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Supporting Information

Synthesis of indolo- and benzothieno[3,2-*c*]quinolines *via* $POCl_3$ mediated tandem cyclization of *o*-alkynylisocyanobenzenes derived from *o*-alkynyl-*N*-phenylformamides

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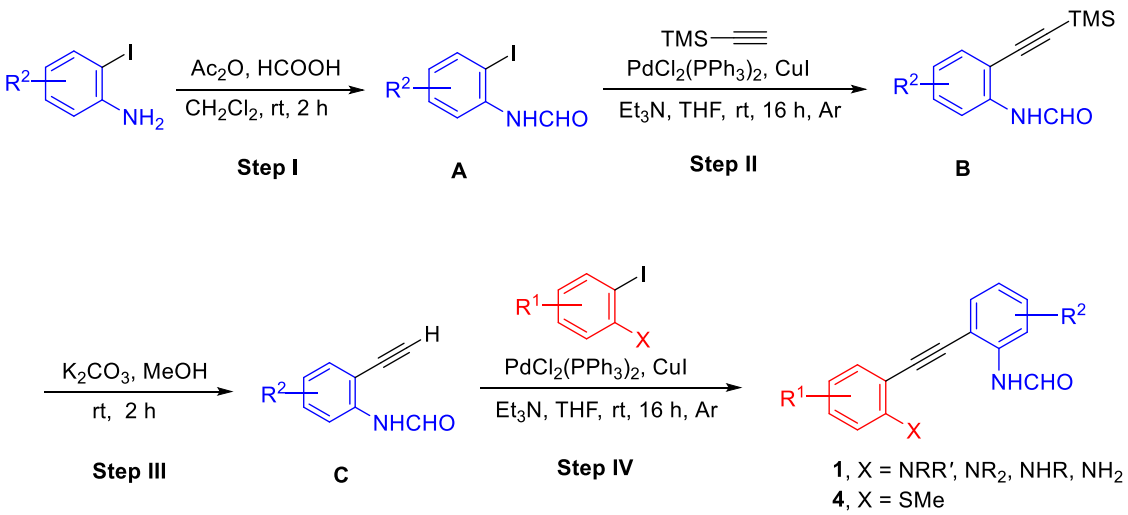
1. General information

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker DPX−400, a Bruker Avance−500 or a JEOL−400 spectrometer using deuterochloroform ($CDCl_3$) or deuterated dimethyl sulfoxide (DMSO-d_6) as the solvents. Chemical shifts for ^{1}H and ^{13}C NMR spectra were reported in parts per million (ppm, δ). The chemical shift of ^{1}H NMR spectra is reported with reference to tetramethylsilane (δ = 0.00 ppm) as the internal reference, while the chemical shift of ^{13}C NMR spectra is reported with reference to $CDCl_3$ at 77.0 ppm or DMSO-d_6 at 39.5 ppm. Coupling constants (J) were reported in hertz (Hz). Infrared spectra were recorded on a Bruker ALPHA FT-IR spectrometer and only partial data were reported in cm^{-1}. High-resolution mass spectra (HRMS) were recorded on a Bruker micro TOF in the electrospray ionization (ESI) mode. Melting points were determined on a Buchi Melting Point M−565 apparatus. UV−vis spectra were recorded on an UV−vis spectrophotometer (Shimadzu UV−2600) and fluorescence spectra were recorded on a spectrofluorometer (Horiba FluoroMax4+, integration time 0.1 sec, slit width 3 nm). The fluorescence quantum yields were measured by comparing between solvents as a blank and sample according to this equation (original from Horiba with sphere cuvette correction): Φ = Δ Area under emission curve /Δ Area under absorption curve the default mode for quantum yield measurement was set at integration time 1.0 sec, slit width 3−5 nm.

All chemicals and solvents were purchased and used without prior purification unless otherwise noted. Reactions were monitored by thin-layer chromatography (TLC) and visualized by UV. *N*-(2-Arylethynyl)phenyl)formamides (**1** or **4**) were synthesized according to literature procedures.[1-2] All reagents and solvents were obtained from commercial sources and used without further purification. Reactions were monitored by Thin-Layer Chromatography (TLC) using silica gel 60 PF_{254} aluminum sheets. Column chromatography was performed using silica gel 60 (particle size 0.06−0.2 mm; 70−230 mesh ASTM).

2. Preparation of formamides 1 and 4[1-2]



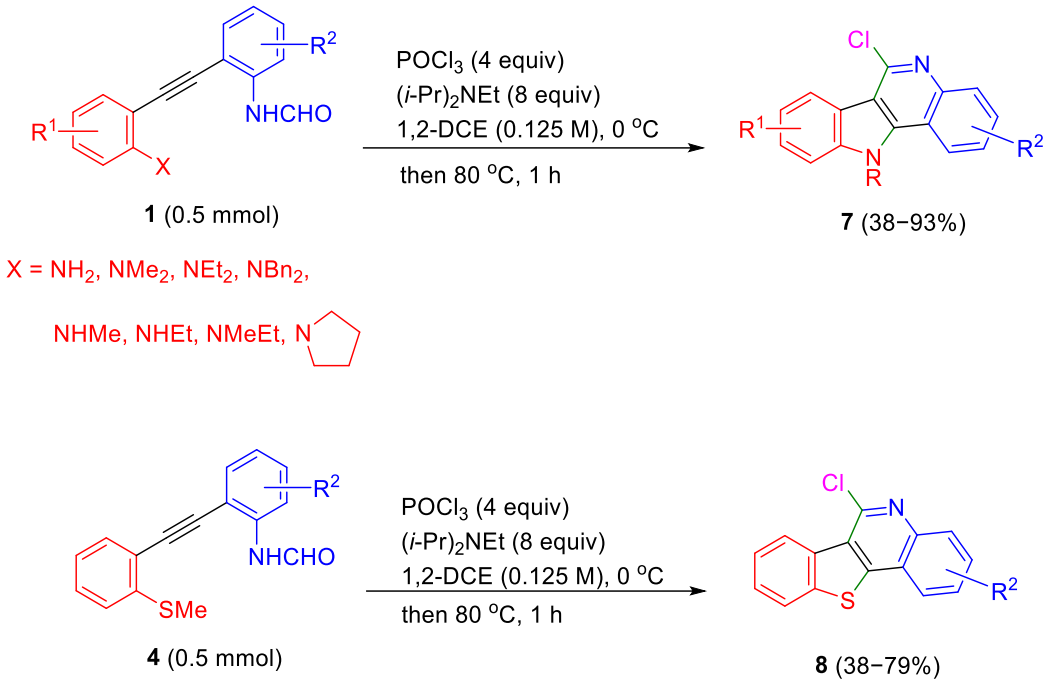
Step I: To a round-bottomed flask filled with formic acid (40.0 mmol, 4.0 equiv) was added Ac_2O (20.0 mmol, 2.0 equiv) at room temperature, and the resulting mixture was stirred for 10 minutes. To this mixture was added a solution of 2-iodoaniline derivative (10.0 mmol, 1.0 equiv) in CH_2Cl_2 (40 mL), and then the reaction mixture was further stirred at room temperature for 2 h. The reaction was quenched with H_2O (20 mL) and the resulting mixture was extracted with CH_2Cl_2 (3 × 20 mL). The combined organic layers were washed with brine (20 mL), dried (anh. Na_2SO_4), filtered and concentrated under reduced pressure (aspirator) to yield the corresponding *N*-(2-iodoaryl)formamide derivative (**A**) which was used in the coupling reaction without prior purification.

Step II: To a two-necked flask containing **A** (10.0 mmol, 1.0 equiv), $PdCl_2(PPh_3)_2$ (91.2 mg, 0.13 mmol, 0.013 equiv), and CuI (19.0 mg, 0.1 mmol, 0.01 equiv) was added Et_3N (10 mL) and THF (10 mL) at room temperature under argon atmosphere. Then, ethynyltrimethylsilane (11.0 mmol, 1.1 equiv) was added dropwise to the reaction mixture. The reaction was allowed to stir at room temperature under argon atmosphere for overnight (16 h). The reaction was quenched with saturated aqueous NH_4Cl (20 mL) and the resulting mixture was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine (20 mL), dried (anh. Na_2SO_4), filtered and concentrated under reduced pressure (aspirator). The crude product was purified by column chromatography on silica gel using EtOAc/hexane as the eluent to afford the corresponding *N*-(2-((trimethylsilyl)ethynyl) phenyl)formamide derivative (**B**).

Step III: To a round-bottomed containing **B** (10.0 mmol, 1.0 equiv) and K_2CO_3 (20.0 mmol, 2.0 equiv) was added MeOH (20 mL). Next, the reaction was stirred at room temperature for 2 h. The reaction was quenched with saturated aqueous NH_4Cl (20 mL) and the resulting mixture was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine (20 mL), dried (anh. Na_2SO_4), filtered and concentrated under reduced pressure (aspirator) to provide the corresponding *N*-(2-ethynylphenyl)formamide derivative (**C**) which was used in the coupling reaction without prior purification.

Step IV: To a two-necked flask containing 2-iodoaniline derivative or (2-iodophenyl)(methyl) sulfane (10.0 mmol, 1.0 equiv), $PdCl_2(PPh_3)_2$ (91.2 mg, 0.13 mmol, 0.013 equiv), and CuI (19.0 mg, 0.1 mmol, 0.01 equiv) was added Et_3N (10 mL) at room temperature under argon atmosphere. Next, a solution of **C** (11.0 mmol, 1.1 equiv) in THF (10.0 mL) was added dropwise to the reaction mixture. The reaction was allowed to stir at room temperature under argon atmosphere for overnight (16 h). The reaction was quenched with saturated aqueous NH_4Cl (20 mL) and the resulting mixture was extracted with EtOAc (3 × 20 mL). The combined organic layers were washed with brine (20 mL), dried (anh. Na_2SO_4), filtered and concentrated under reduced pressure (aspirator). The crude product was purified by column chromatography on silica gel using EtOAc/hexane as the eluent to obtain the corresponding formamide (**1** or **4)**.

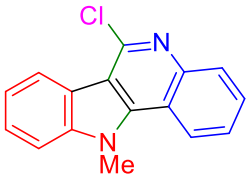
3. Preparation of 6-chloro-indolo[3,2-*c*]quinolines 7 and 6-chloro-benzothieno[3,2-*c*]quinolines 8



To a round-bottomed flask containing **1** or **4** (0.5 mmol, 1.0 equiv) in 1,2-dichloroethane (1,2-DCE) (4.0 mL, 0.125 M) was treated with (*i*-Pr)$_2$NEt (4.0 mmol, 8.0 equiv) and $POCl_3$ (2.0 mmol, 4.0 equiv) at 0 °C. Next, the reaction mixture was stirred at 80 °C for 1 h. The reaction mixture was quenched with H_2O (5 mL) and the residue was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layers were washed with brine (20 mL), dried (anh. Na_2SO_4), filtered and concentrated under reduced pressure (aspirator). The crude product was purified by column chromatography on silica gel using acetone/hexane, CH_2Cl_2/hexane, or EtOAc/hexane as the eluent to provide the corresponding product **7** or **8**.

4. Characterization data of compounds 7–9

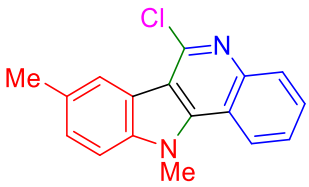
6-Chloro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7a)[3]



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7a** (102.4 mg, 77%) as a pale yellow solid; mp = 139.2−140.5 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.59 (d, J = 7.6 Hz, 1H), 8.40 (d, J = 8.4 Hz, 1H), 8.11 (d, J = 8.8 Hz, 1H), 7.74 (td, J = 7.6, 1.2 Hz, 1H), 7.60 (t, J = 7.8 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.33 (t, J = 7.6 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 146.9, 142.8, 135.6, 129.4, 128.5, 127.8, 124.2, 124.0, 123.6, 122.3, 120.3, 119.8, 115.6, 108.5, 27.8 ppm; IR (ATR): 3051, 2929, 1628, 1600, 1470, 1393, 745 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{12}ClN_2$ 267.0684; found 267.0686.

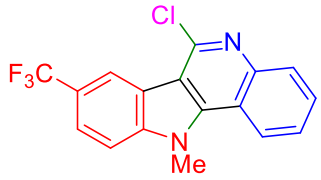
6-Chloro-8,11-dimethyl-11*H*-indolo[3,2-*c*]quinoline (7b)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7b** (96.7 mg, 65%) as a pale yellow solid; mp = 183.6−184.5 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (d, J = 6.8 Hz, 1H), 8.39 (s, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.74 (t, J = 7.6 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.28 (d, J = 8.4 Hz, 1H), 3.94 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 146.8, 140.9, 135.4, 129.8, 129.6, 129.3, 127.6, 124.3, 124.0, 123.5, 122.2, 119.8, 115.5, 108.2, 27.8, 21.5 ppm; IR (ATR): 3060, 2918, 1631, 1605, 1480, 1386, 746 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{14}ClN_2$ 281.0840; found 281.0847.

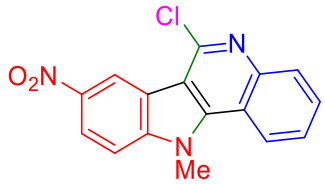
6-Chloro-11-methyl-8-(trifluoromethyl)-11*H*-indolo[3,2-*c*]quinoline (7c)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7c** (148.4 mg, 87%) as an off white solid; mp = 161.8−162.7 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.62 (s, 1H), 8.22 (d, J = 8.4 Hz, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.72−7.66 (m, 2H), 7.46 (t, J = 7.6 Hz, 1H), 7.24 (d, J = 8.4 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.1, 146.9, 144.0, 136.1, 129.8, 127.8, 125.2 (q, $J_{C,F}$ = 3.4 Hz, CH), 124.9 (q, $J_{C,F}$ = 270.0 Hz, CF_3), 124.1, 124.0, 122.6 (q, $J_{C,F}$ = 32.3 Hz, C), 122.1, 121.0 (q, $J_{C,F}$ = 3.9 Hz, CH), 119.2, 114.3, 108.3, 27.8 ppm; IR (ATR): 3045, 2921, 1634, 1610, 1480, 1388, 1242 (-CF_3), 1151 (-CF), 753 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{11}ClF_3N_2$ 335.0557; found 335.0554.

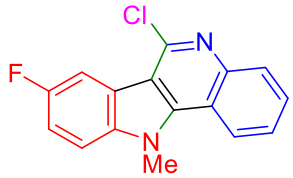
6-Chloro-11-methyl-8-nitro-11*H*-indolo[3,2-*c*]quinoline (7d)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 3:2 v/v) to afford **7d** (71.7 mg, 46%) as a yellow solid; mp = 304.4−305.2 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.45 (d, J = 2.0 Hz, 1H), 8.54 (dd, J = 9.0, 2.2 Hz, 1H), 8.44 (d, J = 8.4 Hz, 1H), 8.16 (d, J = 8.8 Hz, 1H), 7.83 (td, J = 7.6, 1.2 Hz, 1H), 7.63 (td, J = 7.6, 0.8 Hz, 1H), 7.46 (d, J = 9.2 Hz, 1H), 4.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.8, 147.5, 146.2, 141.6, 137.2, 130.5, 128.2, 124.9, 124.5, 124.3, 122.7, 120.3, 119.7, 114.7, 108.2, 28.3 ppm; IR (ATR): 3067, 2921, 1637, 1603, 1488 (-NO), 1471, 1390, 1320 (-NO), 754 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+Na]^+$ calcd for $C_{16}H_{10}ClN_3O_2Na$ 334.0354; found 334.0355.

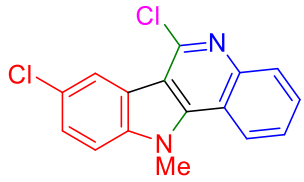
6-Chloro-8-fluoro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7e)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7e** (92.4 mg, 59%) as a pale yellow solid; mp = 180.5−181.7 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, J = 8.4 Hz, 1H), 8.25 (dd, J = 8.8, 2.0 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.75 (td, J = 7.6, 1.2 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.36−7.27 (m, 2H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.6 (d, $J_{C,F}$ = 235.6 Hz, CF), 152.6, 147.2, 138.9, 136.1, 129.8, 127.7, 124.1, 123.8, 122.0, 120.1 (d, $J_{C,F}$ = 9.8 Hz, C), 115.9 (d, $J_{C,F}$ = 24.8 Hz, CH), 115.1, 110.4 (d, $J_{C,F}$ = 25.3 Hz, CH), 108.9 (d, $J_{C,F}$ = 8.8 Hz, CH), 27.9 ppm; IR (ATR): 3031, 2921, 1630, 1609, 1479, 1382, 1114 (-CF), 752 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}ClFN_2$ 285.0589; found 285.0591.

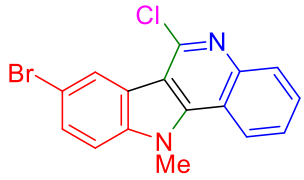
6,8-Dichloro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7f)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7f** (96.5 mg, 58%) as a pale yellow solid; mp = 195.4−196.7 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (d, J = 2.0 Hz, 1H), 8.33 (d, J = 8.4 Hz, 1H), 8.06 (d, J = 8.4 Hz, 1H), 7.73 (td, J = 7.7, 1.0 Hz, 1H), 7.53−7.48 (m, 2H), 7.23 (d, J = 8.4 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.2, 147.1, 140.9, 136.1, 129.8, 128.4, 127.8, 125.7, 124.1, 123.9, 123.6, 122.1, 120.6, 114.5, 109.3, 27.9 ppm; IR (ATR): 3045, 2918, 1633, 1601, 1472, 1387, 752 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}Cl_2N_2$ 301.0294; found 301.0296.

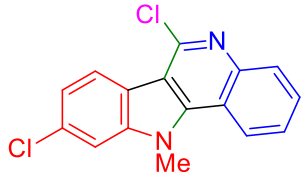
8-Bromo-6-chloro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7g)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7g** (103.5 mg, 54%) as a pale yellow solid; mp = 205.9−206.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 8.30 (d, J = 8.4 Hz, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.72 (t, J = 7.6 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.50 (t, J = 7.6 Hz, 1H), 7.15 (d, J = 8.8 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0, 147.0, 141.1, 136.1, 131.0, 129.8, 127.7, 126.5, 124.0, 123.9, 122.1, 121.1, 114.3, 112.9, 109.8, 27.8 ppm; IR (ATR): 3073, 2919, 1631, 1598, 1470, 1383, 751, 627 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}BrClN_2$ 346.9768; found 346.9763.

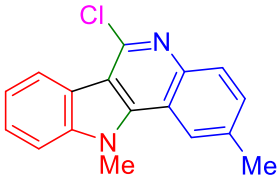
6,9-Dichloro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7h)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7h** (80.4 mg, 52%) as a pale yellow solid; mp = 206.8−207.4 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (d, J = 8.4 Hz, 1H), 8.34 (dd, J = 8.4, 0.8 Hz, 1H), 8.08 (d, J = 8.4 Hz, 1H), 7.74 (ddd, J = 8.3, 6.9, 1.3 Hz, 1H), 7.53 (td, J = 7.6, 1.2 Hz, 1H), 7.32 (d, J = 1.6 Hz, 1H), 7.26 (dd, J = 8.2, 1.8 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 146.8, 143.3, 135.6, 134.5, 129.6, 127.8, 124.8, 124.0, 123.9, 122.3, 120.6, 118.2, 114.8, 108.9, 27.9 ppm; IR (ATR): 3067, 2919, 1632, 1598, 1470, 1392, 745 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}Cl_2N_2$ 301.0294; found 301.0297.

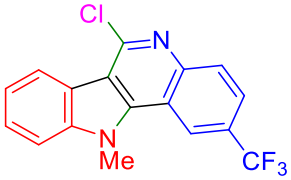
6-Chloro-2,11-dimethyl-11*H*-indolo[3,2-*c*]quinoline (7i)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7i** (114.2 mg, 75%) as a pale yellow solid; mp = 178.7−179.4° C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.59 (d, J = 7.6 Hz, 1H), 8.14 (s, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.61−7.55 (m, 2H), 7.38 (d, J = 8.0 Hz, 1H), 7.32 (t, J = 7.4 Hz, 1H), 3.94 (s, 3H), 2.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0, 145.4, 142.7, 134.9, 133.4, 131.7, 128.4, 127.4, 124.1, 122.8, 122.1, 120.1, 119.8, 115.4, 108.4, 27.8, 21.7 ppm; IR (ATR): 3048, 2917, 1633, 1602, 1473, 1395, 733 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{14}ClN_2$ 281.0840; found 281.0845.

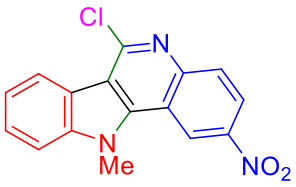
6-Chloro-11-methyl-2-(trifluoromethyl)-11*H*-indolo[3,2-*c*]quinoline (7j)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7j** (165.9 mg, 83%) as a pale yellow solid; mp = 192.4−193.5 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.61 (t, J = 0.8 Hz, 1H), 8.50 (dt, J = 8.0, 1.0 Hz, 1H), 8.11 (dt, J = 8.8, 0.7 Hz, 1H), 7.85 (dd, J = 9.0, 2.2 Hz, 1H), 7.59 (ddd, J = 8.2, 7.3, 1.1 Hz, 1H), 7.35−7.31 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0, 147.7, 142.6, 135.8, 129.1, 128.7, 125.2 (q, $J_{C,F}$ = 32.3 Hz, C), 124.8 (q, $J_{C,F}$ = 2.5 Hz, CH), 124.4 (q, $J_{C,F}$ = 270.1 Hz, CF_3), 124.2, 122.1 (q, $J_{C,F}$ = 4.4 Hz, CH), 121.0, 120.8, 119.1, 116.2, 108.7, 27.7 ppm; IR (ATR): 3064, 2933, 1626, 1605, 1472, 1398, 1248 (-CF_3), 1156 (-CF), 742 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{11}ClF_3N_2$ 335.0557; found 335.0562.

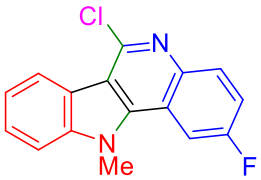
6-Chloro-11-methyl-2-nitro-11*H*-indolo[3,2-*c*]quinoline (7k)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 3:2 v/v) to afford **7k** (80.2 mg, 51%) as a yellow solid; mp = 257.6−258.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.31 (s, 1H), 8.58 (d, J = 7.6 Hz, 1H), 8.45 (dd, J = 9.2, 2.0 Hz, 1H), 8.12 (d, J = 9.2 Hz, 1H), 7.68 (t, J = 7.6 Hz, 1H), 7.46−7.40 (m, 2H), 3.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.0, 149.2, 143.2, 142.9, 136.8, 129.7, 129.0, 124.6, 122.8, 121.7, 121.5, 120.9, 119.2, 117.2, 109.1, 28.0 ppm; IR (ATR): 3084, 2919, 1633, 1603, 1519 (-NO), 1470, 1397, 1326 (-NO), 736 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}ClN_3O_2$ 312.0534; found 312.0538.

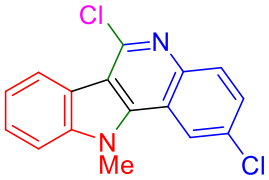
6-Chloro-2-fluoro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7l)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7l** (98.9 mg, 68%) as a pale yellow solid; mp = 151.1−152.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (d, J = 8.0 Hz, 1H), 8.07 (dd, J = 9.2, 5.2 Hz, 1H), 7.98 (dd, J = 10.0, 2.8 Hz, 1H), 7.61 (t, J = 7.8 Hz, 1H), 7.49 (td, J = 8.6, 2.4 Hz, 1H), 7.39−7.32 (m, 2H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.7 (d, $J_{C,F}$ = 243.7 Hz, CF), 151.6, 143.4, 142.6, 134.1, 129.7 (d, $J_{C,F}$ = 9.4 Hz, CH), 128.7, 124.0, 122.3 (d, $J_{C,F}$ = 9.6 Hz, C), 120.2, 119.2, 119.1 (d, $J_{C,F}$ = 25.7 Hz, CH), 115.6, 108.3, 107.3 (d, $J_{C,F}$ = 25.9 Hz, CH), 27.5 ppm; IR (ATR): 3051, 2920, 1633, 1602, 1473, 1396, 1107 (-CF), 739 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}ClFN_2$ 285.0589; found 285.0590.

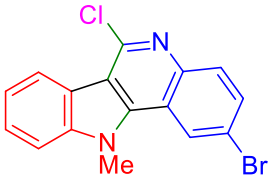
2,6-Dichloro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7m)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7m** (139.2 mg, 89%) as a pale yellow solid; mp = 171.4−172.5 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.54 (d, J = 7.6 Hz, 1H), 8.31 (d, J = 2.4 Hz, 1H), 8.00 (d, J = 8.8 Hz, 1H), 7.65−7.59 (m, 2H), 7.39−7.32 (m, 2H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.3, 145.1, 142.8, 134.3, 130.1, 129.3, 129.2, 128.9, 124.3, 122.9, 122.8, 120.5, 119.4, 116.0, 108.6, 27.8 ppm; IR (ATR): 3058, 2917, 1632, 1603, 1471, 1395, 735 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}Cl_2N_2$ 301.0294; found 301.0297.

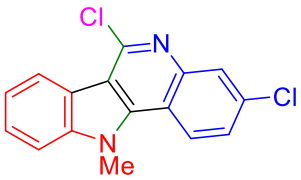
2-Bromo-6-chloro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7n)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 3:2 v/v) to afford **7n** (101.8 mg, 57%) as a pale yellow solid; mp = 193.7−194.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.48 (d, J = 7.6 Hz, 1H), 8.41 (d, J = 1.6 Hz, 1H), 7.88 (d, J = 8.8 Hz, 1H), 7.72 (dd, J = 8.8, 1.6 Hz, 1H), 7.58 (t, J = 7.6 Hz, 1H), 7.33−7.29 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.2, 145.2, 142.7, 134.0, 132.5, 129.3, 128.9, 126.1, 124.2, 123.2, 120.5, 119.3, 117.1, 115.8, 108.6, 27.7 ppm; IR (ATR): 3056, 2919, 1632, 1602, 1470, 1394, 733, 625 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}BrClN_2$ 346.9768; found 346.9765.

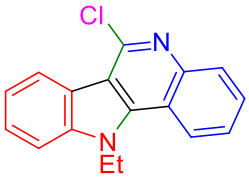
3,6-Dichloro-11-methyl-11*H*-indolo[3,2-*c*]quinoline (7o)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7o** (102.2 mg, 66%) as a pale yellow solid; mp = 188.4−189.6 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (d, J = 7.6 Hz, 1H), 8.19 (d, J = 9.2 Hz, 1H), 7.99 (d, J = 2.0 Hz, 1H), 7.53 (t, J = 7.4 Hz, 1H), 7.36 (dd, J = 9.0, 1.8 Hz, 1H), 7.32−7.19 (m, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.8, 146.1, 141.6, 134.3, 131.0, 127.7, 125.6, 124.3, 123.4, 123.1, 121.7, 119.6, 118.5, 114.6, 107.6, 26.8 ppm; IR (ATR): 3054, 2918, 1631, 1600, 1473, 1392, 738 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}Cl_2N_2$ 301.0294; found 301.0295.

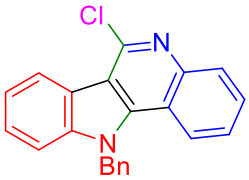
6-Chloro-11-ethyl-11*H*-indolo[3,2-*c*]quinoline (7p)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, acetone/hexane, 2:3 v/v) to afford **7p** (123.5 mg, 85%) as a yellow solid; mp = 131.5−132.7 °C.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.61 (d, J = 7.6 Hz, 1H), 8.39 (dd, J = 8.4, 0.8 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 7.73 (ddd, J = 8.4, 7.0, 1.4 Hz, 1H), 7.59 (td, J = 7.8, 1.1 Hz, 1H), 7.52 (ddd, J = 8.4, 7.1, 1.1 Hz, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.32 (td, J = 7.6, 0.8 Hz, 1H), 4.55 (q, J = 7.2 Hz, 2H), 1.48 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.7, 146.9, 141.8, 135.5, 129.3, 128.4, 127.8, 124.3, 124.0, 123.5, 122.2, 120.1, 119.9, 115.6, 108.7, 36.2, 13.6 ppm; IR (ATR): 3051, 2925, 1632, 1602, 1468, 1396, 735 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{17}H_{14}ClN_2$ 281.0840; found 281.0842.

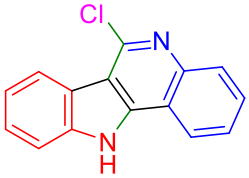
11-Benzyl-6-chloro-11*H*-indolo[3,2-*c*]quinoline (7q)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **7q** (162.6 mg, 93%) as a pale yellow solid; mp = 172.9−173.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (d, J = 8.0 Hz, 1H), 8.44 (dd, J = 8.4, 0.8 Hz, 1H), 8.12 (d, J = 8.4 Hz, 1H), 7.75 (td, J = 7.6, 1.2 Hz, 1H), 7.58−7.49 (m, 2H), 7.34−7.22 (m, 7H), 5.74 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.3, 147.0, 142.0, 137.0, 135.7, 129.4, 128.7 (2C), 128.5, 128.0, 127.5, 127.2 (2C), 124.2, 124.0, 123.8, 122.5, 120.5, 120.1, 115.5, 109.5, 45.1 ppm; IR (ATR): 3065, 2920, 1628, 1602, 1467, 744 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{22}H_{16}ClN_2$ 343.0997; found 343.0996.

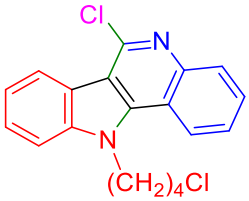
6-Chloro-11*H*-indolo[3,2-*c*]quinoline (7r)[4]



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, acetone/hexane, 2:3 v/v) to afford **7r** (51.2 mg, 38%) as an off white solid; mp = 280.0−281.3 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, DMSO-d_6): δ 12.04 (s, 1H), 8.53 (d, J = 7.6 Hz, 1H), 8.38 (d, J = 8.0 Hz, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.83 (td, J = 7.6, 1.2 Hz, 1H), 7.65−7.60 (m, 2H), 7.55 (d, J = 8.0 Hz, 1H), 7.35 (t, J = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 152.6, 146.6, 141.7, 134.1, 129.7, 129.1, 127.5, 124.1, 123.7, 123.5, 121.4, 120.2, 119.2, 115.2, 111.2 ppm; IR (ATR): 3139 (-NH), 3071, 2927, 1613, 1572, 734 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{15}H_{10}ClN_2$ 253.0527; found 253.0526.

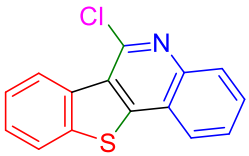
6-Chloro-11-(4-chlorobutyl)-11*H*-indolo[3,2-*c*]quinoline (7s)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 3:2 v/v) to afford **7s** (146.8 mg, 82%) as a pale yellow solid; mp = 121.7−122.9 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, J = 7.6 Hz, 1H), 8.34 (dd, J = 8.8, 1.2 Hz, 1H), 8.06 (d, J = 7.2 Hz, 1H), 7.70 (ddd, J = 8.4, 6.8, 1.6 Hz, 1H), 7.54 (ddd, J = 8.3, 7.3, 1.1 Hz, 1H), 7.49 (ddd, J = 8.3, 6.9, 1.3 Hz, 1H), 7.34 (d, J = 8.0 Hz, 1H), 7.29 (td, J = 7.6, 0.7 Hz, 1H), 4.47 (t, J = 7.0 Hz, 2H), 3.60 (t, J = 6.4 Hz, 2H), 2.11−2.03 (m, 2H), 1.85−1.78 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0, 146.8, 141.8, 135.5, 129.3, 128.4, 127.8, 124.2, 123.9, 123.6, 122.2, 120.2, 119.8, 115.3, 108.6, 44.5, 40.4, 29.7, 25.7 ppm; IR (ATR): 3054, 2924, 1628, 1601, 1466, 744 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{19}H_{17}Cl_2N_2$ 343.0763; found 343.0764.

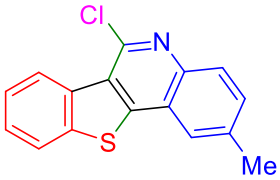
6-Chlorobenzo[4,5]thieno[3,2-*c*]quinoline (8a)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **8a** (107.8 mg, 79%) as an off white solid; mp = 196.2−197.9 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.99−8.97 (m, 1H), 8.47 (dt, J = 8.8, 0.7 Hz, 1H), 8.13 (dt, J = 8.4, 0.4 Hz, 1H), 7.86−7.84 (m, 1H), 7.81 (ddd, J = 8.3, 6.9, 1.3 Hz, 1H), 7.66 (ddd, J = 8.3, 6.9, 1.3 Hz, 1H), 7.57 (td, J = 7.1, 1.6 Hz, 1H), 7.53 (td, J = 7.2, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.1, 147.3, 138.4, 137.3, 132.2, 130.3, 128.6, 128.2, 126.5, 126.4, 125.2, 125.0, 124.3, 124.1, 122.8 ppm; IR (ATR): 3056, 2921, 1614, 1574, 1482, 727 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{15}H_9ClNS$ 270.0139; found 270.0142.

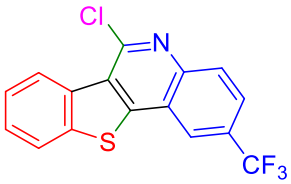
6-Chloro-2-methylbenzo[4,5]thieno[3,2-*c*]quinoline (8b)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **8b** (102.0 mg, 72%) as a white solid; mp = 167.6−168.4 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.91 (dd, J = 8.0, 0.8 Hz, 1H), 8.15 (s, 1H), 7.97 (d, J = 8.8 Hz, 1H), 7.81 (dd, J = 6.8, 1.2 Hz, 1H), 7.57 (dd, J = 8.4, 1.6 Hz, 1H), 7.54−7.46 (m, 2H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.1, 146.0, 138.5, 136.6, 136.5, 132.7, 132.3, 128.5, 128.0, 126.5, 125.1, 125.0, 124.0, 123.0, 122.8, 22.0 ppm; IR (ATR): 3057, 2911, 1623, 1574, 1490, 1462, 1373, 722 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_{11}ClNS$ 284.0295; found 284.0300.

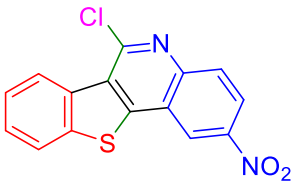
6-Chloro-2-(trifluoromethyl)benzo[4,5]thieno[3,2-*c*]quinoline (8c)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **8c** (99.3 mg, 58%) as a white solid; mp = 186.6−187.7 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.96−8.94 (m, 1H), 8.76 (t, J = 0.8 Hz, 1H), 8.21 (d, J = 9.2 Hz, 1H), 7.95 (dd, J = 9.0, 1.8 Hz, 1H), 7.87−7.84 (m, 1H), 7.60 (td, J = 7.5, 1.3 Hz, 1H), 7.55 (td, J = 7.6, 1.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.6, 148.0, 138.6, 137.9, 131.7, 129.6, 129.3, 128.3 (q, $J_{C,F}$ = 32.7 Hz, C), 126.8, 126.7 (q, $J_{C,F}$ = 271.7 Hz, CF_3), 126.3, 126.0 (q, $J_{C,F}$ = 3.2 Hz, CH), 125.5, 123.3, 123.0, 122.7 (q, $J_{C,F}$ = 4.8 Hz, CH) ppm; IR (ATR): 3062, 1629, 1574, 1499, 1243 (-CF_3), 1115 (-CF), 728 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{16}H_8ClF_3NS$ 338.0013; found 338.0012.

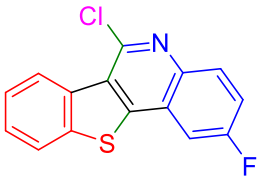
6-Chloro-2-nitrobenzo[4,5]thieno[3,2-*c*]quinoline (8d)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **8d** (58.8 mg, 38%) as a pale yellow solid; mp = 295.1−296.4 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 9.46 (d, J = 2.4 Hz, 1H), 9.03−9.01 (m, 1H), 8.57 (dd, J = 9.2, 2.8 Hz, 1H), 8.25 (d, J = 9.2 Hz, 1H), 7.92−7.90 (m, 1H), 7.67 (td, J = 7.5, 1.5 Hz, 1H), 7.62 (td, J = 7.6, 1.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.3, 148.8, 145.3, 138.6, 138.5, 131.3, 130.2, 129.7, 127.0, 126.9, 125.8, 123.7, 123.3, 123.1, 121.9 ppm; IR (ATR): 3065, 2839, 1619, 1578, 1516 (-NO), 1475, 1335 (-NO), 738 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{15}H_8ClN_2O_2S$ 314.9990; found 314.9993.

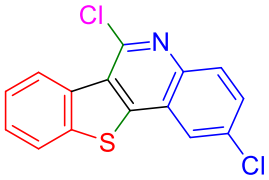
6-Chloro-2-fluorobenzo[4,5]thieno[3,2-*c*]quinoline (8e)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **8e** (95.7 mg, 65%) as a white solid; mp = 200.3−201.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.92 (dt, J = 8.4, 0.8 Hz, 1H), 8.10 (dd, J = 9.4, 5.4 Hz, 1H), 8.04 (dd, J = 10.2, 3.0 Hz, 1H), 7.83 (ddd, J = 7.9, 1.3, 0.5 Hz, 1H), 7.59−7.50 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4, 160.6 (d, $J_{C,F}$ = 247.1 Hz, CF), 144.3, 138.8, 136.2, 131.8, 130.8 (d, $J_{C,F}$ = 9.2 Hz, CH), 129.0, 126.7, 125.7, 125.2, 125.0 (d, $J_{C,F}$ = 10.0 Hz, C), 122.9, 120.7 (d, $J_{C,F}$ = 26.1 Hz, CH), 108.0 (d, $J_{C,F}$ = 24.9 Hz, CH) ppm; IR (ATR): 3052, 2914, 1625, 1574, 1489, 1185 (-CF), 725 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{15}H_8ClFNS$ 288.0045; found 288.0047.

