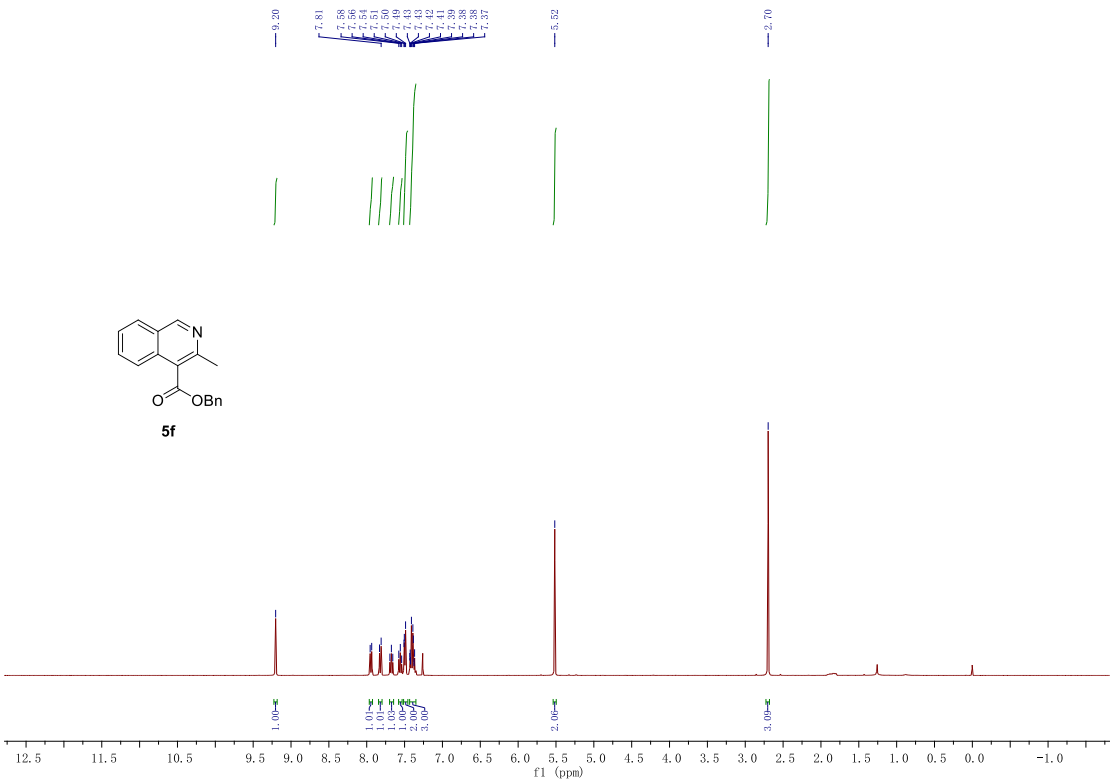

169.14
152.83
148.86
136.83
133.78
131.59
126.69
126.66
123.52
122.74
52.45
22.94
21.53
N
O
OMe
5c
f1 (ppm)

