Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information

Indium(III)-catalyzed solvent-free multicomponent [2+2+1+1]-annulation to polycyclic functionalized fused pyridines as potential optical chemosensors

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General remarks

All experiments were carried out in open-air unless stated otherwise. Merck precoated silica gel plates (Art. 5554) treated with a fluorescent indicator were used for analytical thin-layer chromatography (TLC). Column chromatography was performed using silica gel 9385 (Merck). Melting points are uncorrected and were determined using Fisher-Johns Melting Point Apparatus. ^{1}H NMR and ^{13}C NMR spectra were recorded on VNS (600 and 150 MHz or 300 and 75 MHz) spectrometers at the core research support center for natural products and medical materials of Yeungnam University. The NMR spectra recorded in $CDCl_3$ using δ = 7.24 and 77.00 ppm as the residual solvent chemical shifts. All chemical shifts (δ) are expressed in units of ppm and *J* values are given in Hz. Multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or overlap of nonequivalent resonances, and dd = doublet of doublets. Infrared (IR) spectra were recorded on a PerkinElmer Spectrum Two^{TM} IR spectrometer with frequencies expressed in cm^{-1}, and high-resolution mass spectrometry (HRMS) was carried out using a JEOL JMS-700 spectrometer (Magnetic sector-Electric sector double focusing mass analyzer) at the Korea Basic Science Institute. The compound **10a-k**, **11**, and **12** was analyzed for HRMS using Thermo Fisher Q exactive orbitrap mass spectrometer. The crystal structures were determined by single-crystal diffraction methods at the Korea Basic Science Institute (KBSI, Western Seoul Center, Korea).

For UV absorption studies an OPTIZEN 3220UV UV-Visible spectrophotometer was used, and for fluorescence measurements, a Hitachi-7000 F fluorescence spectrometer with Quartz cells (10 mm) was used to acquiring the absorption and emission spectral data. All the fluorescence (Hitachi-7000 F) measurements were carried out after 5 min of incubation at room temperature at 260 nm (excitation wavelength) with 5 nm of slit width, 250 V of photomultiplier tube voltage, and a scan speed of 240 nm/min. The absorption spectra of samples in solution were obtained in the range of 220-500 nm at 1 nm interval in triplicates. All solutions were prepared using spectroscopic grade solvents without further purification.

General procedure for the synthesis of 5a-k, 7a-l, 9a-e, and 10a-k

In an oven-dried schlenk flask, all the staring material in calculated amount including α-tetralone **1a** (0.5mmol), *N*,*N*-dimethylformamide dimethyl acetal **2** (1 mmol, 2 eq), dimedone **3a** (0.5mmol,

1eq), and NH_4OAc **4** (1.5 mmol, 3 eq) with 5 mol% of $In(OTf)_3$ was stirred and heated on an oil bath at 100 ℃ temperature. Whereas, for dimerization starting Indanones or tetralones were used as 2 mmol (2 eq) in the absence of 1,3-cyhexanediones with *N*,*N*-dimethylformamide dimethyl acetal **2** (1 mmol, 2 eq), and NH_4OAc (1.5 mmol, 3 eq) and 5 mol% of $In(OTf)_3$ and heated at 100 ℃ temperature. The reaction progress was monitored *via* TLC continuously. After 4 h the reaction was completed as no starting materials remained as shown in TLC analysis. The reaction was cooled to RT and directly run into column chromatography to get the pure product in eluent of EtOAc: Hex (1:9).

Gram scale synthesis of 5a

In an oven-dried schlenk flask, all the staring material in calculated amount including *α*-tetralone (**1a**) (1.02g, 7 mmol), *N*,*N*-dimethylformamide dimethyl acetal (**2**) (1.86 mL, 2 eq), dimedone (**3a**) (0.98g, 7 mmol, 1 eq), and NH_4OAc (**4**) (1.6g, 3 eq) with 5 mol% of $In(OTf)_3$ were stirred and heated on an oil bath at 100 ℃ temperature. The reaction progress was monitored *via* TLC continuously. After 4 h the reaction was completed as no starting materials remained as shown in TLC analysis. The reaction was cooled to RT and directly run into column chromatography to get the pure product **5a** in eluent of EtOAc: Hex (1:9) in 89% (1.7 g) yield.

Gram scale synthesis of 10a

In an oven-dried schlenk flask, all the staring material in calculated amount including *α*-tetralone (**1a**) (1.2 g, 8 mmol), *N*,*N*-dimethylformamide dimethyl acetal (**2**) (2.12 mL, 2 eq) with NH_4OAc (**4**) (1.8 g, 3 eq) and 5 mol% of $In(OTf)_3$ were stirred and heated on an oil bath at 100 ℃ temperature. The reaction progress was monitored *via* TLC continuously. After 4 h the reaction was completed as no starting materials remained as shown in TLC analysis. The reaction was cooled to RT and directly run into column chromatography to get the pure product **10a** in eluent of EtOAc: Hex (1:9) with 78% (1.76 g) yield.

Control Experiments

a. **Procedure for the synthesis of Intermediate 11**

In an oven-dried schlenk flask, α-tetralone (**1a**) (73 mg, 0.5 mmol), *N*,*N*-dimethylformamide dimethyl acetal (**2**) (0.13 mL, 2 eq) and 5 mol % of $In(OTf)_3$ are placed together and heated on an

oil bath at 100 ℃ temperature. The reaction progress was monitored *via* TLC continuously. After 6 h the reaction was completed as maximum starting materials were finished as shown in TLC analysis. The reaction was cooled to RT and directly run into column chromatography to get the pure product **11** in eluent of EtOAc: Hex (4:6).

b. **Procedure for the synthesis of 5a *via* intermediate 11**

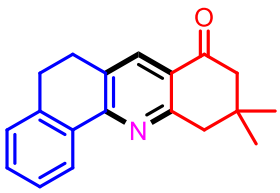
In an oven-dried schlenk flask, intermediate **11** (50 mg, 0.25 mmol), dimedone (**3a**) (35 mg, 1 eq), and NH_4OAc (**4**) (58 mg, 3 eq) with 5 mol% of $In(OTf)_3$ was refluxed in toluene (2 mL) on an oil bath. The reaction progress was monitored *via* TLC continuously. After 12 h the reaction was completed as no starting materials remained as shown in TLC analysis. The reaction was cooled to RT and directly run into column chromatography to get the pure product **5a** in eluent of EtOAc: Hex (1:9) in 64% (44 mg) yield.

c. **Procedure for the synthesis of compound 12**

In an oven-dried schlenk flask, intermediate **11** (50 mg, 0.25 mmol), dimedone (**3a**) (35 mg, 1 eq), and 5 mol% of $In(OTf)_3$ were stirred and heated in DMF (2 mL) on an oil bath at 100 ℃ temperature. The reaction progress was monitored *via* TLC continuously. After 16 h reaction was completed as no starting materials remained as shown in TLC analysis. The reaction was cooled to RT and directly run into column chromatography to get the pure product **12** in eluent of EtOAc: Hex (2:8).

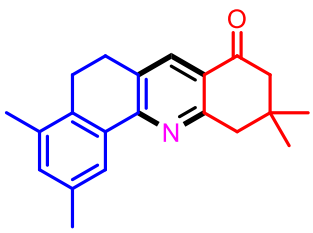
Characterization data of synthesized compounds

10,10-Dimethyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5a)



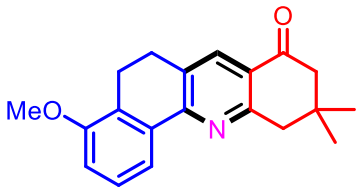
Pale yellow solid; EtOAc:Hex (1:9); Yield: 94% (130 mg); mp 180-182 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (d, J = 7.2 Hz, 1H), 8.02 (s, 1H), 7.36-7.29 (m, 2H), 7.20 (d, J = 6.6 Hz, 1H), 3.04 (s, 2H), 2.93-2.89 (m, 4H), 2.50 (s, 2H), 1.10 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.0, 160.4, 156.2, 139.0, 133.6, 133.4, 130.1, 130.1, 127.8, 127.1, 125.9, 125.5, 52.0, 46.2, 32.9, 28.2, 27.7, 27.4; IR (ATR) 2953, 2867, 1676, 1589, 1452, 1417, 1326, 1313, 1280, 1119, 944, 764, 742, 669, 579, 485, 454 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{19}H_{19}NO$: 277.1467. Found: 277.1467.

2,4,10,10-Tetramethyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5b)



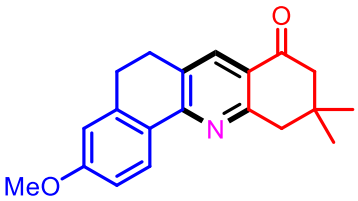
Pale solid; EtOAc:Hex (1:9); Yield: 94% (143 mg); mp 190-192 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.90 (s, 1H), 6.69 (s, 1H), 3.98 (s, 3H), 3.90 (s, 3H), 3.03 (s, 2H), 2.91-2.88 (m, 2H), 2.85-2.82 (m, 2H), 2.49 (s, 2H), 1.09 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.0, 160.5, 156.3, 150.8, 148.2, 133.1, 132.8, 129.2, 126.3, 124.8, 110.5, 108.5, 56.0, 55.8, 52.0, 46.3, 32.9, 28.2, 27.6, 27.5; IR (ATR) 2943, 2889, 1672, 1584, 1557, 1417, 1408, 1317, 1278, 1172, 1095, 938, 868, 780, 697, 583cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{21}H_{23}NO$: 305.1780. Found: 305.1783.

4-Methoxy-10,10-dimethyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5c)



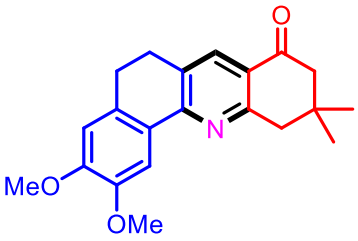
Pale yellow solid; EtOAc:Hex (1:9); Yield: 93% (143 mg); mp 138-140 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (d, J = 11.4 Hz, 2H), 7.28 (t, J = 8.4 Hz, 1H), 6.90 (d, J = 8.4 Hz, 1H), 3.82 (s, 3H), 3.01 (s, 2H), 2.90-2.86 (m 4H), 2.49 (s, 2H), 1.08 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.9, 160.2, 156.2, 156.1, 134.7, 133.3, 130.0, 127.6, 127.1, 125.4, 118.2, 111.8, 55.4, 51.9, 46.2, 32.8, 28.2, 26.8, 19.7; IR (ATR) 2932, 2838, 1682, 1580, 1552, 1418, 1313, 1253, 1055, 802, 759, 725, 565 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{20}H_{21}NO_2$: 307.1572. Found: 307.1570.

3-Methoxy-10,10-dimethyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5d)



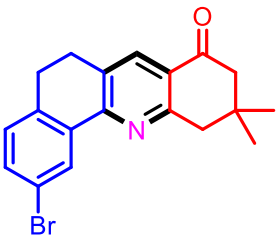
Pale yellow solid; EtOAc:Hex (1:9); Yield: 95% (146 mg); mp 168-170 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.26 (d, J = 9.0 Hz, 1H), 7.94 (s, 1H), 6.84 (d, J = 7.8 Hz, 1H), 6.70 (s, 1H), 3.80 (s, 3H), 2.98 (s, 2H), 2.92-2.81 (m, 4H), 2.47 (s, 2H), 1.07 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.9, 161.4, 160.4, 156.3, 141.2, 133.5, 129.3, 128.0, 124.9, 113.1, 112.8, 55.3, 52.0, 46.1, 28.2, 28.2, 27.5; IR (ATR) 2927, 1668, 1584, 1415, 1332, 1263, 1151, 1115, 1035, 862, 772, 648, 491 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{20}H_{21}NO_3$: 307.1572. Found: 307.1574.

2,3-Dimethoxy-10,10-dimethyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5e)



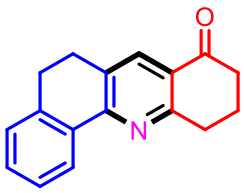
Pale yellow solid; EtOAc:Hex (2:8); Yield: 90% (152 mg); mp 180-180 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (s, 1H), 8.02 (s, 1H), 7.05 (s, 1H), 3.05 (s, 2H), 2.91-2.89 (m, 2H), 2.82-2.80 (m, 2H), 2.51 (s, 2H), 2.36 (s, 3H), 2.29 (s, 3H), 1.11 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.1, 160.3, 156.8, 136.0, 135.0, 134.7, 133.4, 133.2, 133.0, 129.9, 125.3, 124.3, 52.0, 46.3, 32.9, 28.2, 27.2, 23.4, 21.0, 19.5; IR (ATR) 2924, 2853, 1739, 1670, 1582, 1509, 1449, 1336, 1256, 1218, 1189, 1124, 1010, 980 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{21}H_{23}NO_3$: 337.1678. Found: 337.1680.

2-Bromo-10,10-dimethyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5f)



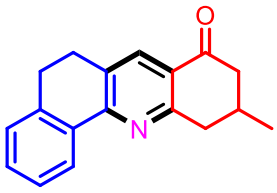
Pale yellow solid; EtOAc:Hex (2:8); Yield: 88% (156 mg); mp 168-170 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.02 (s, 1H), 7.41 (d, J = 6.6 Hz, 1H), 7.08 (d, J = 7.8 Hz, 1H), 3.03 (s, 2H), 2.93-2.90 (m, 2H), 2.87-2.84 (m, 2H), 2.51 (s, 2H), 1.10 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.9, 160.6, 154.8, 137.7, 135.5, 133.7, 132.7, 130.1, 129.5, 128.8, 125.9, 121.1, 52.0, 46.2, 32.9, 28.2, 27.3, 27.1; IR (ATR) 2949, 2930, 1677, 1585, 1574, 1479, 1427, 1306, 1259, 1200, 1135, 1077, 819, 732, 688, 580 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{19}H_{18}BrNO$: 355.0572. Found: 355.0573.