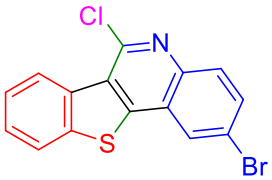
2,6-Dichlorobenzo[4,5]thieno[3,2-*c*]quinoline (8f)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **8f** (92.0 mg, 60%) as a white solid; mp = 245.9−246.7 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.94 (d, J = 8.0 Hz, 1H), 8.42 (d, J = 2.4 Hz, 1H), 8.04 (d, J = 8.8 Hz, 1H), 7.85 (dd, J = 7.2, 1.2 Hz, 1H), 7.71 (dd, J = 9.2, 2.4 Hz, 1H), 7.58 (td, J = 7.5, 1.3 Hz, 1H), 7.53 (td, J = 7.6, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.5, 145.7, 138.7, 132.6, 131.9, 131.3, 129.9, 129.1, 126.8, 125.9, 125.3, 124.9, 123.3 (2C), 123.0 ppm; IR (ATR): 3042, 2965, 1604, 1570, 1472, 725 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{15}H_8Cl_2NS$ 303.9749; found 303.9752.

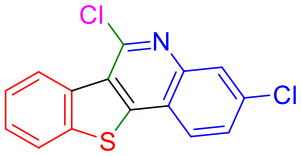
2-Bromo-6-chlorobenzo[4,5]thieno[3,2-*c*]quinoline (8g)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **8g** (118.3 mg, 67%) as a pale brown solid; mp = 241.6−242.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.97 (dt, J = 8.2, 0.9 Hz, 1H), 8.62 (d, J = 2.0 Hz, 1H), 7.99 (d, J = 8.8 Hz, 1H), 7.88−7.84 (m, 2H), 7.60 (td, J = 7.5, 1.3 Hz, 1H), 7.55 (td, J = 7.7, 1.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.5, 145.8, 138.7, 136.0, 133.8, 131.9, 129.9, 129.1, 129.0, 126.8, 126.6, 125.9, 125.3, 123.0, 120.7 ppm; IR (ATR): 3037, 2919, 1600, 1571, 1471, 725, 644 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{15}H_8BrClNS$ 347.9244; found 347.9253.

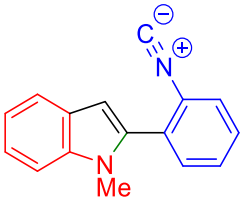
3,6-Dichlorobenzo[4,5]thieno[3,2-*c*]quinoline (8h)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **8h** (109.9 mg, 72%) as an off white solid; mp = 219.9−221.3 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.92 (dd, J = 8.0, 1.2 Hz, 1H), 8.37 (d, J = 9.2 Hz, 1H), 8.09 (d, J = 2.0 Hz, 1H), 7.84 (dd, J = 7.6, 1.2 Hz, 1H), 7.59−7.51 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.4, 147.4, 138.4, 137.2, 136.5, 131.9, 128.9, 127.4, 127.1, 126.5, 125.7, 125.4, 125.2, 122.9, 122.6 ppm; IR (ATR): 3078, 1601, 1573, 1476, 726 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{15}H_8Cl_2NS$ 303.9749; found 303.9756.

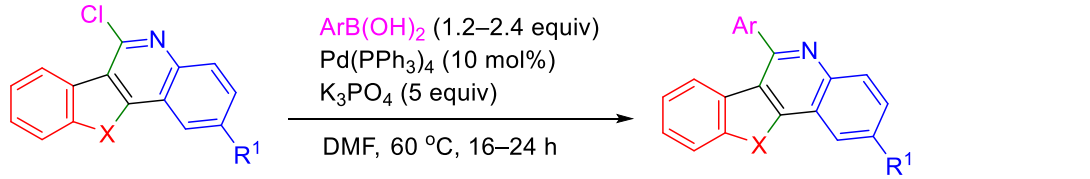
2-(2-Isocyanophenyl)-1-methyl-1*H*-indole (9a)[5-6]



Compound **9a** was prepared according to the standard reaction conditions except for the reaction was carried out at 0 °C for 1 h. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **9a** (37.5 mg, 32%) as brown oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.67 (d, J = 8.0 Hz, 1H), 7.54−7.44 (m, 4H), 7.39 (d, J = 8.0 Hz, 1H), 7.29 (ddd, J = 7.6, 7.6, 0.8 Hz, 1H), 7.17 (t, J = 7.5 Hz, 1H), 6.64 (s, 1H), 3.67 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 167.2, 138.2, 135.7, 132.1, 130.4, 129.3, 129.3, 127.7, 127.6, 126.3, 122.3, 120.9, 120.1, 109.8, 103.7, 31.1 ppm; HRMS (ESI−TOF) m/z: $[M+H]^+$ calcd for $C_{16}H_{13}N_2$ 233.1074; found 233.1075.

5. Preparation of 10aa, 10ab, 10ac, 10nb, 10pb, and 11aa (Suzuki–Miyaura cross-coupling)[7]

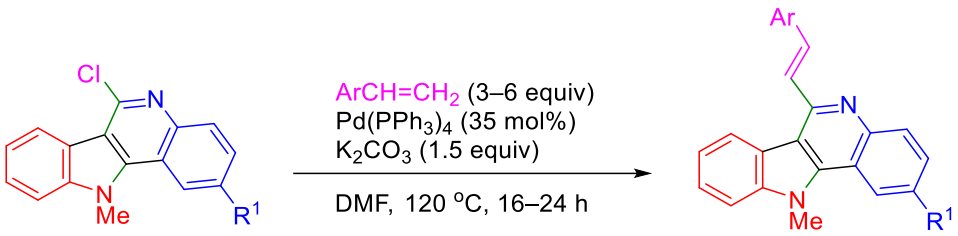


7; X = NR (0.5 mmol)
8a; X = S (0.5 mmol)

10; X = NR (32–74%)
11aa; X = S, R^1 = H, Ar = H (32%)

To a two-necked flask containing **7** or **8** (0.5 mmol, 1.0 equiv), arylboronic acid (0.6–1.2 mmol, 1.2–2.4 equiv), K_3PO_4 (2.5 mmol, 5.0 equiv), and $Pd(PPh_3)_4$ (0.05 mmol, 0.1 equiv) was added DMF (5.0 mL) at room temperature. Next, the reaction mixture was stirred at 60 °C under an argon atmosphere for 16–24 h. The reaction mixture was cooled to room temperature and the resulting mixture was extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine (20 mL), dried (anh. Na_2SO_4), filtered and concentrated under reduced pressure (aspirator). The crude product was purified by column chromatography on silica gel using CH_2Cl_2/hexane or EtOAc/hexane as the eluent to obtain the corresponding product **10** or **11**.

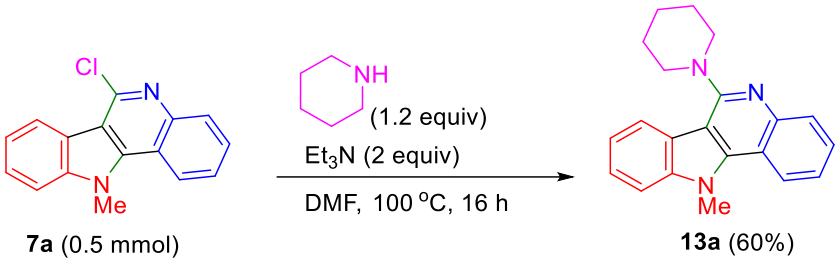
6. Preparation of 12aa, 12ab, 12ac and 12na (Heck cross-coupling)[8]



7 **12** (23–48%)

To a two-necked flask containing **7** (0.5 mmol, 1.0 equiv), K_2CO_3 (0.75 mmol, 1.5 equiv), and $Pd(PPh_3)_4$ (0.175 mmol, 0.35 equiv) was added DMF (3.0 mL) at room temperature under argon atmosphere. Next, a solution of styrene derivatives (1.5–3.0 mmol, 3.0–6.0 equiv) in DMF (2.0 mL) was added through the septum by using a syringe. The reaction mixture was heated at 120 °C under argon atmosphere for 16–24 h. After that, the reaction mixture was cooled to room temperature and the resulting mixture was extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine (20 mL), dried (anh. Na_2SO_4), filtered and concentrated under reduced pressure (aspirator). The crude product was purified by column chromatography on silica gel using EtOAc/hexane as the eluent to yield the corresponding product **12**.

7. Preparation of 11-methyl-6-(piperidin-1-yl)-11*H*-indolo[3,2-*c*]quinoline (13a)[9]

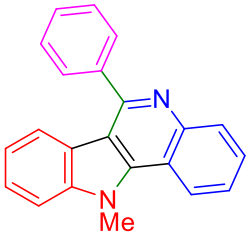


7a (0.5 mmol) **13a** (60%)

To a two-necked flask containing of **7a** (0.5 mmol, 1.0 equiv), piperidine (0.6 mmol, 1.2 equiv), and Et_3N (1.0 mmol, 2.0 equiv) was added DMF (5.0 mL) at room temperature. Next, the reaction mixture was stirred at 100 °C for overnight (16 h). The reaction mixture was cooled to room temperature and the resulting mixture was extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine (20 mL), dried (anh. Na_2SO_4), filtered and concentrated under reduced pressure (aspirator). The crude product was purified by column chromatography on silica gel using CH_2Cl_2/hexane as the eluent to give the corresponding product **13a**.

8. Characterization data of compounds 10, 11 and 13

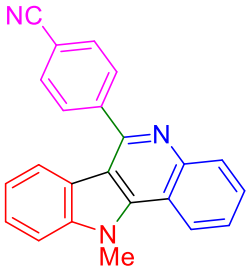
11-Methyl-6-phenyl-11*H*-indolo[3,2-*c*]quinoline (10aa)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 2:3 v/v) to afford **10aa** (99.2 mg, 64%) as a yellow solid; mp = 175.8−177.0 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, J = 8.4 Hz, 1H), 7.74−7.62 (m, 5H), 7.52−7.45 (m, 3H), 7.37−7.32 (m, 2H), 7.06 (d, J = 7.6 Hz, 1H), 6.98 (t, J = 7.4 Hz, 1H), 4.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 146.8, 142.3, 136.6, 130.0, 129.4 (2C), 128.9 (2C), 128.7, 128.5, 127.7, 127.5, 126.4, 123.7, 123.0, 122.7, 120.5, 119.7, 115.4, 108.4, 27.7 ppm; IR (ATR): 3056, 2920, 1626, 1605, 1473, 1389 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{22}H_{17}N_2$ 309.1386; found 309.1384.

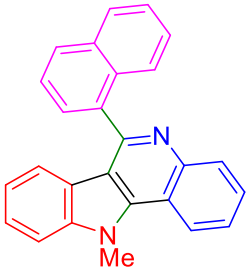
4-(11-Methyl-11*H*-indolo[3,2-*c*]quinoline-6-yl)benzonitrile (10ab)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 3:2 v/v) to afford **10ab** (125.5 mg, 74%) as a yellow solid; mp = 154.4−155.7 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.4 Hz, 2H), 7.74 (td, J = 7.6, 1.3 Hz, 1H), 7.69 (d, J = 8.4 Hz, 2H), 7.59−7.52 (m, 2H), 7.44−7.37 (m, 2H), 7.04 (t, J = 7.2 Hz, 1H), 6.98 (d, J = 7.6 Hz, 1H), 4.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.2, 146.7, 143.1, 139.0, 138.2, 134.1, 133.0, 132.3, 130.0, 129.0, 128.3, 127.9, 125.5, 123.4, 123.0, 122.6, 120.0, 119.9, 118.4, 115.9, 113.5, 108.8, 27.8 ppm; IR (ATR): 3028, 2927, 2228 (-CN), 1626, 1596, 1472, 1394 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{23}H_{16}N_3$ 334.1339; found 334.1340.

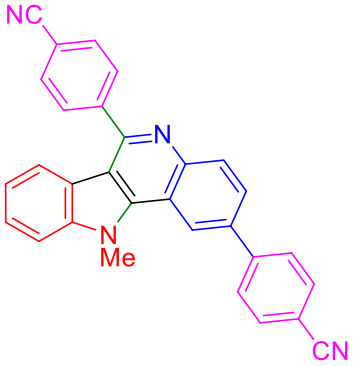
11-Methyl-6-(naphthalen-1-yl)-11*H*-indolo[3,2-*c*]quinoline (10ac)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 3:2 v/v) to afford **10ac** (112.9 mg, 63%) as an off white solid; mp = 212.3−213.4 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (dd, J = 8.4, 0.4 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 8.03 (d, J = 8.4 Hz, 1H), 7.74−7.69 (m, 2H), 7.59 (dd, J = 6.8, 1.2 Hz, 1H), 7.52−7.48 (m, 2H), 7.42 (td, J = 7.6, 1.1 Hz, 1H), 7.37 (d, J = 7.6 Hz, 1H), 7.28−7.19 (m, 3H), 6.81 (td, J = 7.4, 1.2 Hz, 1H), 6.54 (d, J = 7.6 Hz, 1H), 4.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.5, 146.8, 142.9, 140.6, 134.2, 133.7, 131.7, 128.9, 128.8, 128.4, 127.7, 127.6, 127.3, 126.7, 126.6, 126.4, 125.8 (2C), 124.4, 123.1, 122.9, 120.4, 119.8, 117.0, 108.3, 27.8 ppm; IR (ATR): 3048, 2920, 1626, 1601, 1471, 1392 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{26}H_{19}N_2$ 359.1543; found 359.1540.

4,4'-(11-Methyl-11*H*-indolo[3,2-*c*]quinoline-2,6-diyl)dibenzonitrile (10nb)

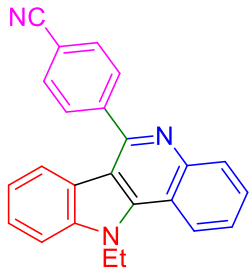


Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:4 v/v) to afford **10nb** (69.9 mg, 32%) as a yellow solid; mp = 321.2−322.7 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (dd, J = 8.8, 0.4 Hz, 1H), 8.02−7.99 (m, 2H), 7.96 (dd, J = 8.8, 2.4 Hz, 1H), 7.74−7.70 (m, 5H), 7.67−7.64 (m, 2H), 7.56 (ddd, J = 8.4, 7.2, 1.2 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.07 (td, J = 7.6, 0.8 Hz, 1H), 6.97 (ddd, J = 7.7, 1.1, 0.7 Hz, 1H), 4.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ NMR (101 MHz,) δ 152.5, 146.6, 145.2,

143.2, 141.3, 139.8, 133.9, 133.1 (2C), 132.7 (2C), 130.5 (2C), 128.8, 128.7, 128.0, 127.8 (2C), 123.9, 122.8, 122.7, 120.3, 119.7, 118.9, 118.5, 116.3, 113.1, 110.8, 109.0, 27.8 ppm; IR (ATR): 3055, 2920, 2228 (-CN), 1724, 1595, 1474, 1395 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{30}H_{19}N_4$ 435.1604; found 435.1605.

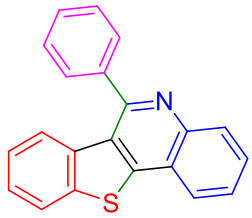
4-(11-Ethyl-11*H*-indolo[3,2-*c*]quinoline-6-yl)benzonitrile (10pb)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 3:2 v/v) to afford **10pb** (106.0 mg, 61%) as a pale yellow solid; mp = 215.5−216.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.0 Hz, 2H), 7.72 (ddd, J = 8.4, 6.8, 1.4 Hz, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.56 (dd, J = 8.4, 0.8 Hz, 1H), 7.51 (td, J = 7.5, 1.4 Hz, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.36 (ddd, J = 8.1, 6.9, 1.1 Hz, 1H), 7.02 (td, J = 7.4, 0.8 Hz, 1H), 6.97 (d, J = 7.2 Hz, 1H) 4.62 (q, J = 7.2 Hz, 2H), 1.52 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.5, 146.7, 142.1, 141.8, 139.5, 132.8 (2C), 130.5 (2C), 128.9, 128.2, 128.0, 125.5, 123.2, 122.8 (2C), 120.0, 119.7, 118.6, 115.5, 112.6, 108.9, 36.1, 13.6 ppm; IR (ATR): 3061, 2923, 2224 (-CN), 1626, 1595, 1466, 1398 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{18}N_3$ 348.1495; found 348.1498.

6-Phenylbenzo[4,5]thieno[3,2-*c*]quinoline (11aa)

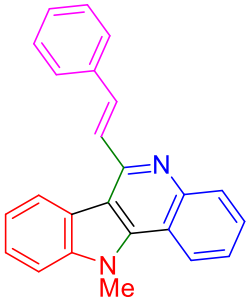


Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:9 v/v) to afford **11aa** (50.2 mg, 32%) as an off white solid; mp = 218.1−219.4 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, J = 8.4 Hz, 1H), 7.81−7.74 (m, 2H), 7.68−7.60 (m, 4H), 7.47−7.37 (m, 4H), 7.09 (t, J = 7.4 Hz, 1H), 6.78 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100

MHz, $CDCl_3$): δ 163.2, 147.1, 143.7, 138.5, 136.3, 133.0, 130.2, 129.6, 129.4 (2C), 129.0 (2C), 128.8, 128.1, 127.8, 126.6, 125.9, 125.4, 125.3, 124.6, 122.9 ppm; IR (ATR): 3036, 2917, 1568, 1553, 1479, 1441 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{14}NS$ 312.0841; found 312.0842.

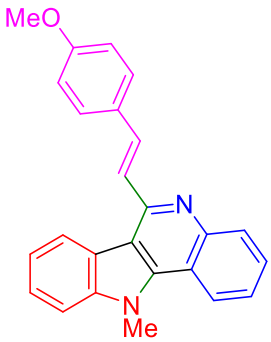
(*E*)-11-Methyl-6-styryl-11*H*-indolo[3,2-*c*]quinoline (12aa)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:19 v/v) to afford **12aa** (75.7 mg, 45%) as a yellow solid; mp = 162.9−164.2 °C (CH_2Cl_2/hexane).

^1H NMR (400 MHz, $CDCl_3$): δ 8.33 (d, J = 8.0 Hz, 1H), 8.24 (d, J = 7.6 Hz, 1H), 8.15 (d, J = 8.4 Hz, 1H), 7.90 (d, J = 16.8 Hz, 1H), 7.75−7.71 (m, 3H), 7.57−7.41 (m, 6H), 7.23−7.19 (m, 2H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.5, 146.8, 142.9, 139.1, 138.0, 136.6, 129.0 (2C), 128.8, 128.7, 127.9, 127.7, 126.9 (2C), 125.5, 123.7, 123.0, 122.8 (2C), 120.9, 119.8, 115.1, 108.5, 27.7 ppm; IR (ATR): 3057, 2922, 1635, 1589, 1470, 1389 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{19}N_2$ 335.1543; found 335.1542.

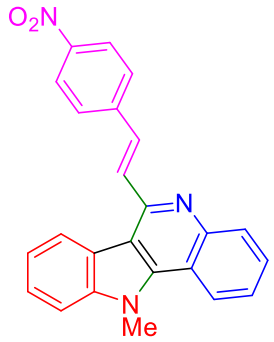
(*E*)-6-(4-Methoxystyryl)-11-methyl-11*H*-indolo[3,2-*c*]quinoline (12ab)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:19 v/v) to afford **12ab** (87.7 mg, 48%) as a yellow solid; mp = 159.4−160.6 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.31 (d, J = 8.4 Hz, 1H), 8.21 (d, J = 8.0 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 7.71 (td, J = 7.6, 1.6 Hz, 1H), 7.70 (d, J = 16.4 Hz, 1H), 7.63 (d, J = 8.8 Hz, 2H), 7.53 (td, J = 7.6, 0.8 Hz, 1H), 7.43 (td, J = 7.6, 1.2 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.21−7.14 (m, 2H), 7.01 (d, J = 8.8 Hz, 2H), 3.97 (s, 3H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.1, 152.5, 146.8, 142.8, 139.5, 137.5, 129.4, 128.7, 128.2 (2C), 127.8, 127.5, 125.5, 123.7, 123.0, 122.7, 121.0, 120.4, 119.8, 114.9, 114.4 (2C), 108.5, 55.4, 27.6 ppm; IR (ATR): 3063, 2929, 1635, 1591, 1474, 1395, 1252 (-C-O-C-) cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{25}H_{21}N_2O$ 365.1648; found 365.1645.

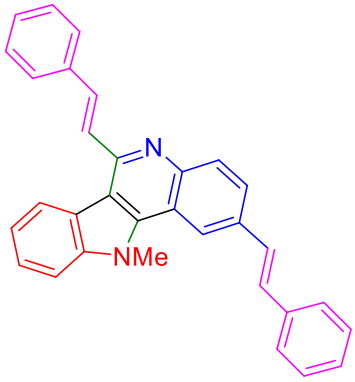
(*E*)-11-Methyl-6-(4-nitrostyryl)-11*H*-indolo[3,2-*c*]quinoline (12ac)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:19 v/v) to afford **12ac** (77.4 mg, 38%) as a orange solid; mp = 230.9−232.4 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 8.8 Hz, 2H), 8.27 (d, J = 7.6, 1H), 8.18 (d, J = 8.0 Hz, 1H), 8.14 (d, J = 7.8 Hz, 1H), 8.08 (d, J = 16.8 Hz, 1H), 7.84 (d, J = 8.4 Hz, 2H), 7.76 (ddd, J = 8.3, 6.9, 1.3 Hz, 1H), 7.59 (dt, J = 7.8, 0.8 Hz, 1H), 7.49 (dt, J = 7.6, 1.2 Hz, 1H), 7.45 (d, J = 8.4 Hz, 1H), 7.30 (d, J = 16.8 Hz, 1H), 7.23 (dt, J = 7.6, 0.8 Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 147.6, 146.8, 143.1, 142.7, 137.5, 135.7, 129.0, 128.1 (2C), 127.6, 127.4 (2C), 125.0, 124.5 (2C), 123.4, 123.2, 122.5, 120.5, 120.0, 115.1, 108.8, 27.7 ppm; IR (ATR): 3057, 2919, 1580, 1489 (-NO), 1471, 1392, 1342 (-NO) cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{24}H_{18}N_3O_2$ 380.1394; found 380.1392.

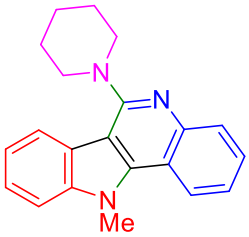
11-Methyl-2,6-di((*E*)-styryl)-11*H*-indolo[3,2-*c*]quinoline (12na)



Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, EtOAc/hexane, 1:19 v/v) to afford **12na** (50.1 mg, 23%) as a yellow solid; mp = 206.5−207.8 °C (CH_2Cl_2/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (br dd, J = 9.4, 2.0 Hz, 2H), 8.12 (d, J = 8.8 Hz, 1H), 8.03 (dd, J = 9.0, 1.8 Hz, 1H), 7.90 (d, J = 16.8 Hz, 1H), 7.75 (d, J = 7.2 Hz, 2H), 7.57−7.51 (m, 5H), 7.46−7.34 (m, 4H), 7.30−7.18 (m, 5H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 146.7, 142.8, 139.0, 138.1, 137.5, 136.6, 131.9, 129.1 (2C), 128.9, 128.8, 128.7 (2C), 128.3, 128.2, 127.7, 127.5, 127.0 (2C), 126.5 (2C), 126.0, 124.6, 123.7, 123.0, 122.7, 120.9, 120.0, 115.3, 108.6, 27.7 ppm; IR (ATR): 3024, 2919, 1586, 1472, 1391 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{32}H_{25}N_2$ 437.2013; found 437.2012.

11-Methyl-6-(piperidin-1-yl)-11*H*-indolo[3,2-*c*]quinoline (13a)

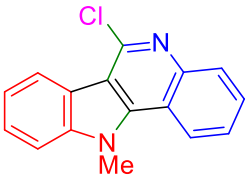


Prepared according to standard reaction conditions. Purification by column chromatography (SiO_2, CH_2Cl_2/hexane, 3:2 v/v) to afford **13a** (93.8 mg, 60%) as a yellow solid; mp = 128.7−130.5 °C (chloroform/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.52 (d, J = 7.6 Hz, 1H), 8.46 (d, J = 8.4 Hz, 1H), 8.12 (d, J = 8.4 Hz, 1H), 7.67 (td, J = 7.6, 1.2 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.43−7.37 (m, 2H), 7.31 (t, J = 7.6 Hz, 1H), 3.96 (s, 3H), 3.54 (t, J = 5.2 Hz, 4H), 1.97−1.85 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.5, 152.2, 148.4, 142.4, 128.5, 128.1, 127.2, 125.2, 124.9, 123.9, 121.8, 120.3, 119.6, 114.5, 108.2, 51.9 (2C), 27.8, 27.1 (2C), 24.7 ppm; IR (ATR): 3051, 2929,

1620, 1587, 1475, 1392 cm^{-1}; HRMS (ESI−TOF) *m/z*: $[M+H]^+$ calcd for $C_{21}H_{22}N_3$ 316.1808; found 316.1806.

9. Photophysical properties of 7a, 10ab, 10nb, 12aa and 12na



7a

ε = 22,195 $cm^{-1}M^{-1}$

λ_{abs} = 385 nm

λ_{em} = 440 nm

Φ_F = 0.05

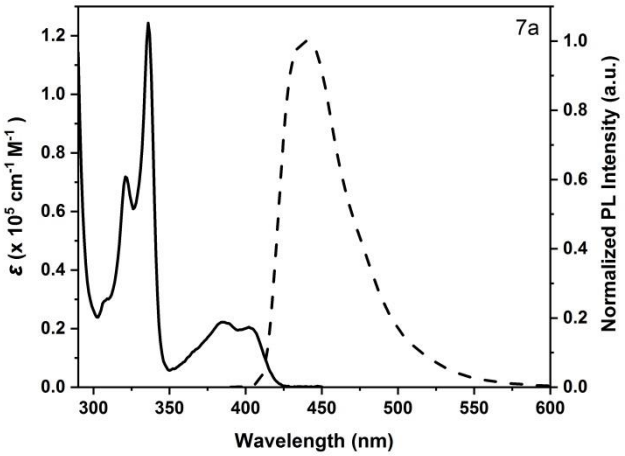
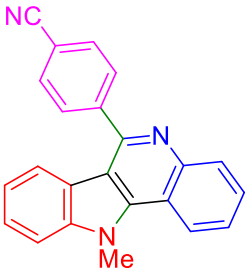


Figure S1. UV–vis absorption spectra (solid line) and fluorescence spectra (dashed line) observed for compound **7a** in $CHCl_3$ solution.



10ab

ε = 38,141 $cm^{-1}M^{-1}$

λ_{abs} = 403 nm

λ_{em} = 461 nm

Φ_F = 0.28

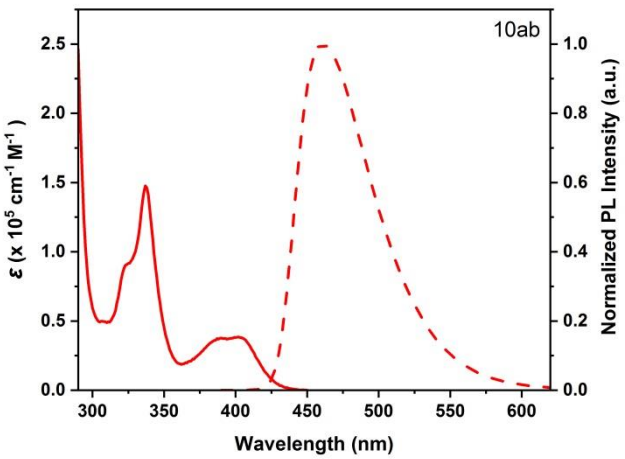
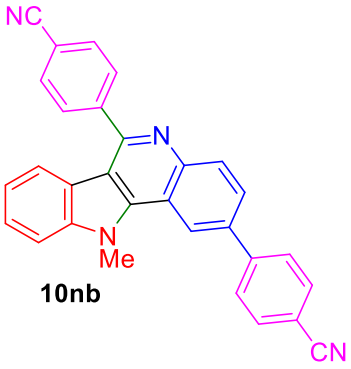


Figure S2. UV–vis absorption spectra (solid line) and fluorescence spectra (dashed line) observed for compound **10ab** in $CHCl_3$ solution.



10nb

ε = 46,783 $cm^{-1}M^{-1}$

λ_{abs} = 410 nm

λ_{em} = 466 nm

Φ_F = 0.42

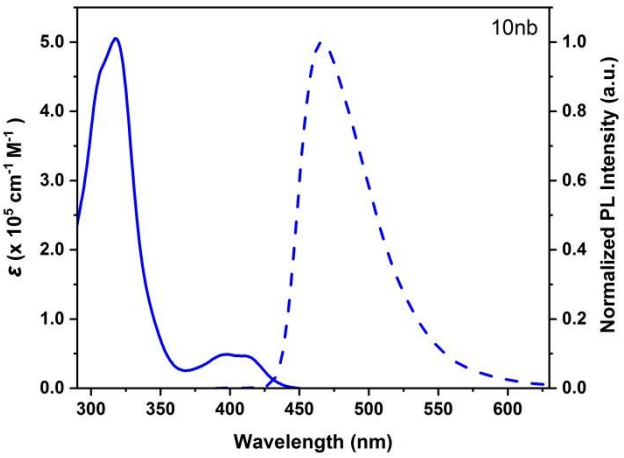
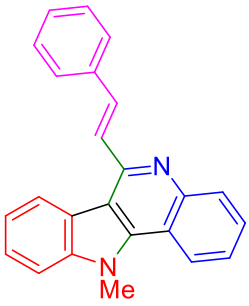


Figure S3. UV–vis absorption spectra (solid line) and fluorescence spectra (dashed line) observed for compound **10nb** in $CHCl_3$ solution.



12aa

ε = 51,417 $cm^{-1}M^{-1}$

λ_{abs} = 405 nm

λ_{em} = 486 nm

Φ_F = 0.19

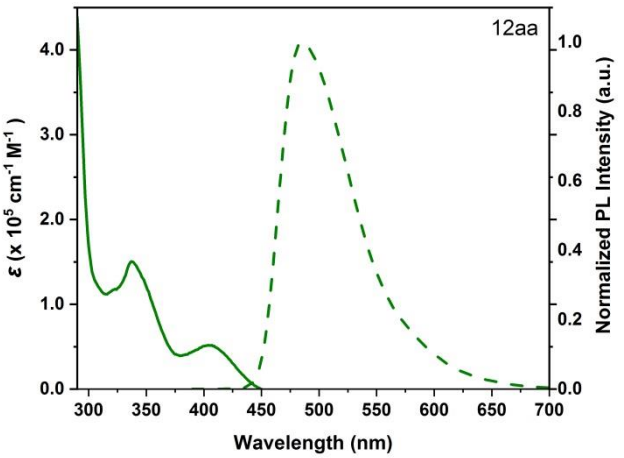
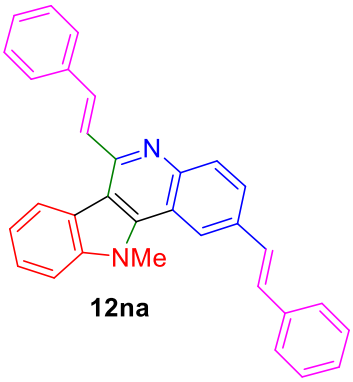


Figure S4. UV–vis absorption spectra (solid line) and fluorescence spectra (dashed line) observed for compound **12aa** in $CHCl_3$ solution.



12na

ε = 51,935 $cm^{-1}M^{-1}$

λ_{abs} = 440 nm

λ_{em} = 546 nm

Φ_F = 0.56

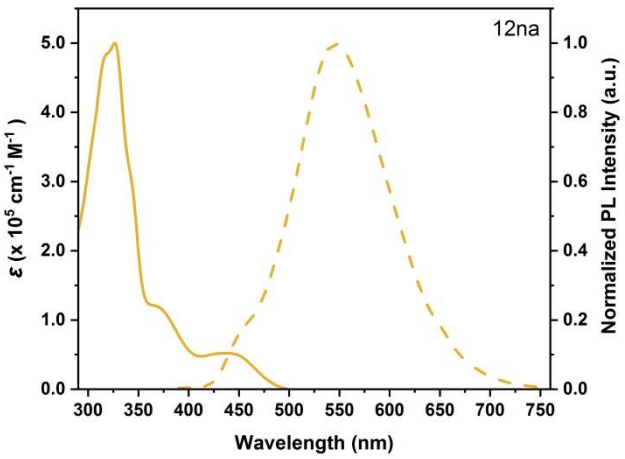


Figure S5. UV–vis absorption spectra (solid line) and fluorescence spectra (dashed line) observed for compound **12na** in $CHCl_3$ solution.

10. Computation details

Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations were carried out to elucidate electronic structures and electronic transition energies of **10ab**, **10nb**, **12aa**, and **12na** using Gaussian 16 package.[10] Ground-state geometry optimizations were calculated in gas phase with B3LYP functional[11-13] and 6-31++G(d,p)[14-19] basis set. The true minima nature of each stationary point was verified with the frequency calculations (no presence of imaginary-frequency mode). The TD-DFT was performed for ten singlet excited states using CPCM solvation model[20] using B3LYP/6-311++G(d,p)[14-19] in $CHCl_3$. Molecular orbitals were plotted and visualized using Multiwfn[21] program and VMD[22] program, respectively. In general, the calculated absorption wavelengths shift slightly from the experimental absorption wavelength (~ 20–40 nm), similar to what found in other works.[23-26]

Table S1. Calculated electronic transition energies (in eV and nm) and oscillator strength (*f*) of **12ab, 12n, 14aa,** and **14n** using B3LYP/6-311++G(d,p).