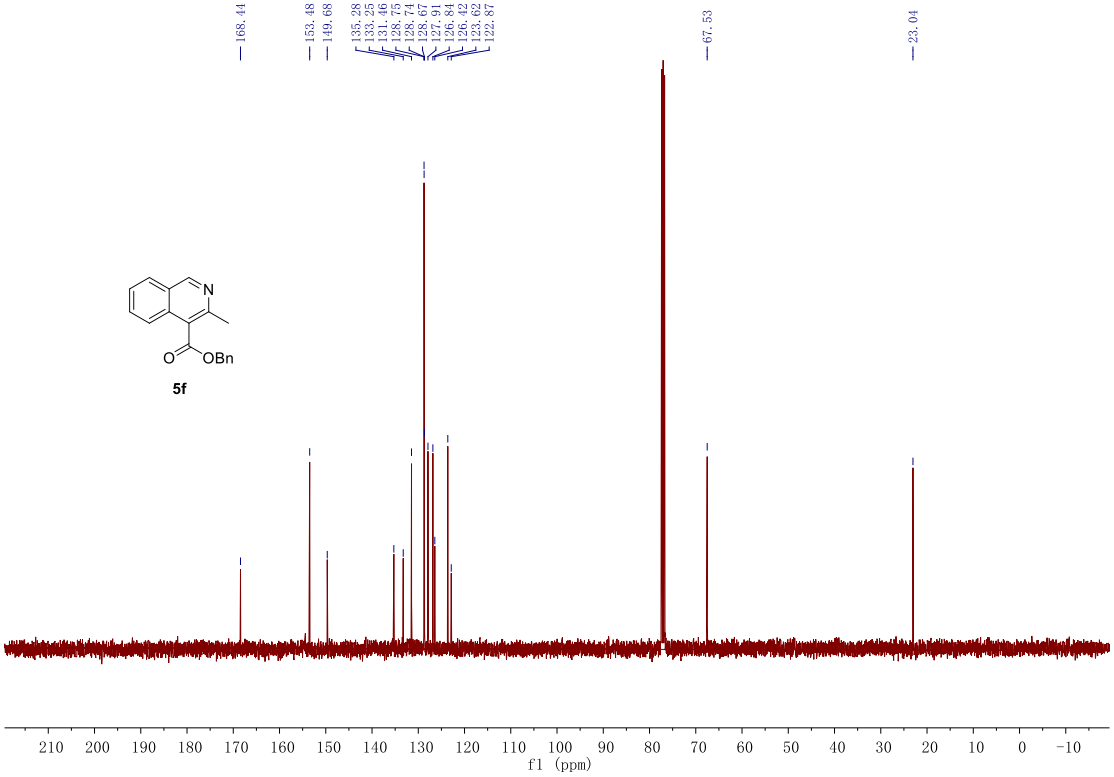

9.64
7.77
7.76
7.75
7.63
7.61
7.60
7.60
7.59
4.06
2.75
Cl
N
O
OMe
5d
1.00
1.09
2.01
3.02
3.01
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)


168.64
150.64
150.30
134.70
132.99
131.31
127.21
123.58
122.88
82.67
23.01
Cl
N
O
OMe
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


9.20
7.95
7.93
7.88
7.86
7.72
7.70
7.70
7.68
7.58
7.56
7.54
4.56
4.55
4.53
4.51
2.74
1.48
1.46
1.44
N
O
OEt
5e
1.00
1.03
1.01
1.00
1.00
2.01
3.00
3.07
f1 (ppm)


168.57
153.30
149.45
133.22
131.42
127.90
126.82
126.43
123.63
123.23
61.69
22.96
14.33
N
O
OEt
5e
f1 (ppm)