6,9,10,11-Tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5g)



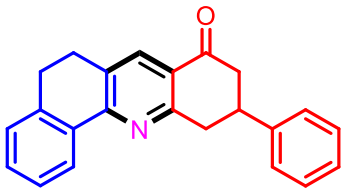
Brown solid; EtOAc:Hex (1:9); Yield: 76% (95 mg); mp 200-202 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (d, J = 7.2 Hz, 1H), 8.04 (s, 1H), 7.35-7.31 (m, 2H), 7.22 (d, J = 6.6 Hz, 1H), 3.15 (t, J = 6.0 Hz, 2H), 2.95-2.89 (m, 4H), 2.67 (t, J = 6.0 Hz, 2H), 2.18 (p, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.0, 161.9, 155.9, 139.1, 133.9, 133.7, 130.3, 130.2, 127.9, 127.2, 126.5, 126.0, 38.5, 32.5, 27.8, 27.5, 22.0; IR (ATR) 2938, 2851, 1670, 1585, 1459, 1416, 1282, 1101, 1030, 927, 755, 735, 655, 577, 446 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{17}H_{15}NO$: 249.1154. Found: 249.1152.

10-Methyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5h)



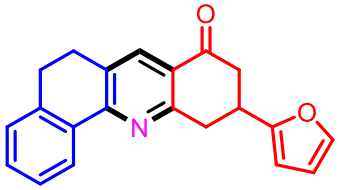
Brown solid; EtOAc:Hex (2:8); Yield: 81% (106 mg); mp 143-145 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (d, J = 7.2 Hz, 1H), 8.05 (s, 1H), 7.37-7.32 (m, 2H), 7.23 (d, J = 6.6 Hz, 1H), 3.27 (d, J = 15.6 Hz, 1H), 2.98-2.90 (m, 4H), 2.84 (dd, J = 9.6, 6.6 Hz, 1H), 2.74 (d, J = 13.2 Hz, 1H), 2.42-2.31 (m, 2H), 1.18 (d, J = 4.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.0, 161.3, 156.1, 139.2, 133.9, 130.3, 127.9, 127.2, 126.0, 46.6, 40.8, 29.4, 27.9, 27.5, 21.2; IR (ATR) 2922, 2949, 1674, 1583, 1412, 1310, 1277, 1202, 1030, 930, 745, 578 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{18}H_{17}NO$: 263.1310. Found: 263.1312.

10-Phenyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5i)



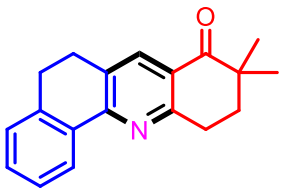
Brown solid; EtOAc:Hex (2:8); Yield: 84% (137 mg); mp 168-170 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (d, J = 6.6 Hz, 1H), 8.09 (s, 1H), 7.38-7.33 (m, 4H), 7.31 (d, J = 7.8 Hz, 2H), 7.27 (t, J = 7.2 Hz, 1H), 7.23 (d, J = 6.0 Hz, 1H), 3.50 (t, J = 13.2 Hz, 2H), 3.37-3.30 (m, 1H), 3.01-2.92 (m, 5H), 2.89-2.82 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.2, 160.9, 156.4, 142.9, 139.2, 133.9, 133.6, 130.5, 130.3, 128.7, 127.9, 127.2, 126.9, 126.6, 126.0, 125.9, 45.5, 40.2, 39.8, 27.8, 27.5; IR (ATR) 2923, 2852, 1676, 1589, 1456, 1415, 1311, 1275, 1017, 747, 696, 563, 499 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{23}H_{19}NO$: 325.1467. Found: 325.1465.

10-(Furan-2-yl)-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5j)



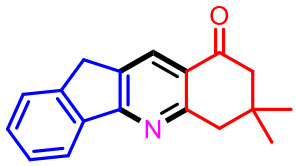
Brown solid; EtOAc:Hex (2:8); Yield: 86% (135 mg); mp 198-200 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (d, J = 6.6 Hz, 1H), 8.06 (s, 1H), 7.39-7.30 (m, 3H), 7.23 (d, J = 6.0 Hz, 1H), 6.28 (dd, J = 3.0, 1.8 Hz, 1H), 6.08 (d, J = 3.0 Hz, 1H), 3.66-3.61 (m, 1H), 3.56 (dd, J = 16.8, 4.2 Hz, 1H), 3.38 (dd, J = 16.8, 9.6 Hz, 1H), 3.05 (dd, J = 16.8, 4.0 Hz, 1H), 2.97-2.91 (m, 4H), 2.86 (dd, J = 16.8, 10.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.4, 160.0, 156.4, 156.0, 141.6, 139.2, 133.9, 133.4, 130.6, 130.4, 127.9, 127.2, 126.1, 126.0, 110.1, 104.9, 42.6, 37.0, 33.2, 27.8, 27.5; IR (ATR) 2941, 2851, 1676, 1588, 1415, 1313, 1154, 1008, 929, 808, 750, 732, 599, 585, 464 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{21}H_{17}NO_2$: 315.1259. Found: 315.1261.

9,9-Dimethyl-6,9,10,11-tetrahydrobenzo[*c*]acridin-8(5*H*)-one (5k)



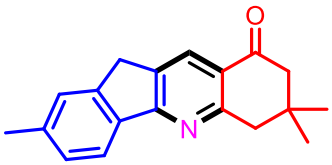
Yellow solid; EtOAc:Hex (1:9); Yield: 92% (127 mg); mp 160-162 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (d, J = 6.6 Hz, 1H), 8.08 (s, 1H), 7.38-7.31 (m, 2H), 7.22 (d, J = 7.2 Hz, 1H), 3.19 (t, J = 6.6 Hz, 2H), 2.97-2.90 (m, 4H), 2.02 (t, J = 6.0 Hz, 2H), 1.23 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 202.5, 160.8, 155.8, 139.2, 134.9, 130.3, 130.2, 127.9, 127.2, 126.0, 125.3, 41.4, 35.5, 28.8, 27.9, 27.5, 24.2; IR (ATR) 2930, 2860, 1671, 1588, 1451, 1422, 1380, 1254, 1135, 1047, 939, 772, 743, 621 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{19}H_{19}NO$: 277.1467. Found: 277.1468.

7,7-Dimethyl-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7a)



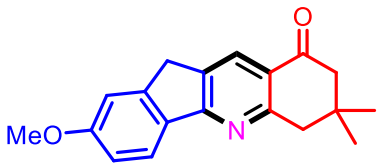
Pale yellow solid; EtOAc:Hex (1:9); Yield: 93% (122 mg); mp 128-130 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.16 (d, J = 8.4 Hz, 1H), 7.58 (d, J = 9.0 Hz, 1H), 7.48-7.43 (m, 2H), 3.88 (s, 2H), 3.13 (s, 2H), 2.55 (s, 2H), 1.12 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.1, 164.4, 161.9, 145.5, 139.7, 135.1, 130.4, 130.0, 127.5, 125.4, 125.0, 122.0, 52.1, 46.6, 34.2, 33.0, 28.2; IR (ATR) 2920, 2851, 1672, 1598, 1467, 1391, 1331, 1225, 1202, 1123, 1002, 963, 755, 730, 572, 485 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{18}H_{17}NO$: 263.1310. Found: 263.1312.

2,7,7-Trimethyl-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7b)



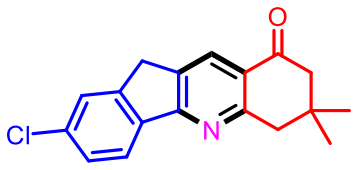
Yellow solid; EtOAc:Hex (1:9); Yield: 86% (119 mg); mp 179-181 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.29 (s, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.36 (s, 1H), 7.26 (d, J = 7.8 Hz, 1H), 3.81 (s, 2H), 3.10 (s, 2H), 2.53 (s, 2H), 2.43 (s, 3H), 1.11 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.0, 164.5, 161.8, 145.9, 140.5, 137.1, 134.9, 130.2, 128.5, 126.0, 124.5, 121.7, 52.1, 46.5, 34.0, 33.0, 28.2, 21.8; IR (ATR) 2957, 2834, 1673, 1608, 1558, 1389, 1279, 1244, 1137, 1093, 1027, 820, 779, 511, 415 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{19}H_{19}NO$: 277.1467. Found: 277.1463.

2-Methoxy-7,7-dimethyl-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7c)



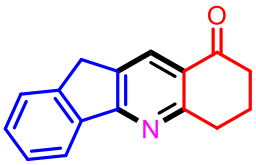
Yellow solid; EtOAc:Hex (1:9); Yield: 81% (119 mg); mp 173-175 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.25 (s, 1H), 8.08 (s, 1H), 7.05 (d, J = 2.4 Hz, 1H), 6.98 (d, J = 8.4 Hz, 1H), 3.85 (s, 3H), 3.80 (s, 2H), 3.10 (s, 2H), 2.52 (s, 2H), 1.10 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.8, 162.0, 147.9, 134.6, 130.0, 124.0, 123.4, 114.3, 110.3, 55.5, 55.4, 52.0, 46.3, 34.2, 33.0, 28.2; IR (ATR) 2959, 2838, 1673, 1592, 1386, 1312, 1276, 1094, 1027, 834, 777, 611, 524, 415 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{19}H_{19}NO_2$: 293.1416. Found: 293.1418.

2-Chloro-7,7-dimethyl-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7d)



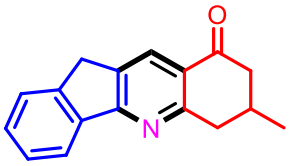
White solid; EtOAc:Hex (2:8); Yield: 88% (131 mg); mp 215-217 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.33 (s, 1H), 8.04 (d, J = 7.8 Hz, 1H), 7.54 (s, 1H), 7.42 (d, J = 7.8 Hz, 1H), 3.85 (s, 2H), 3.11 (s, 2H), 2.55 (s, 2H), 1.11 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.9, 163.3, 162.1, 157.7, 146.9, 138.3, 136.0, 134.8, 130.5, 128.0, 125.7, 125.1, 122.9, 52.1, 46.6, 34.1, 33.0, 28.2; IR (ATR) 2956, 2867, 1676, 1595, 1469, 1384, 1344, 1279, 1165, 1070, 867, 836, 775, 608, 587cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{18}H_{16}ClNO$: 297.0920. Found: 297.0919.

6,7,8,11-Tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7e)



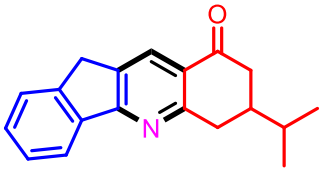
White solid; EtOAc:Hex (1:9); Yield: 76% (89 mg); mp 125-127 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.13 (d, J = 6.0 Hz, 1H), 7.57 (d, J = 7.8 Hz, 1H), 7.48-7.43 (m, 2H), 3.87 (s, 2H), 3.23 (t, J = 6.0 Hz, 2H), 2.69 (t, J = 6.0 Hz, 2H), 2.23-2.17 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.1, 163.3, 145.5, 135.1, 130.7, 130.0, 127.5, 125.9, 125.4, 122.0, 38.6, 34.2, 32.8, 22.1; IR (ATR) 2953, 2920, 2851, 1671, 1598, 1552, 1467, 1391, 1201, 755, 730 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{16}H_{13}NO$: 235.0997. Found: 235.0999.

7-Methyl-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7f)



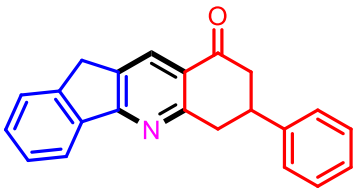
White solid; EtOAc:Hex (2:8);Yield: 86% (107 mg); mp 168-170 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (s, 1H), 8.11 (d, J = 7.8 Hz, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.46-7.41 (m, 2H), 3.83 (s, 2H), 3.28 (d, J = 16.8 Hz, 1H), 2.87 (dd, J = 16.8, 9.6 Hz, 1H), 2.74 (d, J = 14.4 Hz, 1H), 2.41-2.30 (m, 2H), 1.17 (d, J = 6.0 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.0, 164.2, 162.7, 145.5, 139.7, 135.0, 130.5, 129.9, 127.4, 125.3, 125.3 121.9, 46.6, 41.0, 34.1, 29.4, 21.1; IR (ATR) 2922, 2860, 1669, 1596, 1553, 1388, 1291, 968, 754, 742, 581, 492 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{17}H_{15}NO$: 249.1154. Found: 249.1156.

7-Isopropyl-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7g)



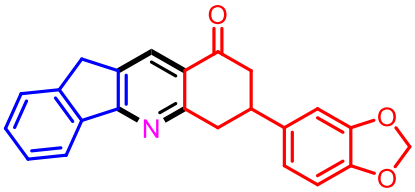
White solid; EtOAc:Hex (2:8); Yield: 81% (112 mg); mp 190-192 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.33 (s, 1H), 8.15 (s, 1H), 7.60-7.54 (m, 1H), 7.49-7.42 (m, 2H), 3.87 (s, 2H), 3.33 (d, J = 16.8 Hz, 1H), 2.96 (dd, J = 16.8, 12.0 Hz, 1H), 2.79 (d, J = 16.8 Hz, 1H), 2.40 (dd, J = 16.8, 13.2 Hz, 1H), 2.09-2.01 (m, 1H), 1.75-1.69 (m, 1H), 1.01 (t, J = 7.2 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.5, 163.2, 145.5, 135.1, 130.6, 130.1, 127.5, 125.5, 125.4, 122.0, 42.6, 40.6, 36.6, 34.2, 32.0, 19.6, 19.4; IR (ATR) 2960, 2923, 2868, 1673, 1595, 1464, 1395, 1348, 1287, 1187, 1015, 961, 801, 750, 738 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{19}H_{19}NO$: 277.1467. Found: 277.1468.