	Calculation					Experiment	
	Band assignment		**Energy (eV)**	**λ_{abs} (nm)[a]**	**f[b]**	**λ_{abs} (nm)**	**ε[c]**
10ab	H-1 → L+0 (90.26%)	CT	3.57	347.2	0.088	389	37545
	H-0 → L+0 (94.28%)	CT	3.38	366.5	0.078	403	38141
10nb	H-1 → L+0 (88.73%)	CT	3.42	362.3	0.184	397	49045
	H-0 → L+0 (96.31%)	CT	3.20	386.8	0.377	410	46783
12aa	H-1 → L+0 (86.68%)	CT	3.32	373.4	0.351	405	51417
	H-0 → L+0 (92.04%)	π-π*	3.23	383.8	0.410		
12na	H-1 → L+0 (82.69%)	CT	3.15	393.7	0.209	440	51935
	H-0 → L+0 (88.73%)	π-π*	2.78	446.2	1.350		

[a]Absorption wavelength. [b]Oscillation strength. [c]Molar extinction coefficient

Cartesian coordinates

10ab

Total atom = 41

C	0.80669408	2.59061652	-0.26524393
C	-0.33535087	1.78816954	-0.09421106
C	-1.60698785	2.41508151	-0.01841159
C	0.66704620	3.97355853	-0.32609323
C	-0.59955548	4.57641327	-0.21890664
C	-1.75032869	3.80738354	-0.06763545
C	-0.58405579	0.36221660	-0.01442212
N	-2.59340575	1.43350671	0.08319229
C	-1.98532186	0.18986298	0.06796277
C	-4.01776927	1.72138832	0.12836782
C	0.24406905	-0.79774758	-0.05583407
N	-0.26251731	-2.01659651	-0.10493719
C	-1.61714083	-2.19399193	-0.04322089
C	-2.56264008	-1.11882635	0.08309490
C	-3.94157380	-1.44776863	0.19157283
C	-4.36634143	-2.76223759	0.15646951
C	-3.43593730	-3.81461211	0.01164432
C	-2.08976028	-3.53142884	-0.08253720
H	1.78812415	2.14274624	-0.35983930
H	1.54686151	4.59533345	-0.45960189
H	-0.68569994	5.65794367	-0.26176480
H	-2.71967902	4.28890889	0.00239120
H	-4.46249040	1.37956943	1.06796810
H	-4.53896192	1.25580271	-0.71309064
H	-4.16183379	2.79828023	0.05859532
H	-4.68406894	-0.67139896	0.30990345
H	-5.42582240	-2.98424366	0.24301786
H	-3.78166469	-4.84360513	-0.01693044
H	-1.34699626	-4.31646996	-0.17961353
C	4.54349794	-0.75144304	0.09171538

C	3.87329241	-1.49668541	-0.89491482
C	2.48284781	-1.49396038	-0.94017536
C	3.80268588	-0.00863316	1.02718045
C	2.41192122	-0.00118506	0.96095625
C	1.73486177	-0.73687545	-0.02437972
C	5.97723891	-0.75344100	0.14750597
N	7.14063805	-0.75344048	0.19178169
H	4.44590698	-2.07446037	-1.61280963
H	1.96006144	-2.08509420	-1.68412149
H	4.31907316	0.55151279	1.79967659
H	1.84583453	0.56576110	1.69305692

10nb

Total atom = 52

C	3.63903028	2.35634977	-0.27510493
C	2.29335683	1.96799923	-0.14809471
C	1.29074100	2.97239509	-0.12313292
C	3.95528612	3.70928248	-0.34283892
C	2.94804700	4.68995292	-0.28595228
C	1.60596064	4.33576427	-0.17922475
C	1.59477662	0.69974379	-0.07644942
N	0.03641165	2.36314007	-0.05923716
C	0.21060263	0.99073612	-0.04711410
C	-1.21867634	3.09712949	-0.08499750
C	2.00602188	-0.66522680	-0.08730682
N	1.13444510	-1.65667257	-0.16164593
C	-0.20332620	-1.38526161	-0.14950015
C	-0.75705814	-0.06385946	-0.04666823
C	-2.16725938	0.07206559	0.02278047
C	-3.01700997	-1.02668674	-0.03527613
C	-2.45203375	-2.32371577	-0.16808442
C	-1.08730041	-2.49285930	-0.21558001
C	6.07993110	-2.00649786	0.23340080
C	5.24302564	-2.50956194	-0.77868704

C	3.93062855	-2.05928242	-0.88003583
C	5.58418409	-1.05100498	1.13720266
C	4.27411227	-0.59562440	1.01464059
C	3.43373769	-1.08791732	0.00369444
C	7.43316104	-2.46991607	0.34697794
N	8.53173666	-2.84415569	0.43825064
H	4.42612126	1.61468658	-0.33024977
H	4.99289004	4.01234385	-0.44223335
H	3.21756660	5.74066260	-0.33271129
H	0.84231962	5.10522181	-0.14648743
H	-1.78062132	2.95846593	0.84386875
H	-1.83455787	2.79012644	-0.93499204
H	-1.00363613	4.15876581	-0.19372418
H	-2.61278049	1.05324150	0.10081307
H	-3.10359083	-3.19161572	-0.19370592
H	-0.64256504	-3.48005134	-0.28551524
H	5.62512759	-3.25127805	-1.47212522
H	3.27380757	-2.46073335	-1.64395108
H	6.22423170	-0.67673329	1.92925186
H	3.89450339	0.13397160	1.72273937
C	-5.34704881	-1.62134275	-0.77137179
C	-6.72748799	-1.45707198	-0.71911678
C	-7.28986974	-0.50731626	0.15133679
C	-4.48903285	-0.84949373	0.03458414
C	-5.06818484	0.09248952	0.90568947
C	-6.44681656	0.26768992	0.96661263
C	-8.71200417	-0.33120206	0.20931435
N	-9.86615960	-0.18582113	0.25600173
H	-4.92652815	-2.34180416	-1.46569154
H	-7.37455075	-2.05286532	-1.35427418
H	-4.43160071	0.67434887	1.56480505
H	-6.87813857	0.99127118	1.65041276

12aa

Total atom = 44

C	-0.13241034	2.92472723	-0.14437051
C	-1.05268132	1.86489848	-0.04825430
C	-2.43979324	2.17449539	-0.01816789
C	-0.59402996	4.23723297	-0.18347731
C	-1.97060694	4.51913074	-0.13589333
C	-2.90885338	3.49307174	-0.05811470
C	-0.96112578	0.41911111	0.00672986
N	-3.16898505	0.98837868	0.03975641
C	-2.28326021	-0.07773229	0.03460714
C	-4.61835487	0.93540899	0.12987667
C	0.12796850	-0.50865509	0.04206124
N	-0.08601591	-1.81748487	0.04981281
C	-1.35649204	-2.30597457	0.03100094
C	-2.53842469	-1.48445637	0.03183111
C	-3.80588962	-2.12767749	0.00768975
C	-3.90850341	-3.50563439	-0.00690224
C	-2.74761896	-4.31073505	0.00259656
C	-1.50261673	-3.71994930	0.02084664
C	2.58507951	-0.86432955	-0.07353904
C	1.52272135	-0.04859937	0.09550324
H	0.93260096	2.73893605	-0.20753646
H	0.11831536	5.05294617	-0.25966529
H	-2.31090727	5.54967152	-0.17050010
H	-3.96804554	3.72623892	-0.04092756
H	-4.93192723	0.34399748	0.99420585
H	-5.06303609	0.51702633	-0.77911116
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12na

Total atom = 58

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C	1.51334447	1.01394475	-0.02862921
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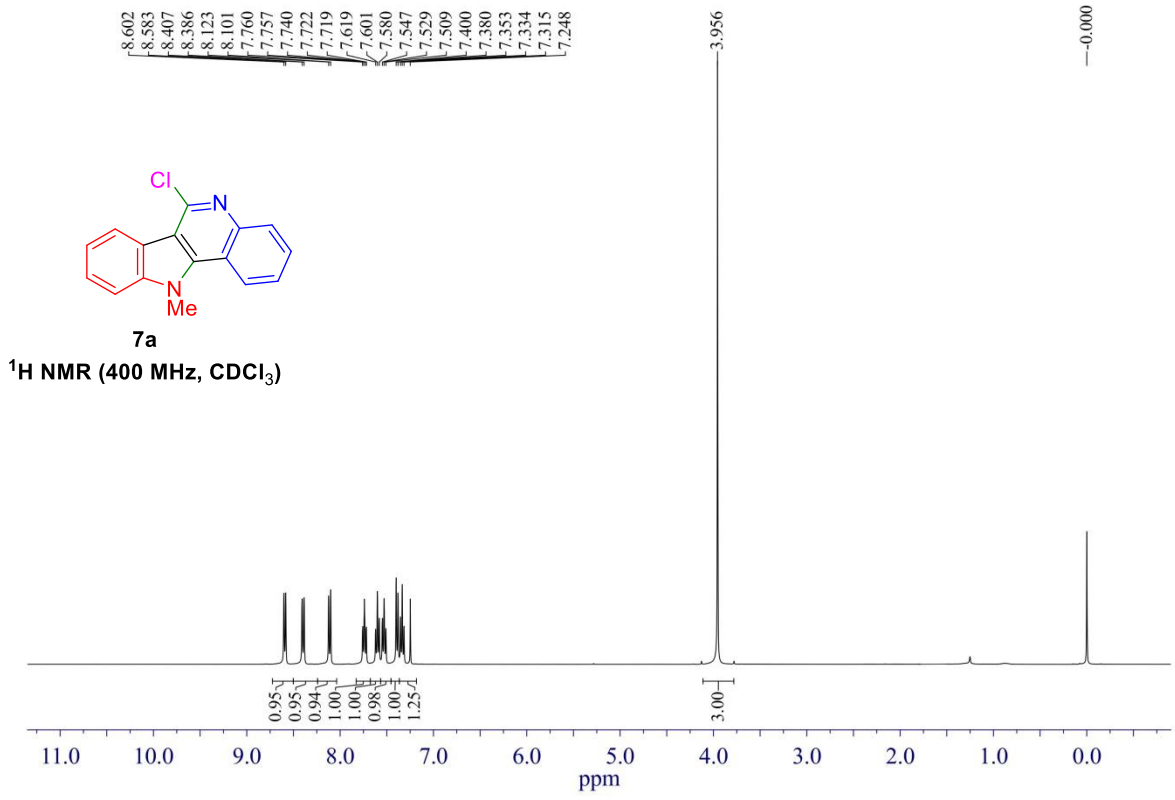
12. NMR spectra



7a

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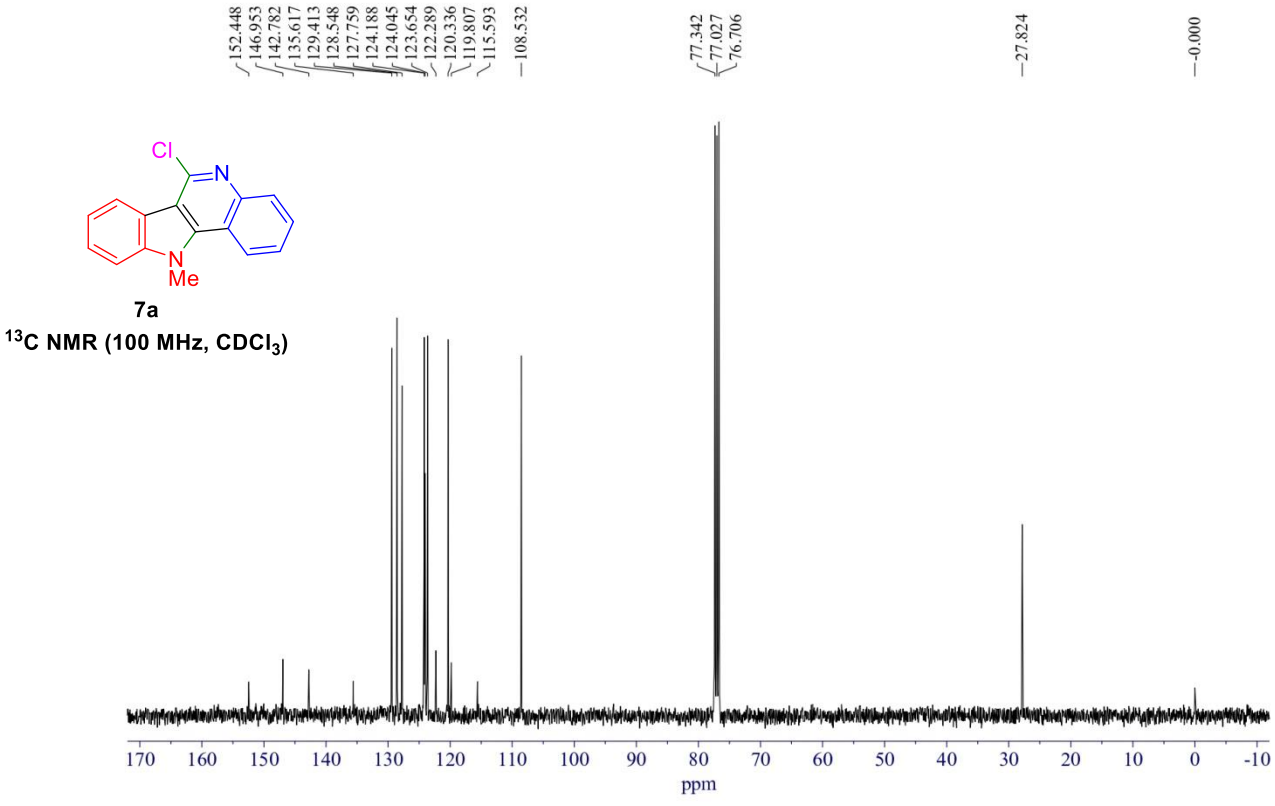

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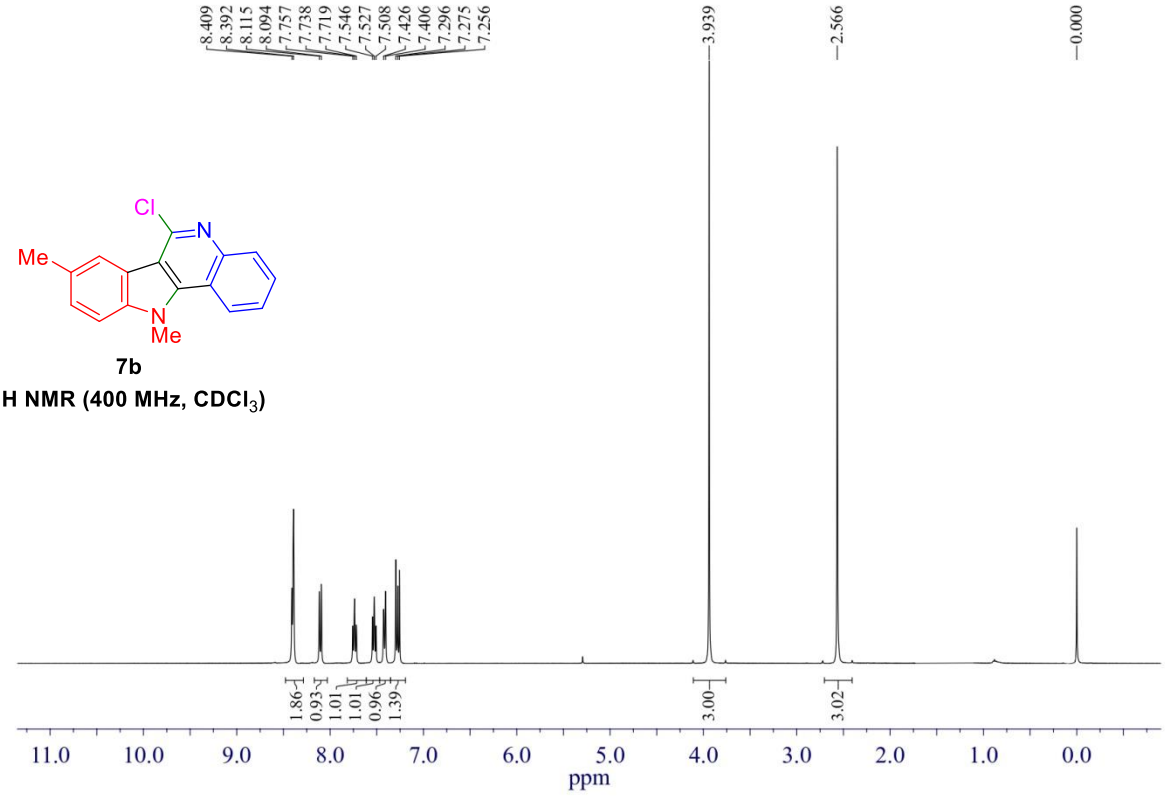

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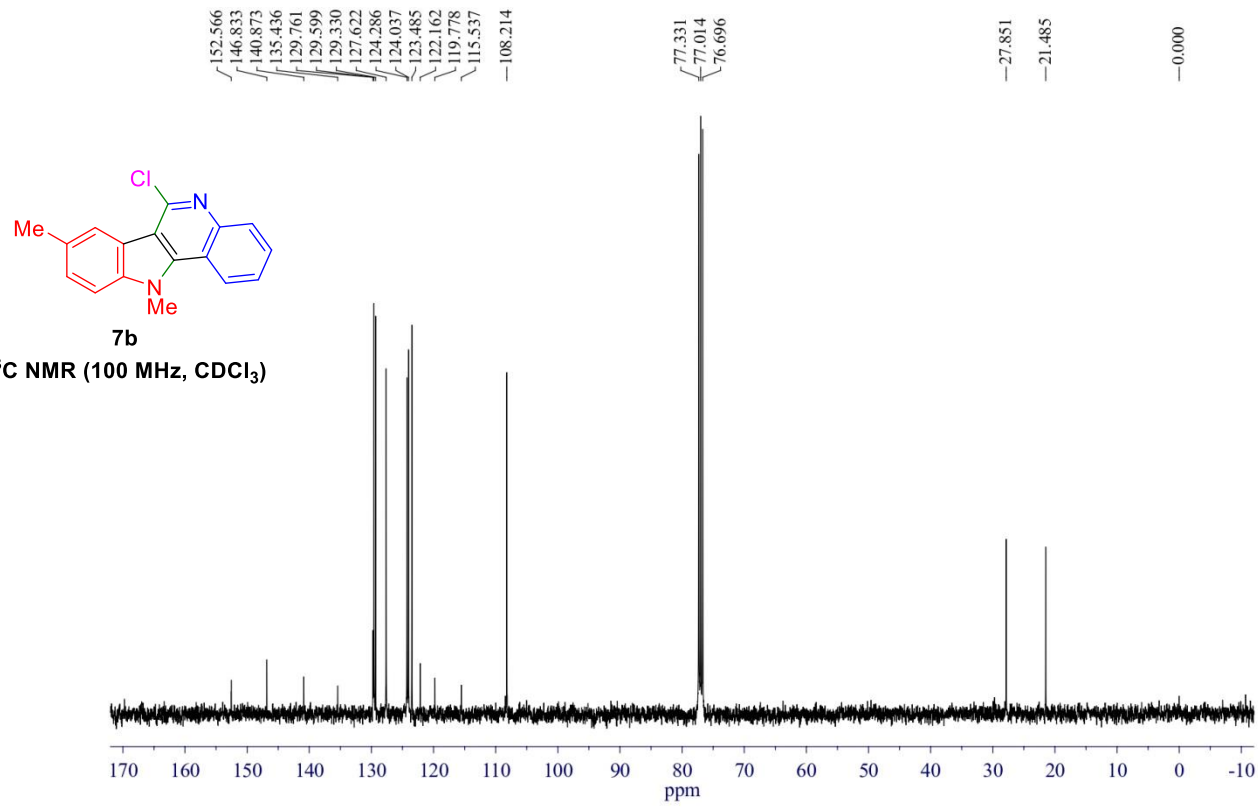

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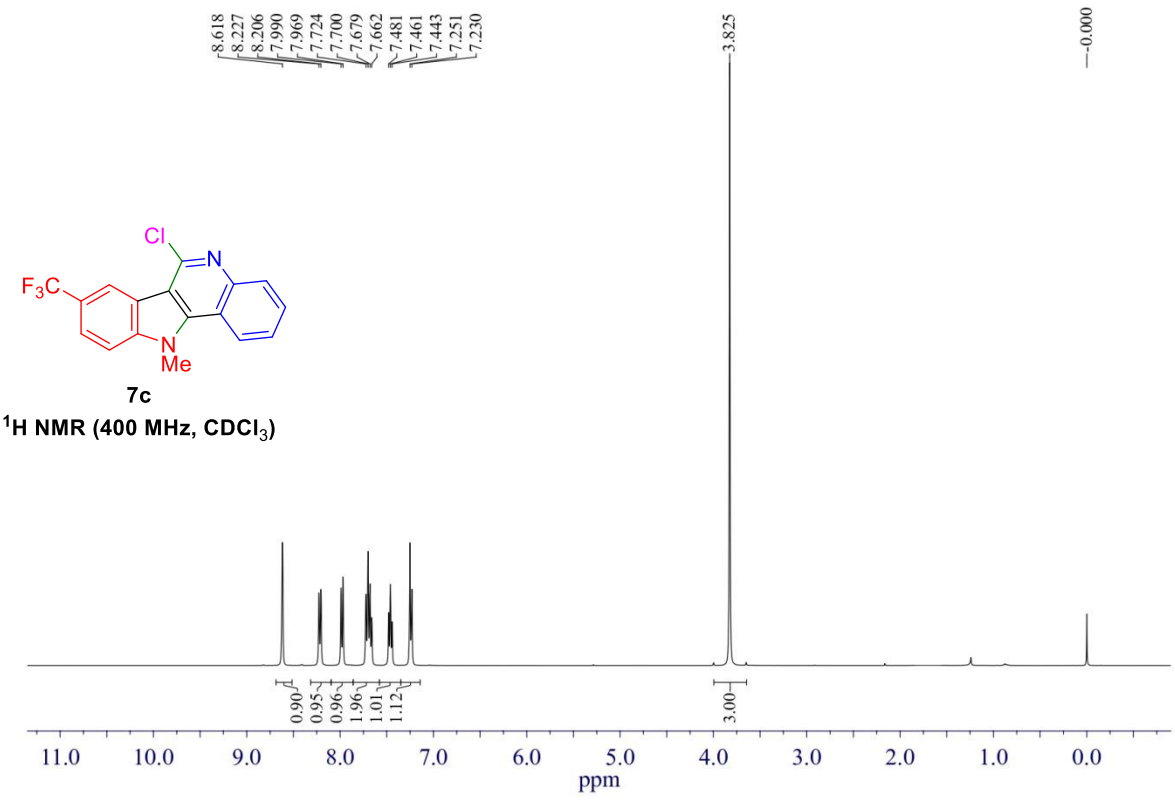

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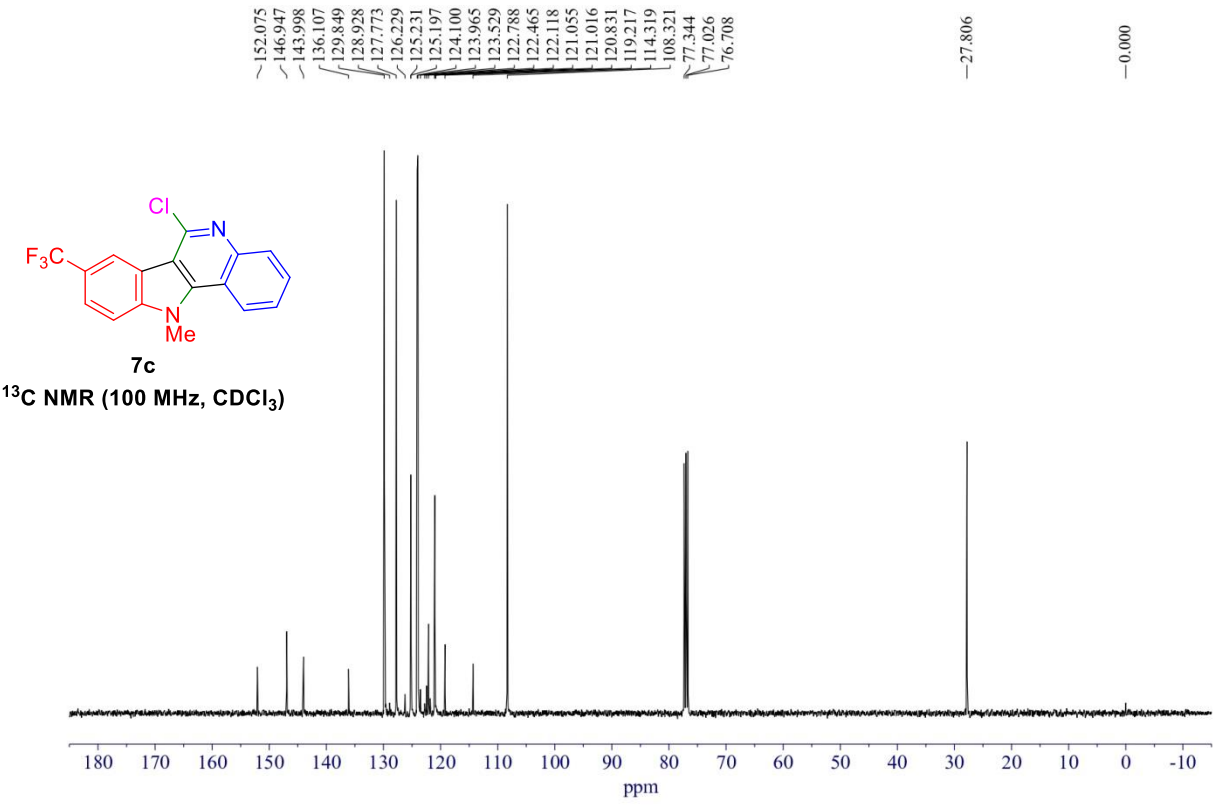

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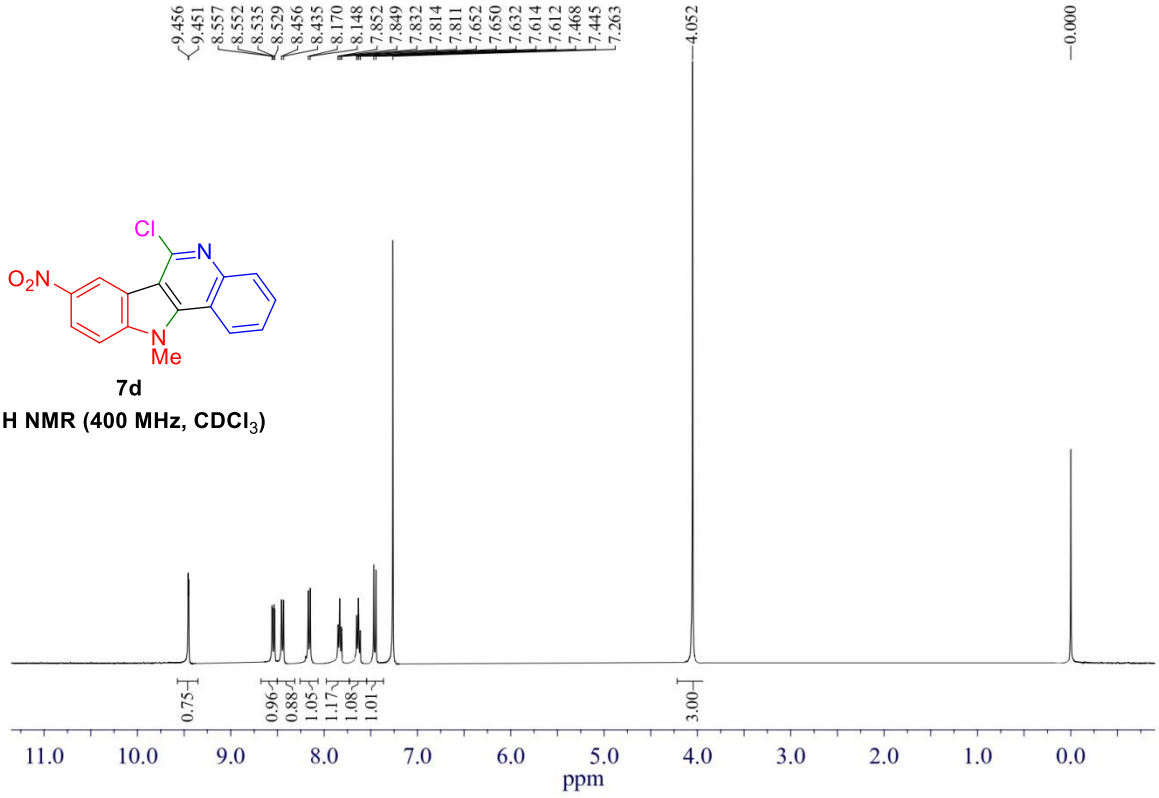

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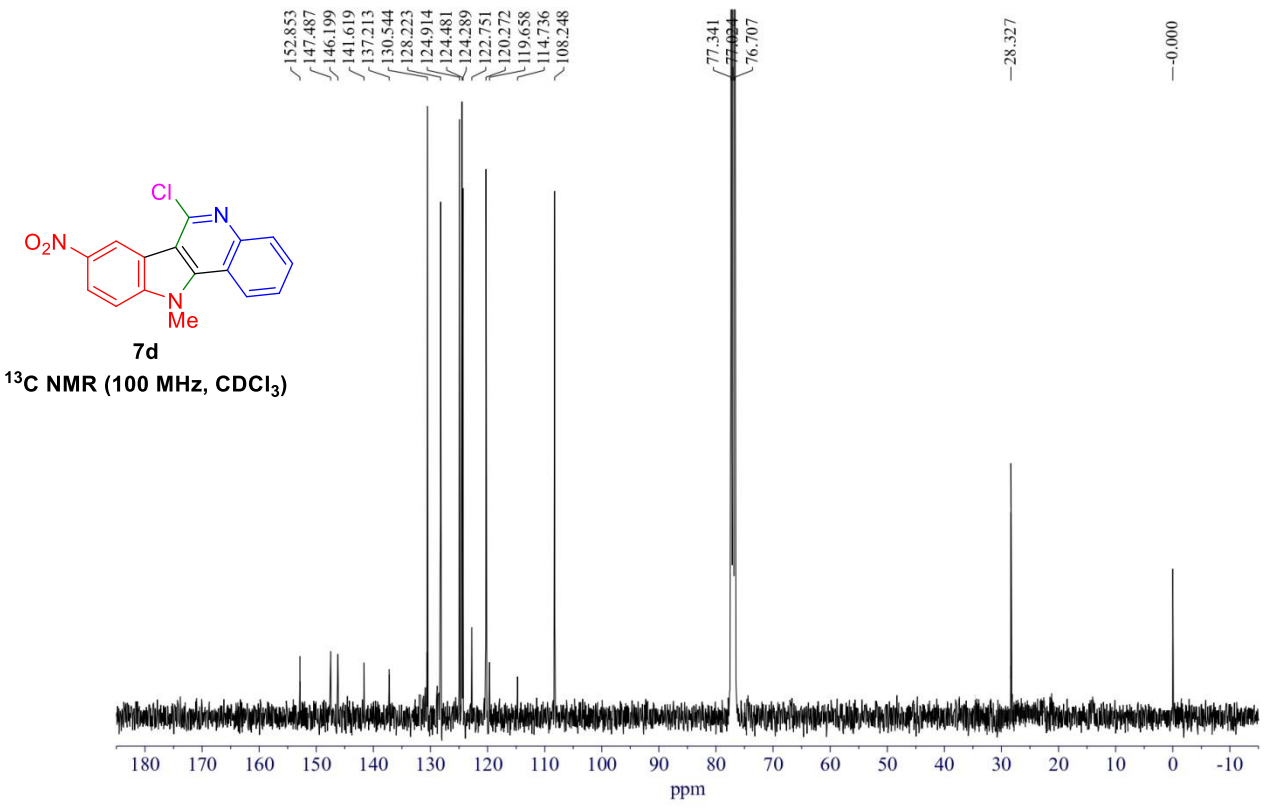

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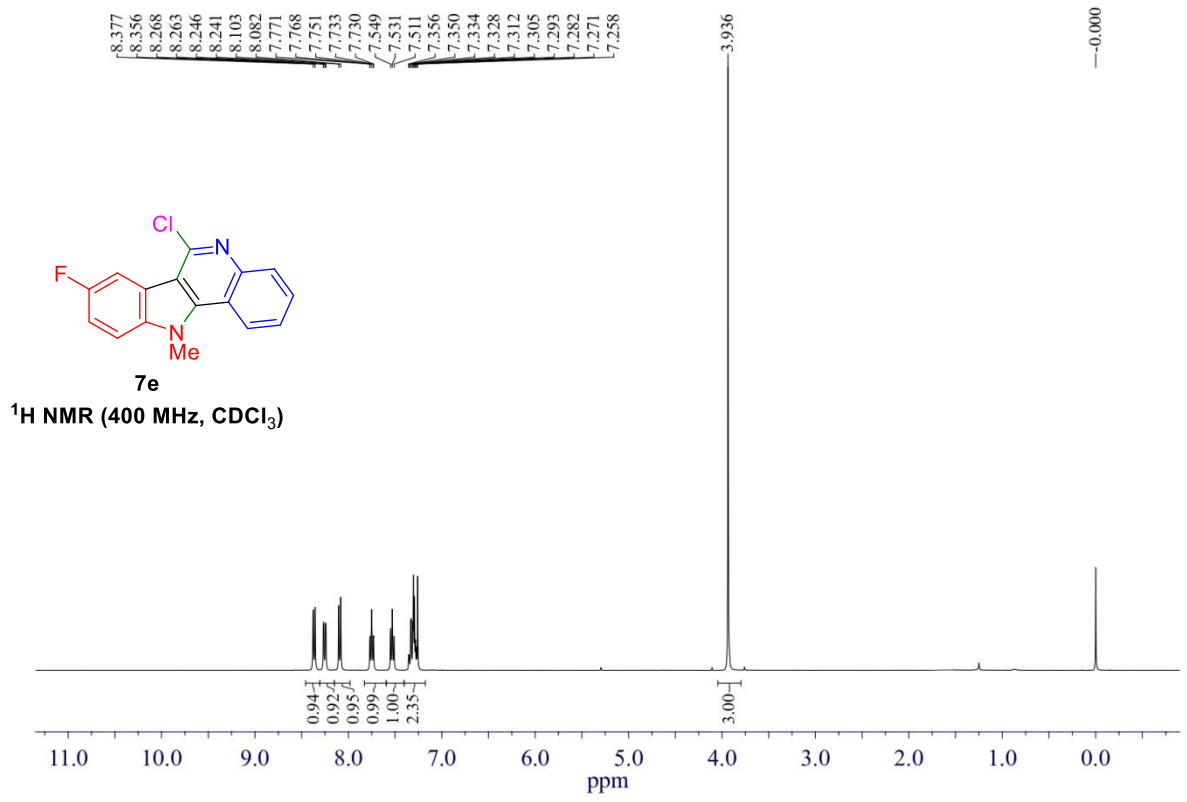

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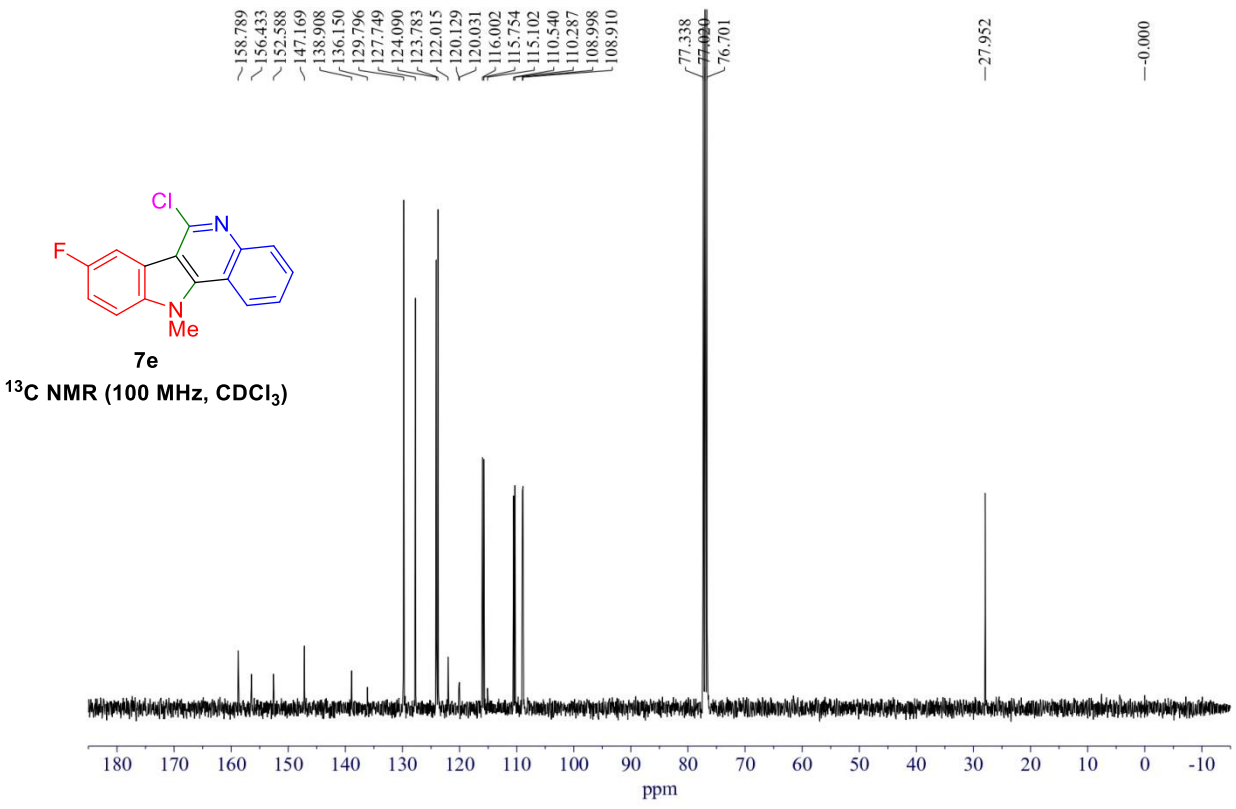

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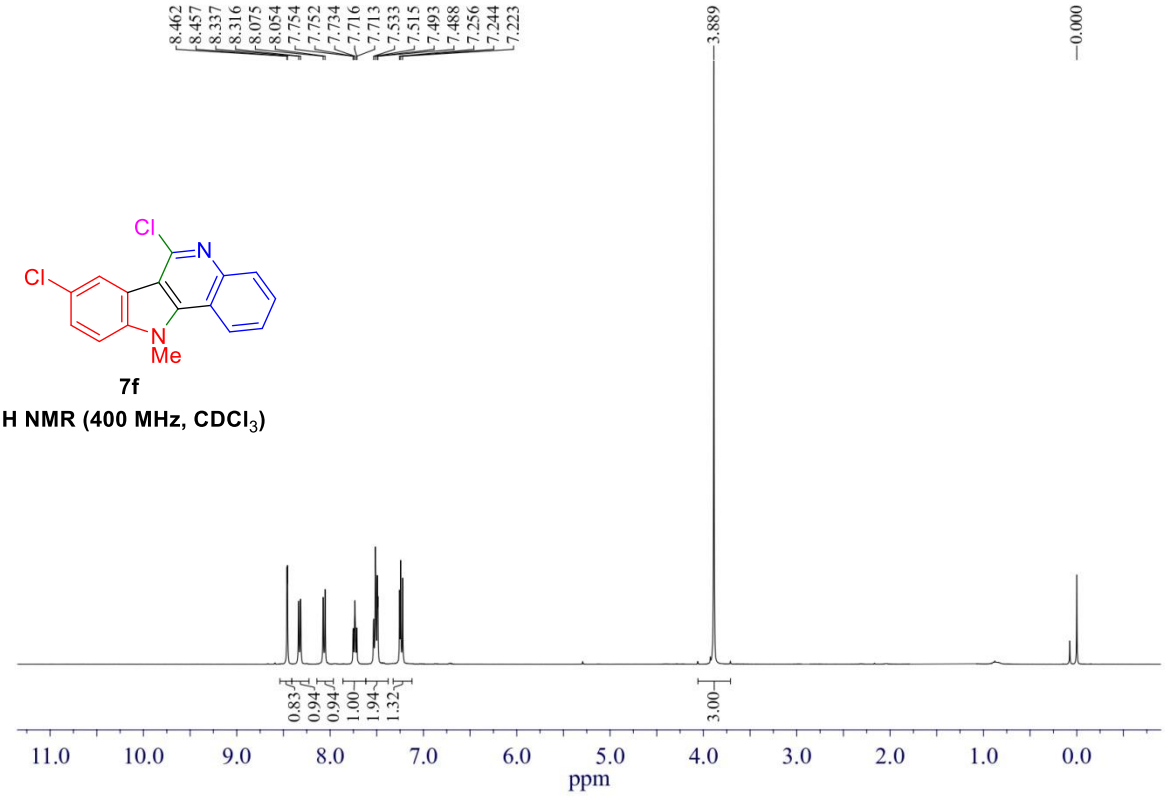

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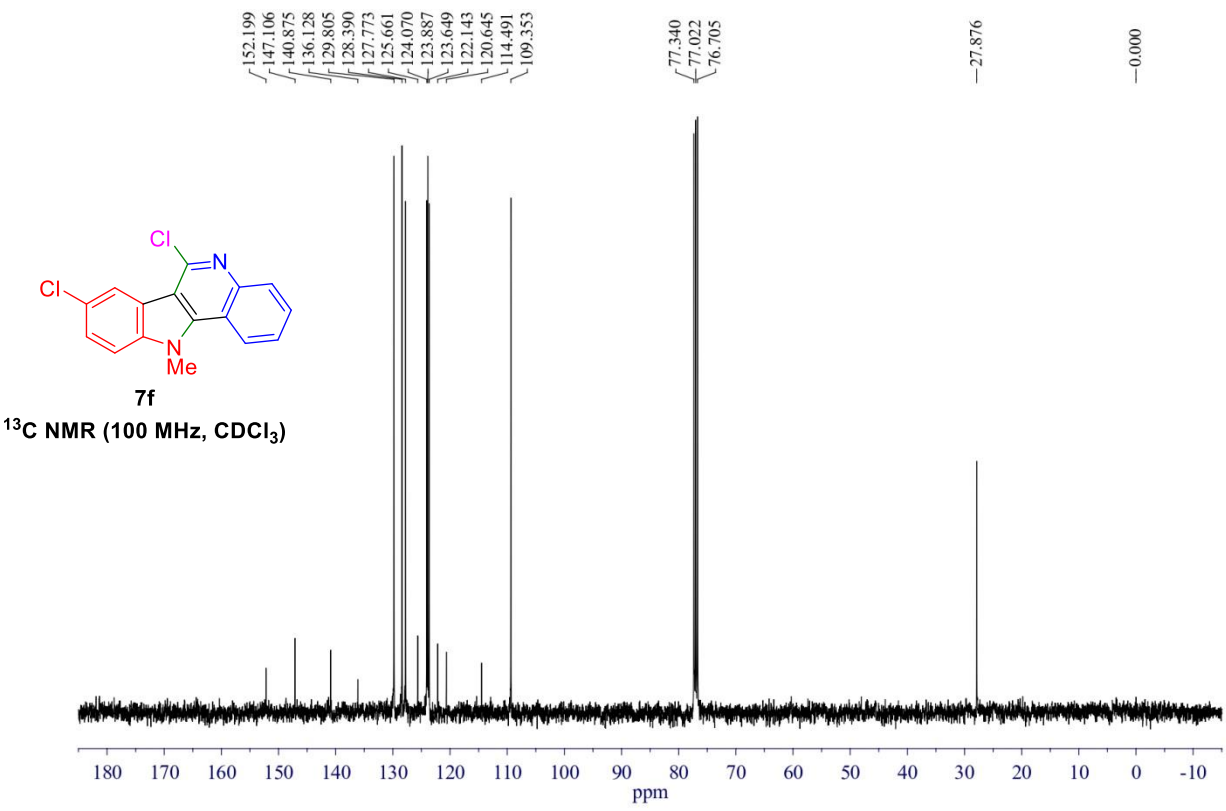