9.20
7.81
7.58
7.56
7.54
7.51
7.50
7.49
7.43
7.43
7.42
7.41
7.39
7.38
7.38
7.37
5.52
2.70
N
O
OBn
5f
1.00
1.01
1.01
1.00
2.00
3.00
2.00
3.00
f1 (ppm)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131.46
128.75
128.74
128.67
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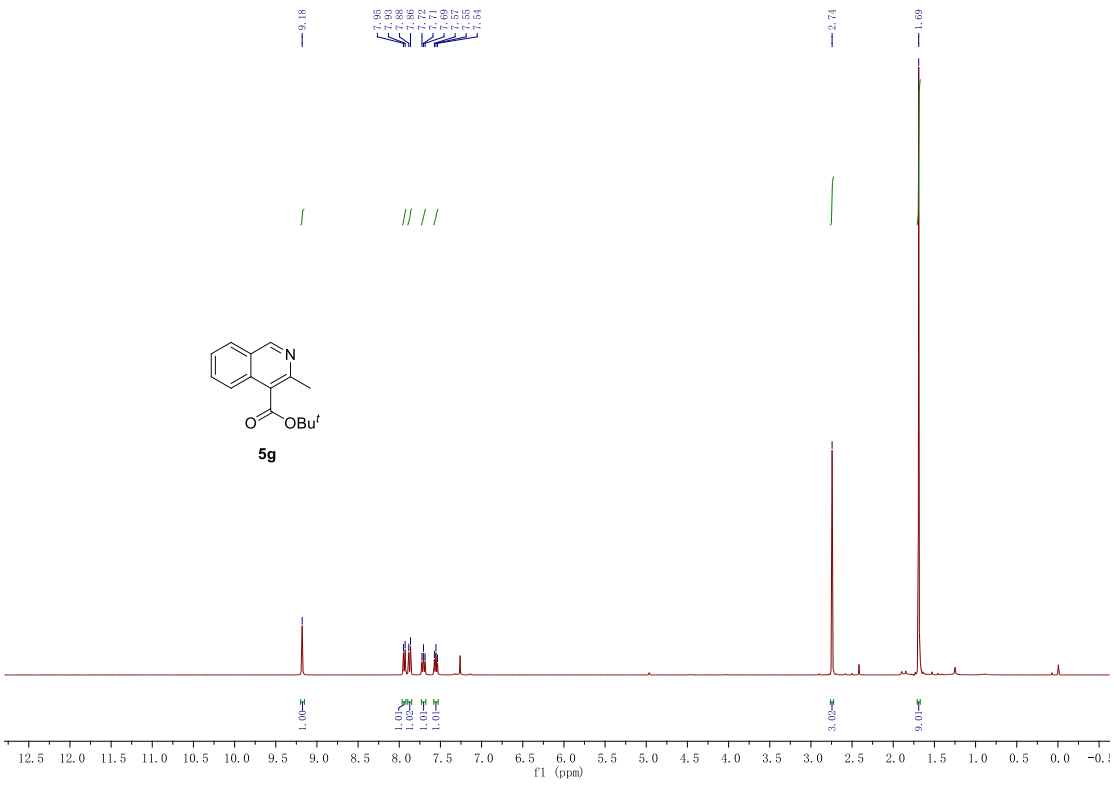
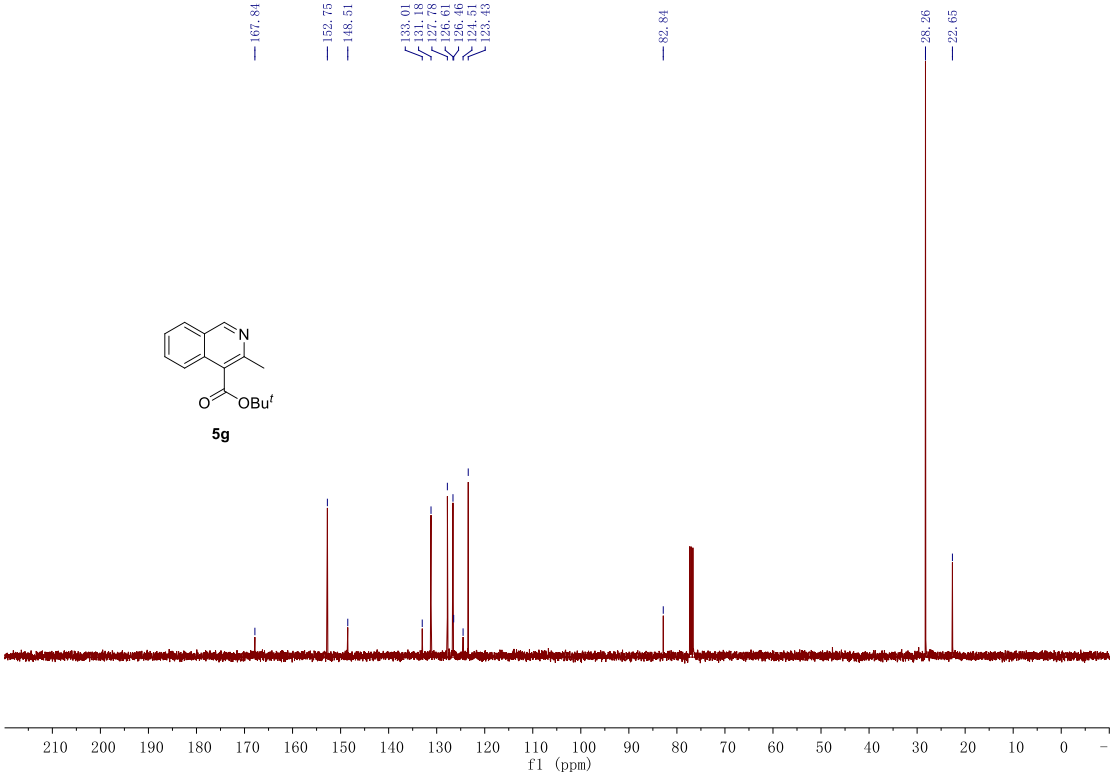
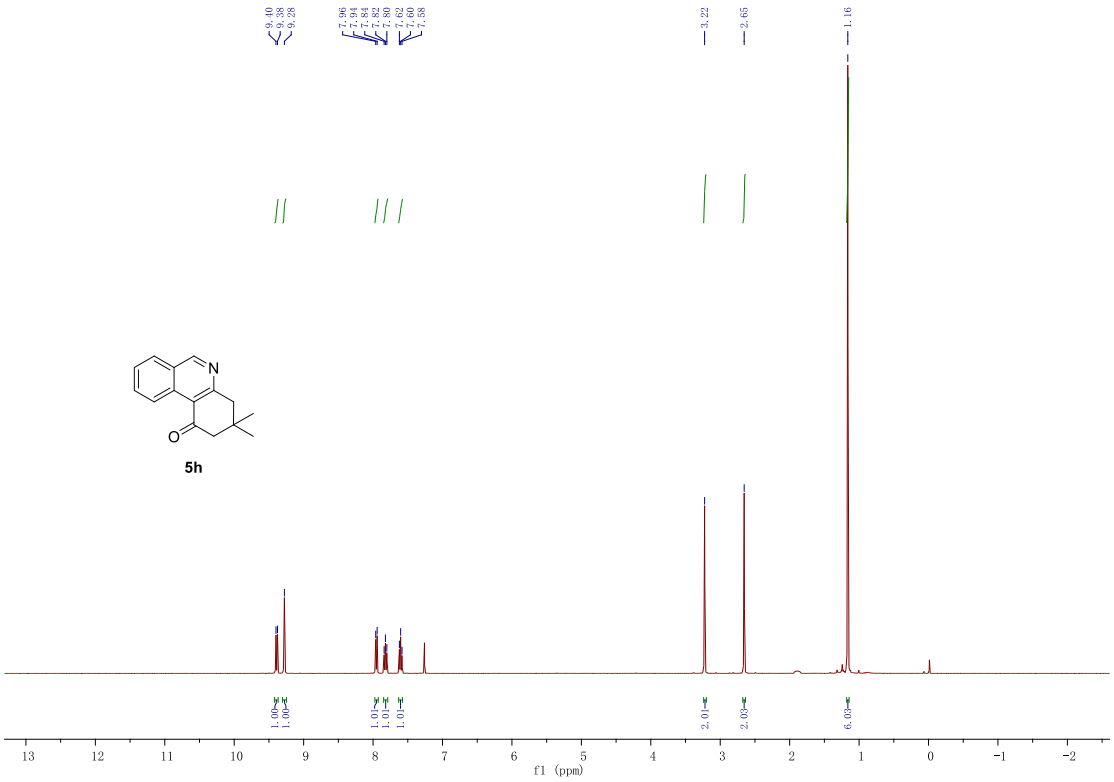
126.42
123.62
122.87
67.53
23.04
N
O
OBn
5f
f1 (ppm)