7-Phenyl-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7h)



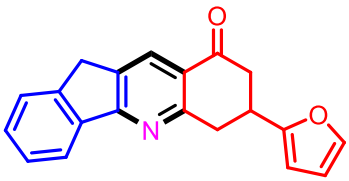
White solid; EtOAc:Hex (2:8); Yield: 79% (123 mg); mp 220-222 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (s, 1H), 8.17 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.47 (d, J = 7.2 Hz, 1H), 7.36 (t, J = 7.8 Hz, 2H), 7.32 (d, J = 7.2 Hz, 2H), 7.27 (t, J = 7.2 Hz, 1H), 3.92 (s, 2H), 3.56 (t, J = 12.0 Hz, 2H), 3.43 (dd, J = 15.6, 13.2 Hz, 1H), 3.03 (d, J = 15.7 Hz, 1H), 2.90 (dd, J = 16.8, 10.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.3, 164.5, 162.3, 145.6, 142.8, 139.6, 135.4, 130.8, 130.2, 128.8, 127.6, 127.0, 126.7, 125.4, 122.2, 45.6, 40.4, 39.8, 34.3; IR (ATR) 3028, 2922, 2852, 1662, 1592, 1555, 1389, 1282, 1182, 1015, 747, 692, 500, 478 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{22}H_{17}NO$: 311.1310. Found: 311.1313.

7-(Benzo[*d*][1,3]dioxol-5-yl)-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7i)



Whit solid; EtOAc:Hex (2:8); Yield: 68% (121 mg); mp 238-240 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.18 (s, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.51-7.45 (m, 2H), 6.80 (s, 1H), 6.77 (q, J = 7.8 Hz, 2H), 5.95 (s, 2H), 3.92 (s, 2H), 3.54 (d, J = 16.2 Hz, 1H), 3.48 (t, J = 11.4 Hz, 1H), 3.37 (dd, J = 16.2, 11.4 Hz, 1H), 3.00-2.96 (m, 1H), 2.87-2.80 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.2, 147.9, 146.4, 145.6, 136.8, 130.8, 130.3, 127.6, 125.4, 122.2, 119.7, 108.4, 107.1, 101.0, 45.9, 40.6, 39.6, 34.3; IR (ATR) 2921, 2854, 1662, 1599, 1488, 1388, 1281, 1242, 1134, 1036, 923, 805, 744, 575, 427 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{23}H_{17}NO_3$: 355.1208. Found: 355.1212.

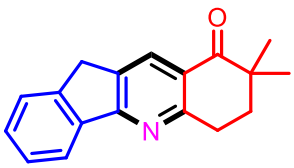
7-(Furan-2-yl)-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7j)



Pale yellow solid; EtOAc:Hex (2:8); Yield: 82% (123 mg); mp 235-237 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.15 (d, J = 7.2 Hz, 1H), 7.57 (d, J = 8.4 Hz, 1H), 7.46 (d, J = 8.7 Hz, 2H), 7.33 (s, 1H), 6.27 (s, 1H), 6.09 (s, 1H), 3.87 (s, 2H), 3.69-3.60 (m, 2H), 3.45 (dd, J = 16.8, 8.4 Hz, 1H), 3.08 (dd, J = 16.8, 9.6 Hz, 1H), 2.89 (dd, J = 16.8, 10.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.4, 164.5, 161.4, 155.9, 145.5, 141.6, 139.6, 135.4, 130.6, 130.2, 127.5, 125.4, 125.4, 122.1, 110.1, 105.0, 42.7, 37.3, 34.2, 33.3; IR (ATR) 2891, 2660, 1671, 1599,

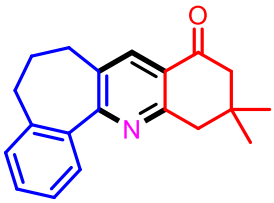
1464, 1390, 1291, 1186, 1011, 928, 752, 732, 705, 597 cm^{-1}; HRMS *m/z* [M^+] calcd for $C_{20}H_{15}NO_2$: 301.1103. Found: 301.1102.

8,8-Dimethyl-6,7,8,11-tetrahydro-9*H*-indeno[1,2-*b*]quinolin-9-one (7k)



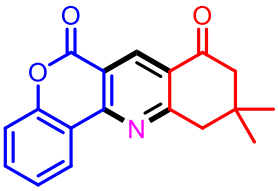
White solid; EtOAc:Hex (1:9); Yield: 92% (121 mg); mp 140-142 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.13 (d, *J* = 7.2 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.45 (dd, *J* = 7.4, 3.1 Hz, 2H), 3.87 (s, 2H), 3.25 (t, *J* = 6.0 Hz, 2H), 2.05 (t, *J* = 6.6 Hz, 2H), 1.24 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 202.6, 163.9, 162.1, 145.5, 139.8, 135.1, 131.6, 129.9, 127.4, 125.3, 124.6, 121.9, 41.4, 35.5, 34.2, 29.1, 24.2; IR (ATR) 2933, 2857, 1608, 1600, 1552, 1381, 1247, 1126, 1042, 769, 741, 502 cm^{-1}; HRMS *m/z* [M^+] calcd for $C_{18}H_{17}NO$: 263.1310. Found: 263.1307.

11,11-Dimethyl-5,6,7,10,11,12-hexahydro-9*H*-benzo[6,7]cyclohepta[1,2-*b*]quinolin-9-one (7l)



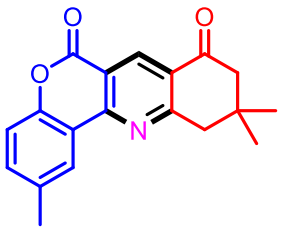
Pale yellow solid; EtOAc:Hex (1:9); Yield: 89% (129 mg); mp 176-178 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.72 (d, *J* = 7.2 Hz, 1H), 7.39-7.32 (m, 2H), 7.22 (d, *J* = 7.2 Hz, 1H), 3.08 (s, 2H), 2.54 (s, 2H), 2.51 (td, *J* = 7.2, 3.0 Hz, 4H), 2.20 (p, *J* = 7.2 Hz, 2H), 1.11 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.3, 163.0, 160.1, 139.6, 139.1, 134.4, 133.6, 129.5, 128.9, 128.6, 126.9, 125.4, 52.0, 46.1, 33.0, 32.6, 30.9, 29.8, 28.2; IR (ATR) 2953, 2870, 1676, 1589, 1452, 1417, 1312, 1230, 1076, 944, 764, 669, 579, 485 cm^{-1}; HRMS *m/z* [M^+] calcd for $C_{20}H_{21}NO$: 291.1623. Found: 291.1620.

10,10-Dimethyl-10,11-dihydro-6*H*-chromeno[4,3-*b*]quinoline-6,8(9*H*)-dione (9a)



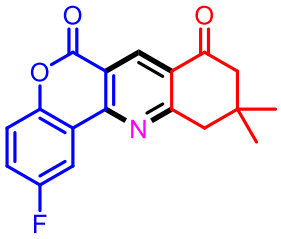
White solid; EtOAc:Hex (2:8); Yield: 75% (110 mg); mp 164-166 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.58 (d, *J* = 7.8 Hz, 1H), 7.59 (t, *J* = 6.6 Hz, 1H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 3.19 (s, 2H), 2.62 (s, 2H), 1.15 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.8, 168.3, 160.3, 154.3, 153.3, 137.7, 133.3, 127.2, 125.6, 124.9, 118.6, 117.3, 116.2, 51.8, 47.1, 32.7, 28.2; IR (ATR) 2963, 2886, 1732, 1687, 1599, 1580, 1406, 1321, 1219, 1138, 1063, 960, 897, 766, 628 cm^{-1}; HRMS *m/z* [M^+] calcd for $C_{18}H_{15}NO_3$: 293.1052. Found: 293.1053.

2,10,10-Trimethyl-10,11-dihydro-6*H*-chromeno[4,3-*b*]quinoline-6,8(9*H*)-dione (9b)



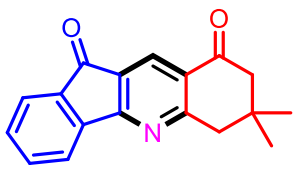
Pale yellow solid; EtOAc:Hex (2:8); Yield: 70% (107 mg); mp 170-172 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.05 (s, 1H), 8.30 (s, 1H), 7.36 (d, J = 8.4 Hz, 1H), 7.19 (d, J = 8.4 Hz, 1H), 3.17 (s, 2H), 2.60 (s, 2H), 2.43 (s, 3H), 1.13 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.8, 168.2, 160.4, 154.3, 151.3, 137.6, 134.7, 134.2, 127.0, 125.2, 118.1, 117.0, 116.1, 51.8, 47.1, 32.6, 28.2, 20.8, 14.1; IR (ATR) 2922, 2852, 1737, 1687, 1600, 1577, 1462, 1221, 1184, 812, 798 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{19}H_{17}NO_3$: 307.1208. Found: 307.1208.

2-Fluoro-10,10-dimethyl-10,11-dihydro-6*H*-chromeno[4,3-*b*]quinoline-6,8(9*H*)-dione (9c)



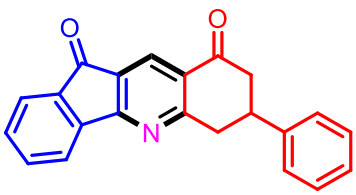
Pale yellow solid; EtOAc:Hex (2:8); Yield: 68% (106 mg); mp 196-198 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.10 (s, 1H), 8.21 (d, J = 8.4 Hz, 1H), 7.34-7.28 (m, 2H), 3.19 (s, 2H), 2.63 (s, 2H), 1.14 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.7, 168.5, 160.2 (C-F, $^{1}J_{C\text{-}F}$ = 243.4 Hz), 158.5, 153.5 (C-F, $^{5}J_{C\text{-}F}$ = 2.8 Hz), 149.3, 137.8, 127.7, 120.7 (C-F, $^{3}J_{C\text{-}F}$ = 24.7 Hz), 119.1 (C-F, $^{2}J_{C\text{-}F}$ = 84 Hz), 119.0 (C-F, $^{4}J_{C\text{-}F}$ = 8.1 Hz), 116.2, 111.3 (C-F, $^{3}J_{C\text{-}F}$ = 24.9 Hz), 51.8, 47.1, 32.7, 28.2, 14.1; IR (ATR) 2955, 2929, 1739, 1689, 1587, 1558, 1460, 1225, 1141, 1074, 979, 890, 828, 797, 735, 606, 587, 420 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{18}H_{14}FNO_3$: 311.0958. Found: 311.0959.

7,7-Dimethyl-7,8-dihydro-6*H*-indeno[1,2-*b*]quinoline-9,11-dione (9d)



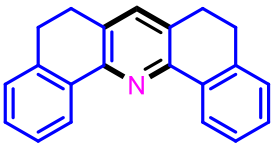
Pale orange solid; EtOAc:Hex (2:8); Yield: 92% (127 mg); mp 164-166 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (s, 1H), 7.94 (d, J = 7.2 Hz, 1H), 7.77 (d, J = 7.8 Hz, 1H), 7.64 (t, J = 7.2 Hz, 1H), 7.51 (t, J = 6.6 Hz, 1H), 3.13 (s, 2H), 2.58 (s, 2H), 1.14 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.5, 190.4, 168.1, 168.0, 142.4, 135.9, 135.3, 132.1, 129.9, 127.2, 126.9, 124.3, 121.9, 51.8, 47.1, 32.8, 28.2; IR (ATR) 2923, 2852, 1709, 1681, 1592, 1508, 1462, 1386, 1274, 1229, 1107, 983, 746, 574 cm^{-1}; HRMS *m/z* [M^{+}] calcd for $C_{18}H_{15}NO_2$: 277.1103. Found: 277.1101.

7-Phenyl-7,8-dihydro-6*H*-indeno[1,2-*b*]quinoline-9,11-dione (9e)



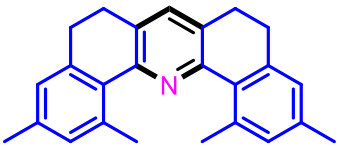
Yellow solid; EtOAc:Hex (2:8); Yield: 74% (120 mg); mp 178-180 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.50 (s, 1H), 7.99 (d, J = 7.8 Hz, 1H), 7.77 (d, J = 7.2 Hz, 1H), 7.64 (t, J = 7.8 Hz, 1H), 7.52 (t, J = 7.2 Hz, 1H), 7.37 (t, J = 7.2 Hz, 2H), 7.32-7.27 (m, 3H), 3.62-3.55 (m, 2H), 3.42 (dd, J = 16.8, 10.8 Hz, 1H), 3.04 (ddd, J = 16.7, 3.8, 2.0 Hz, 1H), 2.91 (dd, J = 16.8, 10.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 195.6, 190.0, 168.1, 167.7, 142.0, 136.0, 135.5, 132.4, 130.5, 128.9, 127.5, 127.5, 127.2, 126.6, 124.4, 122.4, 45.2, 40.5, 39.1; IR (ATR) 2928, 1718, 1680, 1591, 1551, 1390, 1227, 747, 694 cm^{-1}; HRMS ESI *m/z* [MH$^+$] calcd for $C_{22}H_{16}NO_2$: 326.1175. Found: 326.1171.