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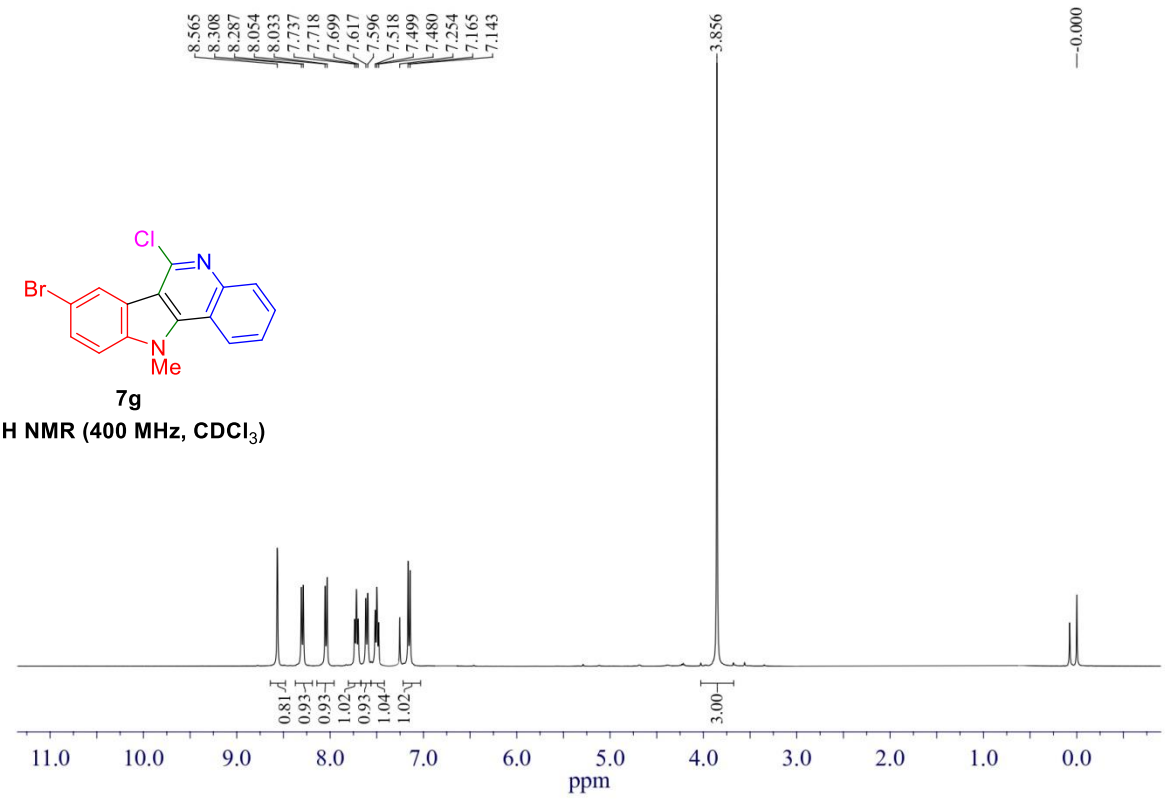

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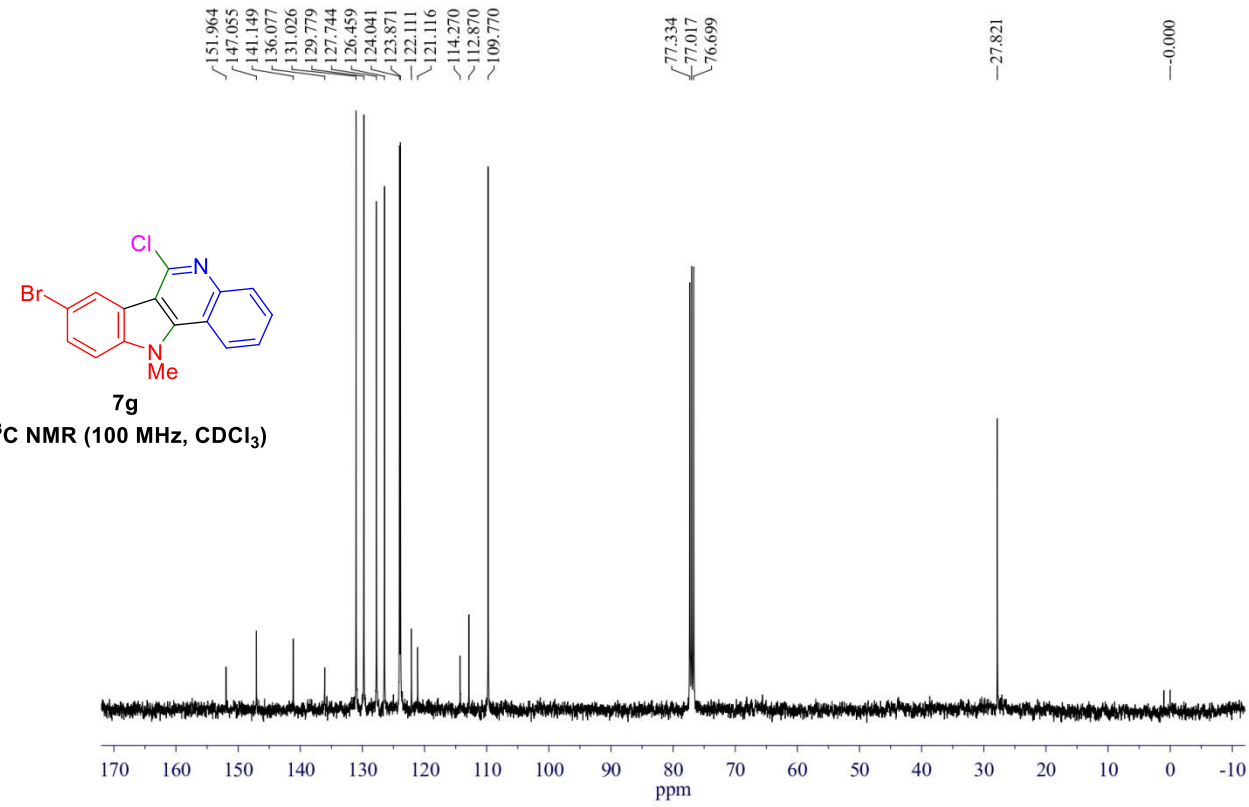

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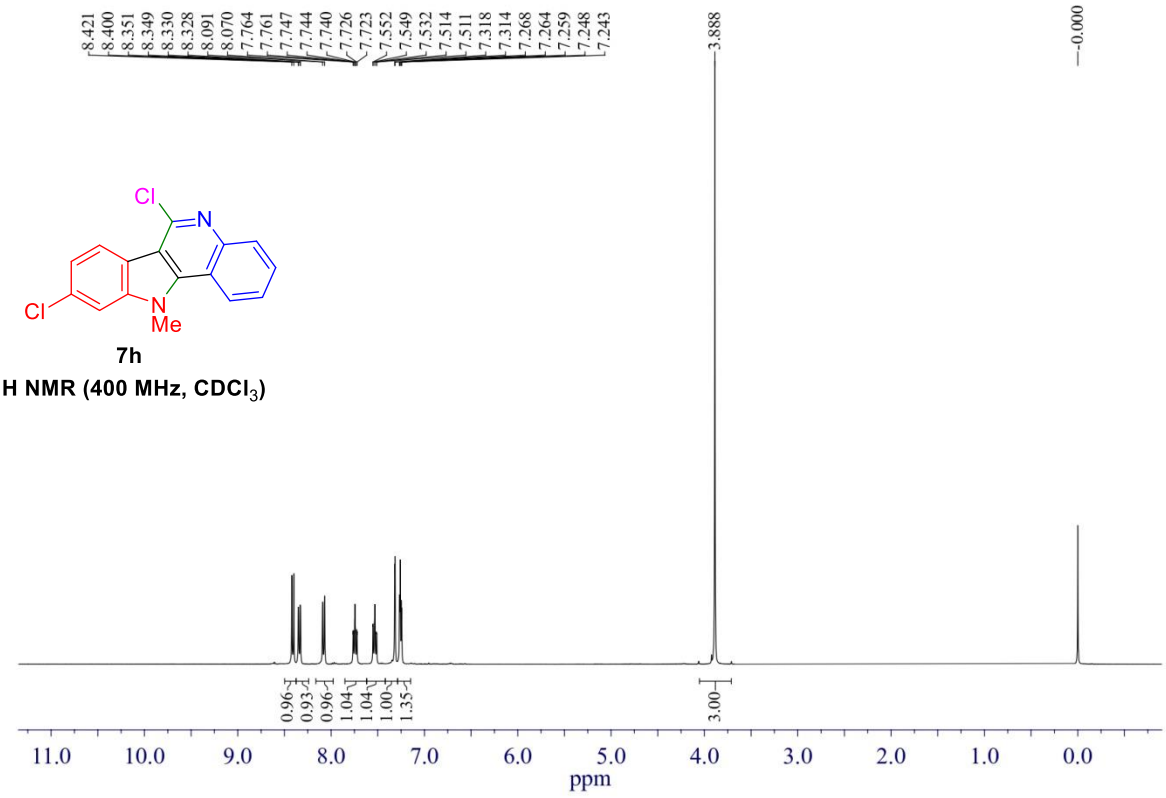

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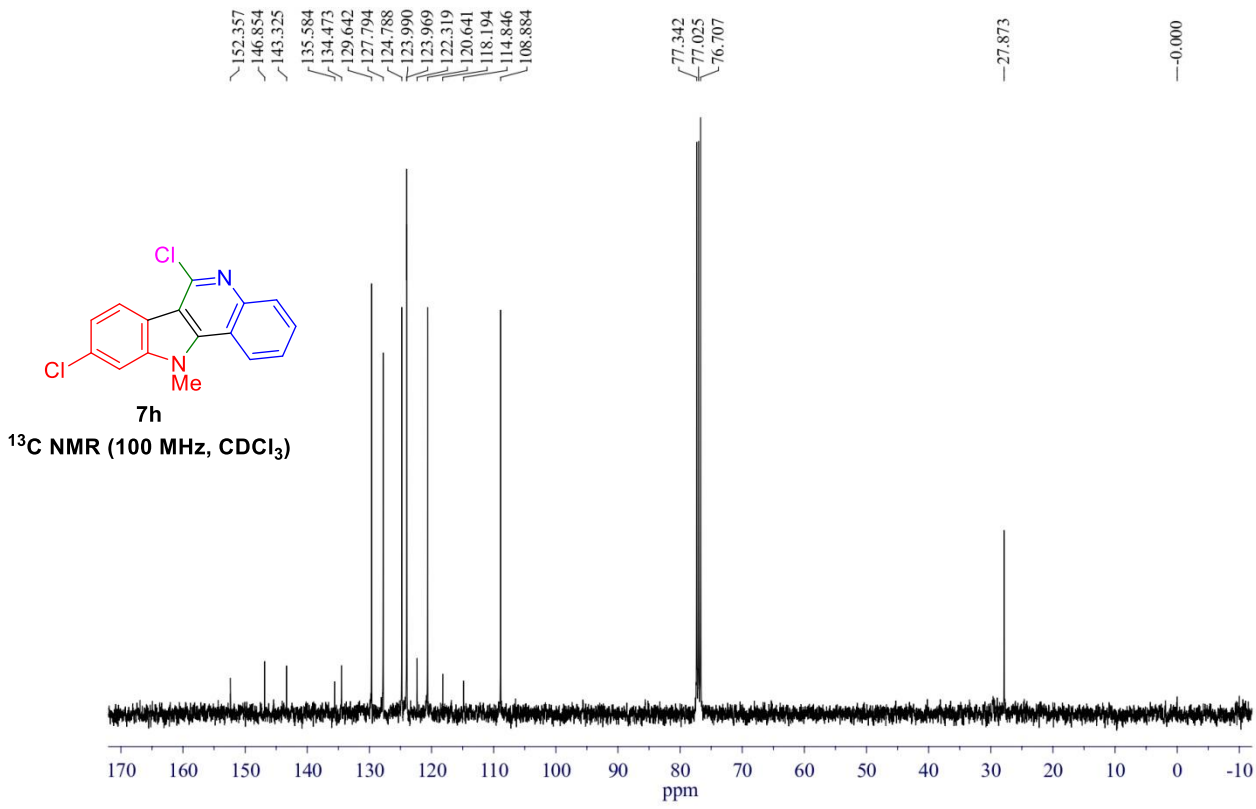

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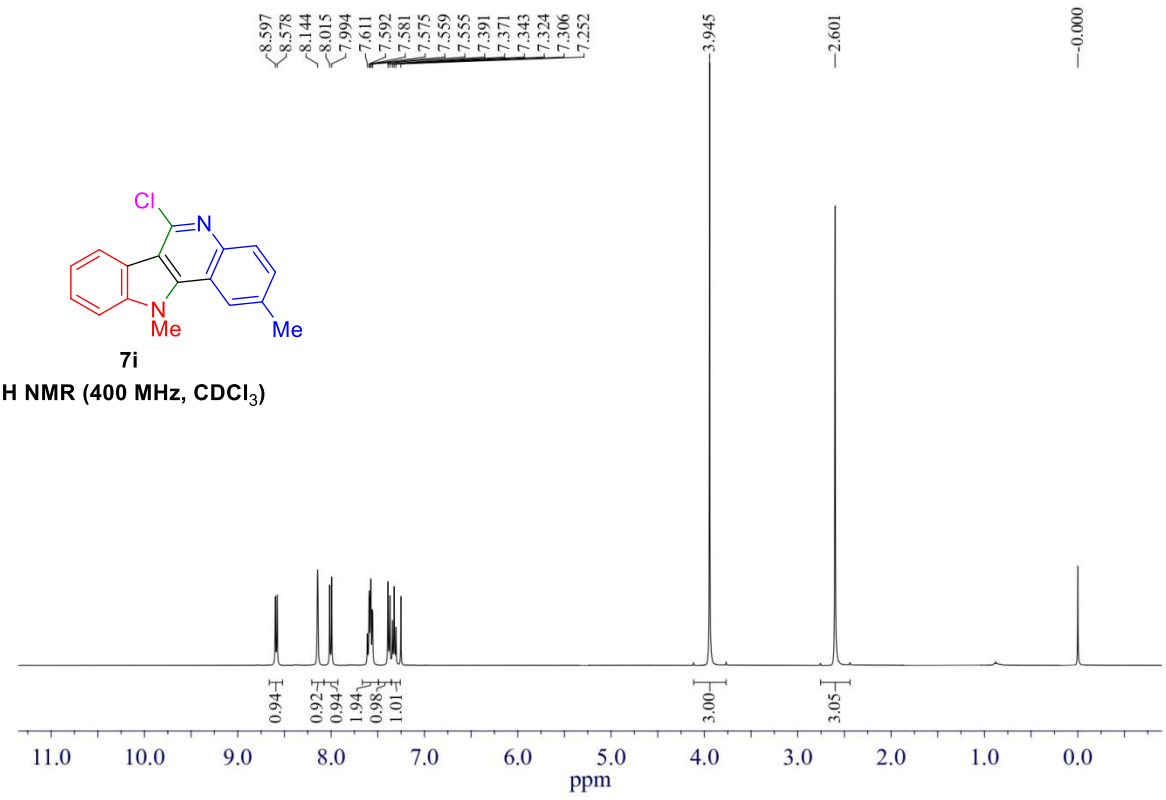

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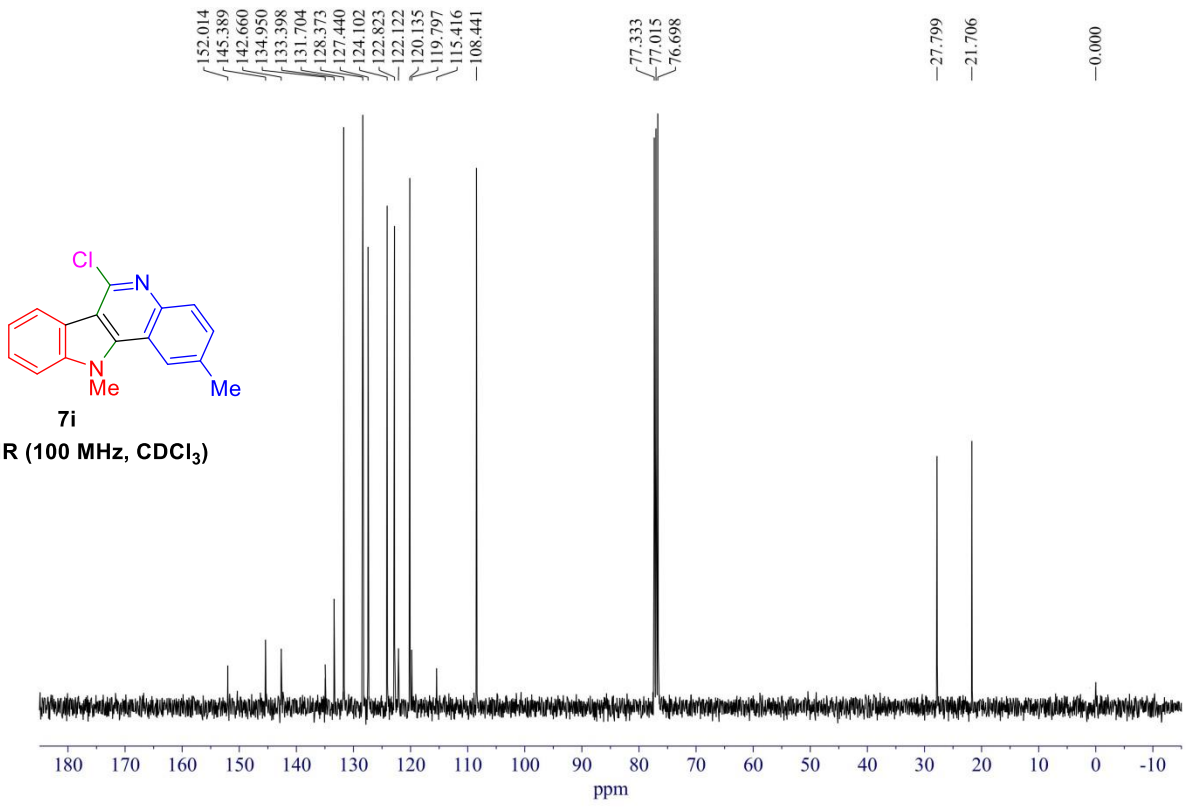

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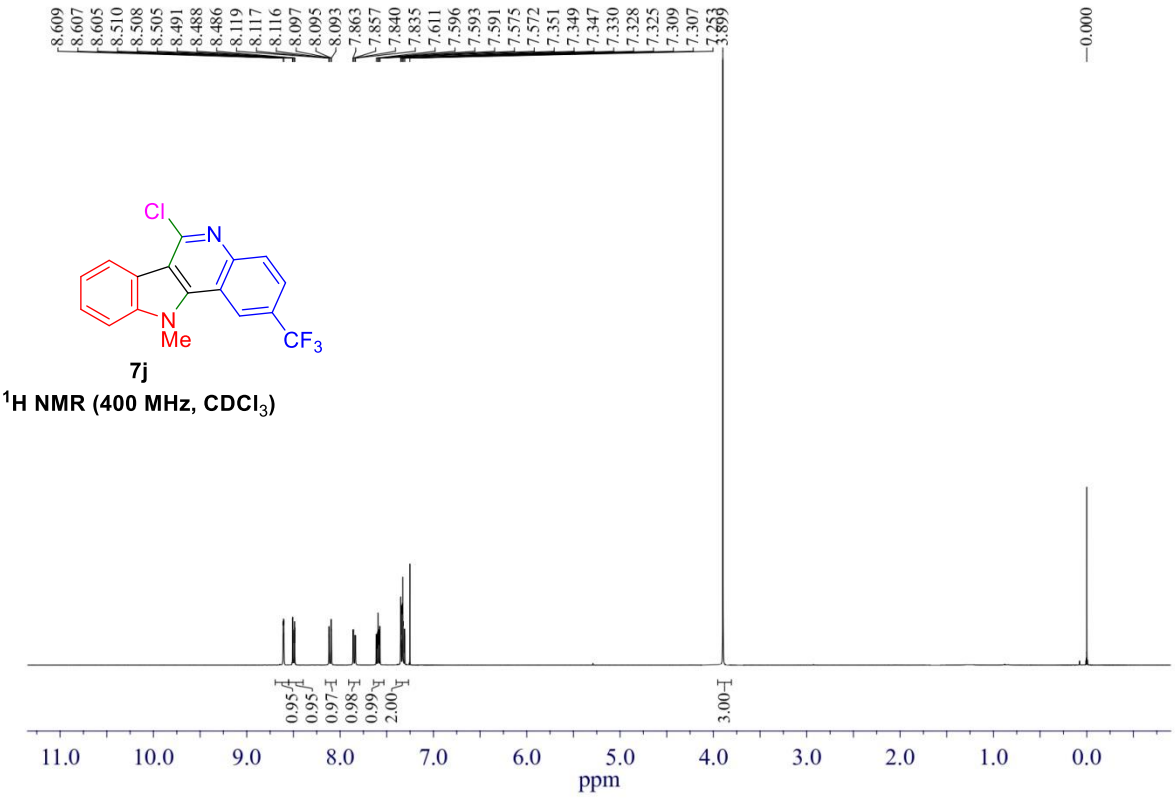

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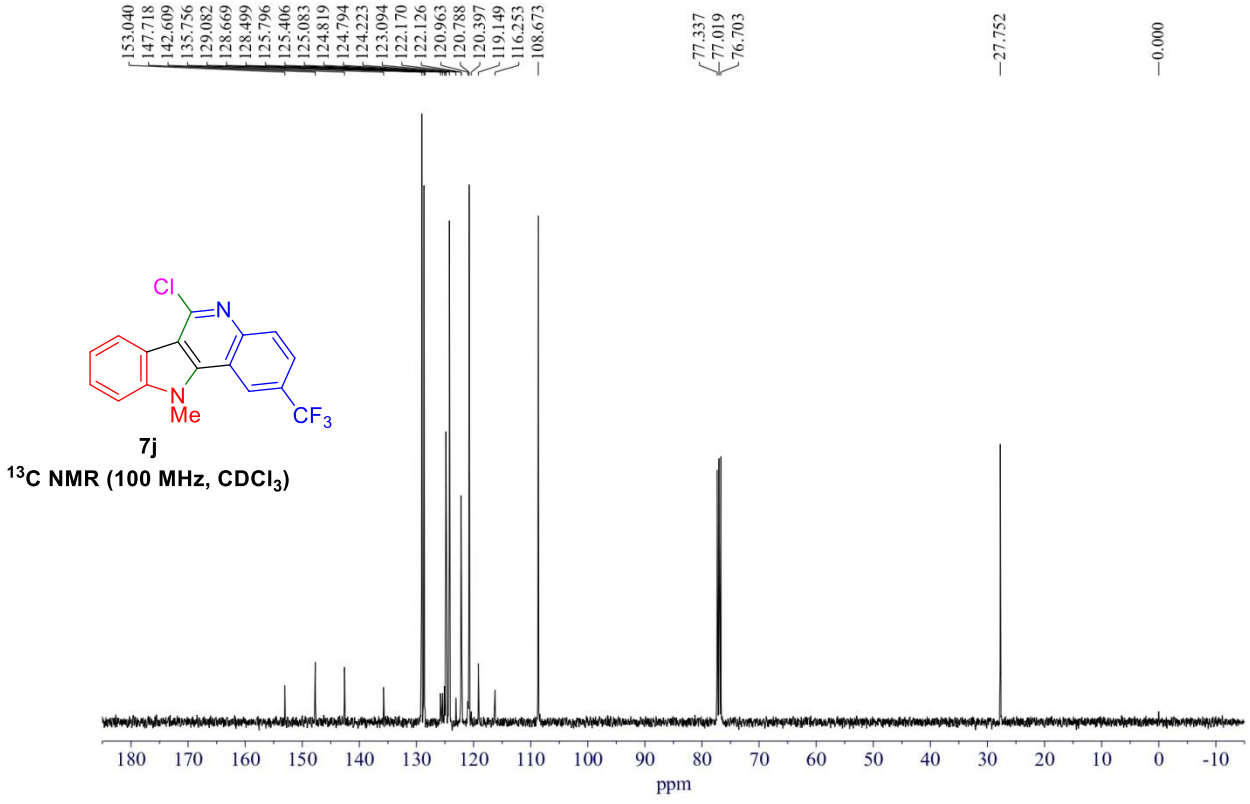

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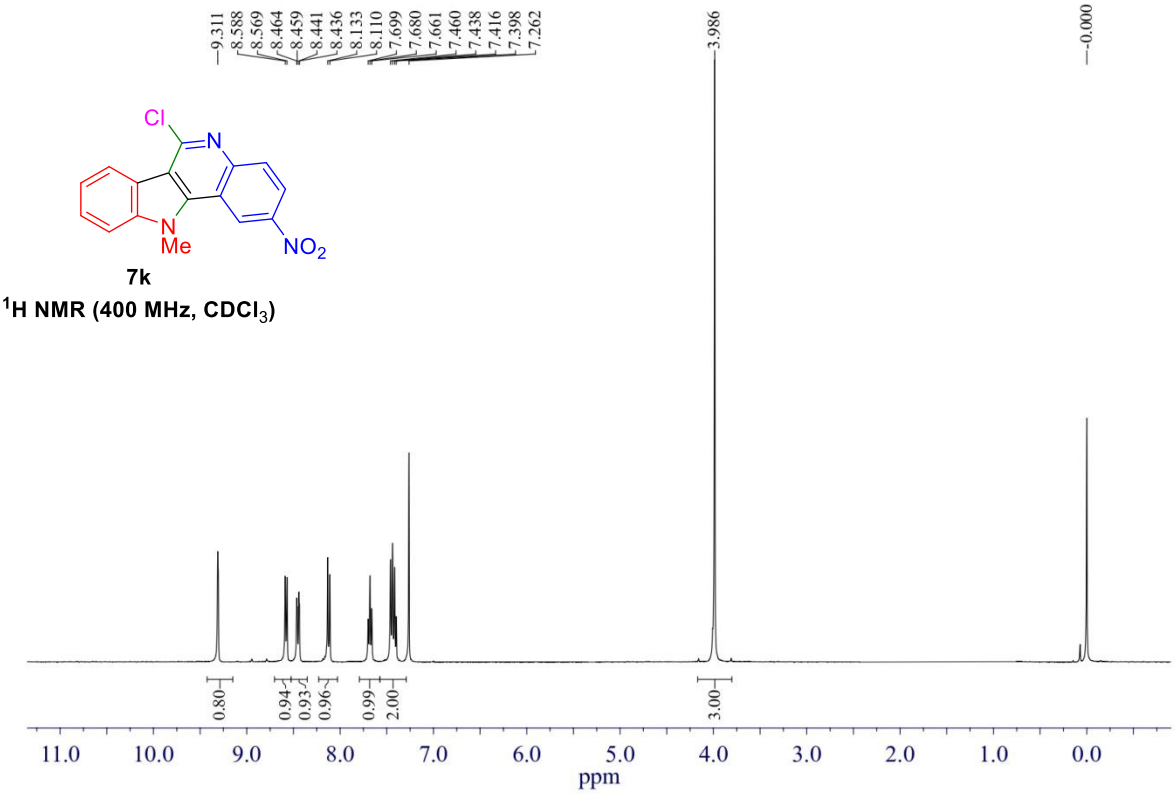

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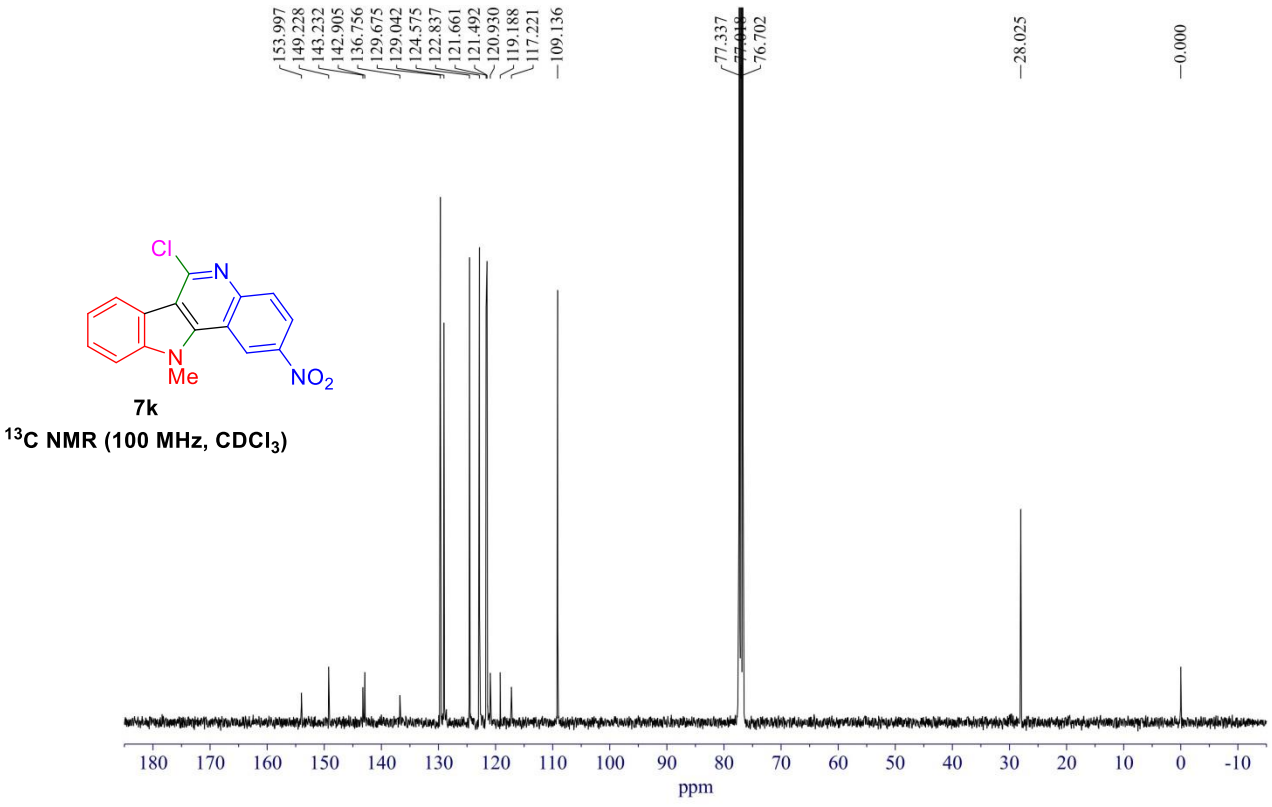

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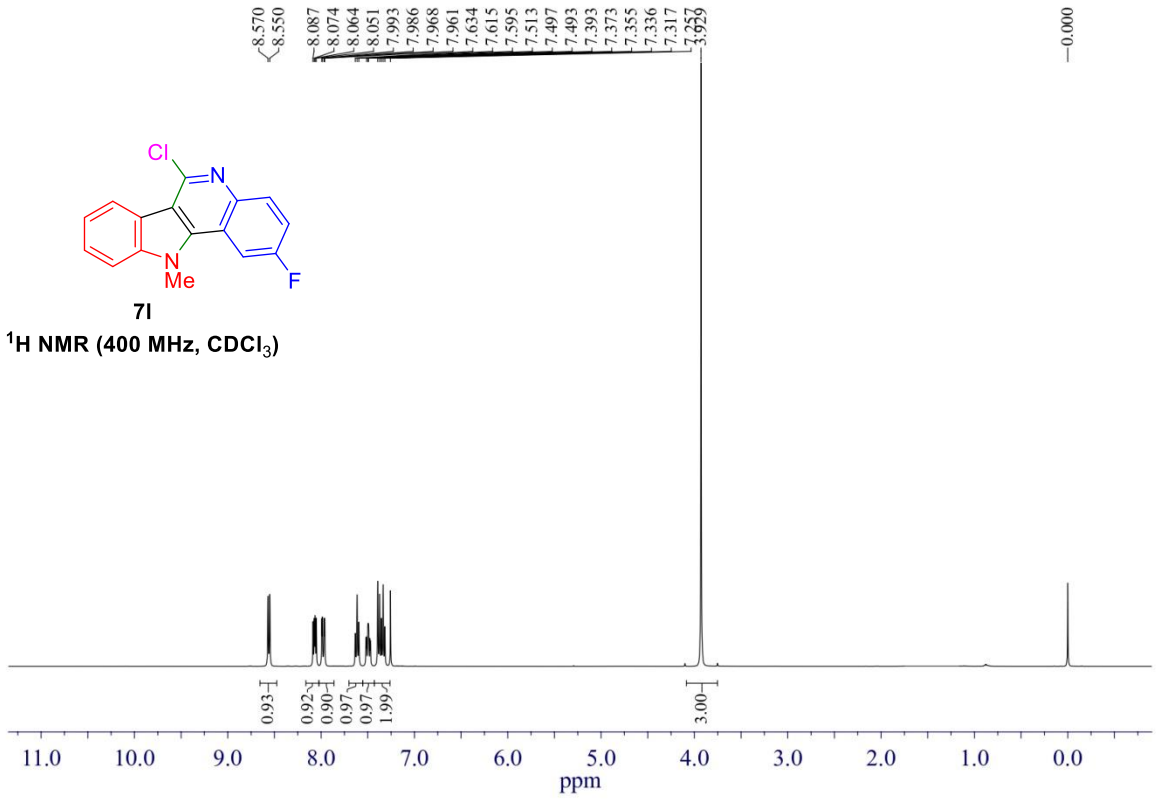

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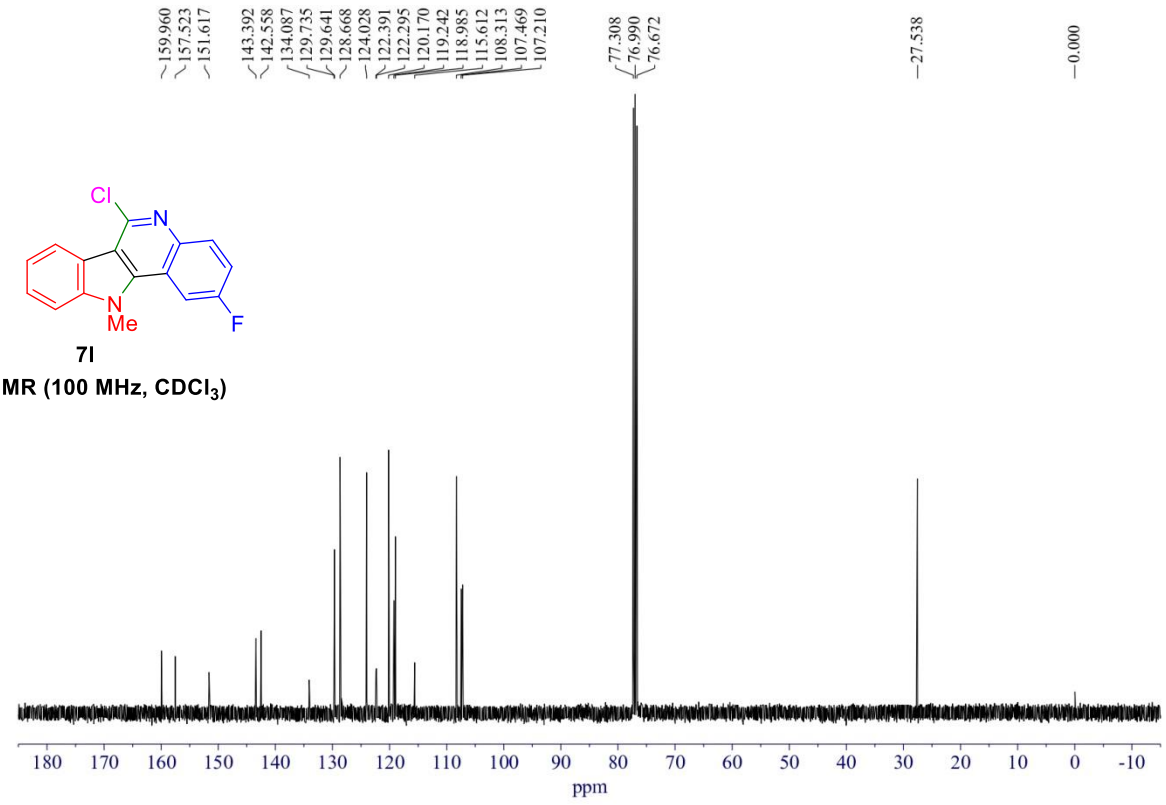
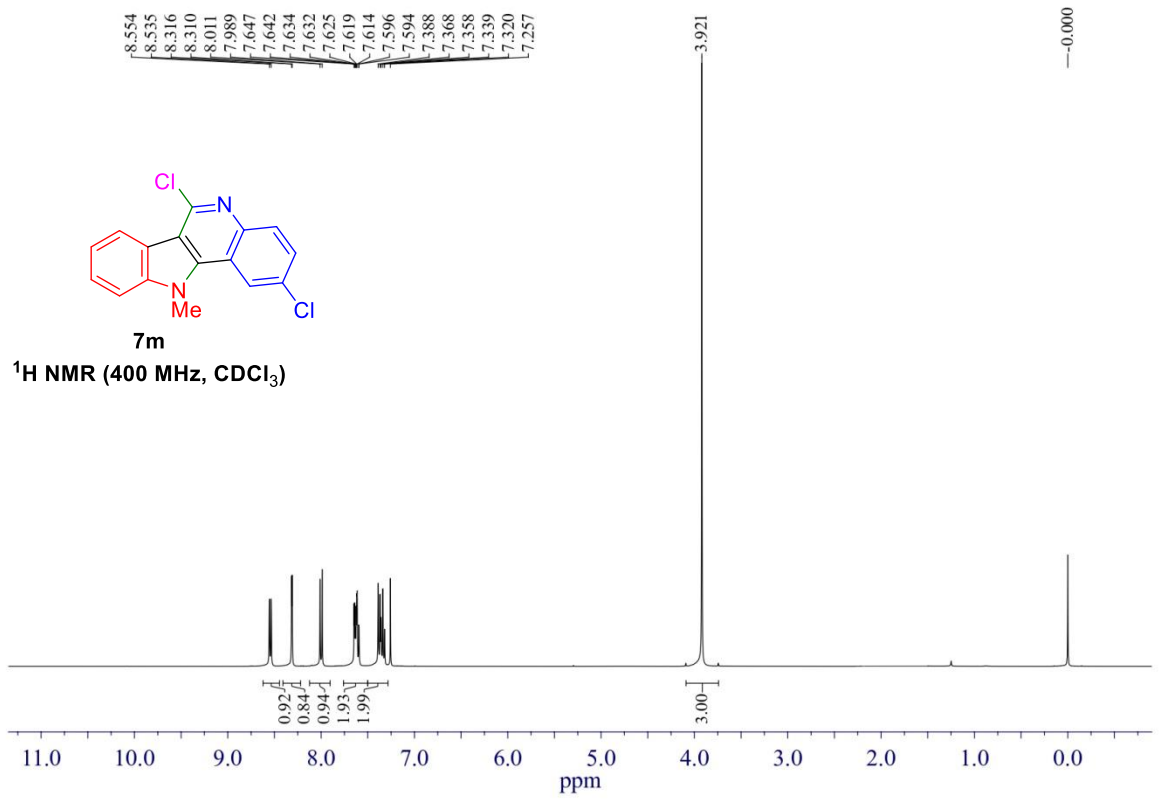