9.18
7.95
7.93
7.88
7.86
7.72
7.71
7.69
7.57
7.55
7.54
2.74
1.69
N
O
OBu^t
1.00
1.05
1.02
1.01
1.01
3.02
9.01
f1 (ppm)

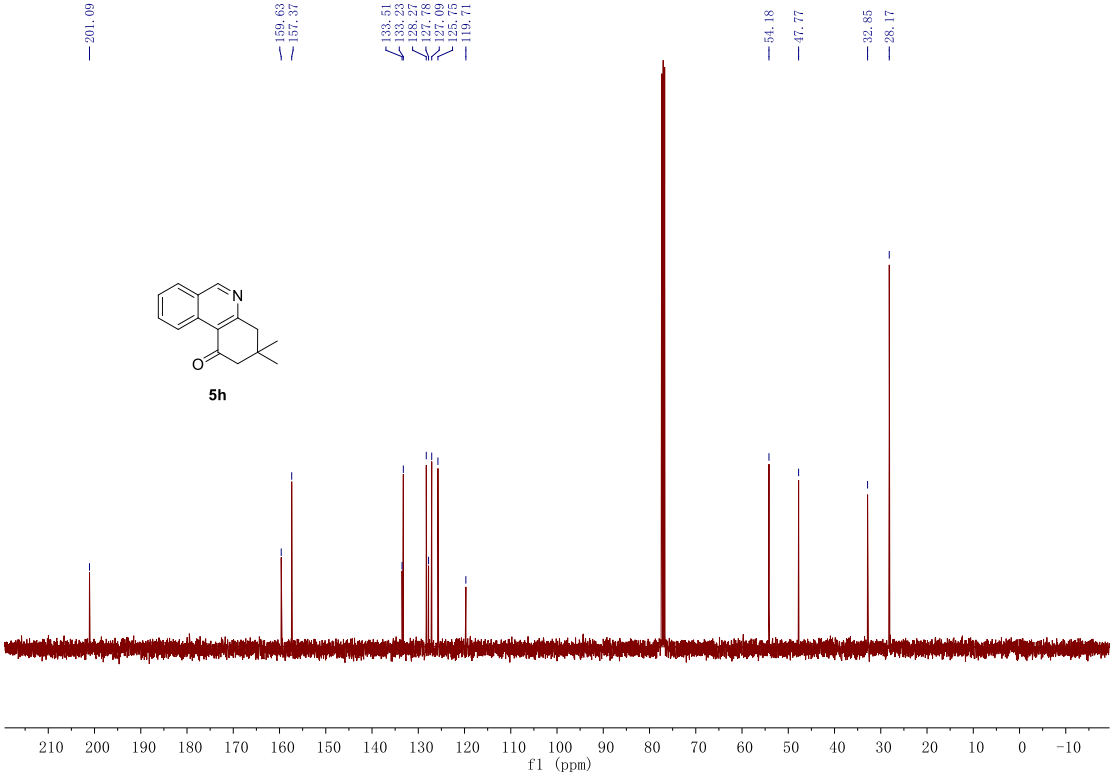
5g


167.84
152.75
148.51
133.01
131.18
127.78
126.61
126.46
124.51
123.43
82.84
28.26
22.65
N
O
OBu^t
f1 (ppm)