5,6,8,9-Tetrahydrodibenzo[*c*,*h*]acridine (10a)



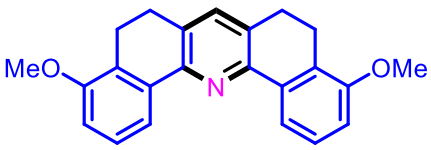
White solid; EtOAc:Hex (1:9); Yield: 90% (127 mg); mp 148-150 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, J = 7.8 Hz, 2H), 7.38 (t, J = 7.8 Hz, 2H), 7.31 (s, 1H), 7.29 (t, J = 7.8 Hz, 2H), 7.22 (d, J = 7.2 Hz, 2H), 2.94 (s, 8H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 150.3, 137.8, 135.3, 134.8, 130.5, 128.6, 127.6, 127.0, 125.0, 28.2, 27.8; IR (ATR) 2927, 1723, 1415, 1271, 1031, 737, 460 cm^{-1}; HRMS ESI *m/z* [MH$^+$] calcd for $C_{21}H_{18}N$: 284.1434. Found: 284.1432.

1,3,11,13-1,3,11,13-Tetramethyl-5,6,8,9-tetrahydrodibenzo[*c*,*h*]acridine (10b)



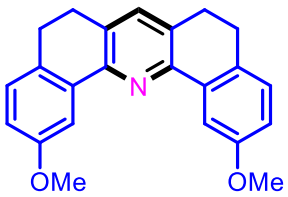
Pale orange solid; EtOAc:Hex (1:9); Yield: 96% (162 mg); mp 140-142 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.26 (s, 2H), 7.30 (s, 1H), 7.04 (s, 2H), 2.93-2.82 (m, 8H), 2.46 (s, 6H), 2.33 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 150.6, 135.7, 134.6, 133.3, 131.4, 130.0, 123.3, 27.6, 23.6, 21.2, 19.6; IR (ATR) 2919, 1430, 1258, 1219, 1032, 910, 868, 748, 563 cm^{-1}; HRMS ESI *m/z* [MH$^+$] calcd for $C_{25}H_{26}NO$: 340.2060. Found: 340.2058.

4,10-Dimethoxy-5,6,8,9-tetrahydrodibenzo[*c*,*h*]acridine (10c)Pale yellow solid; EtOAc:Hex (2:8); Yield: 93% (159 mg); mp 182-184 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 (d, J = 7.8 Hz, 2H), 7.34 (d, J = 7.8 Hz, 2H), 7.31 (s, 1H), 6.89 (d, J = 7.8 Hz, 2H), 3.87 (s, 6H), 2.98-



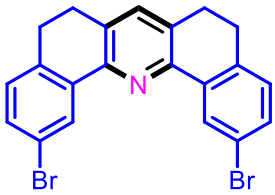
2.85 (m, 8H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.1, 150.1, 135.9, 135.2, 130.6, 127.0, 126.4, 117.5, 110.6, 55.5, 27.2, 20.1; IR (ATR) 2928, 1414, 1264, 1245, 1144, 1117, 903, 819, 777 cm$^-$ HRMS ESI *m/z* [MH^+] calcd for $C_{23}H_{22}NO_2$: 344.1645. Found: 344.1642.

2,12-Dimethoxy-5,6,8,9-tetrahydrodibenzo[*c*,*h*]acridine (10d)



White solid; EtOAc:Hex (1:9); Yield: 90% (154 mg); mp 180-182 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (s, 2H), 7.31 (s, 1H), 7.13 (d, *J* = 7.2 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 2H), 3.91 (s, 6H), 2.94-2.84 (m, 8H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.8, 150.1, 135.8, 135.4, 130.9, 130.2, 128.6, 114.9, 109.4, 55.4, 28.1, 27.3; IR (ATR) 2938, 1493, 1458, 1415, 1215, 1037, 893, 813, 785 cm$^-$ ^{1}; HRMS ESI *m/z* [MH^+] calcd for $C_{23}H_{22}NO_2$: 344.1645. Found: 344.1643.

2,12-Dibromo-5,6,8,9-tetrahydrodibenzo[*c*,*h*]acridine (10e)

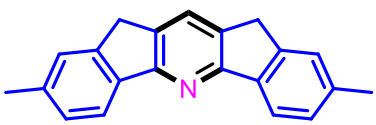


Yellow solid; EtOAc:Hex (2:8); Yield: 88% (192 mg); mp 170-172 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.55 (s, 2H), 7.39 (d, *J* = 7.2 Hz, 2H), 7.30 (s, 1H), 7.07 (d, *J* = 7.8 Hz, 2H), 2.91-2.89 (m, 8H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.2, 136.6, 136.5, 135.5, 131.4, 131.2, 129.3, 127.7, 121.0, 121.0, 27.6; IR (ATR) 2934, 1545, 1442, 1385, 1252, 1029, 895, 781, 553 cm^{-1}; HRMS ESI *m/z* [MH^+] calcd for $C_{21}H_{16}NBr_2$: 441.9624. Found: 441.9623.

10,12-Dihydrodiindeno[1,2-*b*:2',1'-*e*]pyridine (10f)

Yellow solid; EtOAc:Hex (1:9); Yield: 91% (116 mg); mp 218-220 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.90 (s, 1H), 7.54 (d, *J* = 7.8 Hz, 2H), 7.47(t, *J* = 7.8 Hz, 2H), 7.39 (t, *J* = 7.2 Hz, 2H), 3.87 (s, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.9, 135.0, 128.2, 127.1, 125.0, 121.1, 34.5; IR (ATR) 2921, 1388, 1281, 1179, 1010, 728, 410 cm^{-1}; HRMS ESI *m/z* [MH^+] calcd for $C_{19}H_{14}N$: 256.1121. Found: 256.1117.

2,8-Dimethyl-10,12-dihydrodiindeno[1,2-*b*:2',1'-*e*]pyridine (10g)



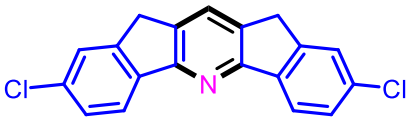
Yellow solid; EtOAc:Hex (1:9); Yield: 89% (125 mg); mp 228-230 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (s, 2H), 7.81 (s, 1H),

7.32 (s, 2H), 7.26 (d, J = 7.8 Hz, 2H), 3.77 (s, 4H), 2.44 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.2, 138.2, 134.5, 128.0, 125.6, 120.7, 34.3, 21.7; IR (ATR) 2925, 1393, 1279, 1185, 1105, 819, 703, 412 cm^{-1}; HRMS ESI m/z [MH$^+$] calcd for $C_{21}H_{18}N$: 284.1434. Found: 284.1430.

3,7-Dimethoxy-10,12-dihydrodiindeno[1,2-*b*:2',1'-*e*]pyridine (10h)

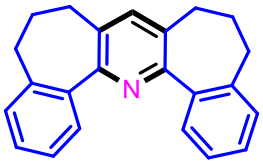
Pale orange solid; EtOAc:Hex (1:9); Yield: 96% (151 mg); mp 108-110 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.75 (s, 2H), 7.42 (d, J = 8.4 Hz, 2H), 6.96 (d, J = 8.4 Hz, 2H), 3.96 (s, 6H), 3.79 (s, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.5, 159.3, 142.4, 136.1, 136.0, 128.9, 125.7, 116.3, 104.2, 55.6, 33.8; IR (ATR) 2925, 1597, 1463, 1244, 1090, 1028, 823, 793 cm^{-1}; HRMS ESI m/z [MH$^+$] calcd for $C_{21}H_{18}NO_2$: 316.1332. Found: 316.1328.

2,8-Dichloro-10,12-dihydrodiindeno[1,2-*b*:2',1'-*e*]pyridine (10i)



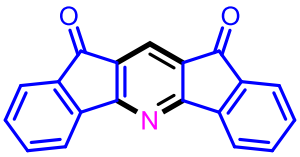
Yellow solid; EtOAc:Hex (2:8); Yield: 84% (135 mg); mp 268-270 °C. (NMR taken with $CDCl_3$ and 1 drop of TFA) ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.25 (d, J = 8.4 Hz, 2H), 7.66 (s, 2H), 7.54 (d, J = 6.6 Hz, 2H), 4.09 (s, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.9, 160.6, 150.6, 146.5, 139.4, 138.4, 137.2, 130.9, 129.6, 126.3, 124.2, 115.3, 113.5, 34.8; IR (ATR) 2903, 1393, 1280, 1168, 1058, 875, 822, 773, 428 cm^{-1}; HRMS ESI m/z [MH$^+$] calcd for $C_{19}H_{12}NCl_2$: 324.0341. Found: 324.0338.

5,6,7,9,10,11-Hexahydrobenzo[6,7]cyclohepta[1,2-*b*]benzo[6,7]cyclohepta[2,1-*e*]pyridine (10j)



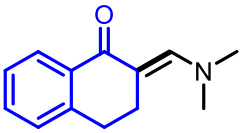
White solid; EtOAc:Hex (1:9); Yield: 85% (132 mg); mp 240-242 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, J = 7.8 Hz, 2H), 7.39 (s, 1H), 7.37 (d, J = 7.2 Hz, 2H), 7.32 (t, J = 7.8 Hz, 2H), 7.23 (d, J = 6.6 Hz, 2H), 2.59 (t, J = 7.2 Hz, 4H), 2.53 (t, J = 7.2 Hz, 4H), 2.26 (p, J = 7.2 Hz, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.1, 139.4, 137.0, 133.4, 129.0, 128.3, 126.7, 33.1, 31.2, 30.0; IR (ATR) 2922, 2856, 1726, 1444, 1418, 1272, 766, 634 cm^{-1}; HRMS ESI m/z [MH$^+$] calcd for $C_{23}H_{22}N$: 312.1747. Found: 312.1745.

Diindeno[1,2-*b*:2',1'-*e*]pyridine-10,12-dione (10k)



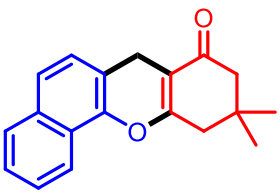
Yellow solid; EtOAc:Hex (2:8); Yield: 89% (125 mg); mp 250-252 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.25 (d, J = 8.4 Hz, 2H), 7.66 (s, 2H), 7.54 (d, J = 6.6 Hz, 2H), 4.09 (s, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 190.1, 170.6, 142.3, 135.5, 135.2, 132.0, 127.8, 126.4, 124.1, 121.9; IR (ATR) 2928, 1710, 1565, 1389, 1260, 1098, 991, 748, 498 cm^{-1}; HRMS ESI *m/z* [MH^{+}] calcd for $C_{19}H_{10}NO_2$: 284.0706. Found: 284.0701.

(*E*)-2-((Dimethylamino)methylene)-3,4-dihydronaphthalen-1(2*H*)-one (11)



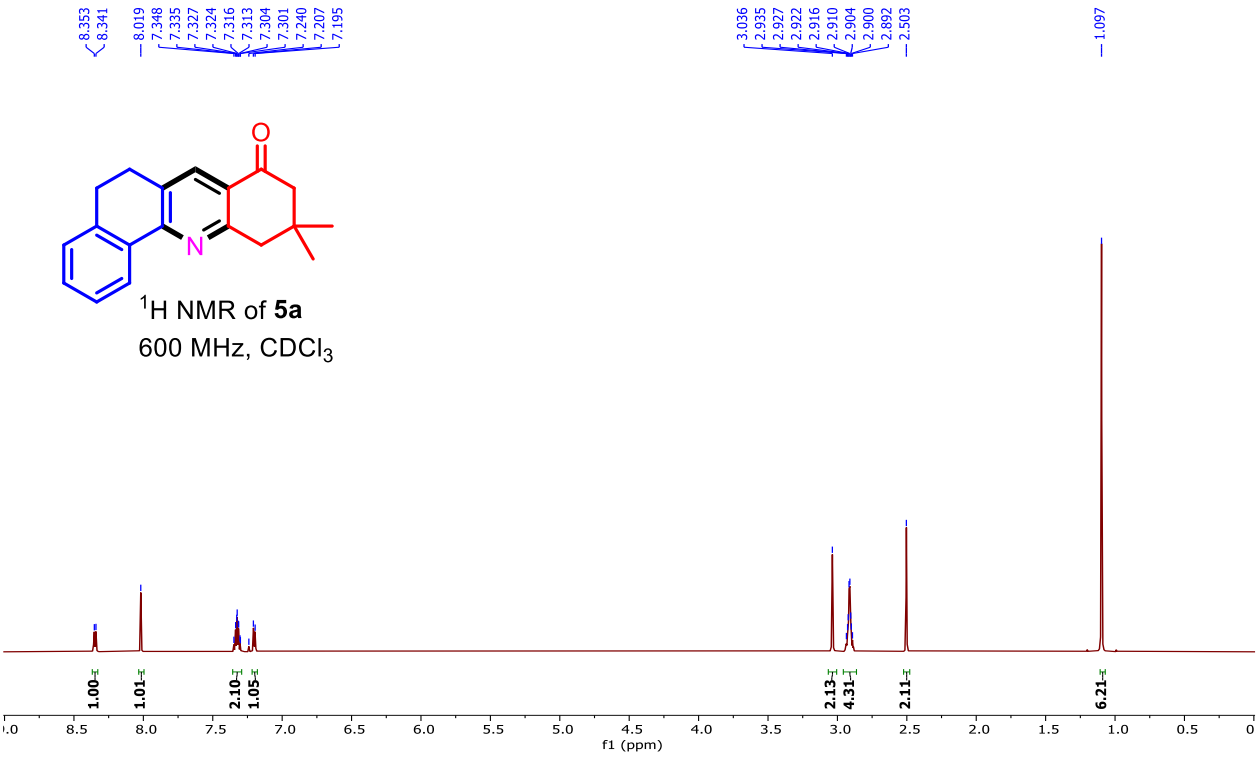
Light brown solid; EtOAc:Hex (4:6); Yield: 88% (176 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 7.8 Hz, 1H), 7.74 (s, 1H), 7.38 (t, J = 7.2 Hz, 1H), 7.31 (t, J = 7.2 Hz, 1H), 7.18 (s, 1H), 3.13 (s, 6H), 2.94 (t, J = 6.6 Hz, 2H), 2.85 (t, J = 6.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.0, 150.1, 141.7, 134.9, 131.0, 127.0, 126.9, 126.3, 103.4, 43.3, 29.1, 24.0; HRMS ESI *m/z* [MH^{+}] calcd for $C_{13}H_{16}NO$: 202.1226. Found: 202.1221.