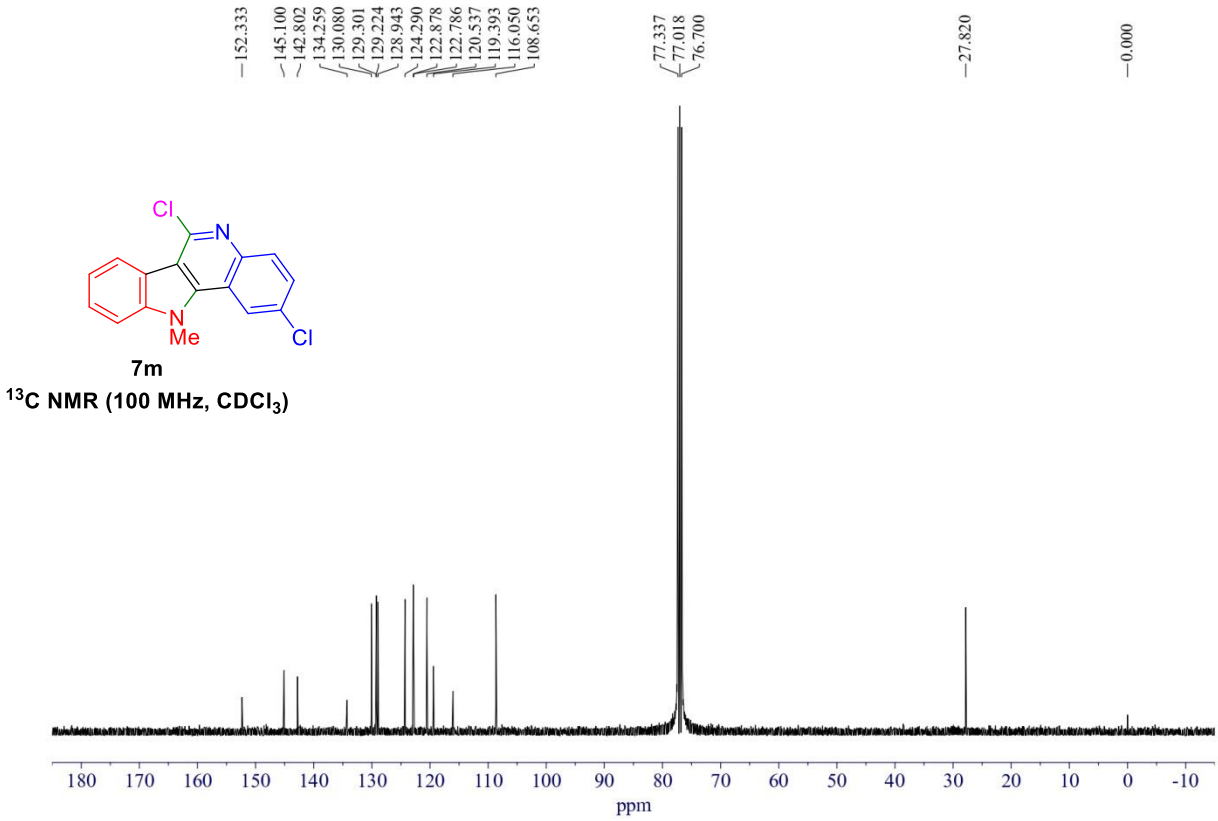
7l

^{13}C NMR (100 MHz, $CDCl_3$)



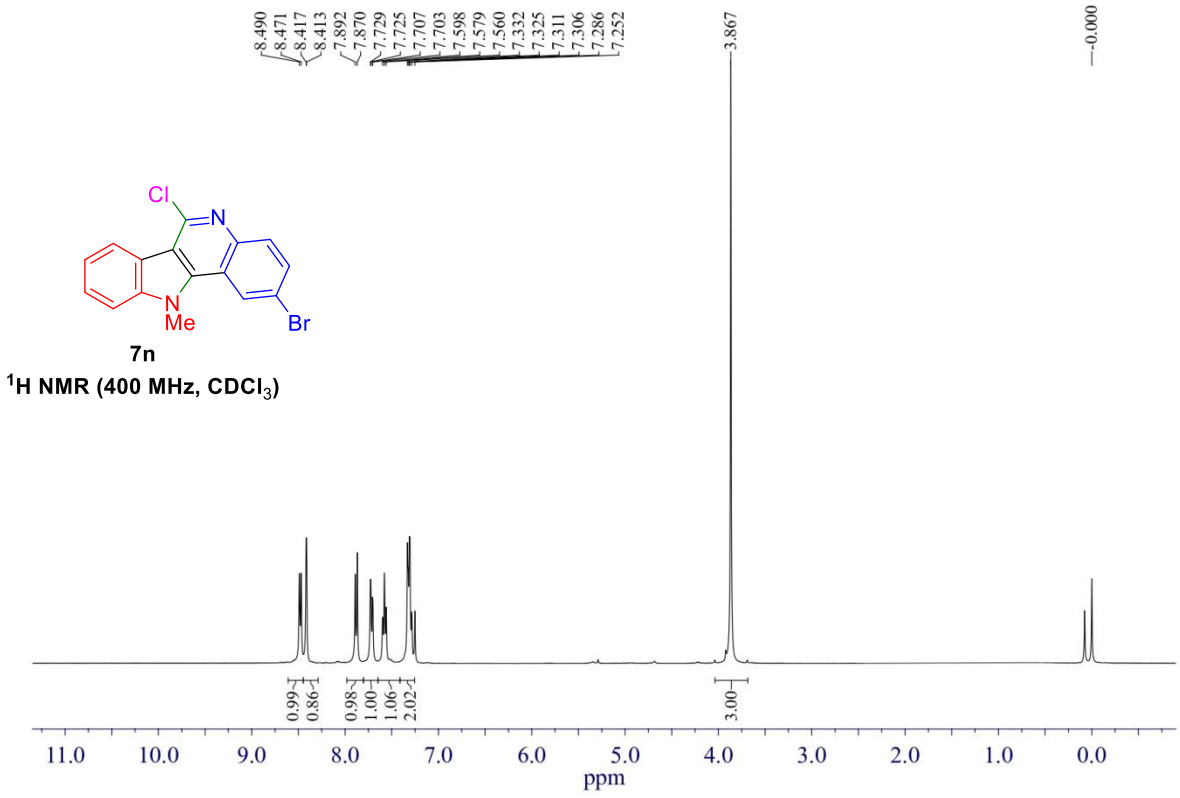
7m

^{1}H NMR (400 MHz, $CDCl_3$)



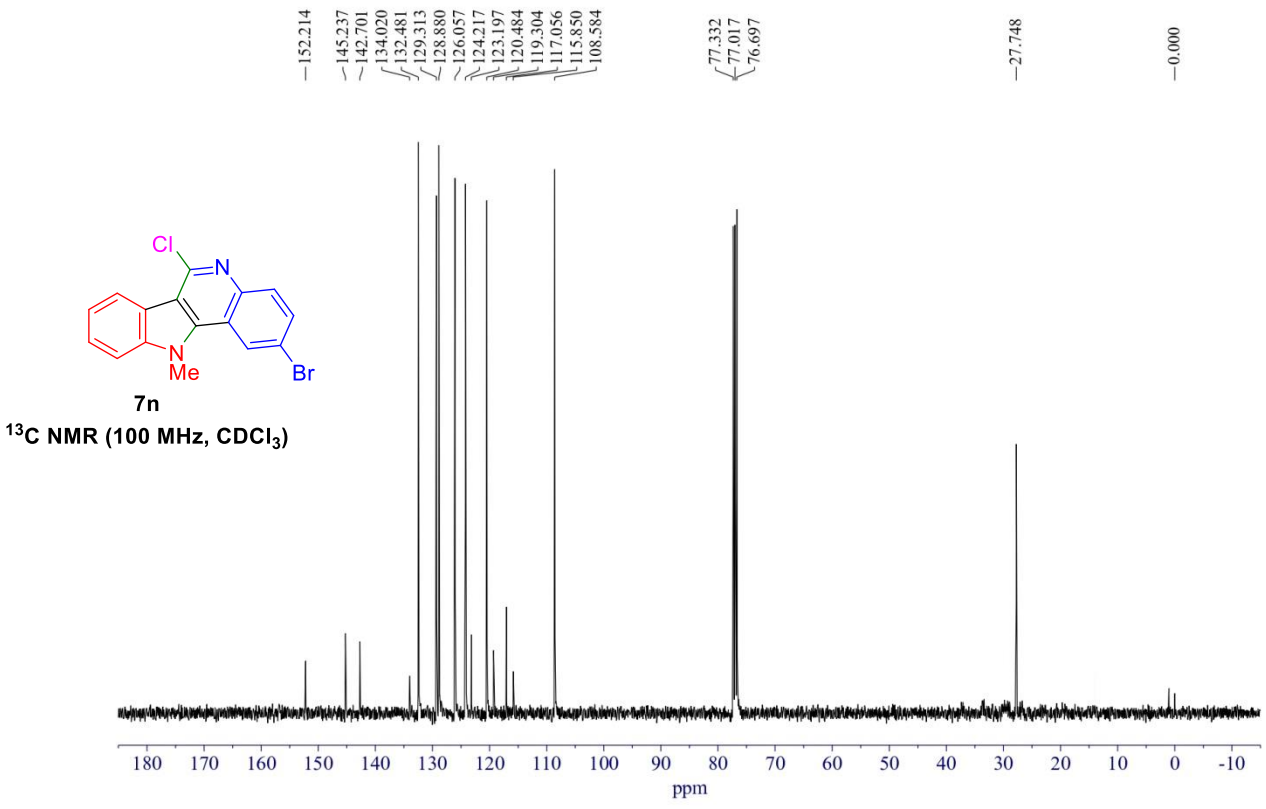
7m

^{13}C NMR (100 MHz, $CDCl_3$)



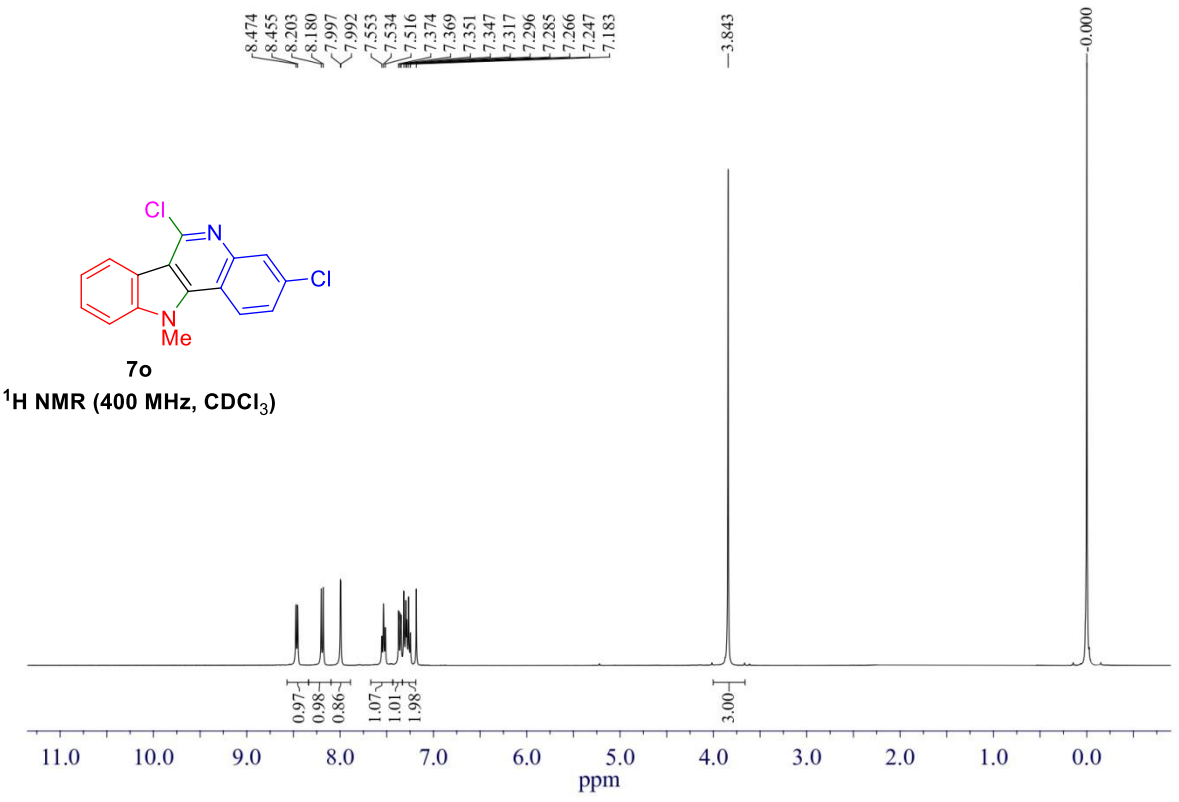
7n

^{1}H NMR (400 MHz, $CDCl_3$)



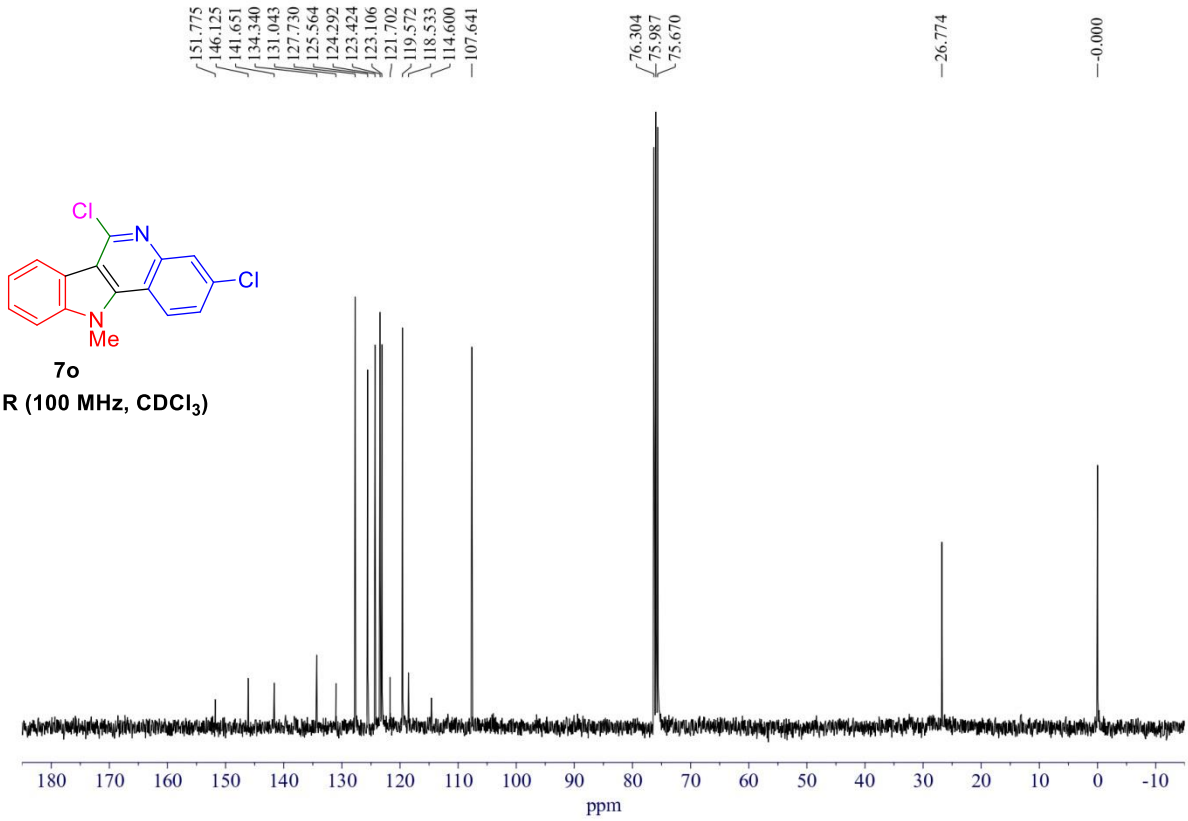
7n

^{13}C NMR (100 MHz, $CDCl_3$)



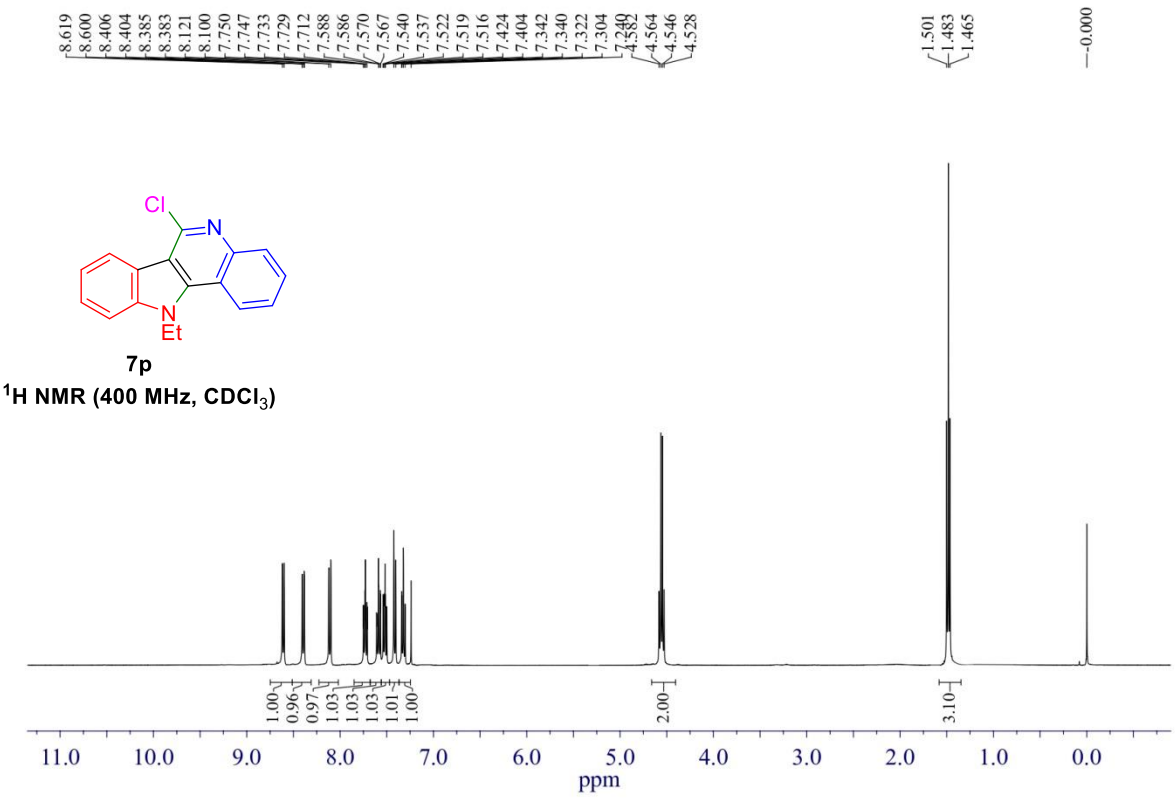
7o

^{1}H NMR (400 MHz, $CDCl_3$)



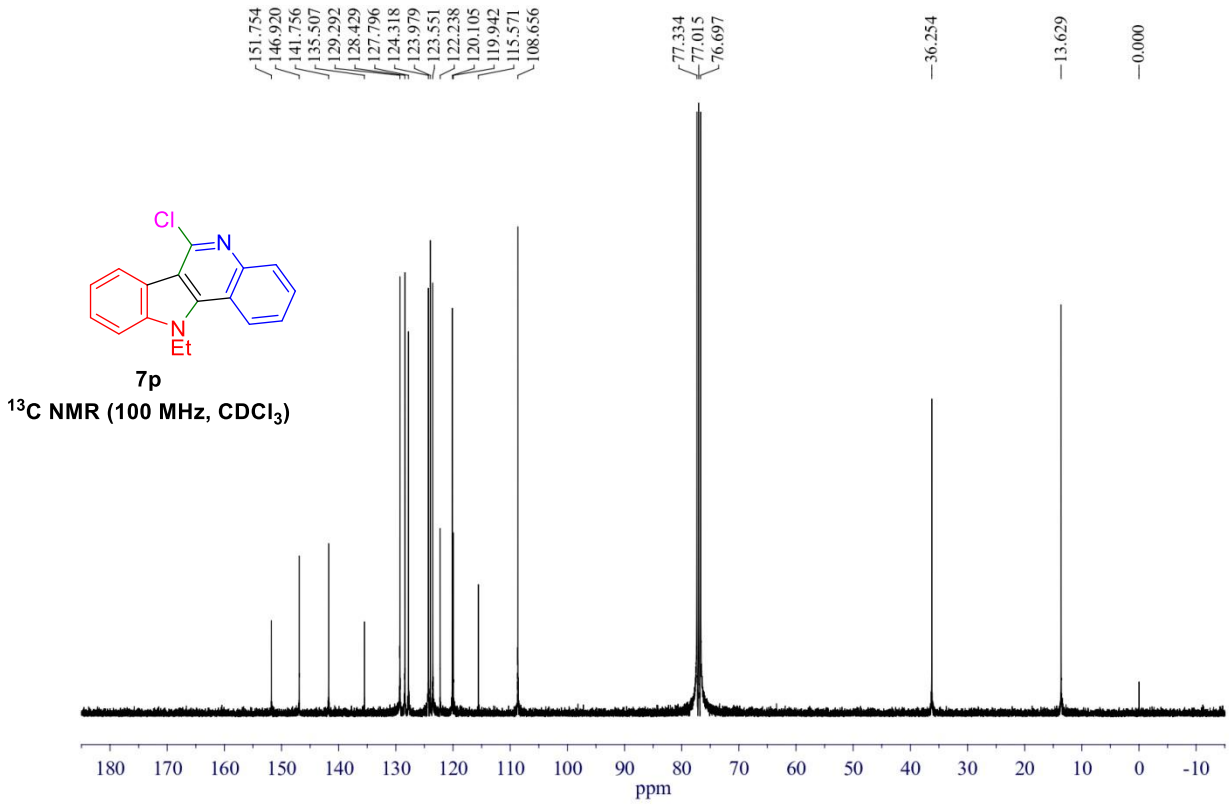
7o

^{13}C NMR (100 MHz, $CDCl_3$)



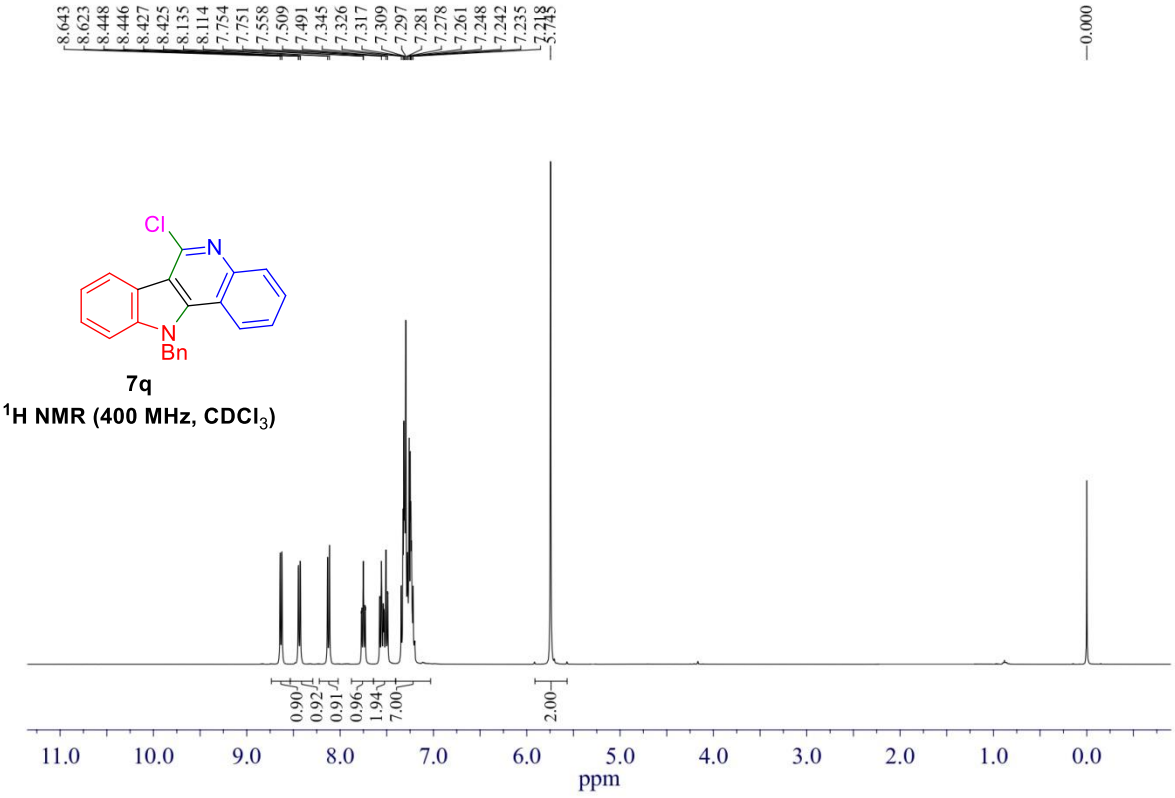
7p

^{1}H NMR (400 MHz, $CDCl_3$)



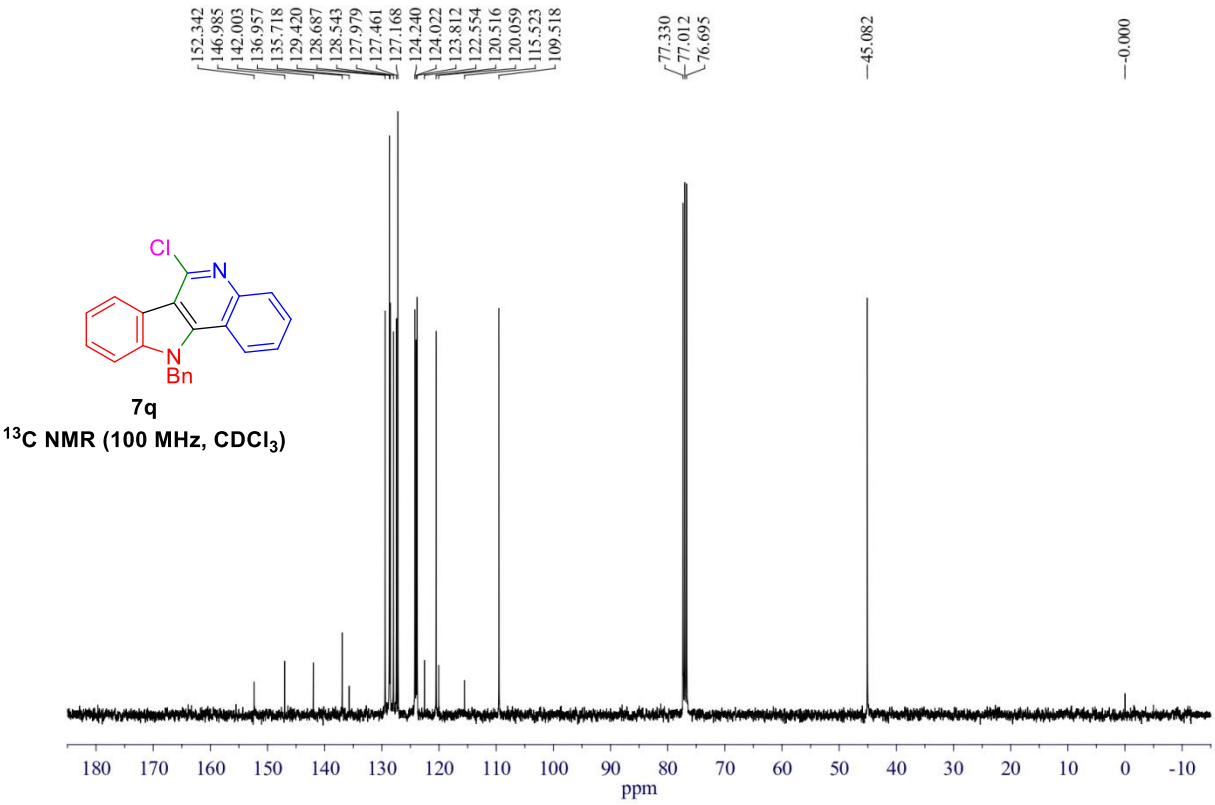
7p

^{13}C NMR (100 MHz, $CDCl_3$)



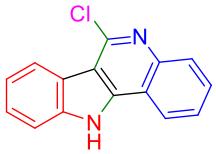
7q

^{1}H NMR (400 MHz, $CDCl_3$)



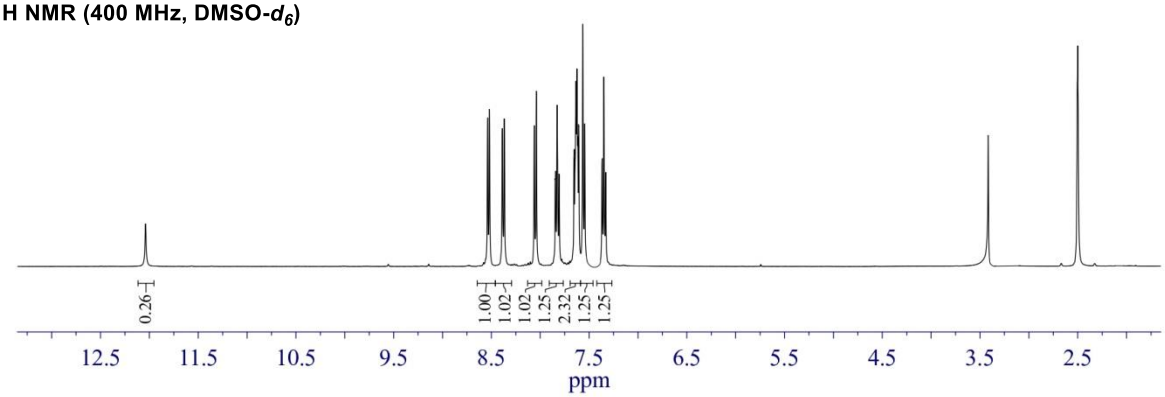
7q

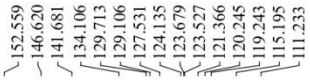
^{13}C NMR (100 MHz, $CDCl_3$)

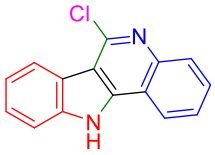


7r

^{1}H NMR (400 MHz, DMSO-d_6)

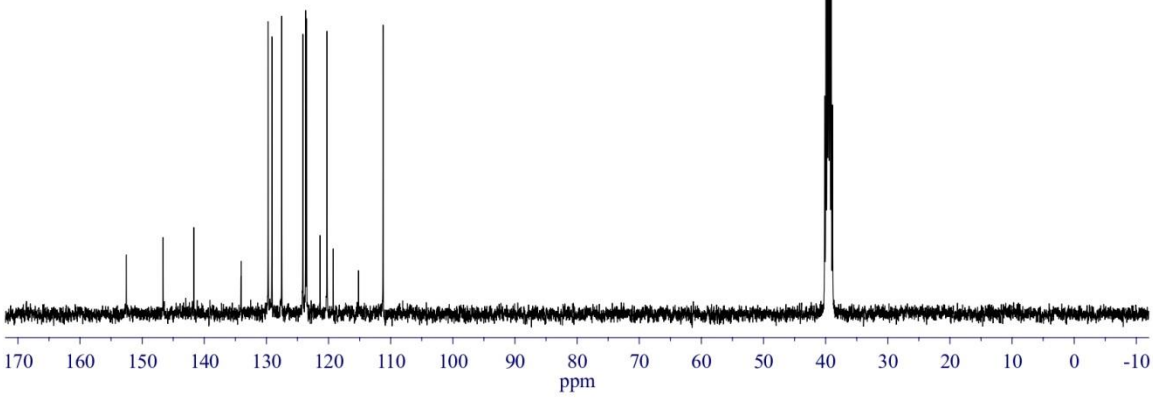


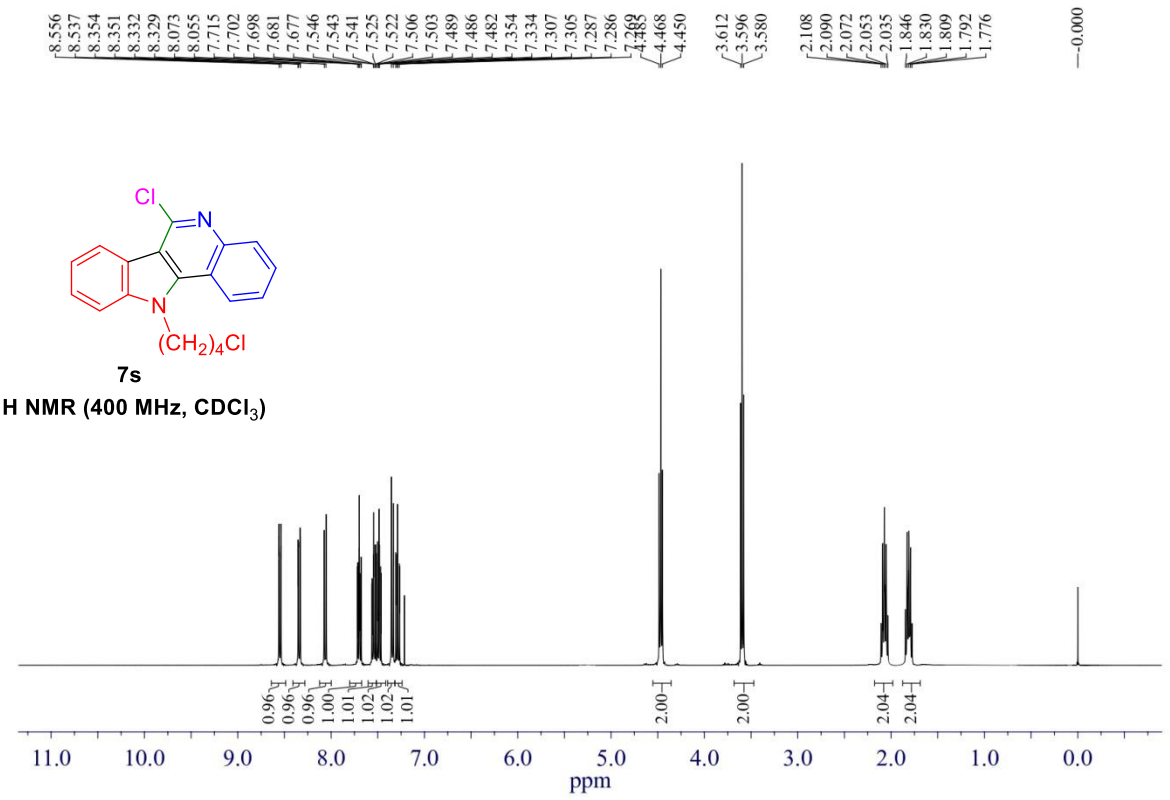




7r

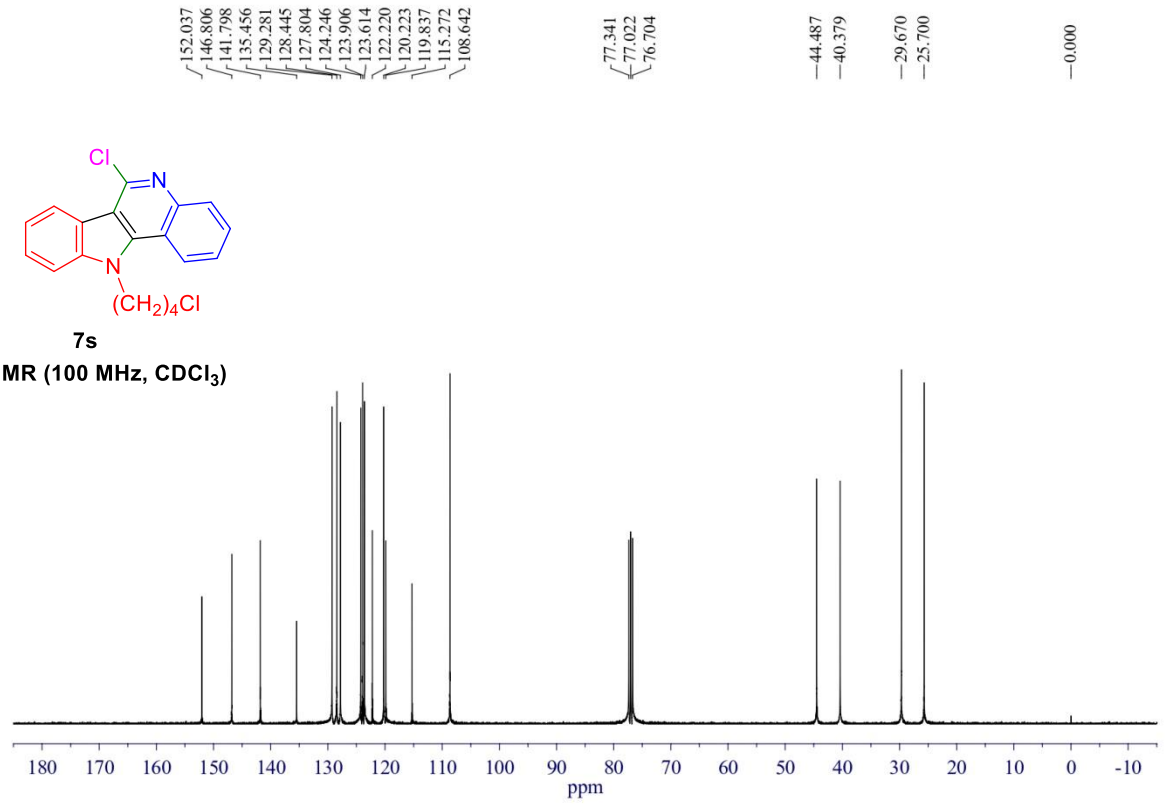
^{13}C NMR (100 MHz, DMSO-d_6)