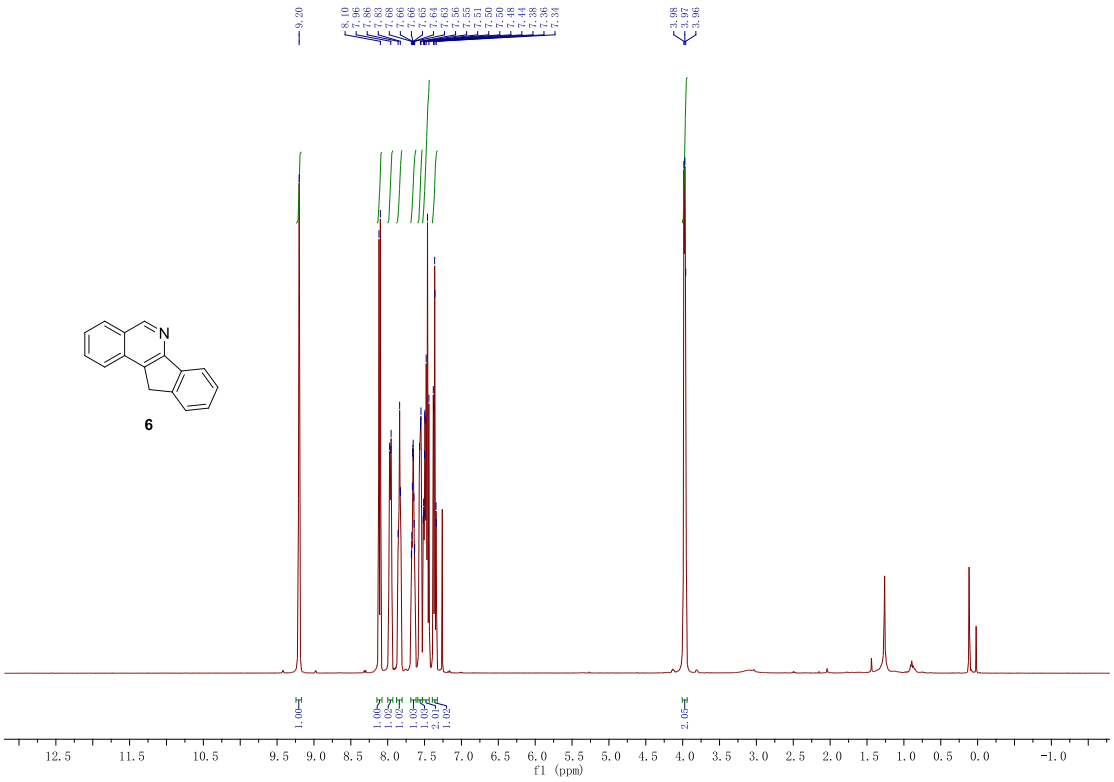
5g

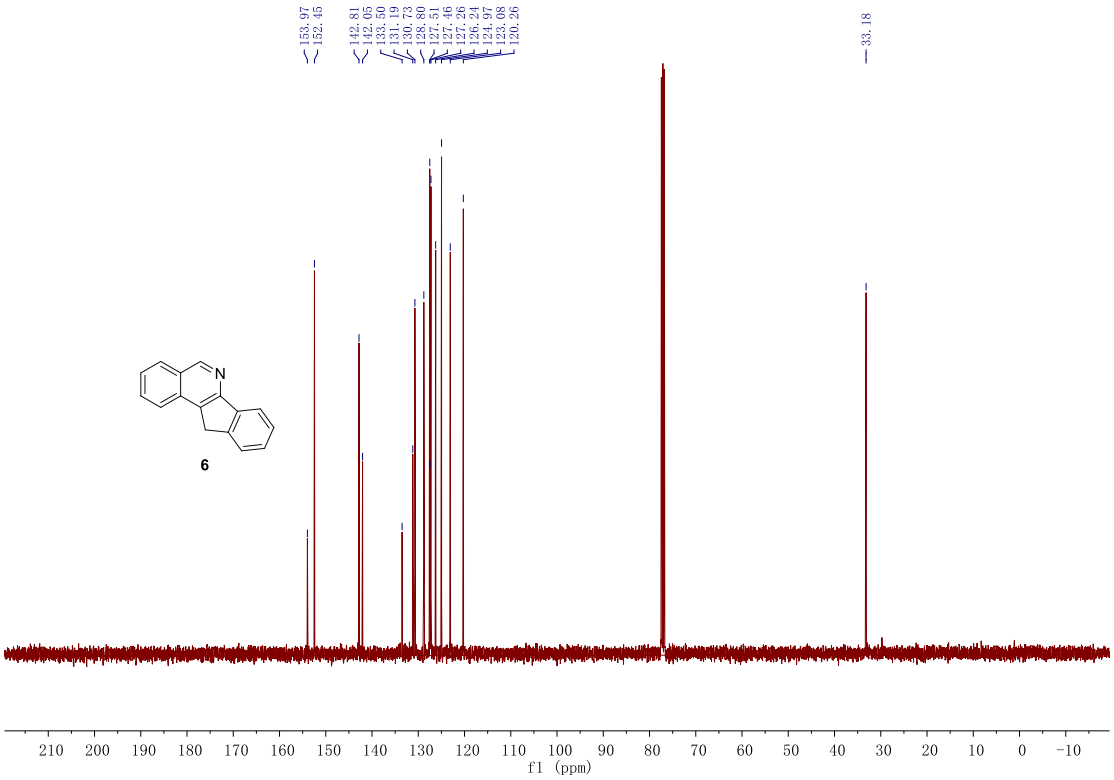

9.40
9.38
9.28
7.96
7.94
7.84
7.82
7.80
7.62
7.60
7.58
3.22
2.65
1.16
1.00
1.00
1.01
1.01
1.01
2.01
2.09
6.05
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

5h


201.09
159.63
157.37
133.51
133.23
128.27
127.78
127.09
125.75
119.71
54.18
47.77
32.85
28.17
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5h


9.20
8.10
7.96
7.88
7.83
7.68
7.66
7.66
7.65
7.64
7.63
7.56
7.55
7.51
7.50
7.48
7.44
7.38
7.36
7.34
3.98
3.97
3.96
1.00
1.00
1.02
1.02
1.00
1.00
1.00
1.02
2.05
N
6
12.5
11.5
10.5
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
-1.0
f1 (ppm)


153.97
152.45
142.81
142.05
133.50
131.19
130.73
128.80
127.51
127.46
127.26
126.24
124.97
123.08
120.26
33.18
N
6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)