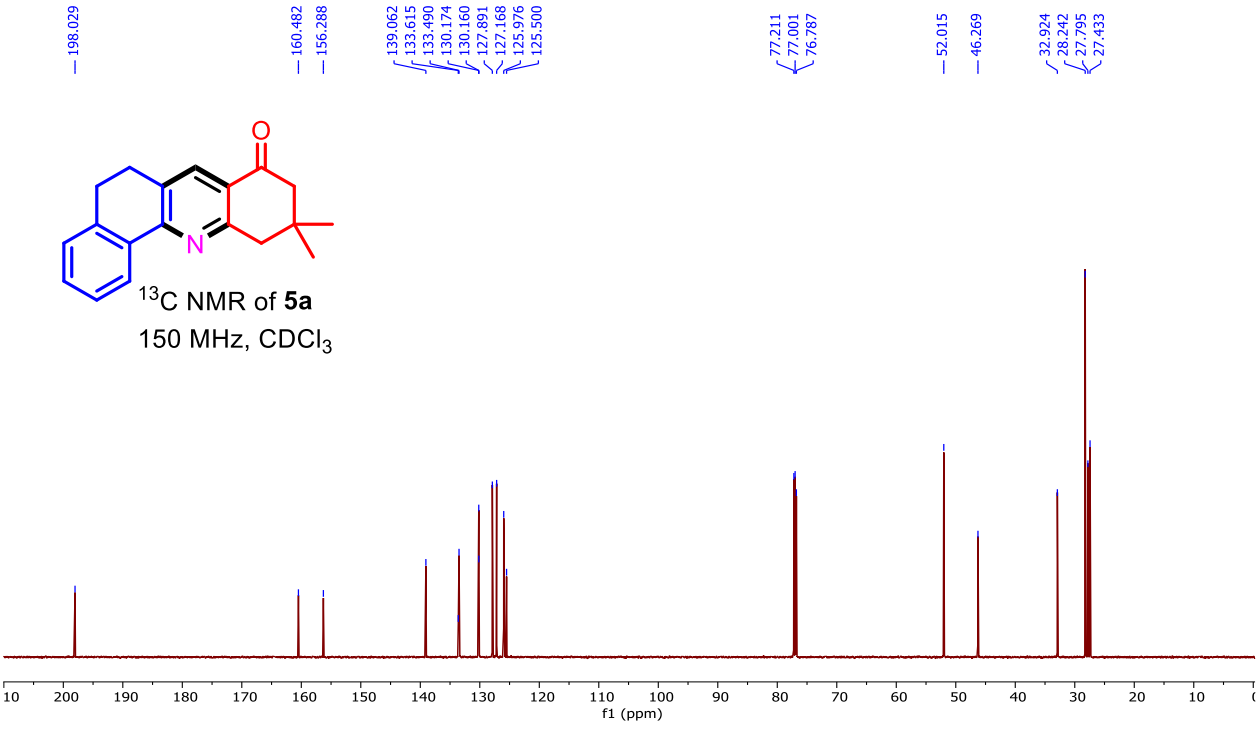
10,10-Dimethyl-7,9,10,11-tetrahydro-8*H*-benzo[*c*]xanthen-8-one (12)

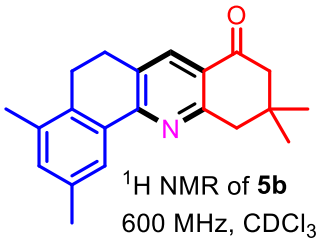


Orange solid; EtOAc:Hex (2:8); Yield: 69% (96 mg); mp 90-92 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 7.8 Hz, 1H), 7.69 (d, J = 9.0 Hz, 1H), 7.56 (t, J = 7.2 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H), 7.15 (d, J = 9.0 Hz, 1H), 3.77 (s, 2H), 2.48 (s, 2H), 2.37 (s, 2H), 1.14 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.2, 164.6, 146.9, 132.0, 130.7, 128.2, 126.9, 124.9, 123.1, 117.0, 113.5, 108.7, 50.6, 41.3, 32.1, 28.4, 18.8; IR (ATR) 2957, 1644, 1597, 1372, 1224, 1178, 809, 731 cm^{-1}; HRMS ESI *m/z* [MH^{+}] calcd for $C_{19}H_{19}O_2$: 279.1379. Found: 279.1375.

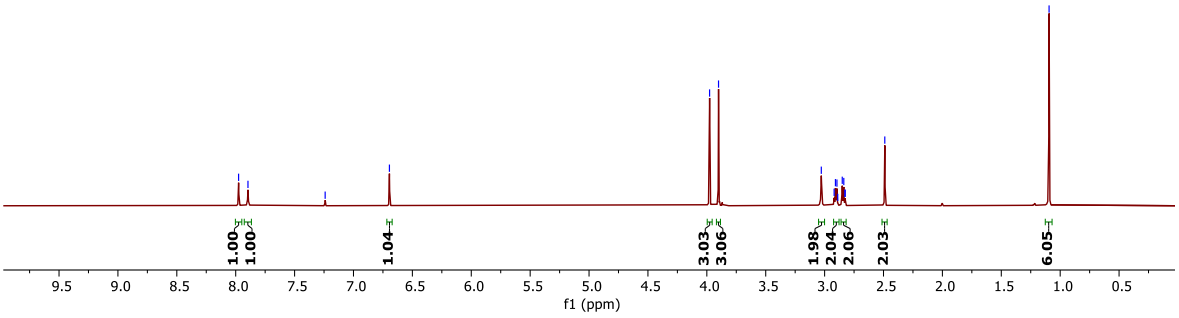
^{1}H NMR and ^{13}C NMR spectra of synthesized compounds