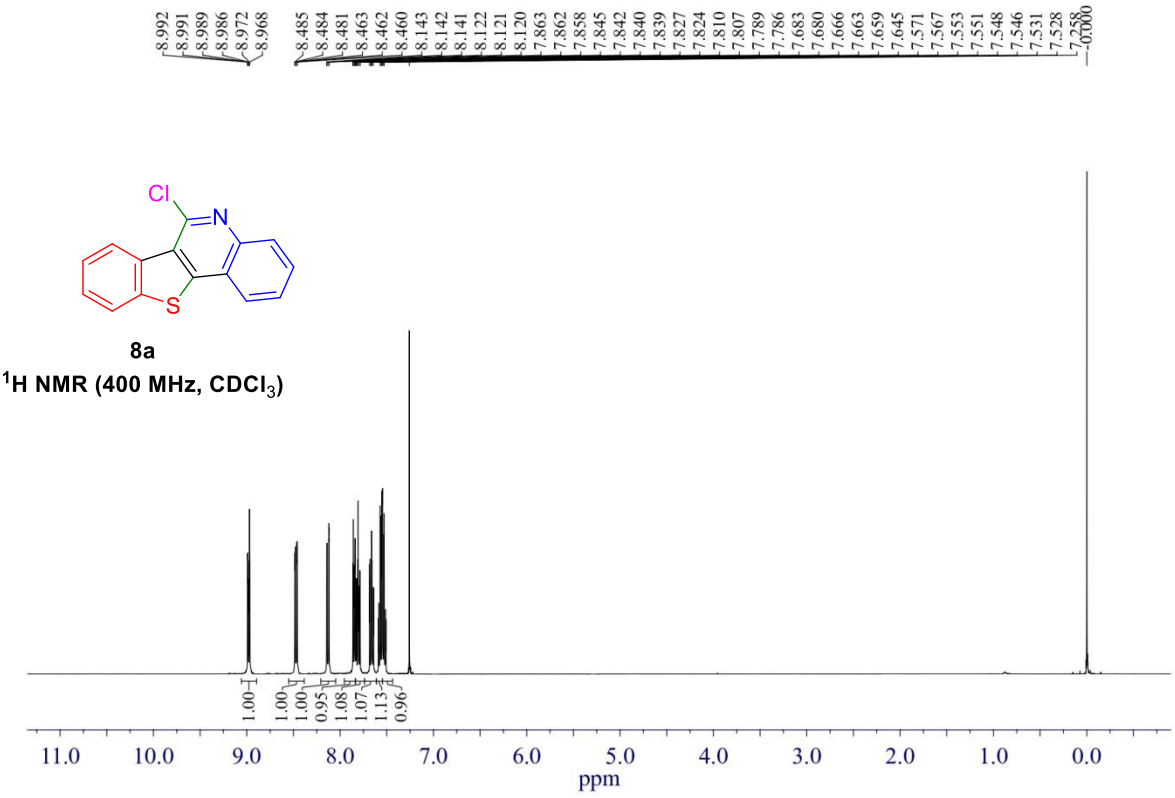
7s

^{1}H NMR (400 MHz, $CDCl_3$)



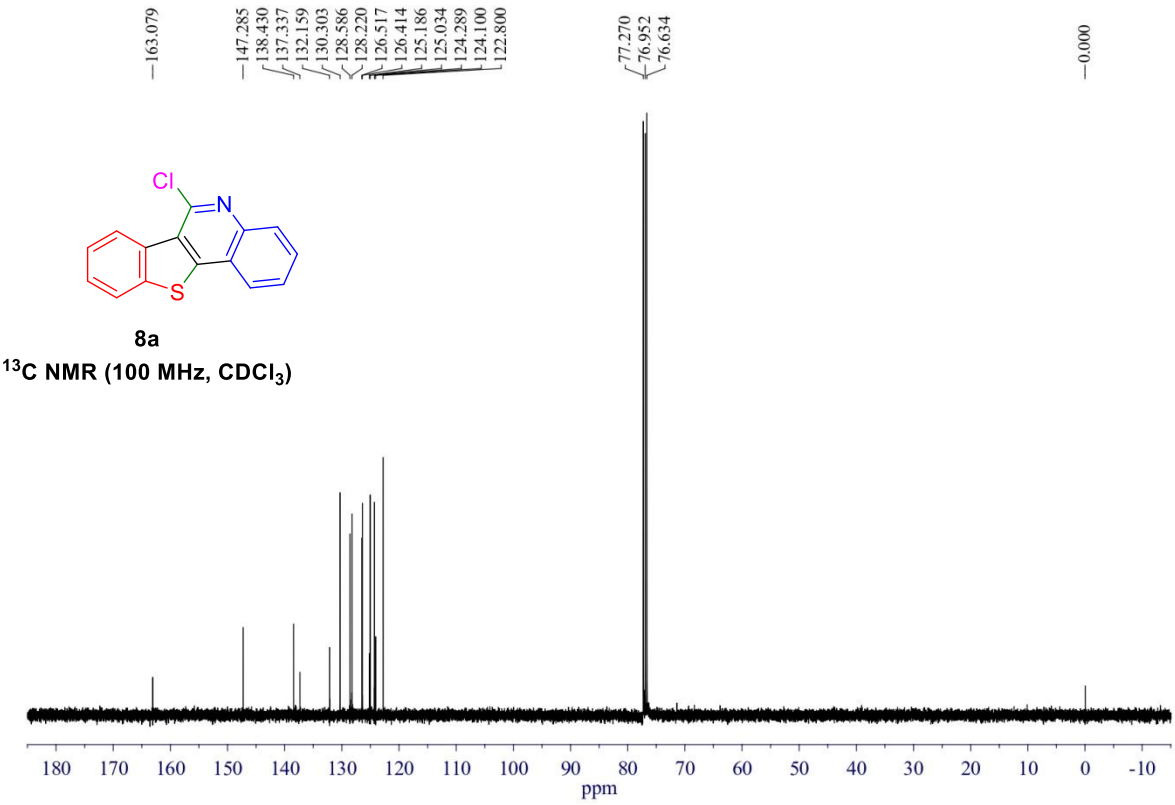
7s

^{13}C NMR (100 MHz, $CDCl_3$)



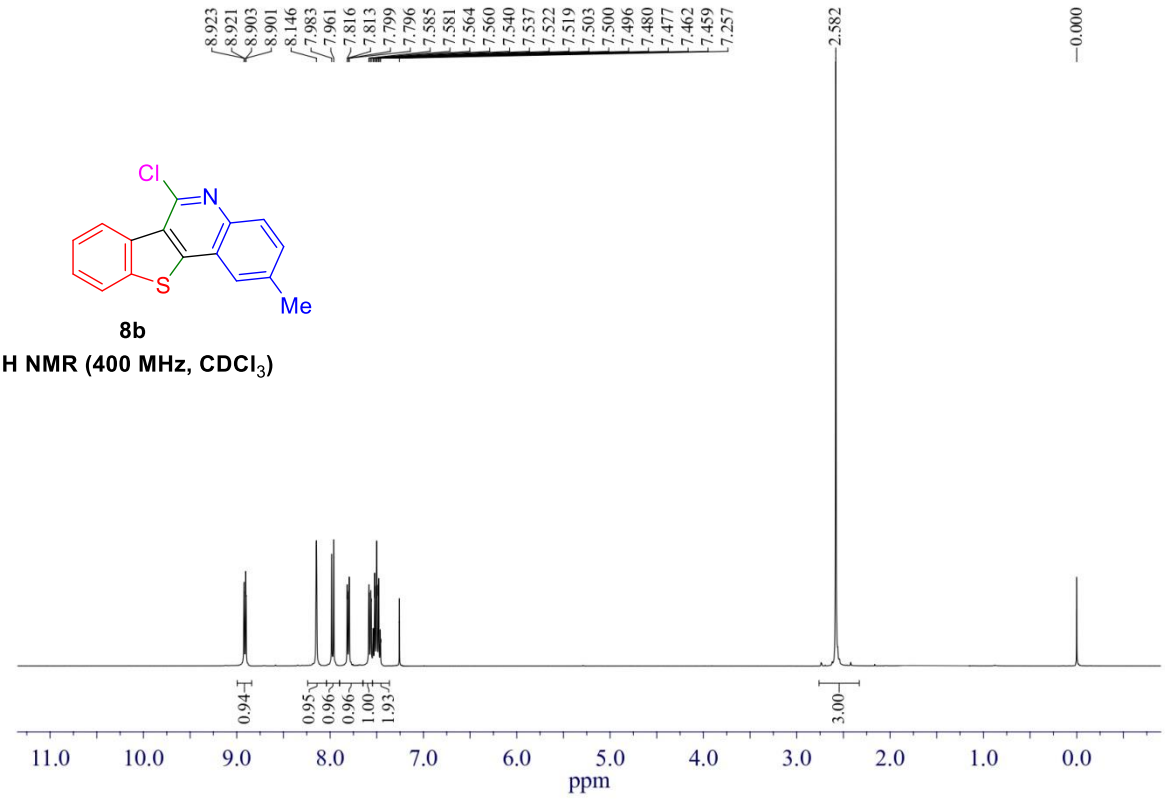
8a

^{1}H NMR (400 MHz, $CDCl_3$)



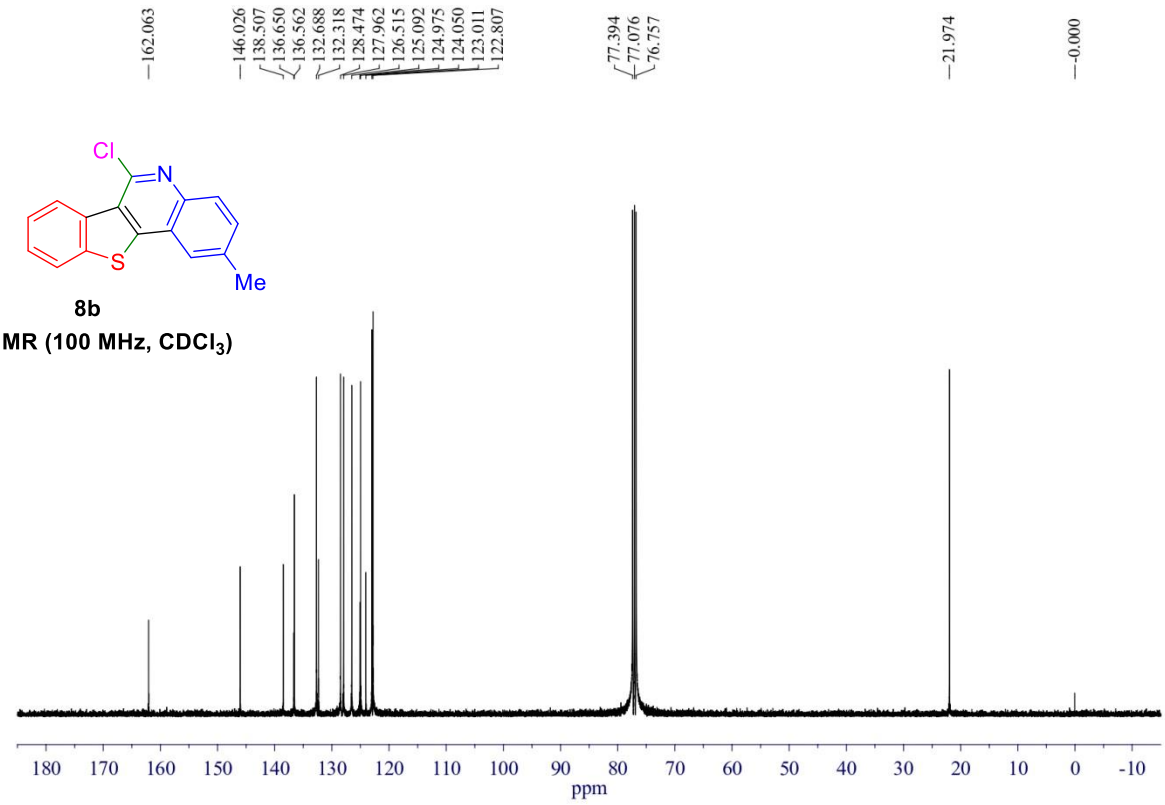
8a

^{13}C NMR (100 MHz, $CDCl_3$)



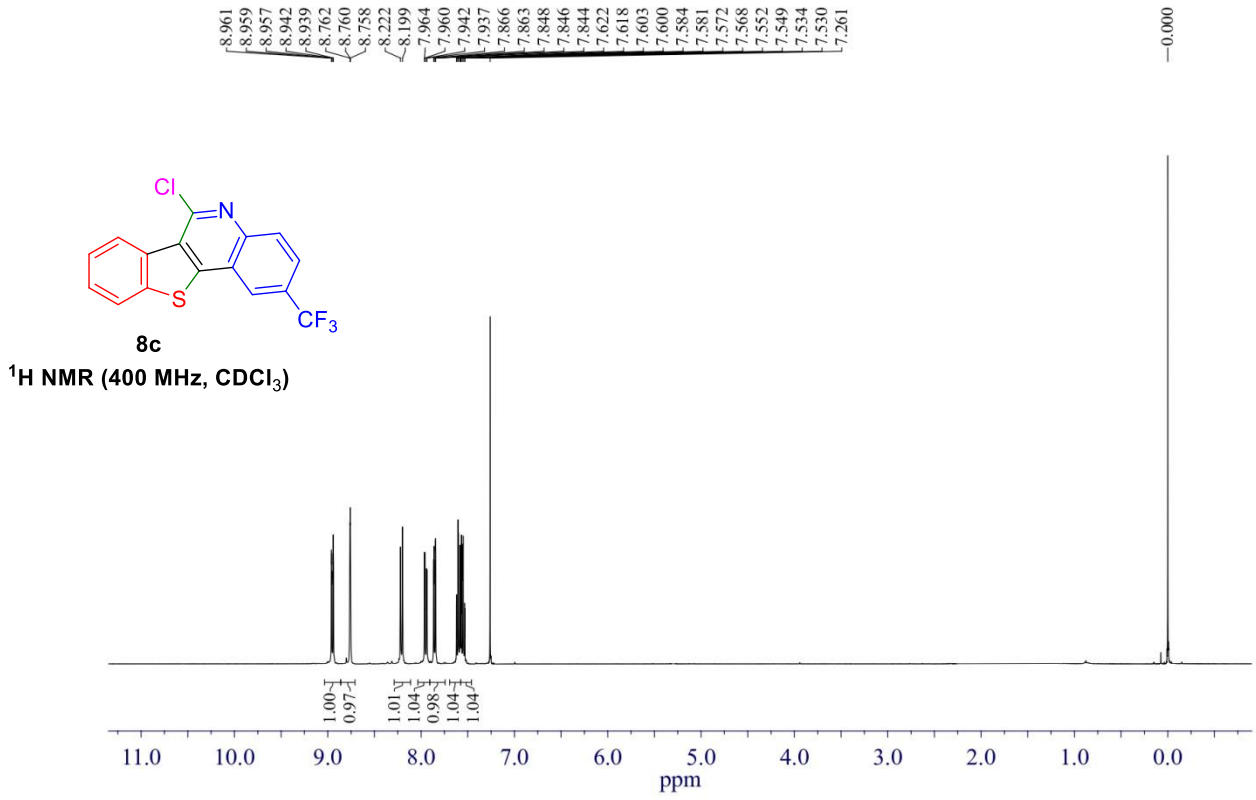
8b

^{1}H NMR (400 MHz, $CDCl_3$)



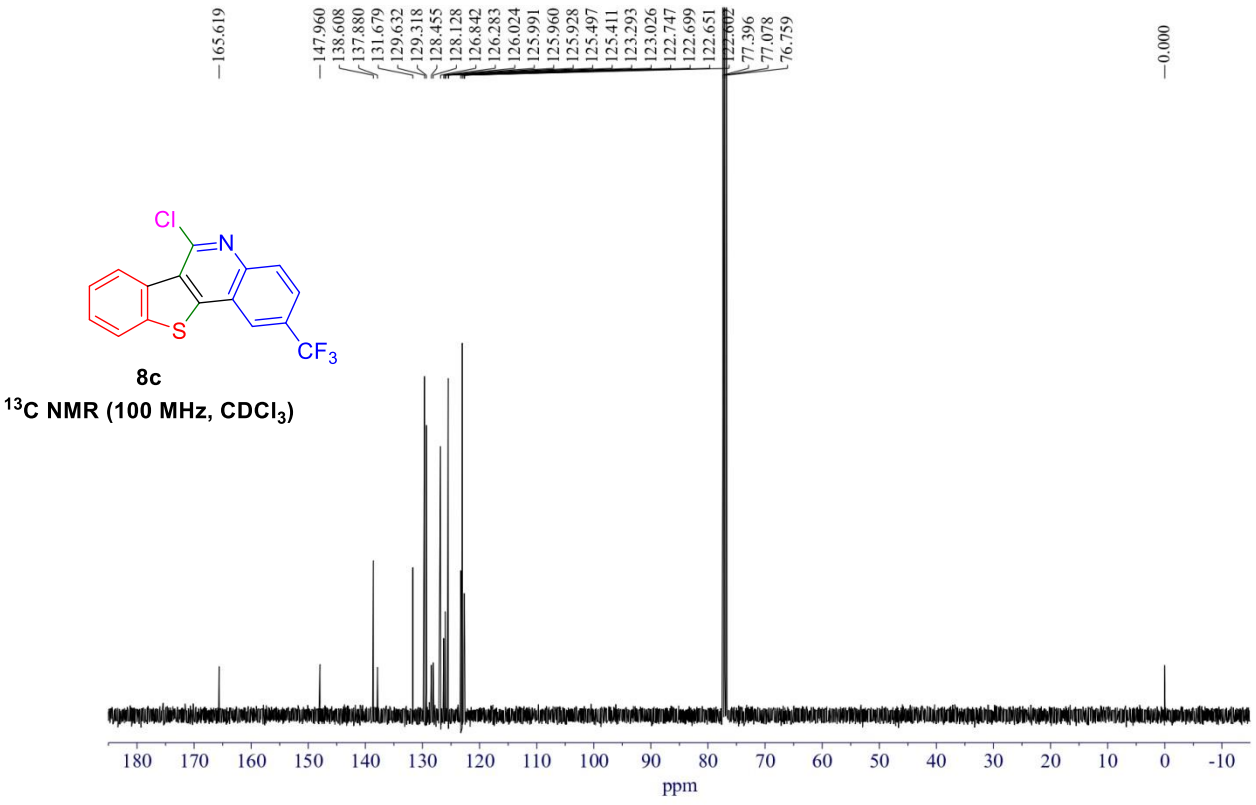
8b

^{13}C NMR (100 MHz, $CDCl_3$)



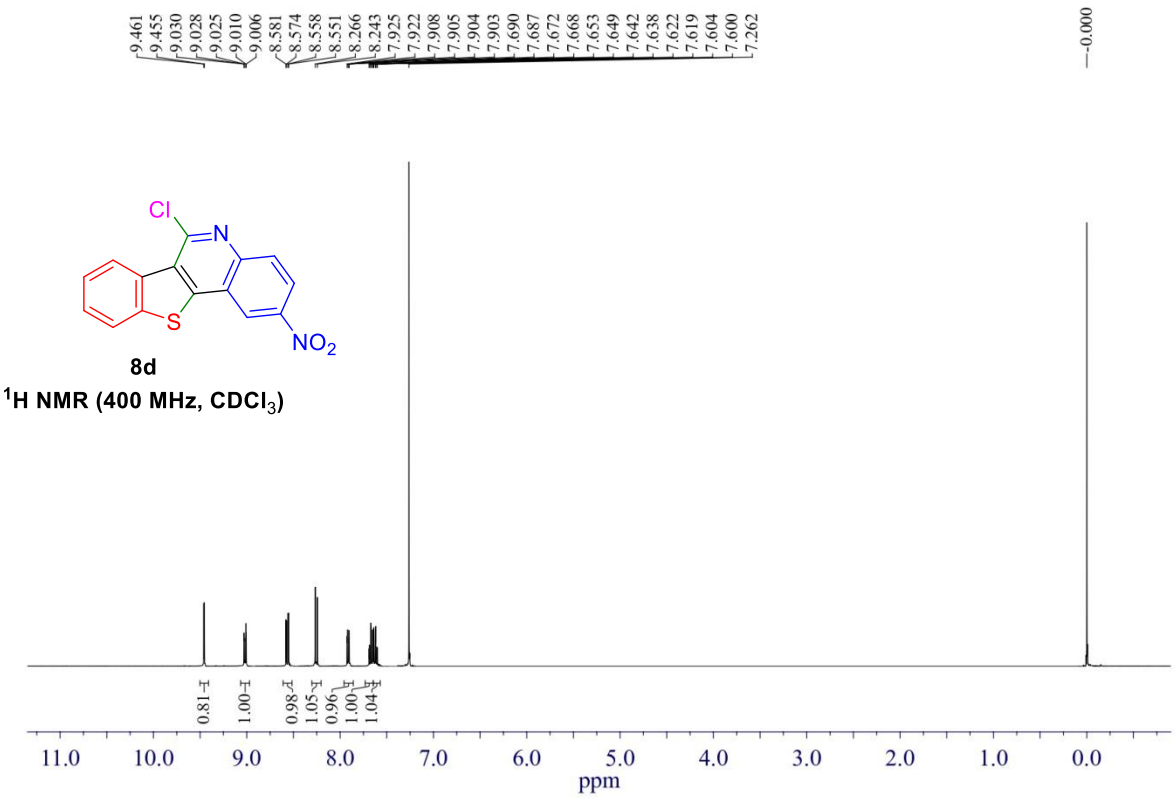
8c

^{1}H NMR (400 MHz, $CDCl_3$)



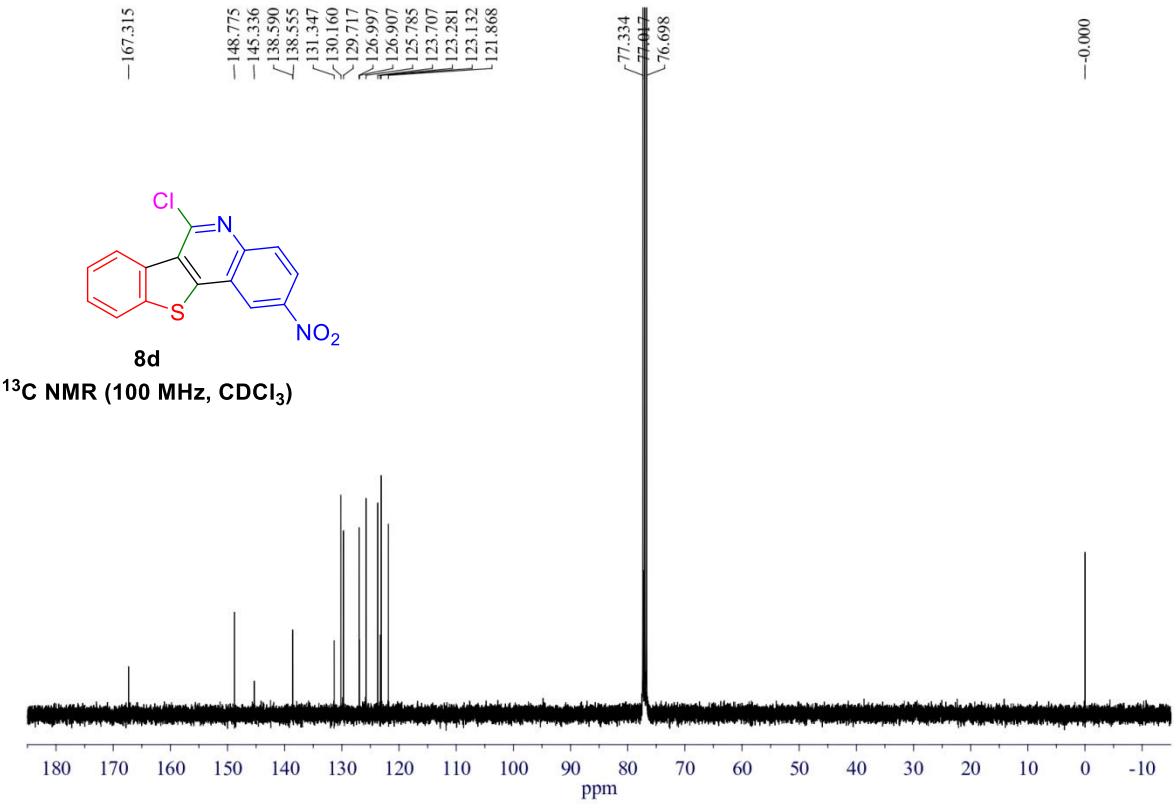
8c

^{13}C NMR (100 MHz, $CDCl_3$)



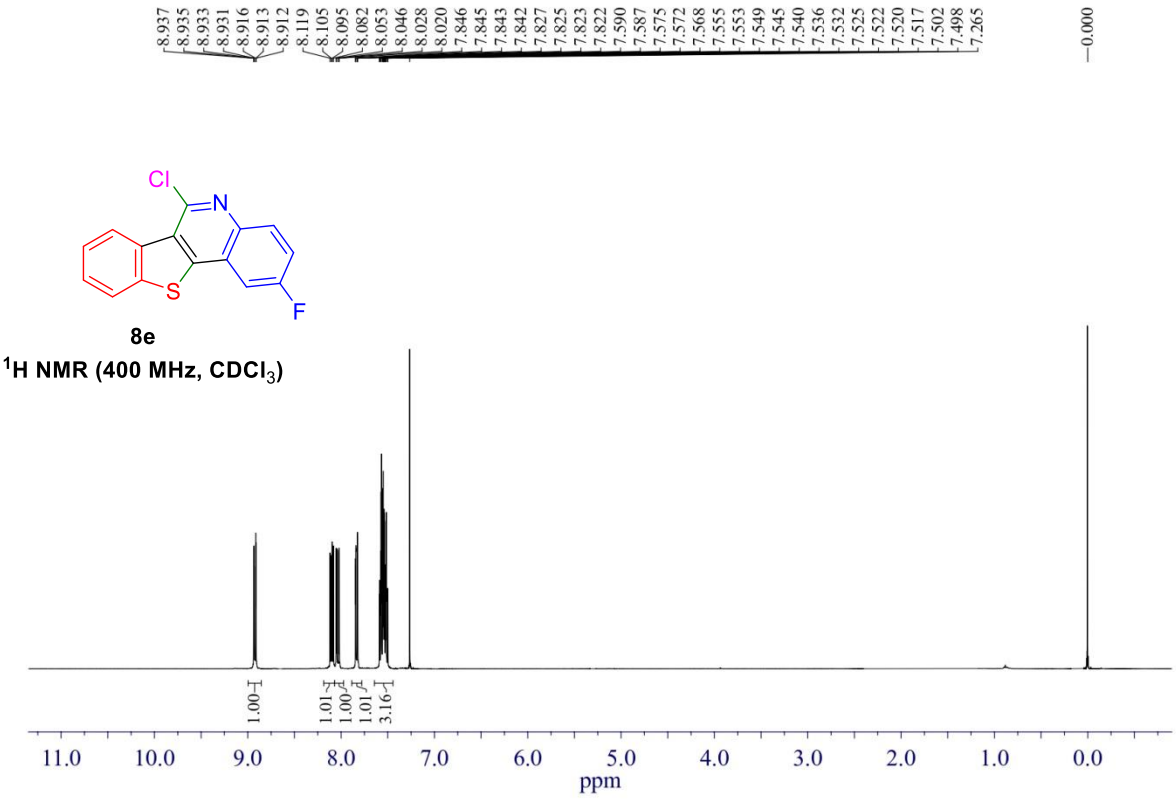
8d

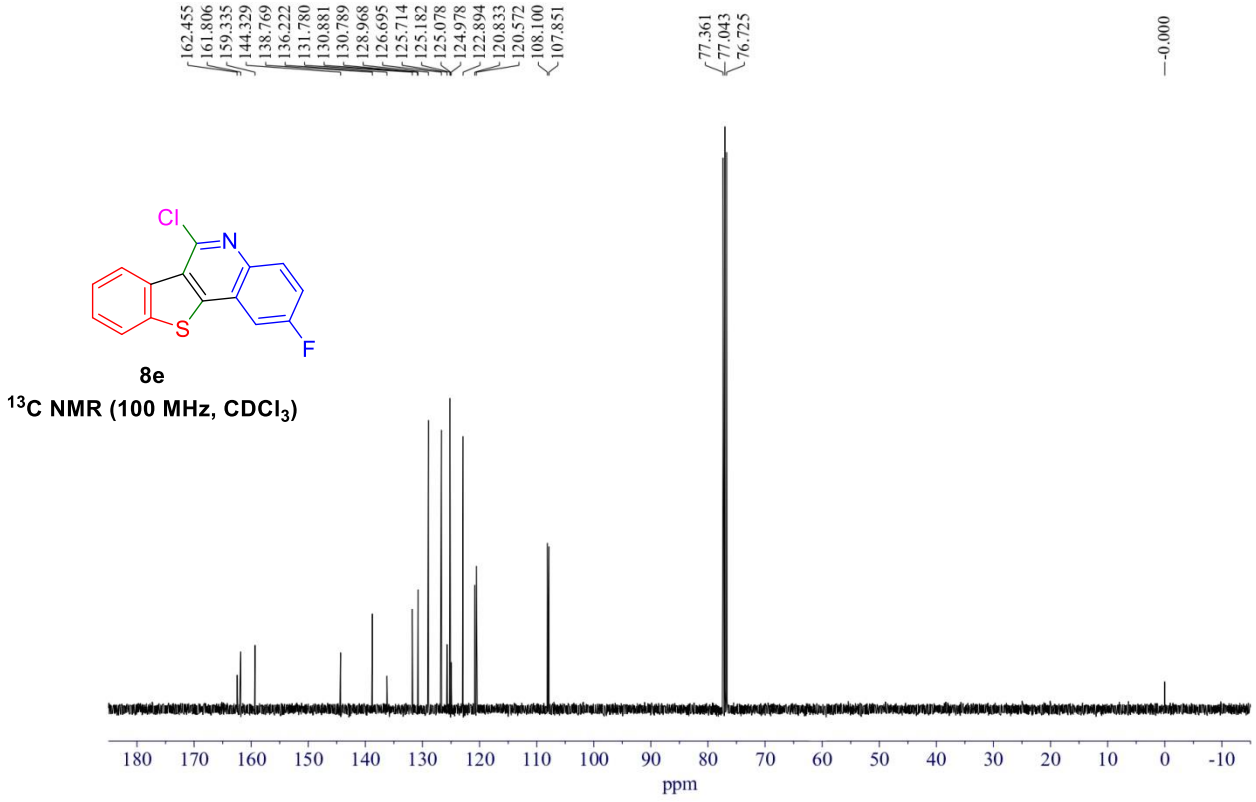
^{1}H NMR (400 MHz, $CDCl_3$)

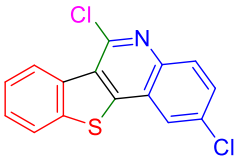


8d

^{13}C NMR (100 MHz, $CDCl_3$)

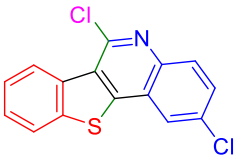

8.937
8.935
8.933
8.931
8.916
8.913
8.912
8.119
8.105
8.095
8.082
8.053
8.046
8.028
8.020
7.846
7.845
7.843
7.842
7.827
7.825
7.823
7.822
7.590
7.587
7.575
7.572
7.568
7.555
7.553
7.549
7.545
7.540
7.536
7.532
7.525
7.522
7.520
7.517
7.502
7.498
7.265
0.000
Cl
N
S
F
8e
1H NMR (400 MHz, CDCl3)
1.00
1.01
1.00
1.01
3.16
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


162.455
161.806
159.335
144.329
138.769
136.222
131.780
130.881
130.789
128.968
126.695
125.714
125.182
125.078
124.978
122.894
120.833
120.572
108.100
107.851
77.361
77.043
76.725
-0.000
Cl
N
S
F
8e
13C NMR (100 MHz, CDCl3)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm



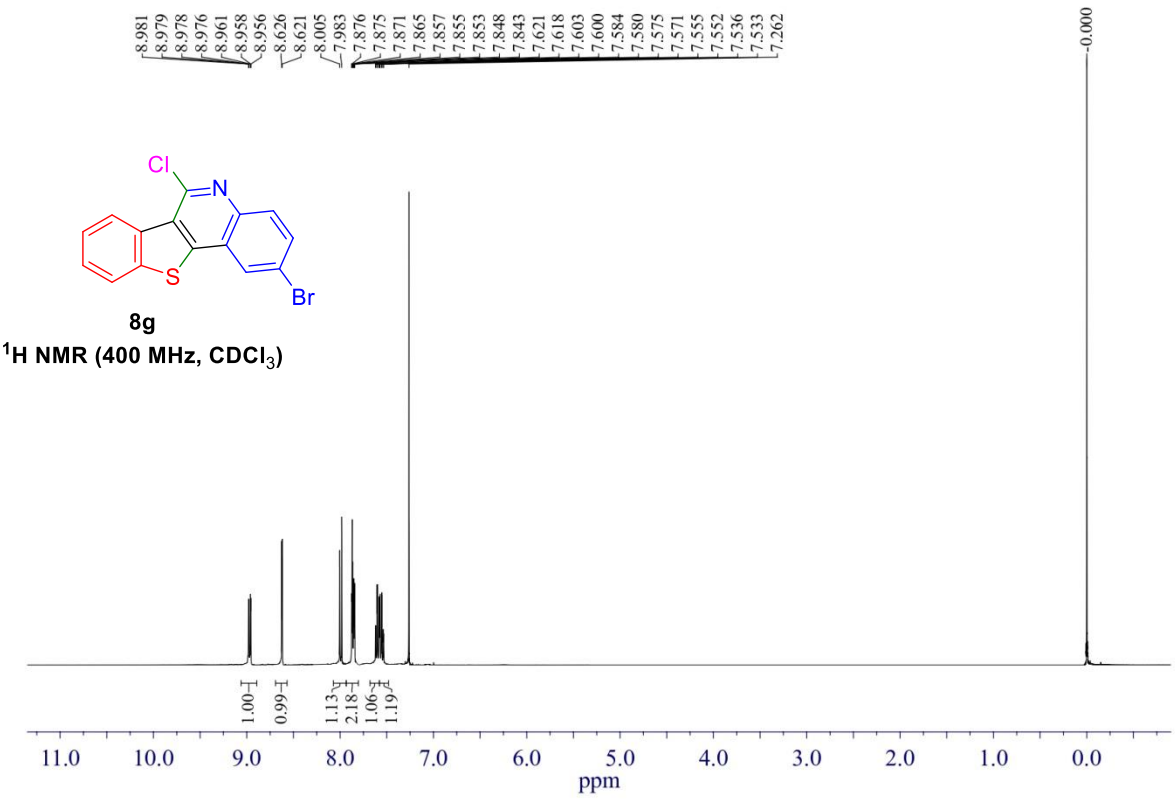
8f

^{1}H NMR (400 MHz, $CDCl_3$)



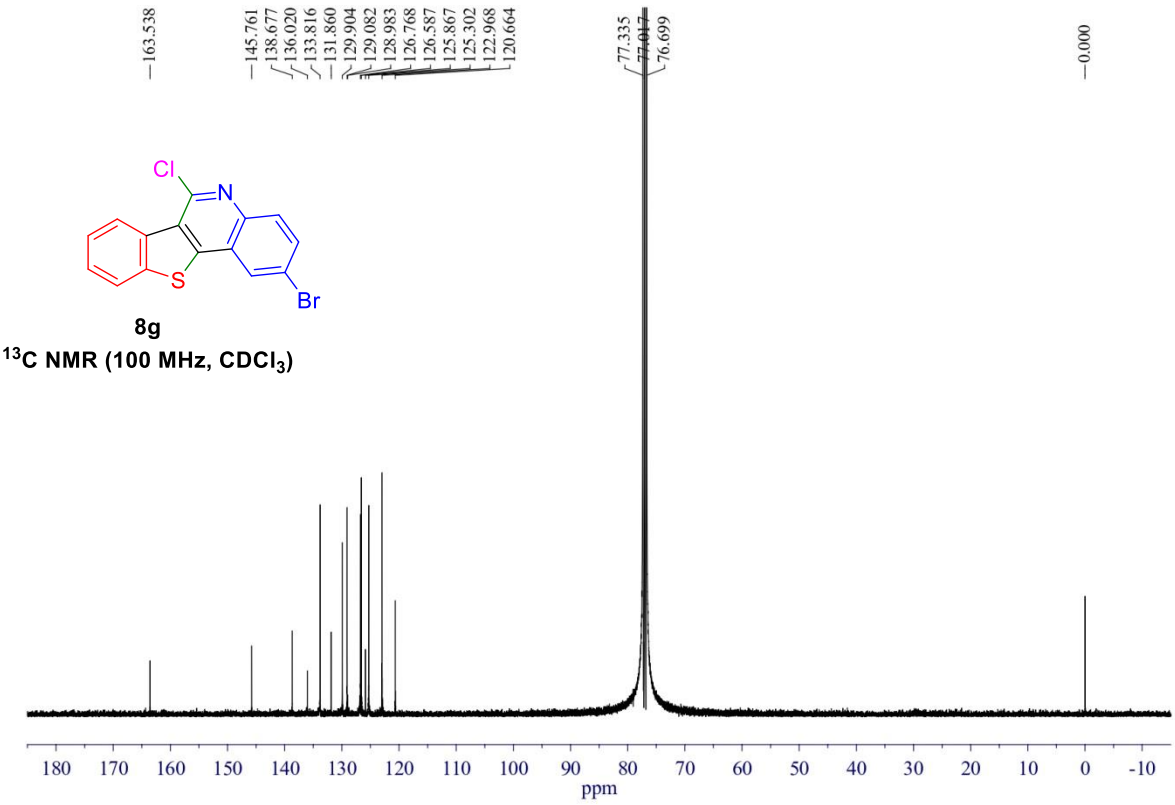
8f

^{13}C NMR (100 MHz, $CDCl_3$)



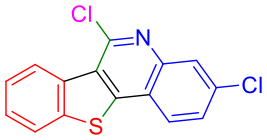
8g

^{1}H NMR (400 MHz, $CDCl_3$)



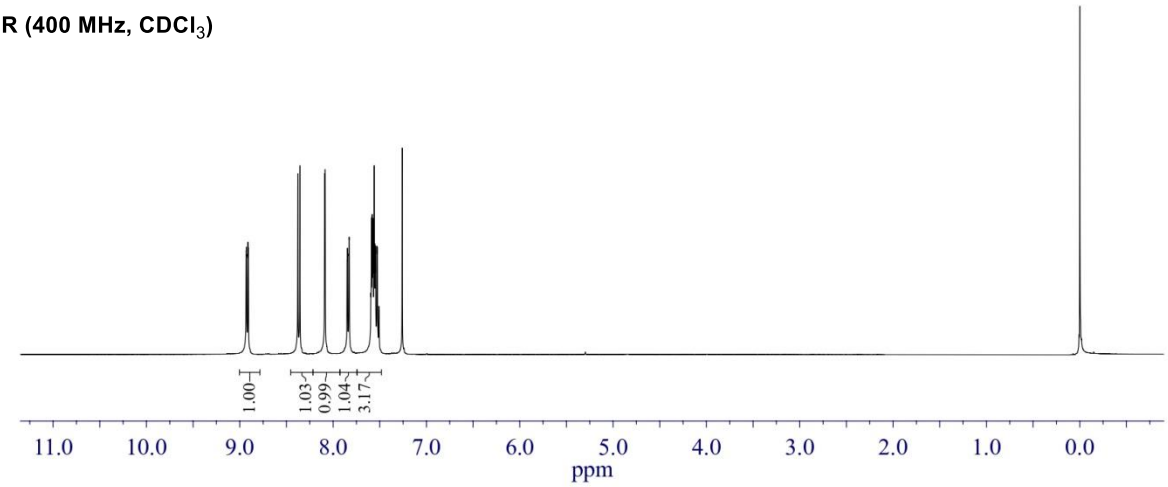
8g

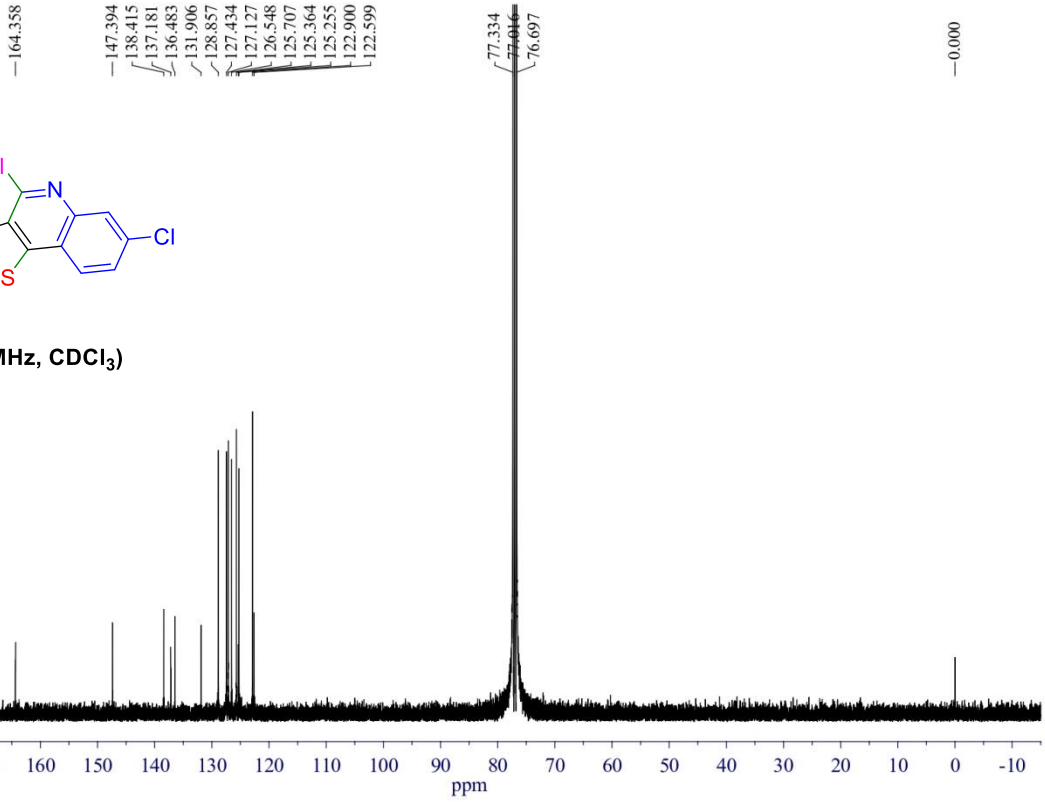
^{13}C NMR (100 MHz, $CDCl_3$)



8h

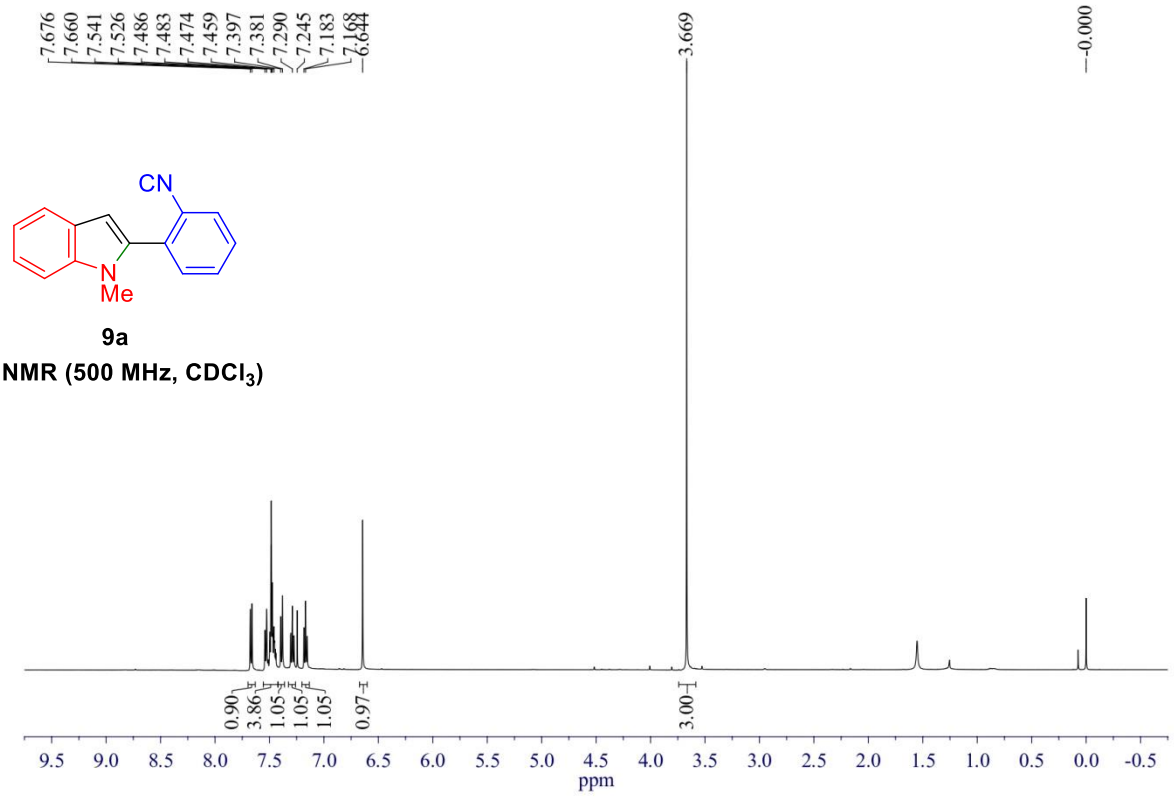
^{1}H NMR (400 MHz, $CDCl_3$)





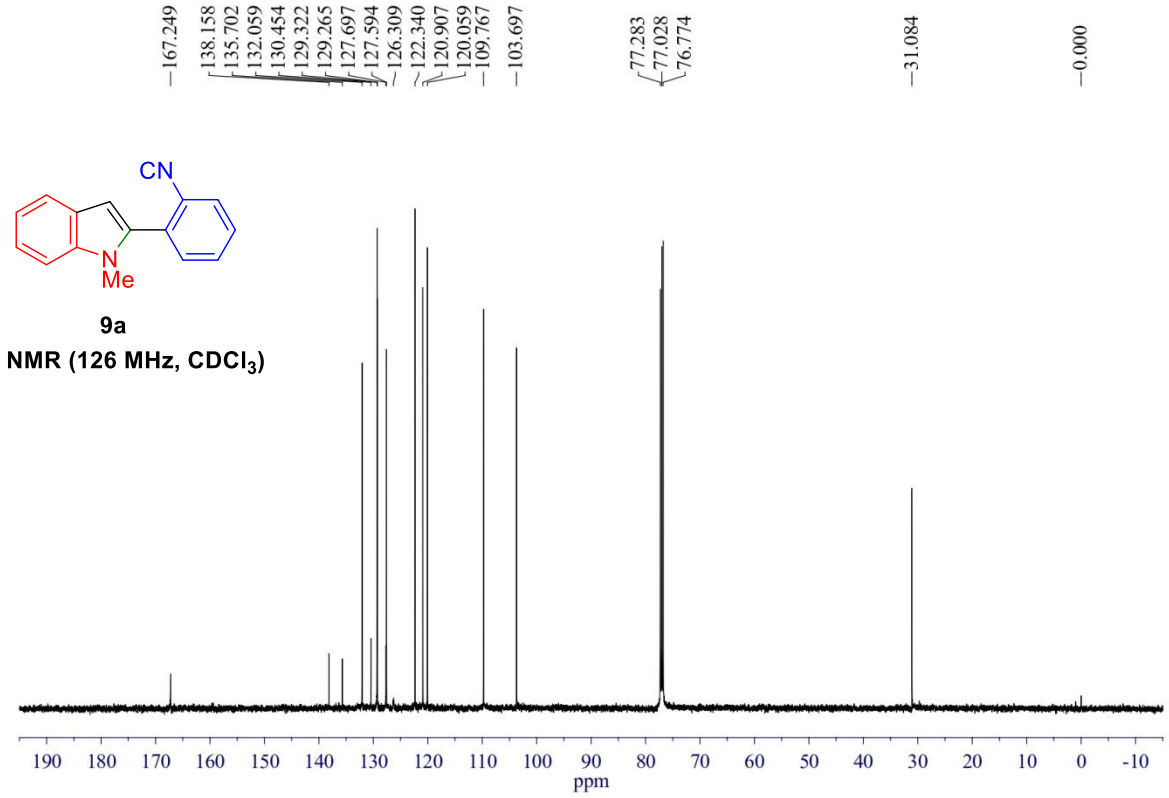
8h

^{13}C NMR (100 MHz, $CDCl_3$)



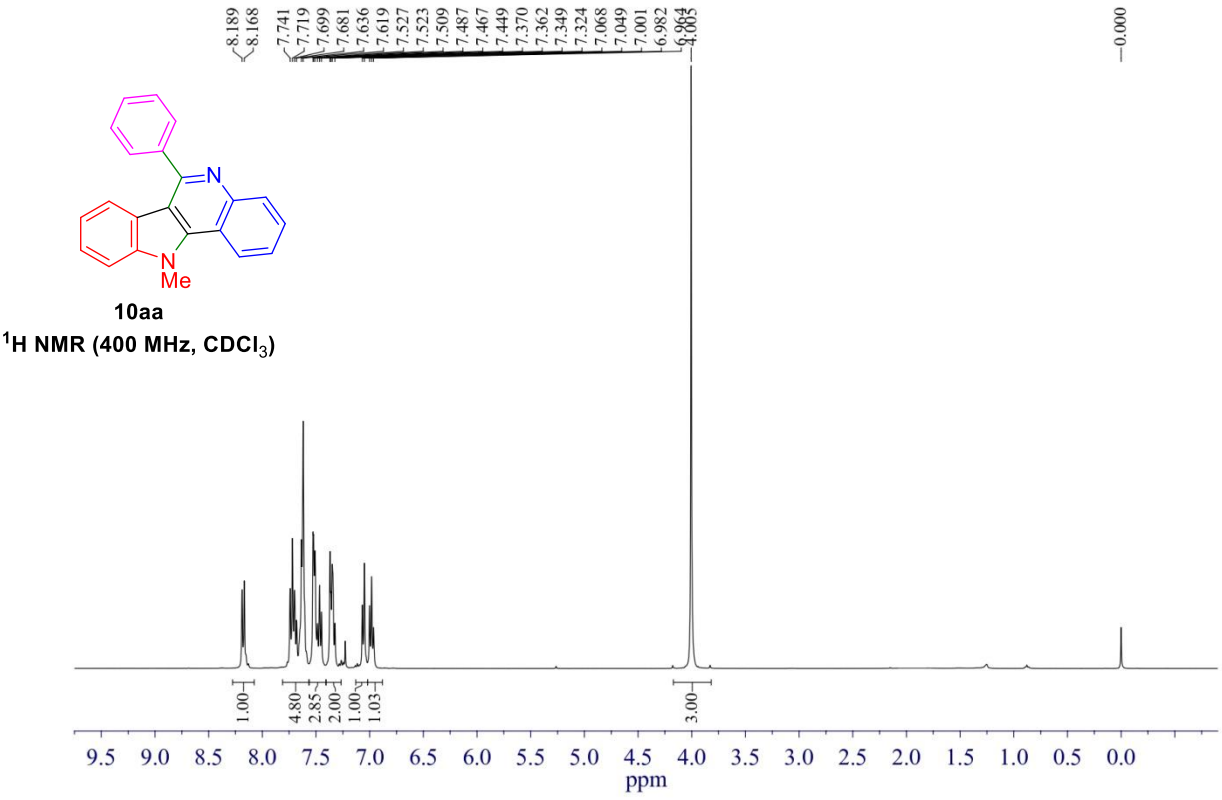
9a

^{1}H NMR (500 MHz, $CDCl_3$)



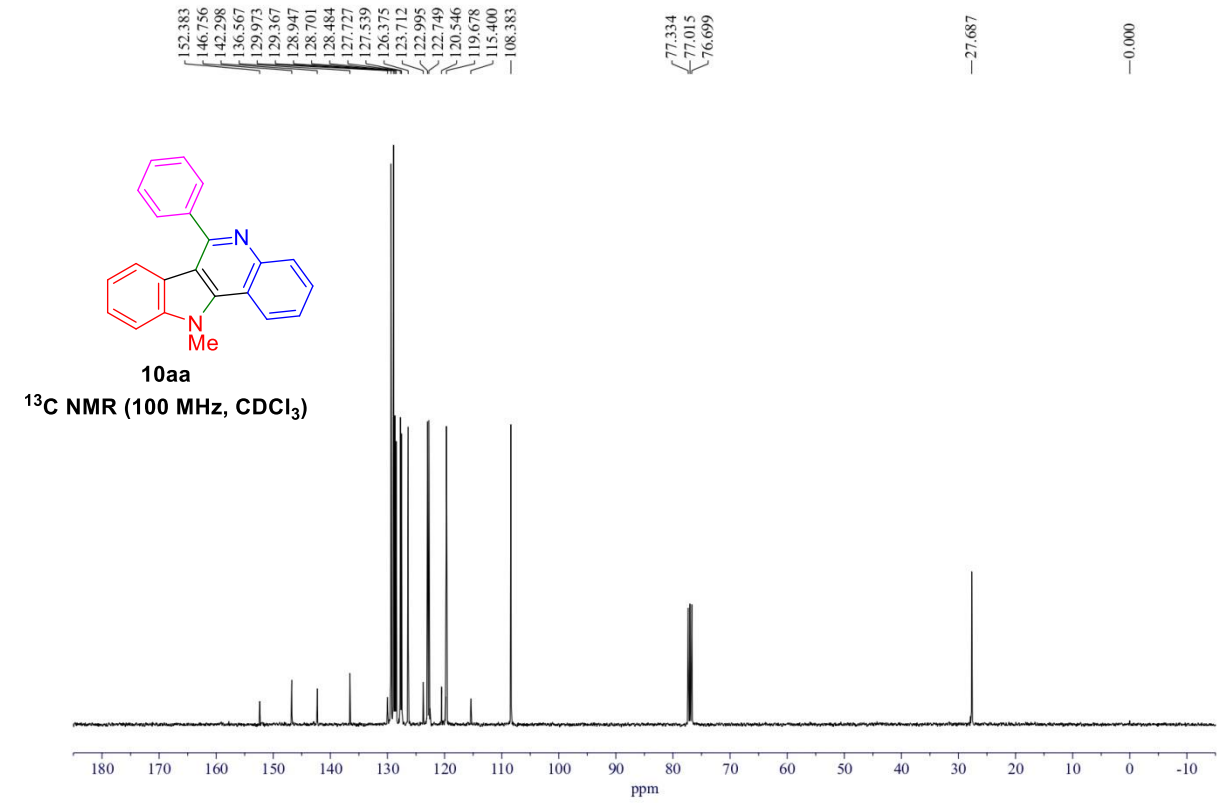
9a

^{13}C NMR (126 MHz, $CDCl_3$)



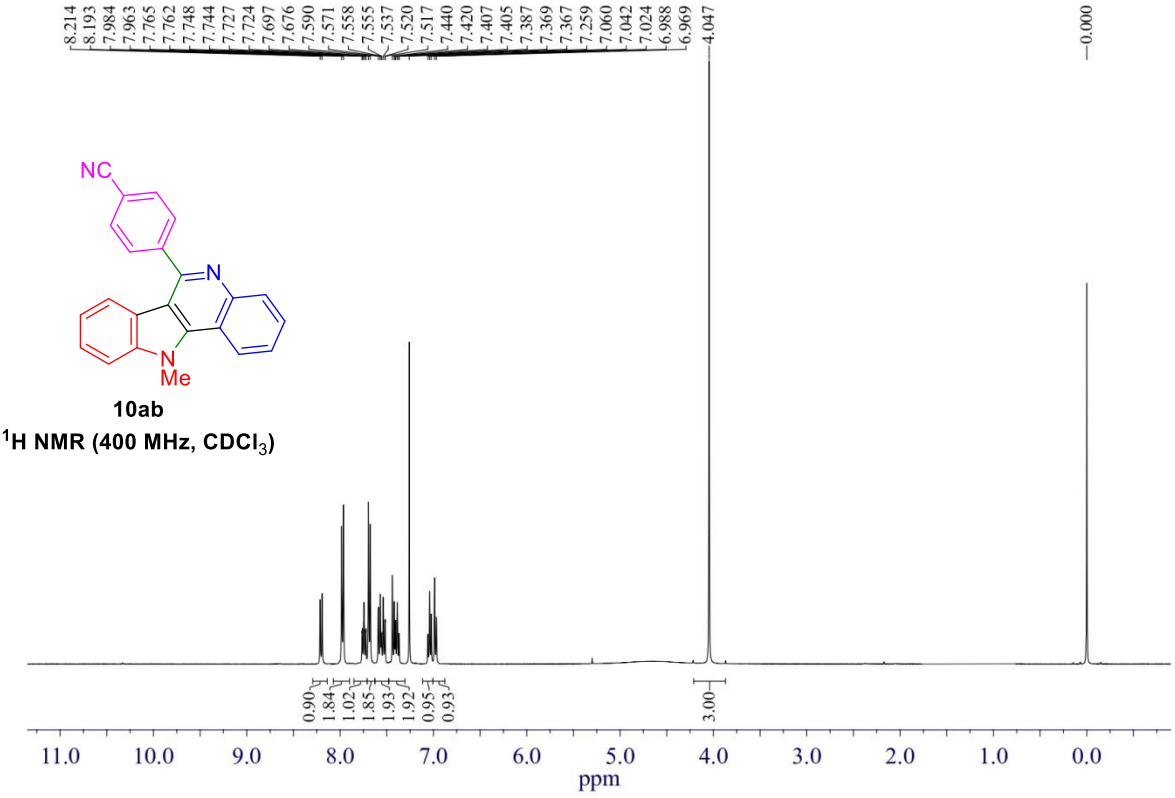
10aa

^{1}H NMR (400 MHz, $CDCl_3$)



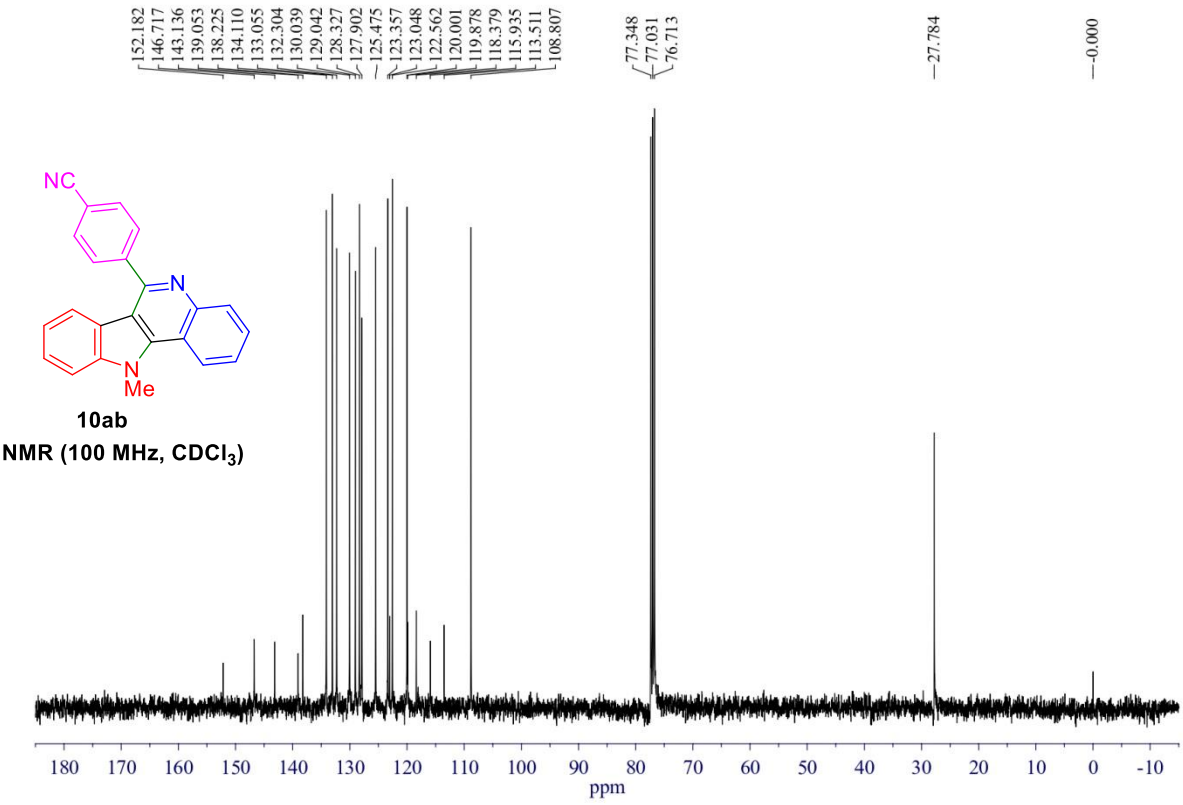
10aa

^{13}C NMR (100 MHz, $CDCl_3$)



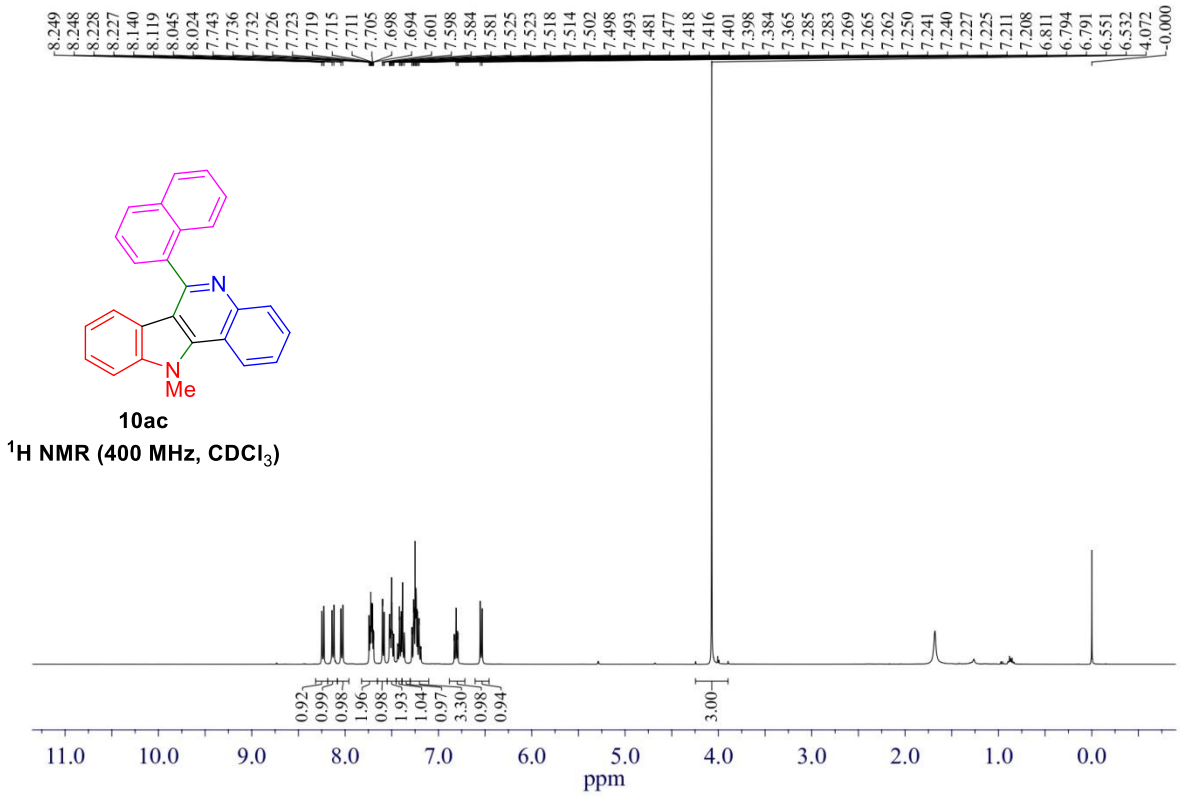
10ab

^{1}H NMR (400 MHz, $CDCl_3$)



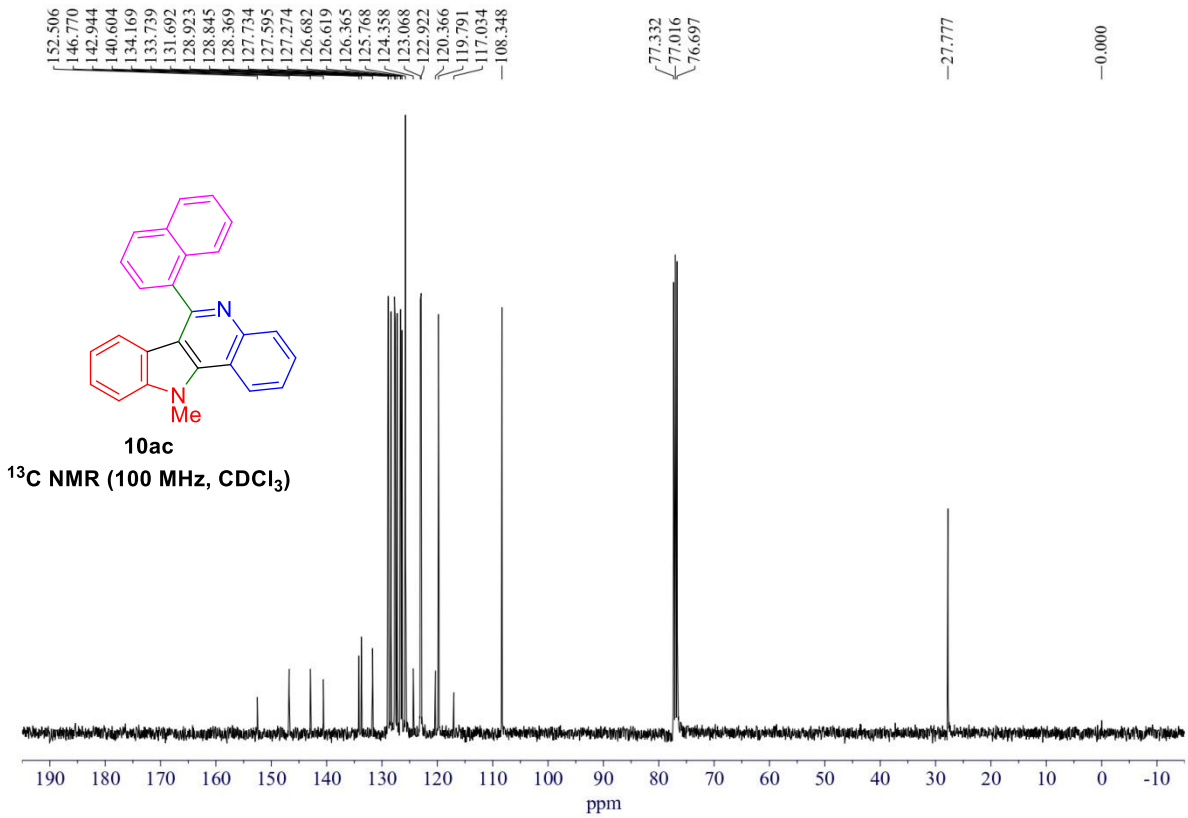
10ab

^{13}C NMR (100 MHz, $CDCl_3$)



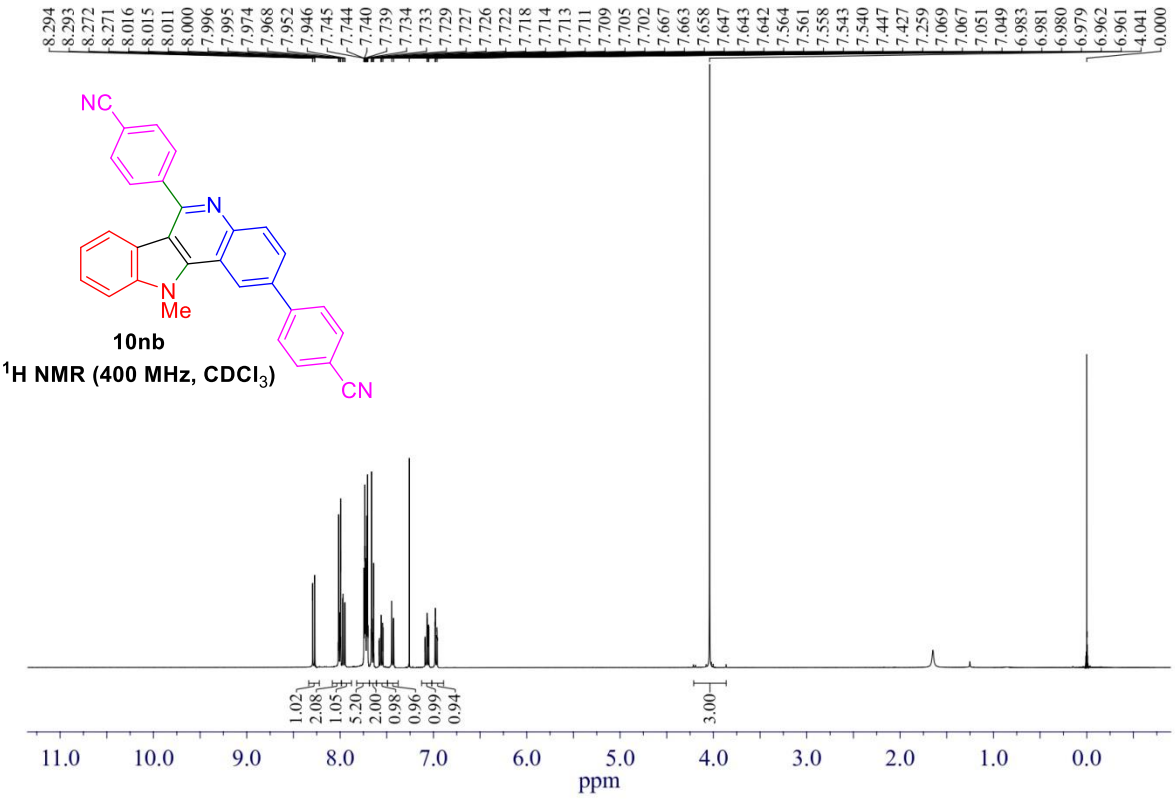
10ac

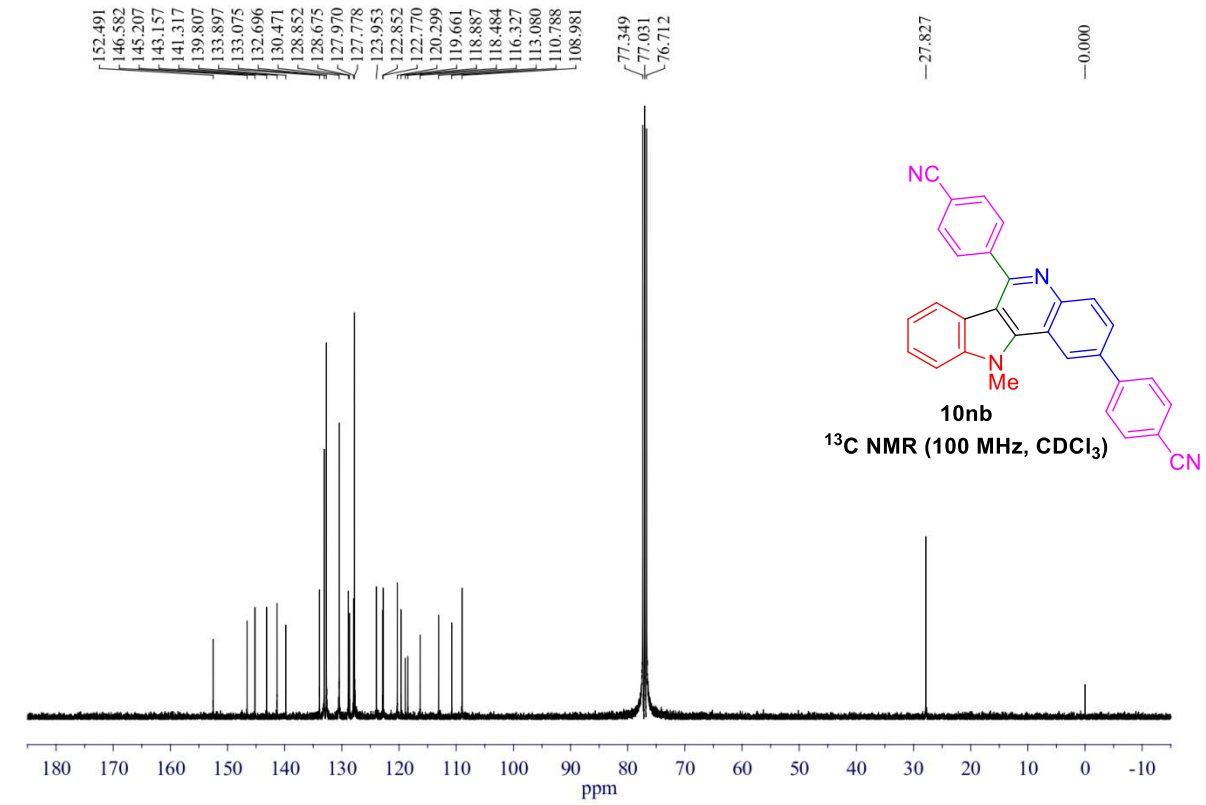
^{1}H NMR (400 MHz, $CDCl_3$)