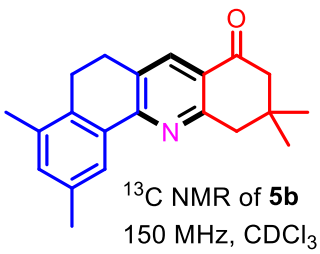




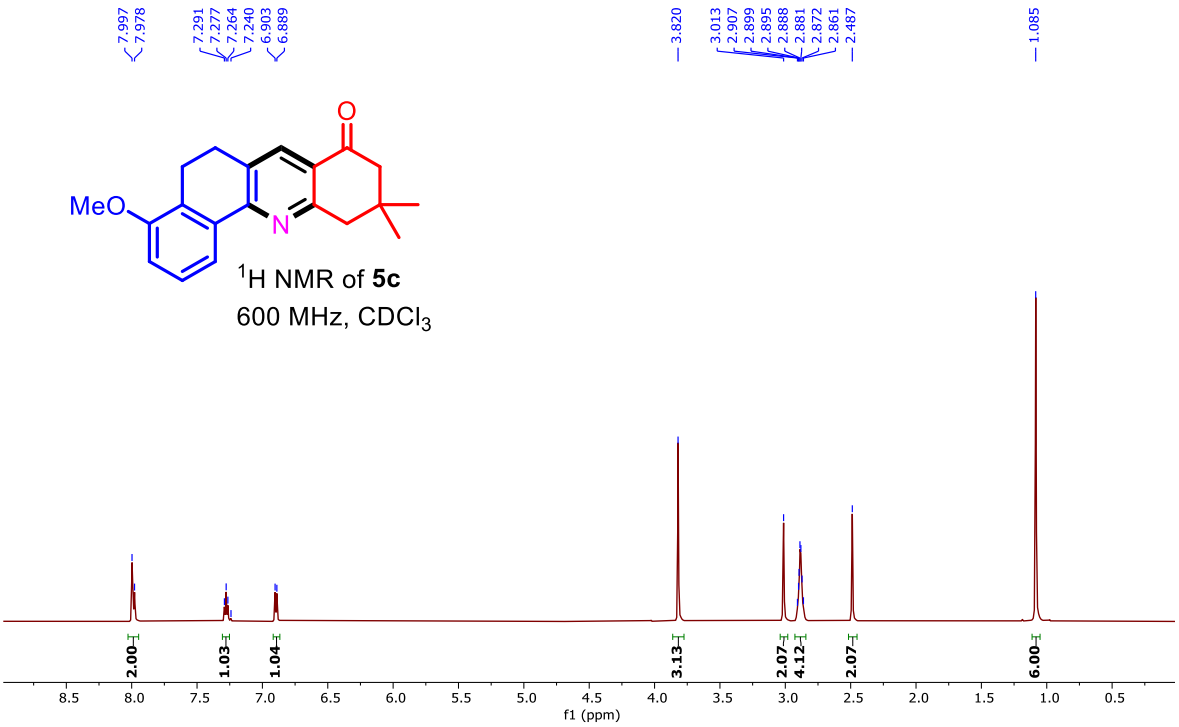


^{1}H NMR of **5b**
600 MHz, $CDCl_3$

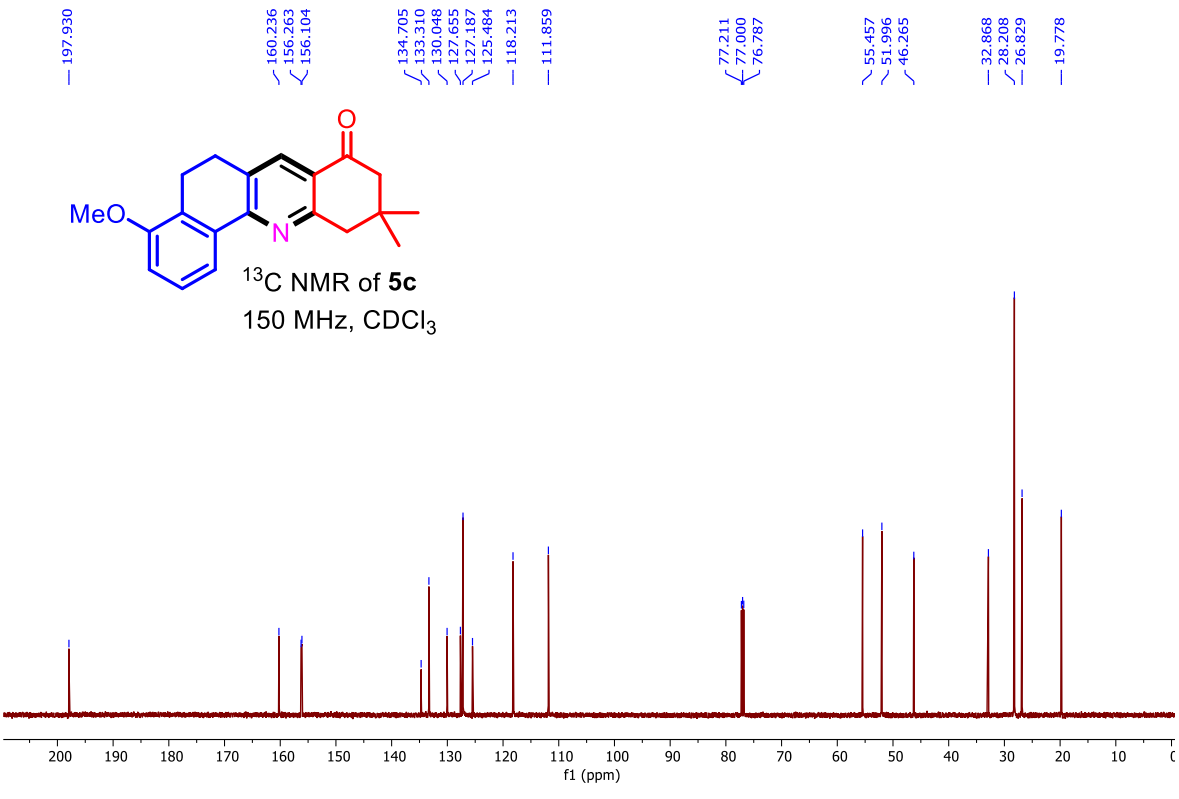




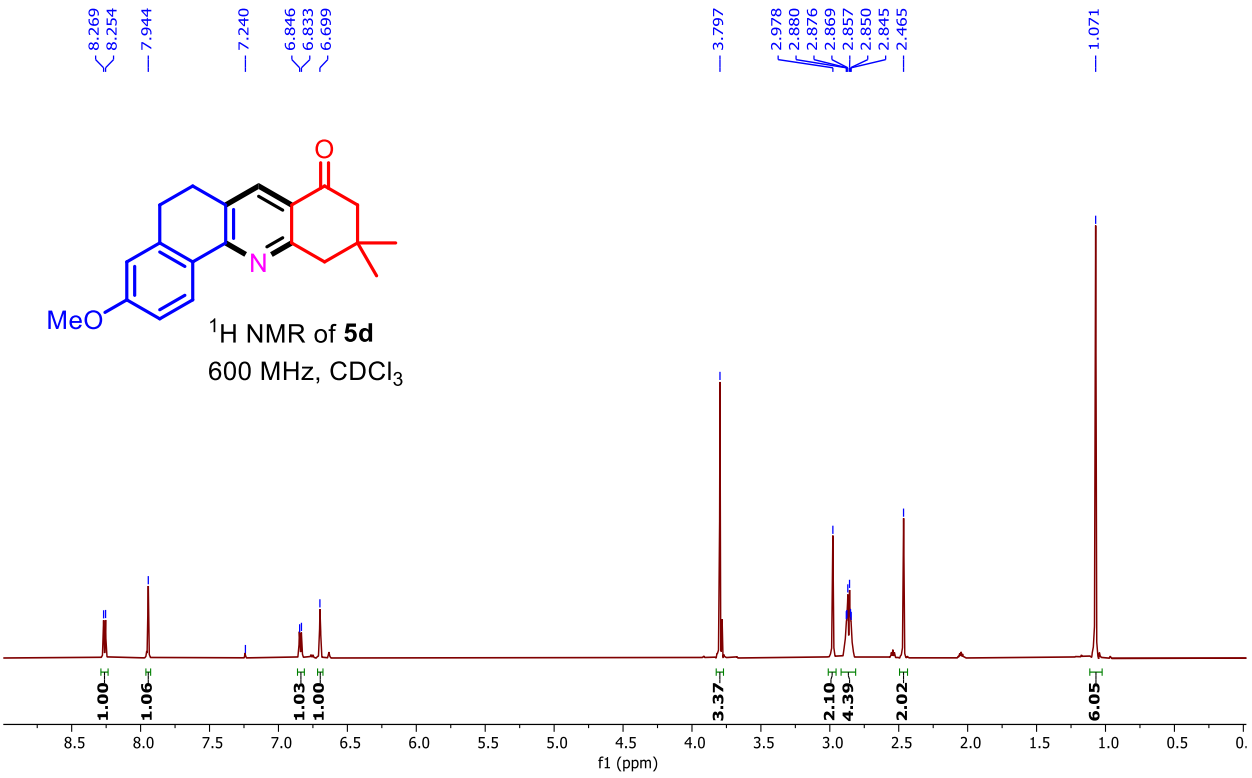
^{13}C NMR of **5b**
150 MHz, $CDCl_3$



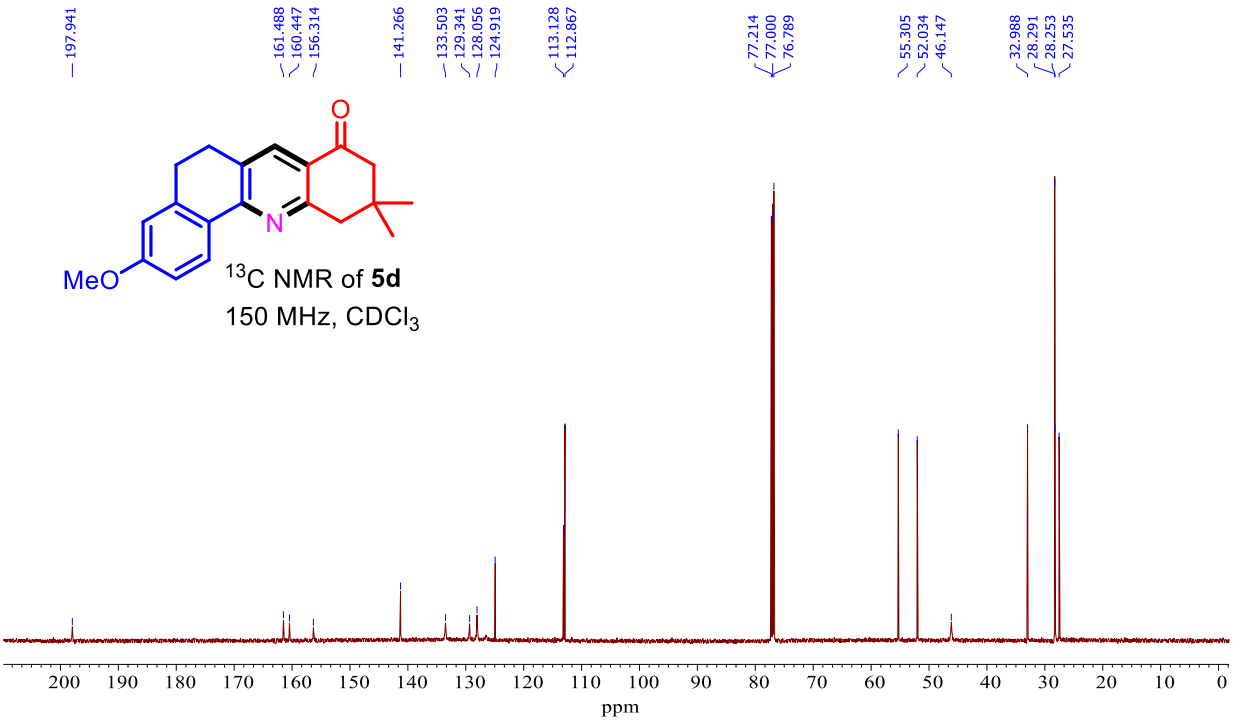
^{1}H NMR of **5c**
600 MHz, $CDCl_3$



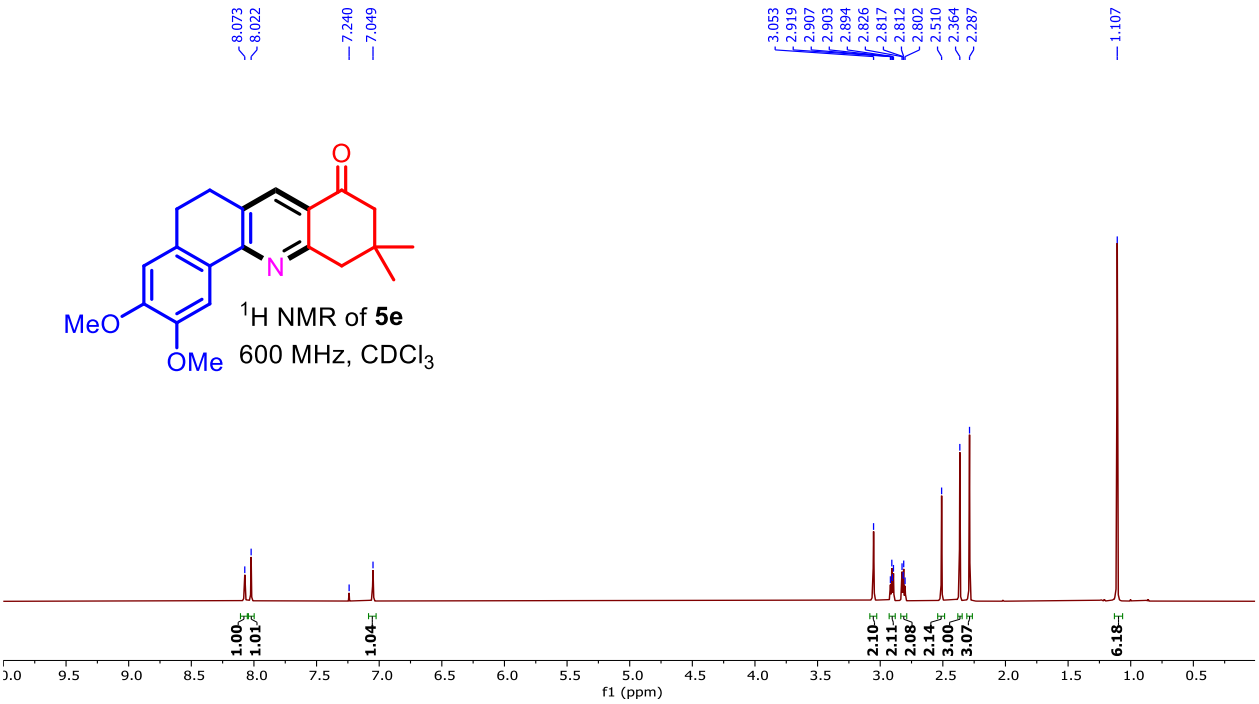
^{13}C NMR of **5c**
150 MHz, $CDCl_3$

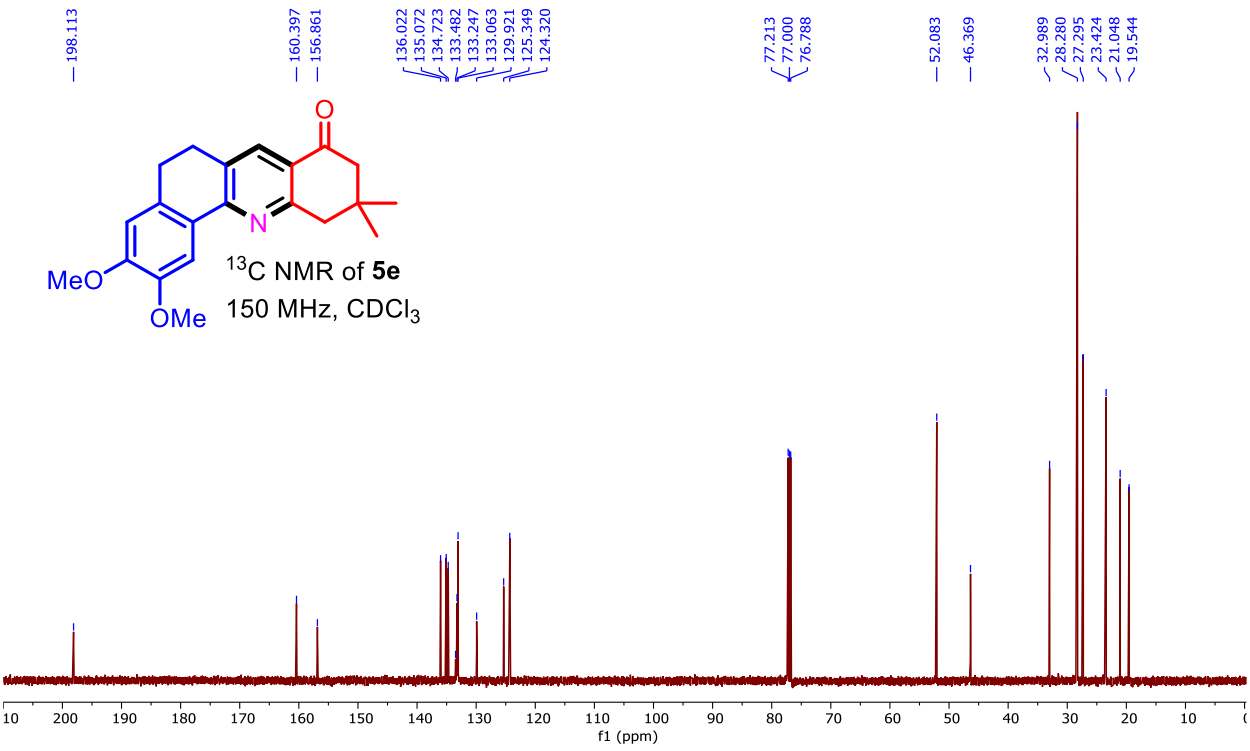


^{1}H NMR of **5d**
600 MHz, $CDCl_3$



^{13}C NMR of **5d**
150 MHz, $CDCl_3$


8.073
8.022
7.240
7.049
3.053
2.919
2.907
2.903
2.894
2.826
2.817
2.812
2.802
2.510
2.364
2.287
1.107
O
N
MeO
OMe
1H NMR of 5e
600 MHz, CDCl3
1.00
1.01
1.04
2.10
2.11
2.08
2.14
3.00
3.07
6.18
f1 (ppm)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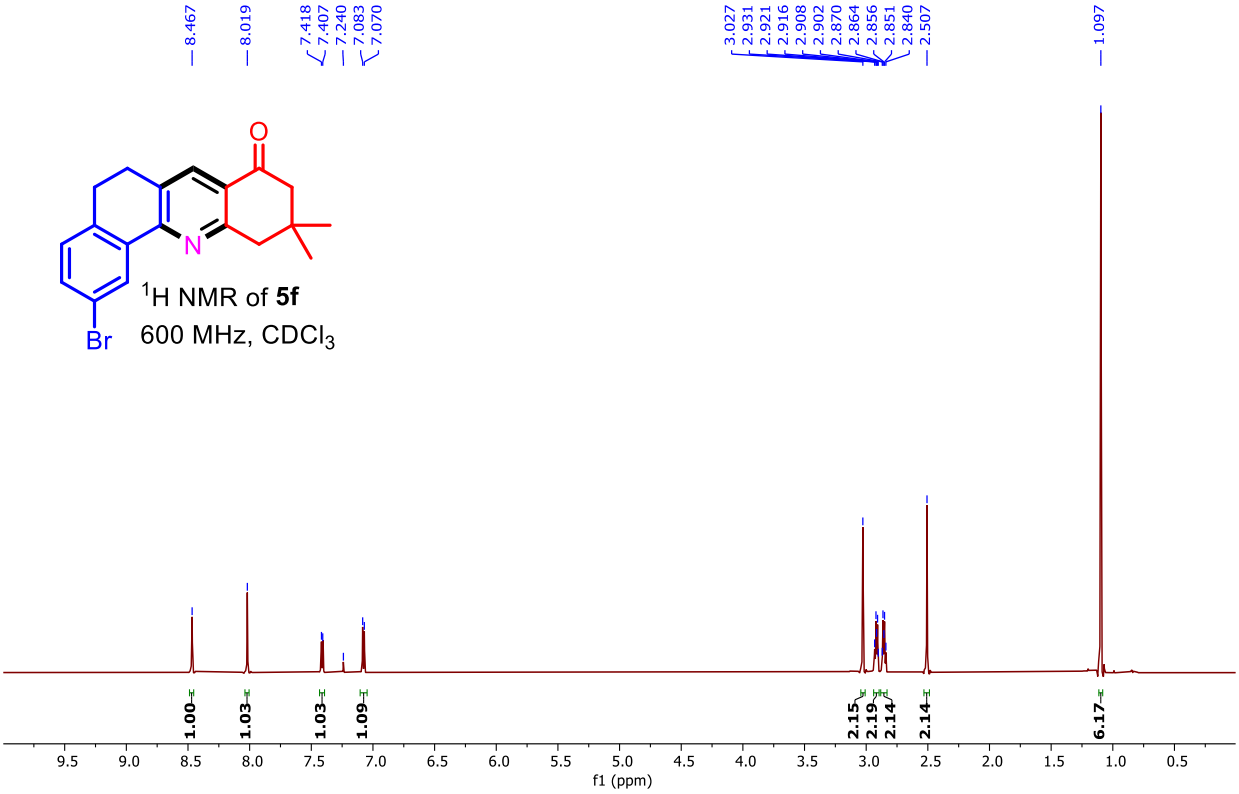
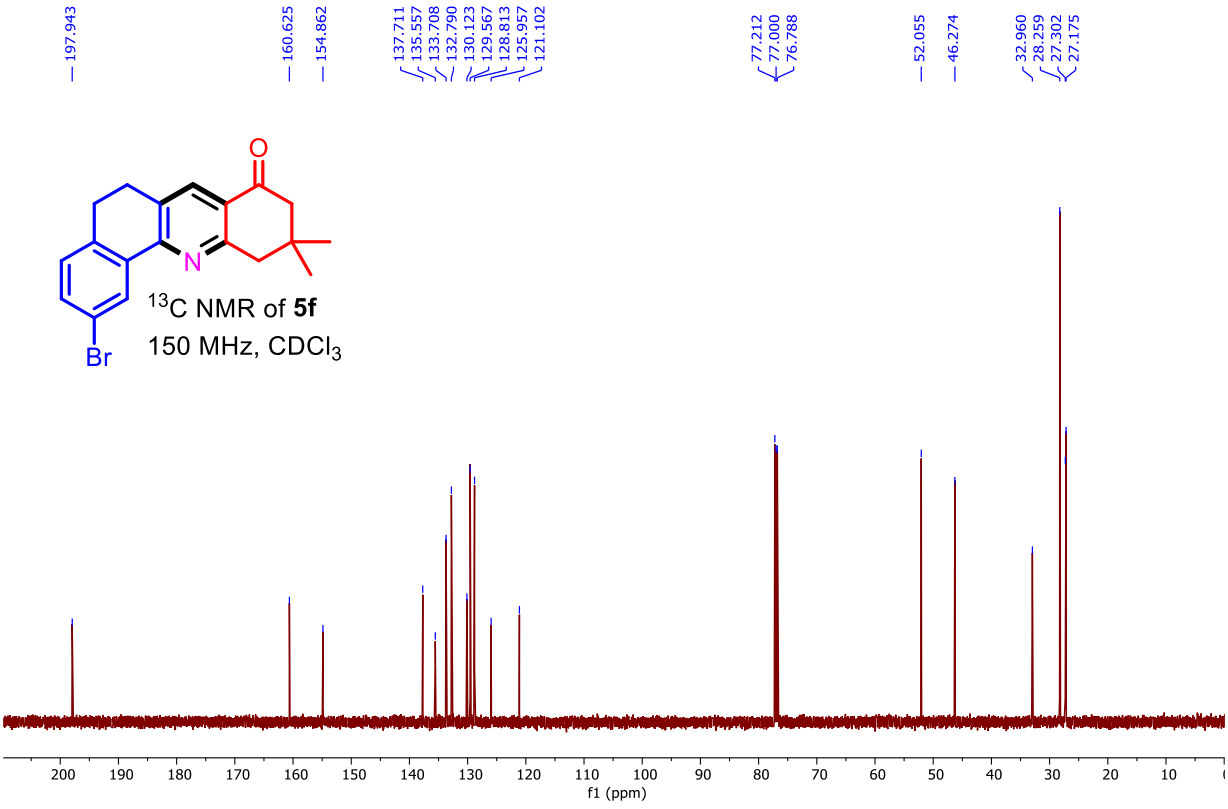
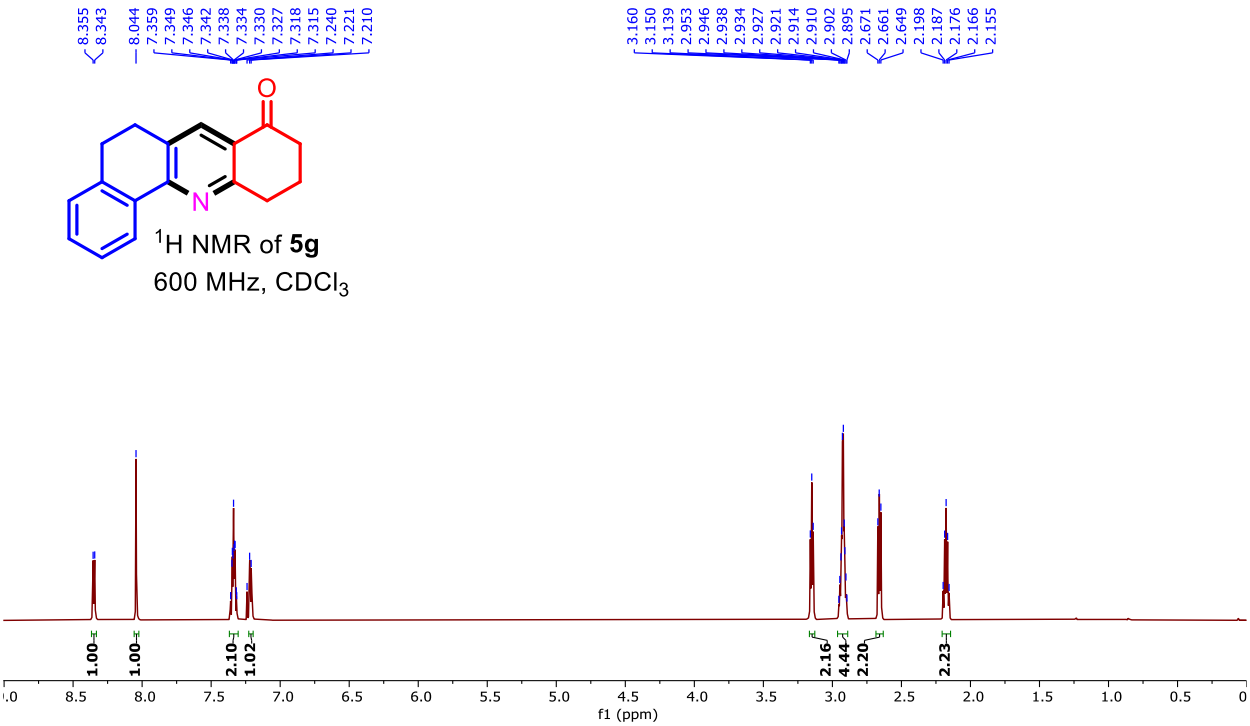
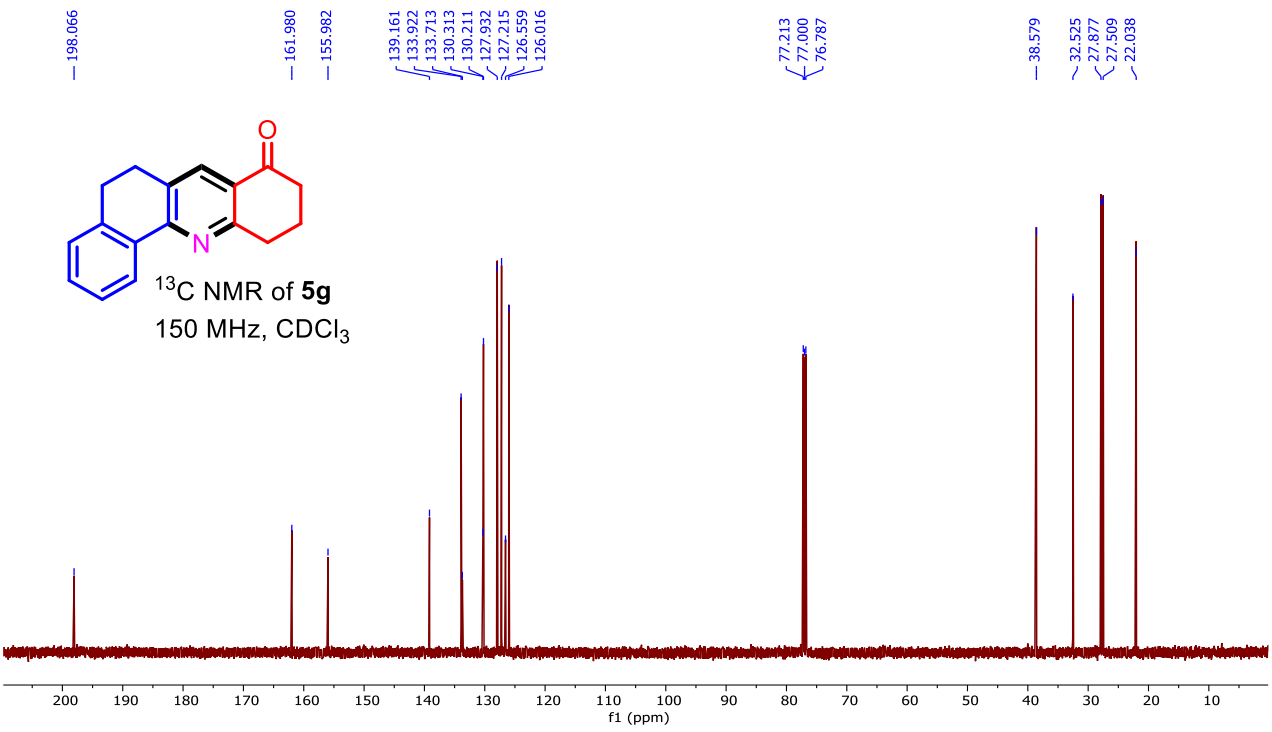
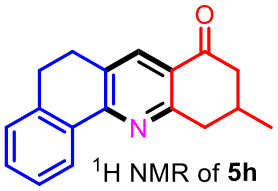
160.397
156.861
136.022
135.072
134.723
133.482
133.247
133.063
129.921
125.349
124.320
77.213
77.000
76.788