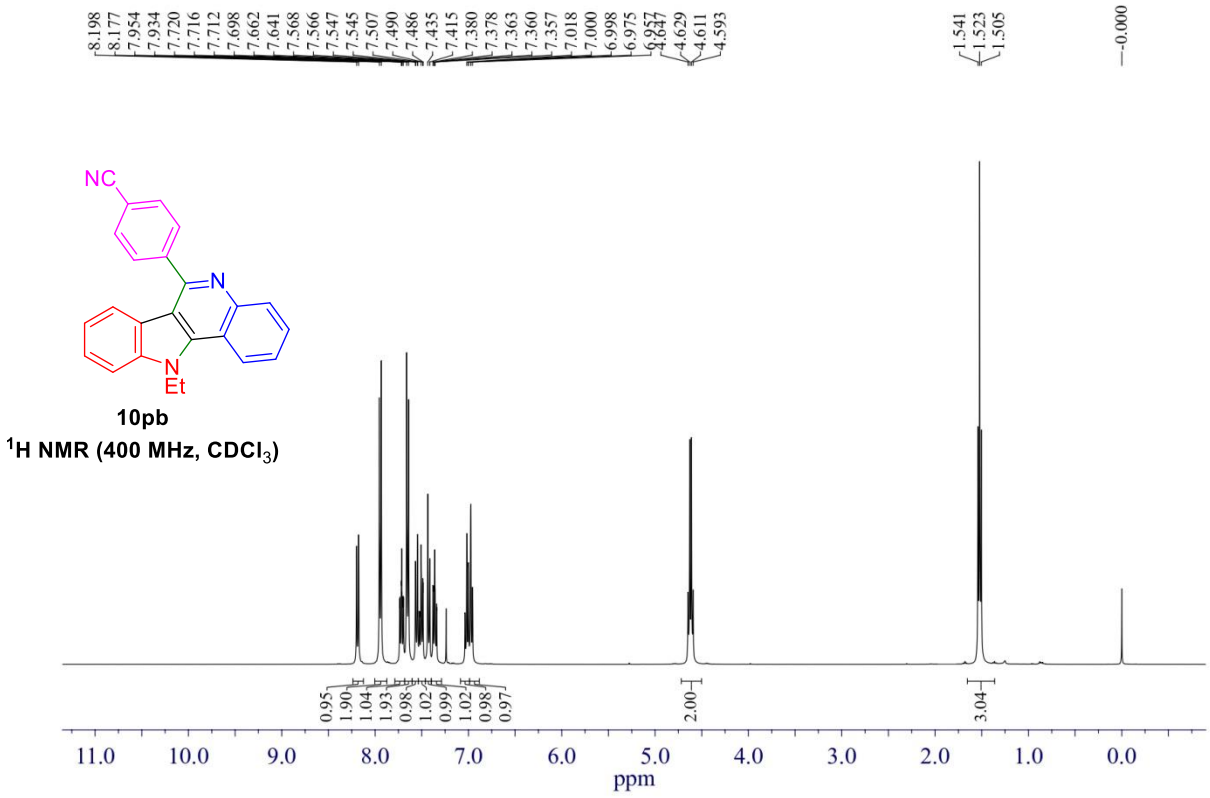


10ac

^{13}C NMR (100 MHz, $CDCl_3$)

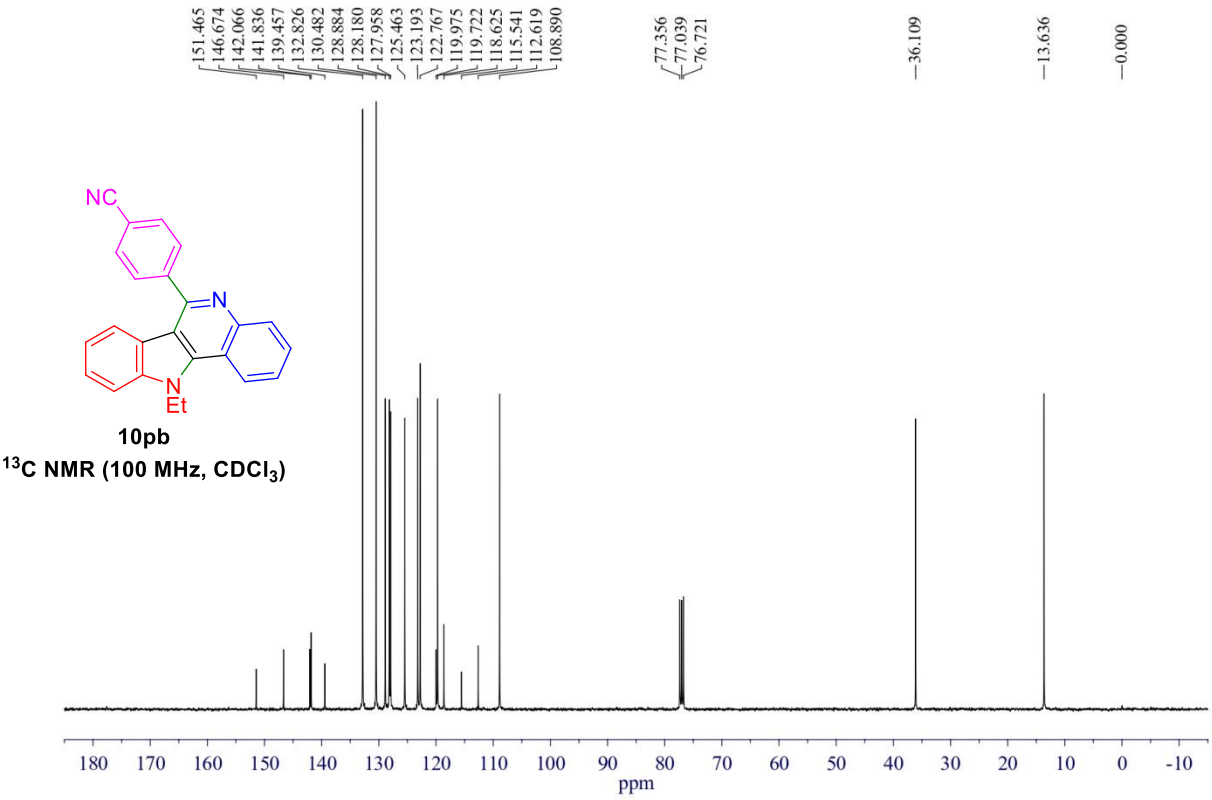

NC
N
N
Me
CN
10nb
^{1}H NMR (400 MHz, CDCl$_3$)
ppm


NC
N
N
Me
CN
10nb
^{13}C NMR (100 MHz, CDCl$_3$)
ppm



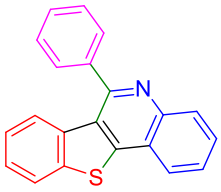
10pb

^{1}H NMR (400 MHz, $CDCl_3$)



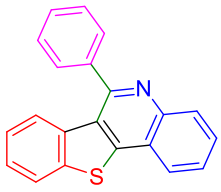
10pb

^{13}C NMR (100 MHz, $CDCl_3$)



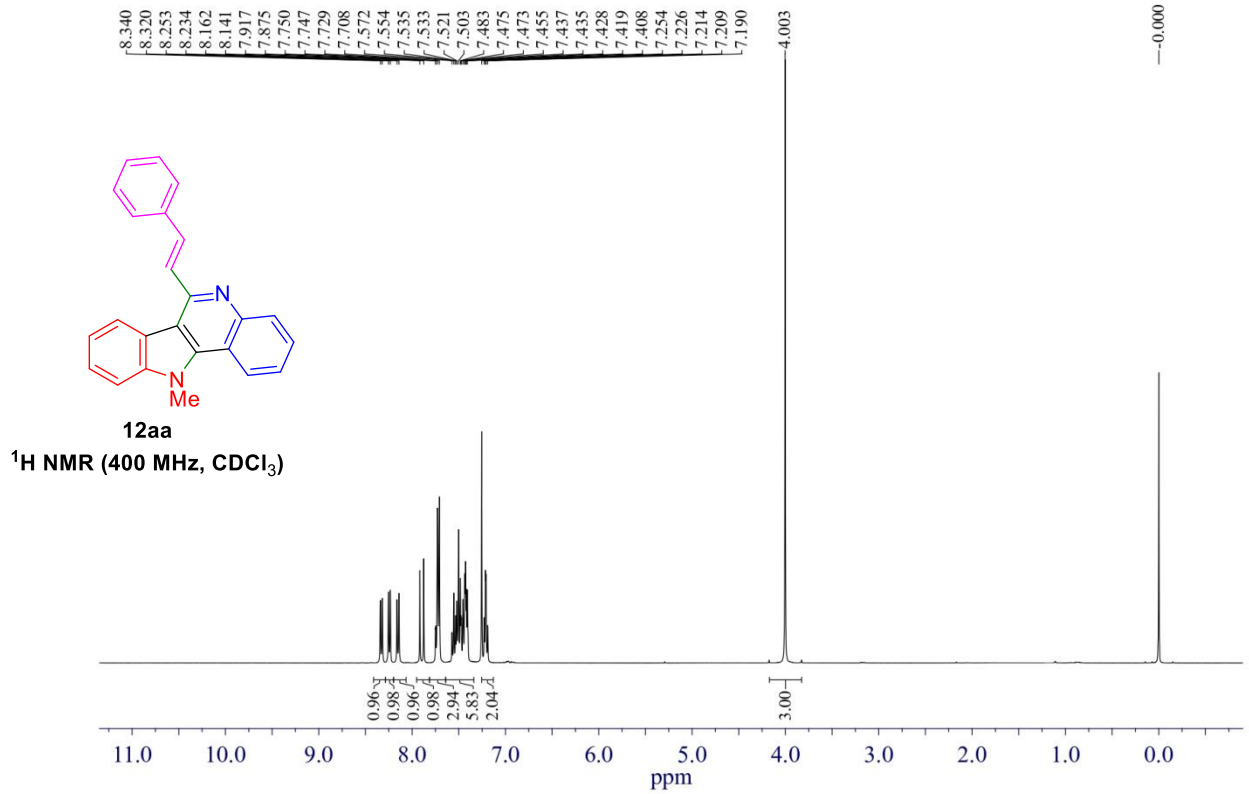
11aa

^{1}H NMR (400 MHz, $CDCl_3$)



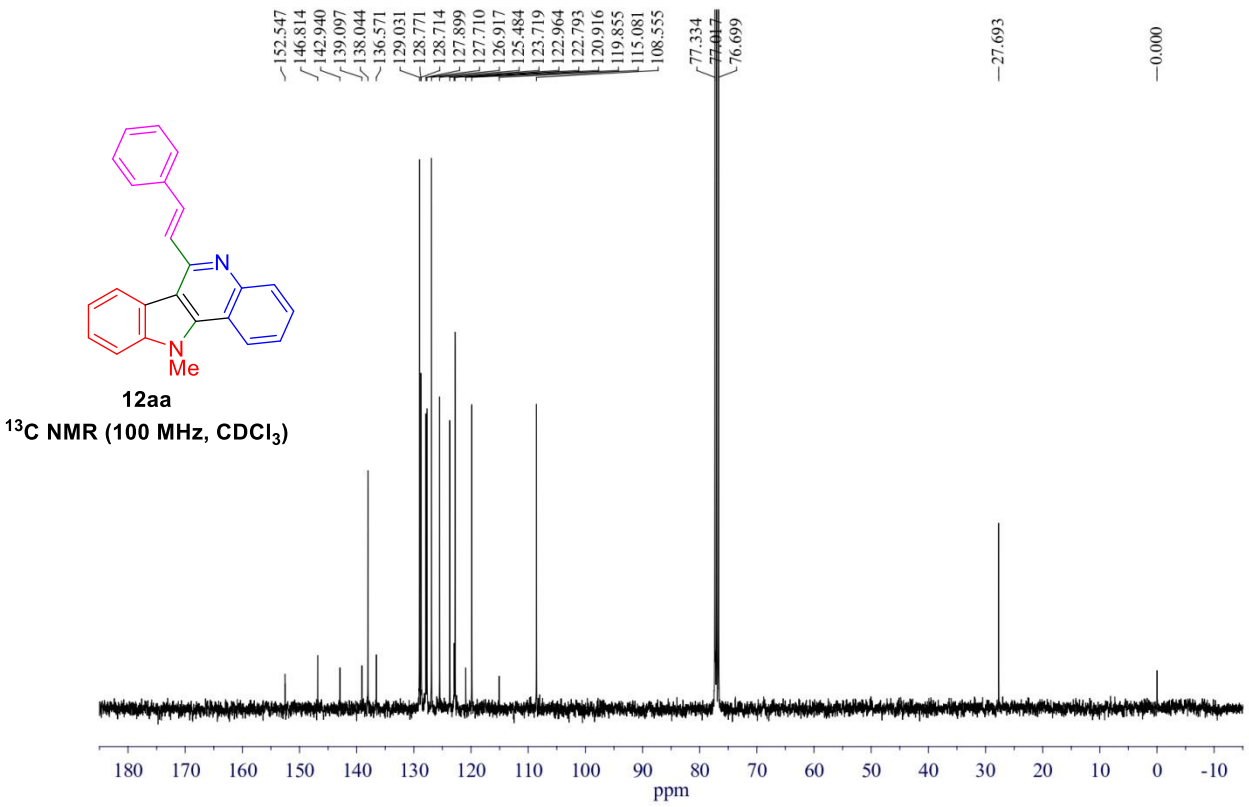
11aa

^{13}C NMR (100 MHz, $CDCl_3$)



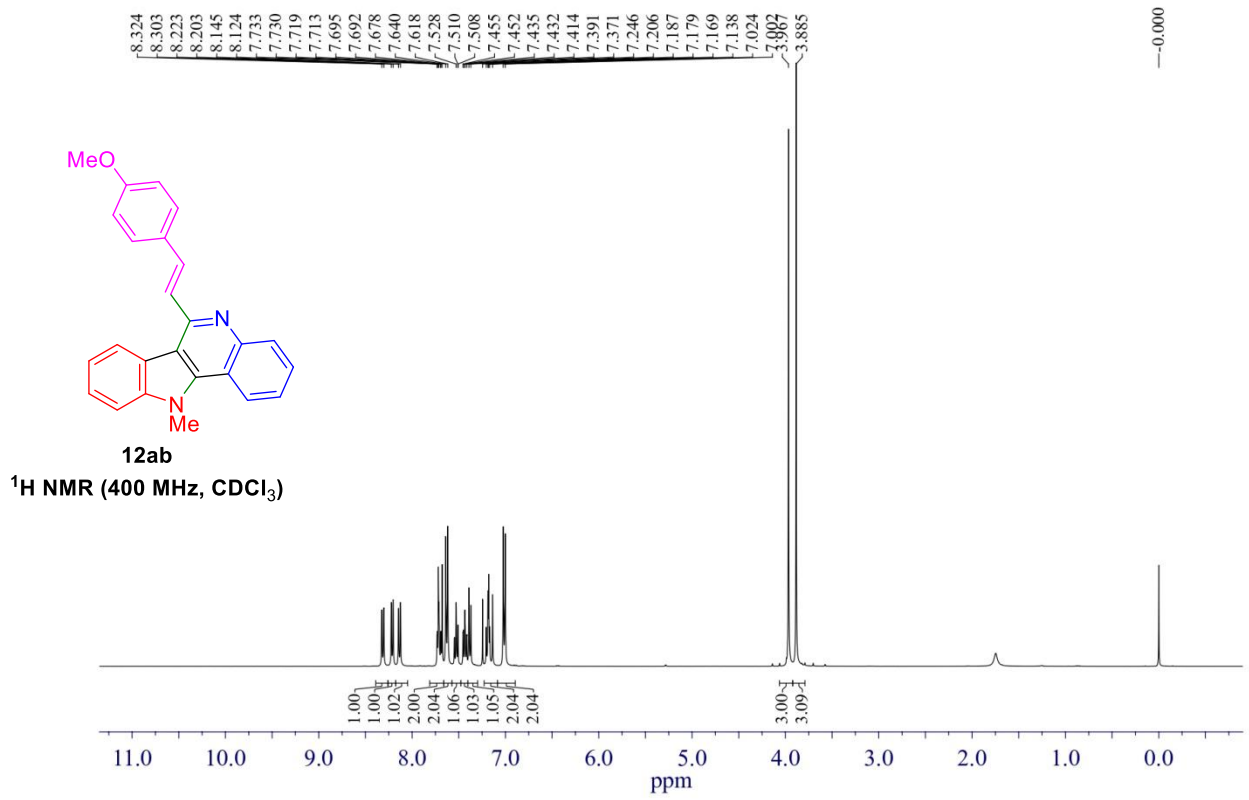
12aa

^{1}H NMR (400 MHz, $CDCl_3$)



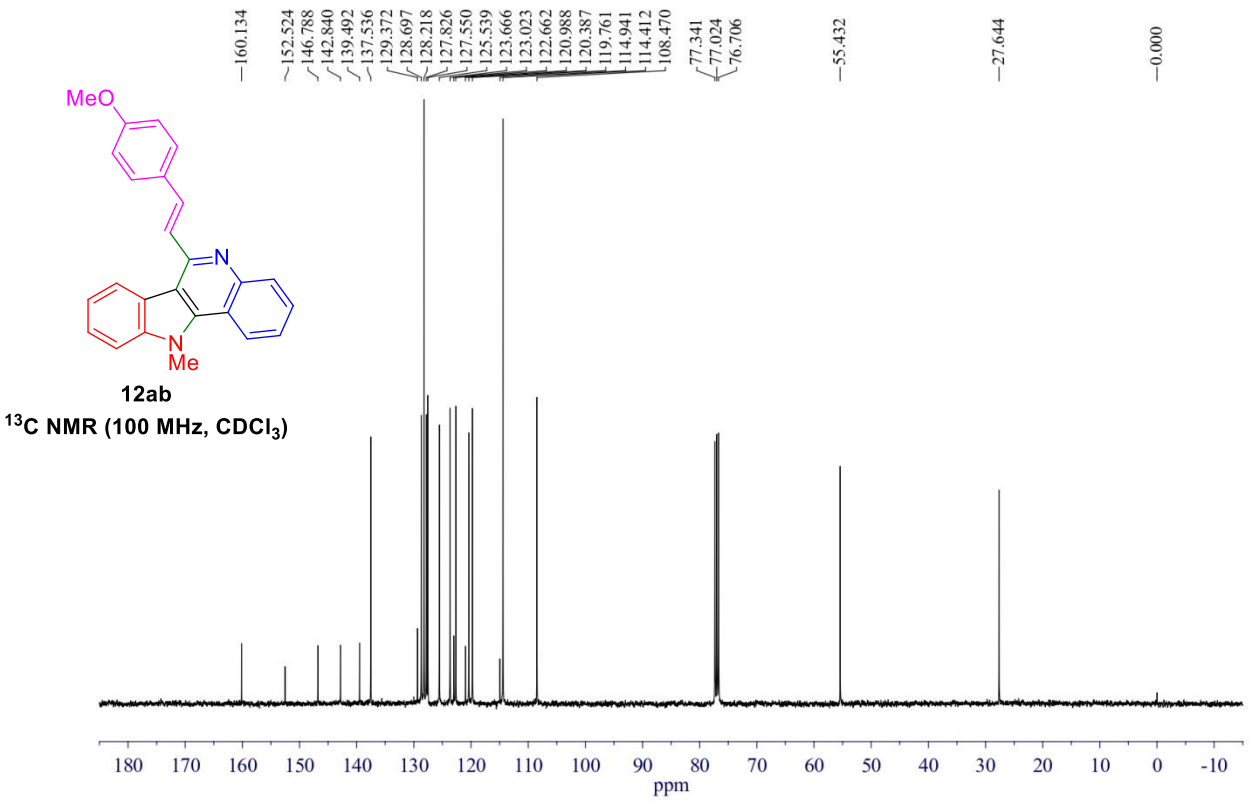
12aa

^{13}C NMR (100 MHz, $CDCl_3$)



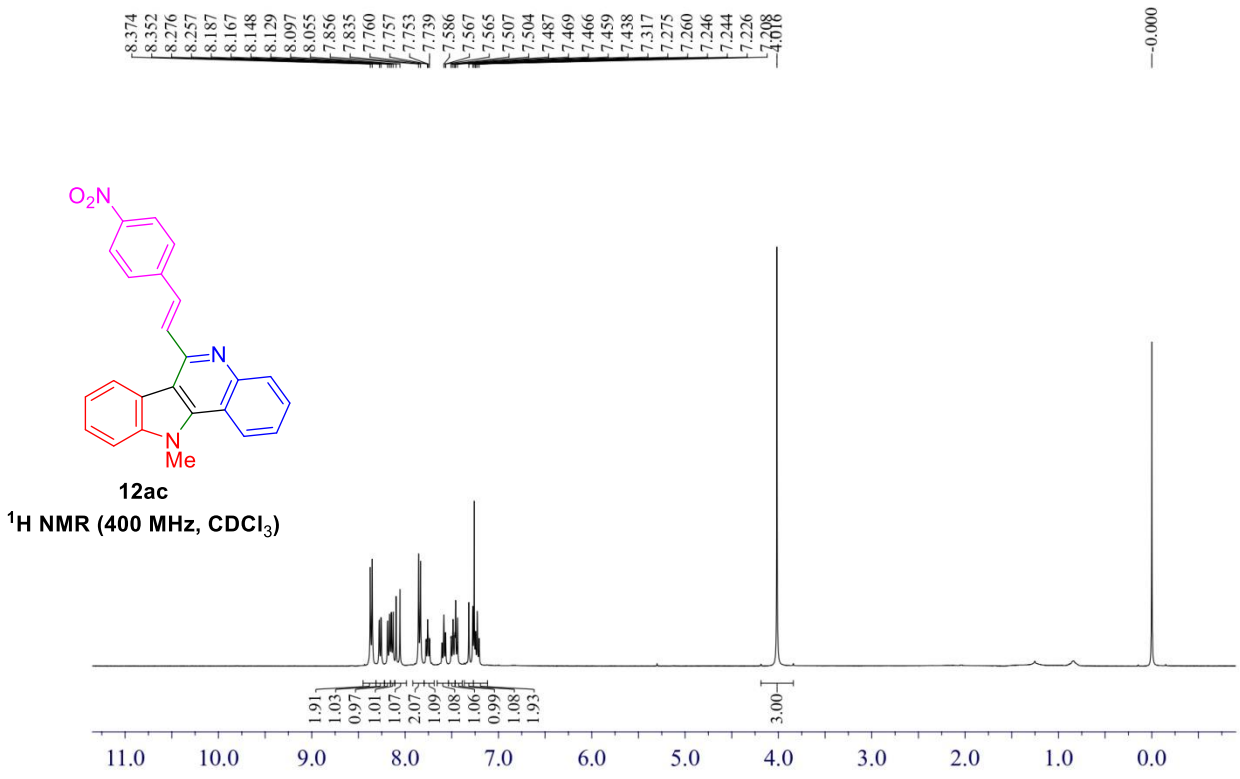
12ab

^{1}H NMR (400 MHz, $CDCl_3$)



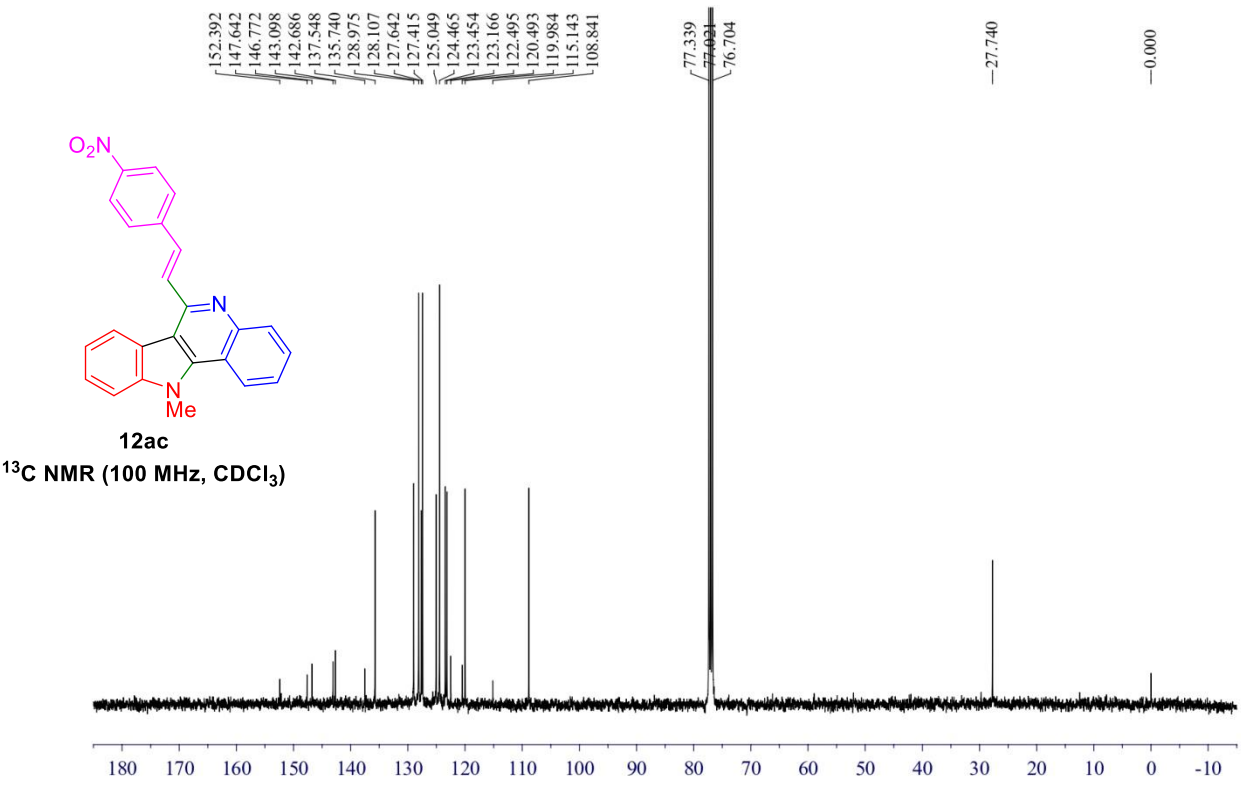
12ab

^{13}C NMR (100 MHz, $CDCl_3$)



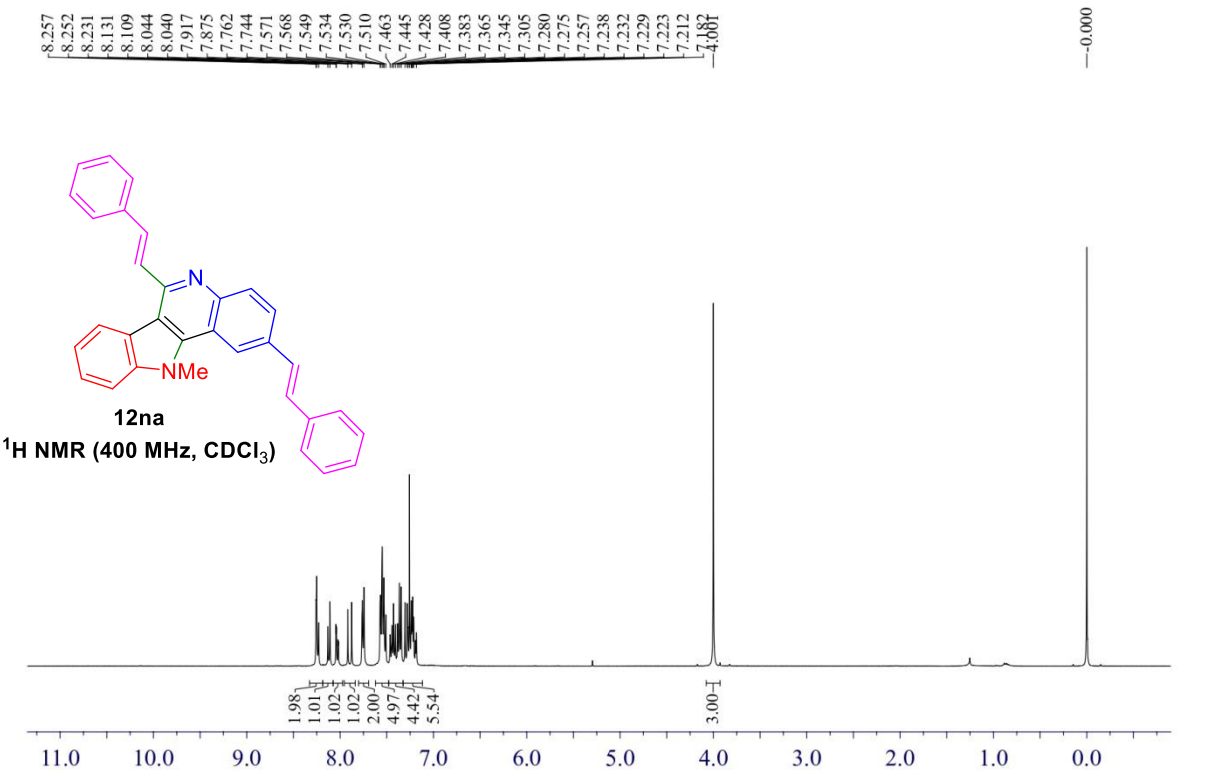
12ac

^{1}H NMR (400 MHz, $CDCl_3$)



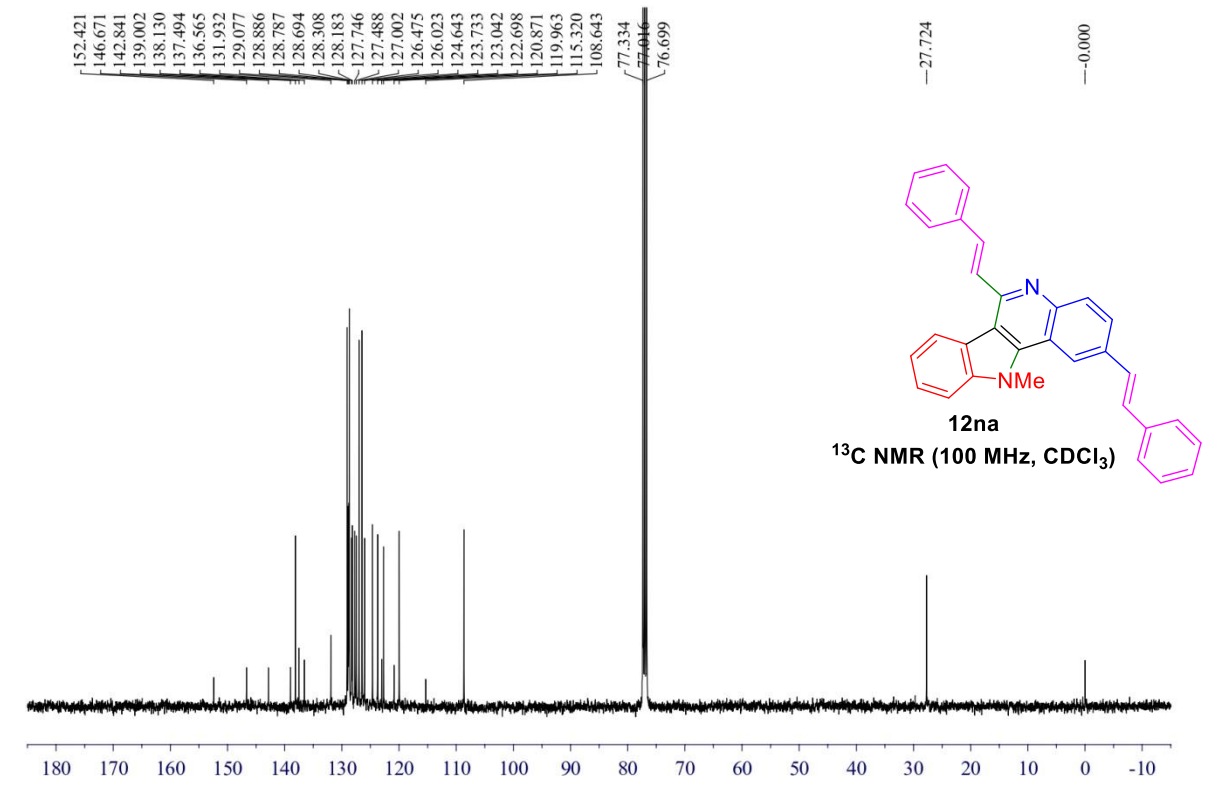
12ac

^{13}C NMR (100 MHz, $CDCl_3$)



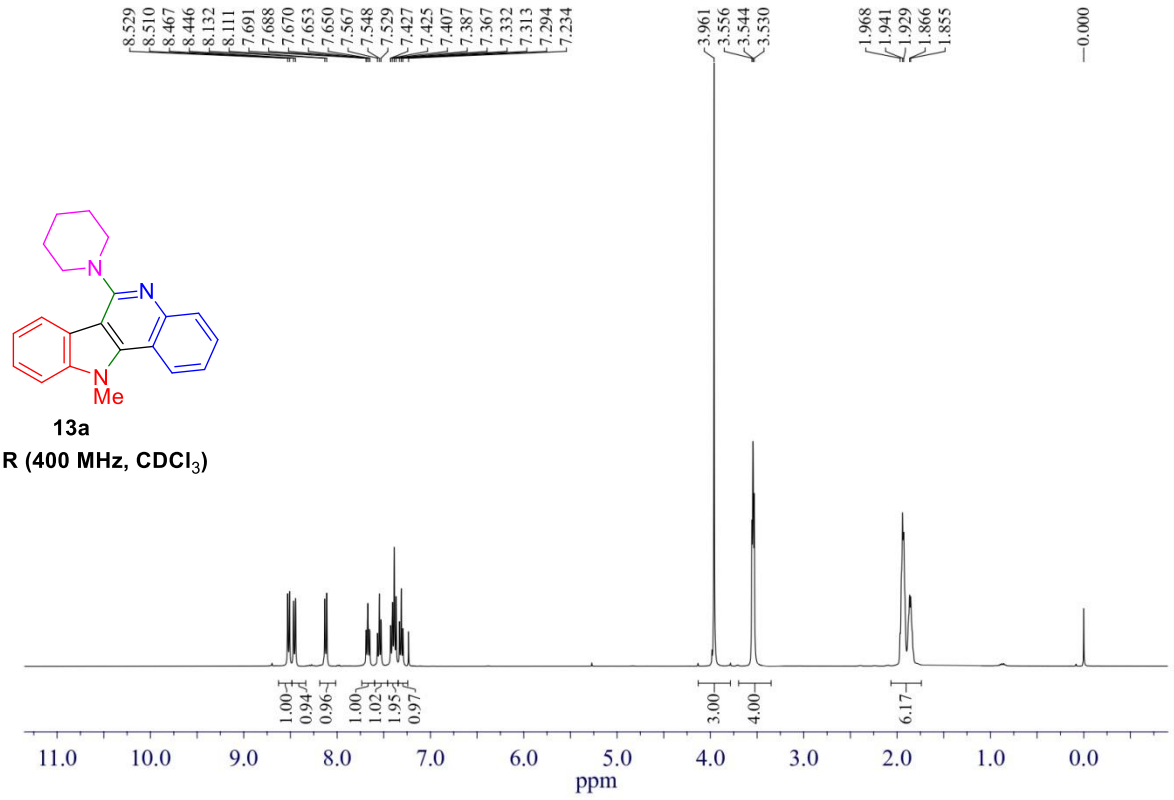
12na

^{1}H NMR (400 MHz, $CDCl_3$)



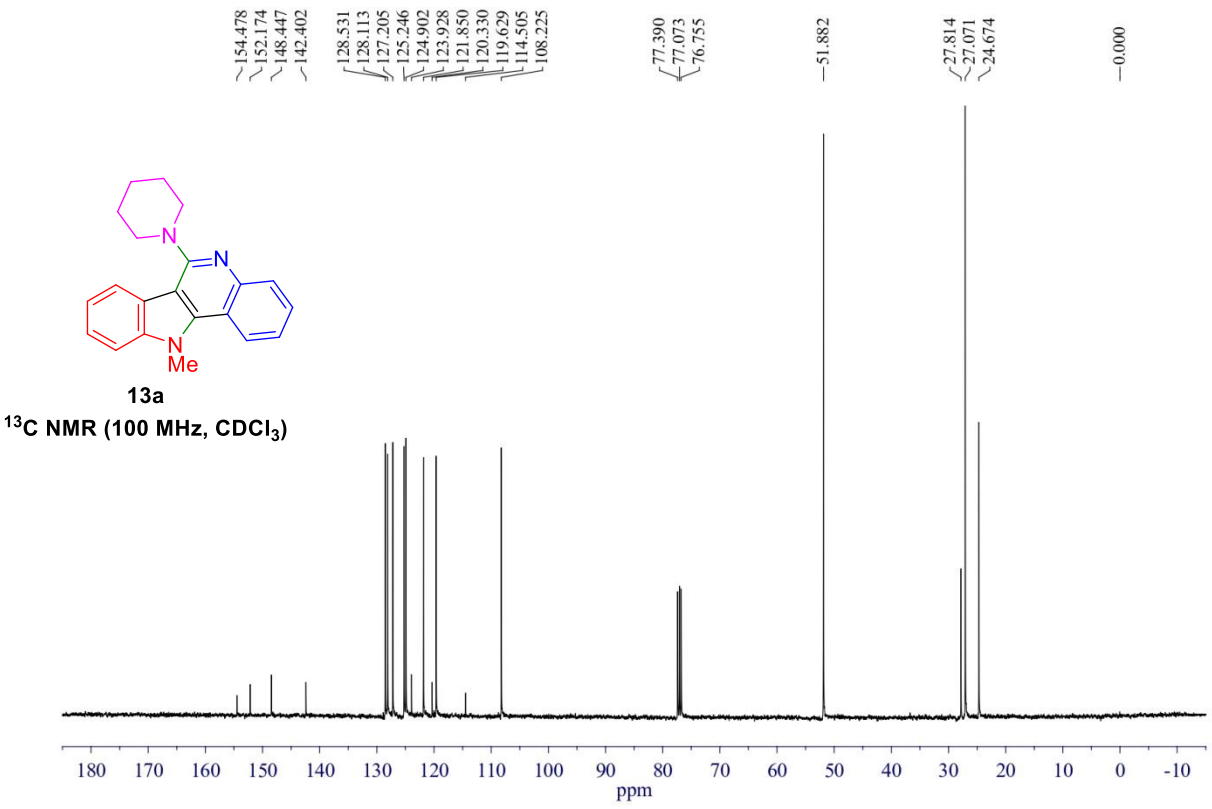
12na

^{13}C NMR (100 MHz, $CDCl_3$)



13a

^{1}H NMR (400 MHz, $CDCl_3$)



13a

^{13}C NMR (100 MHz, $CDCl_3$)