52.083
46.369
32.989
28.280
27.295
23.424
21.048
19.544
O
N
MeO
OMe
13C NMR of 5e
150 MHz, CDCl3
f1 (ppm)


8.467
8.019
7.418
7.407
7.240
7.083
7.070
3.027
2.931
2.921
2.916
2.908
2.902
2.870
2.864
2.856
2.851
2.840
2.507
1.097
O
N
Br
1H NMR of 5f
600 MHz, CDCl3
1.00
1.03
1.03
1.09
2.15
2.19
2.14
2.14
6.17
f1 (ppm)

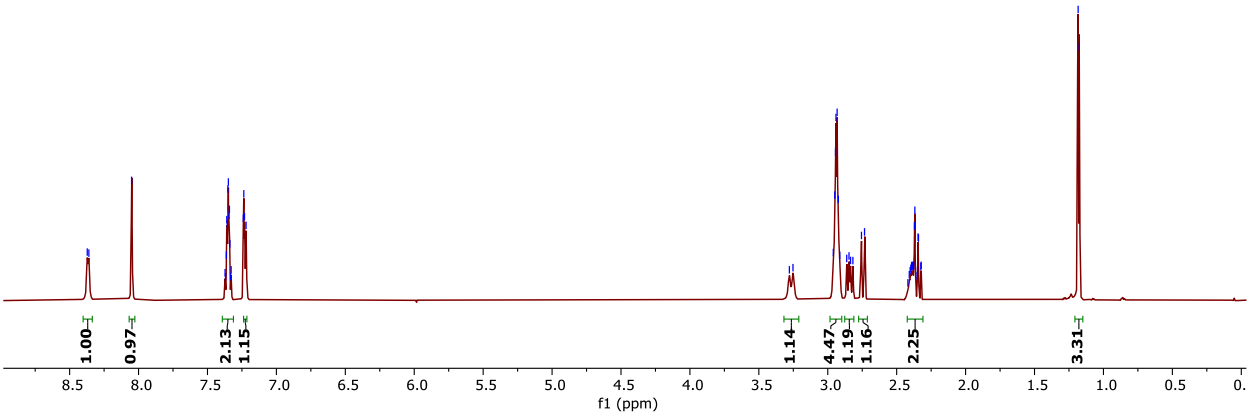

197.943
160.625
154.862
137.711
135.557
133.708
132.790
130.123
129.567
128.813
125.957
121.102
77.212
77.000
76.788
52.055
46.274
32.960
28.259
27.302
27.175
O
N
Br
13C NMR of 5f
150 MHz, CDCl3
f1 (ppm)

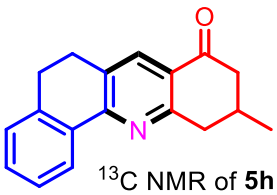

8.355
8.343
8.044
7.359
7.349
7.346
7.342
7.338
7.334
7.330
7.327
7.318
7.315
7.240
7.221
7.210
3.160
3.150
3.139
2.953
2.946
2.938
2.934
2.927
2.921
2.914
2.910
2.902
2.895
2.671
2.661
2.649
2.198
2.187
2.176
2.166
2.155
O
N
1H NMR of 5g
600 MHz, CDCl3
1.00
1.00
2.10
1.02
2.16
4.44
2.20
2.23
f1 (ppm)


198.066
161.980
155.982
139.161
133.922
133.713
130.313
130.211
127.932
127.215
126.559
126.016
77.213
77.000
76.787
38.579
32.525
27.877
27.509
22.038
O
N
13C NMR of 5g
150 MHz, CDCl3
f1 (ppm)

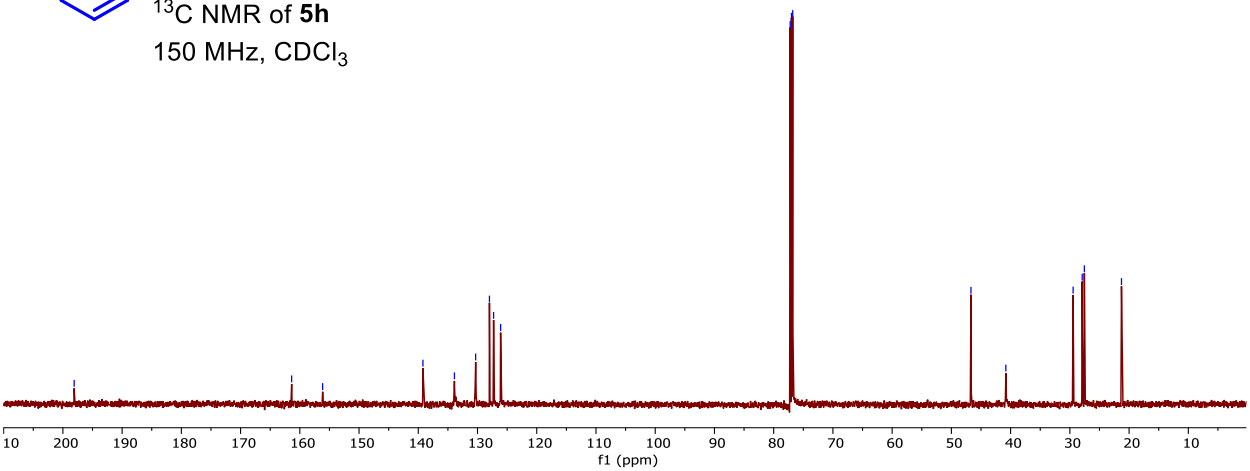


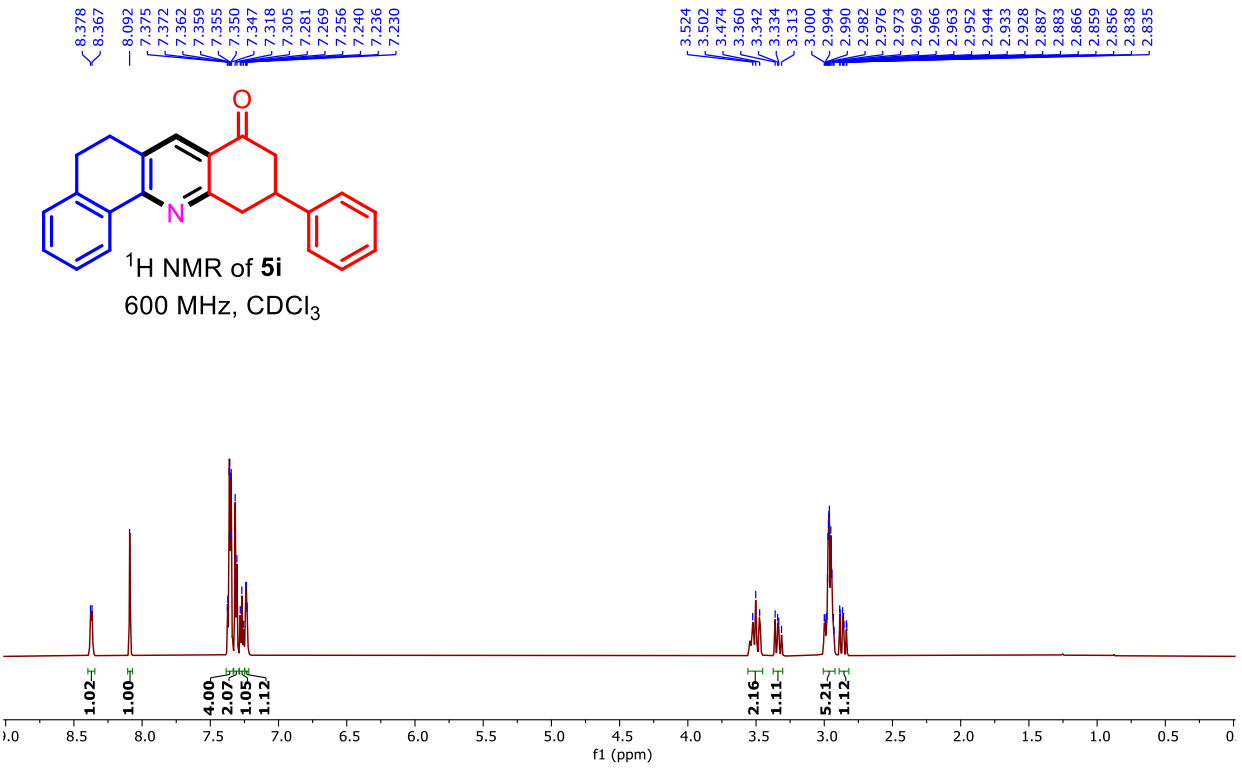
^{1}H NMR of **5h**
600 MHz, $CDCl_3$

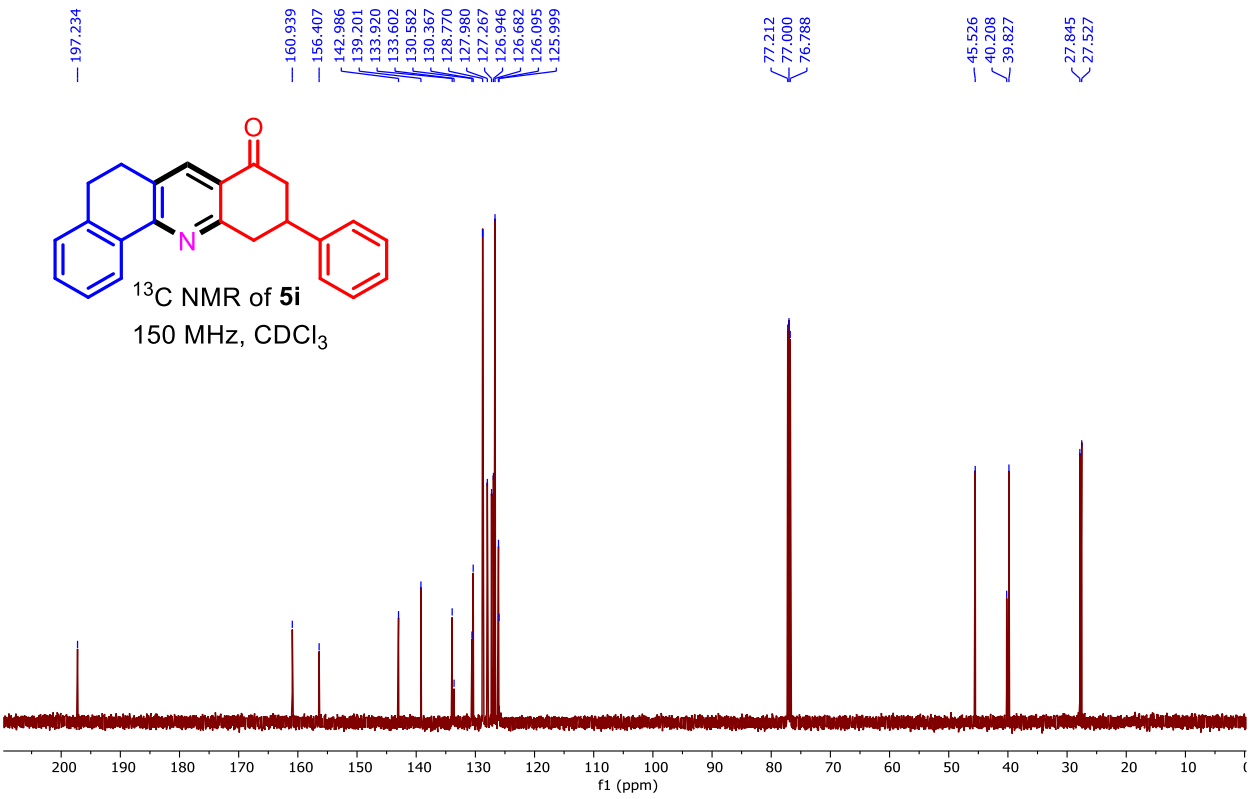


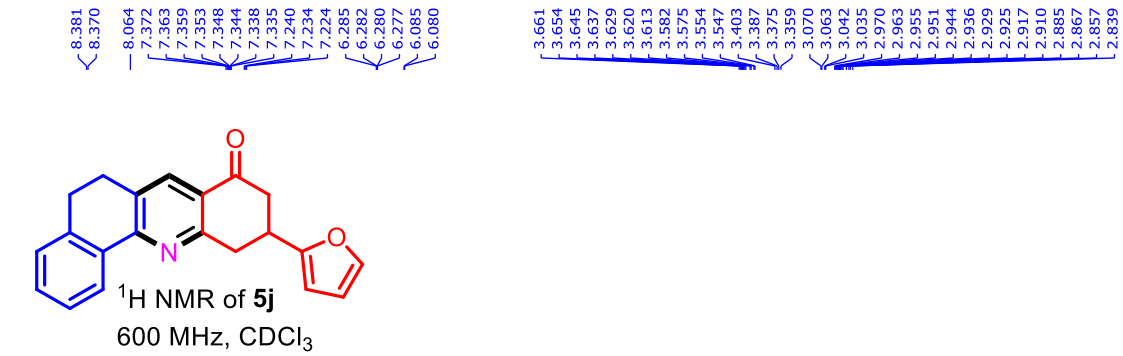


^{13}C NMR of **5h**
150 MHz, $CDCl_3$



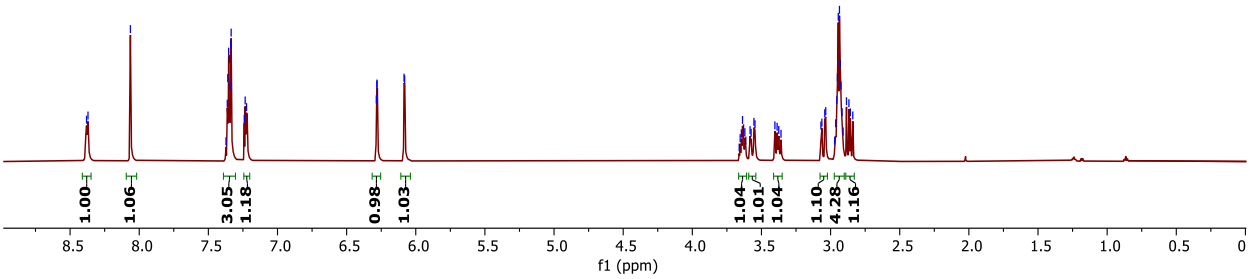

8.378
8.367
8.092
7.375
7.372
7.362
7.359
7.355
7.350
7.347
7.318
7.305
7.281
7.269
7.256
7.240
7.236
7.230
3.524
3.502
3.474
3.360
3.342
3.334
3.313
3.000
2.994
2.990
2.982
2.976
2.973
2.969
2.966
2.963
2.952
2.944
2.933
2.928
2.887
2.883
2.866
2.859
2.856
2.838
2.835
O
N
1H NMR of 5i
600 MHz, CDCl3
1.02
1.00
4.00
2.07
1.05
1.12
2.16
1.11
5.21
1.12
f1 (ppm)

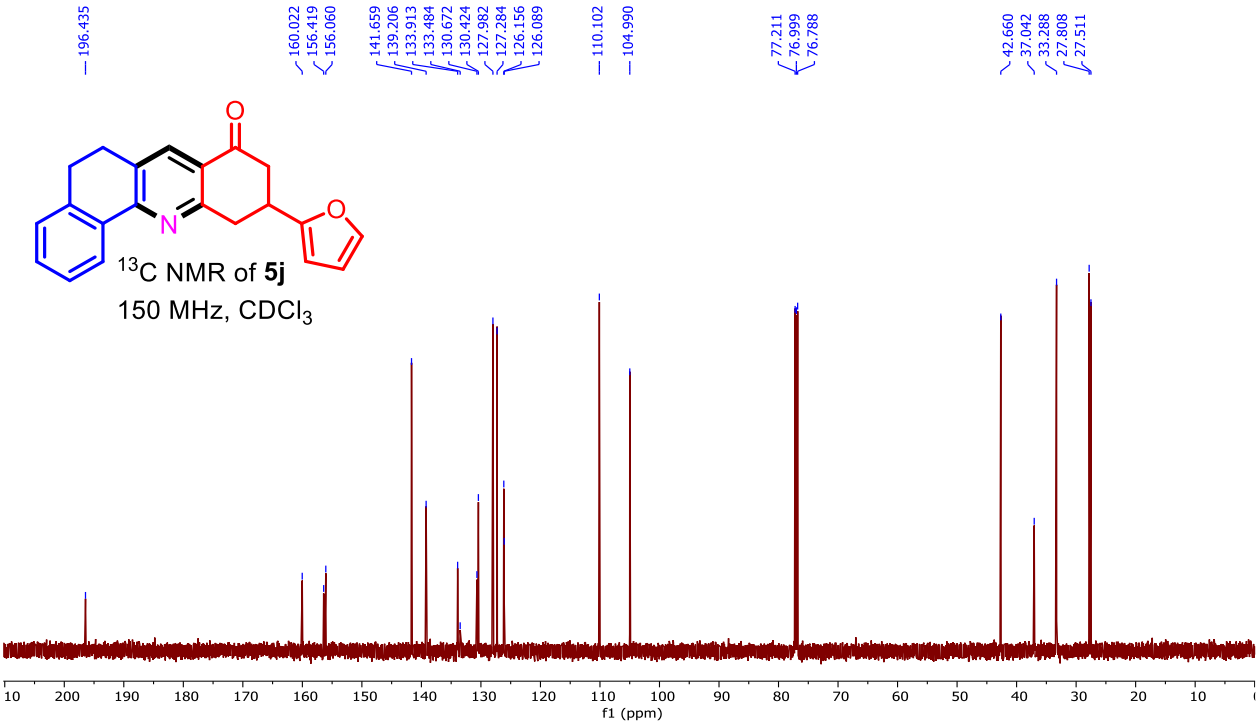

197.234
160.939
156.407
142.986
139.201
133.920
133.602
130.582
130.367
128.770
127.980
127.267
126.946
126.682
126.095
125.999
77.212
77.000
76.788
45.526
40.208
39.827
27.845
27.527
O
N
13C NMR of 5i
150 MHz, CDCl3
f1 (ppm)



^{1}H NMR of **5j**

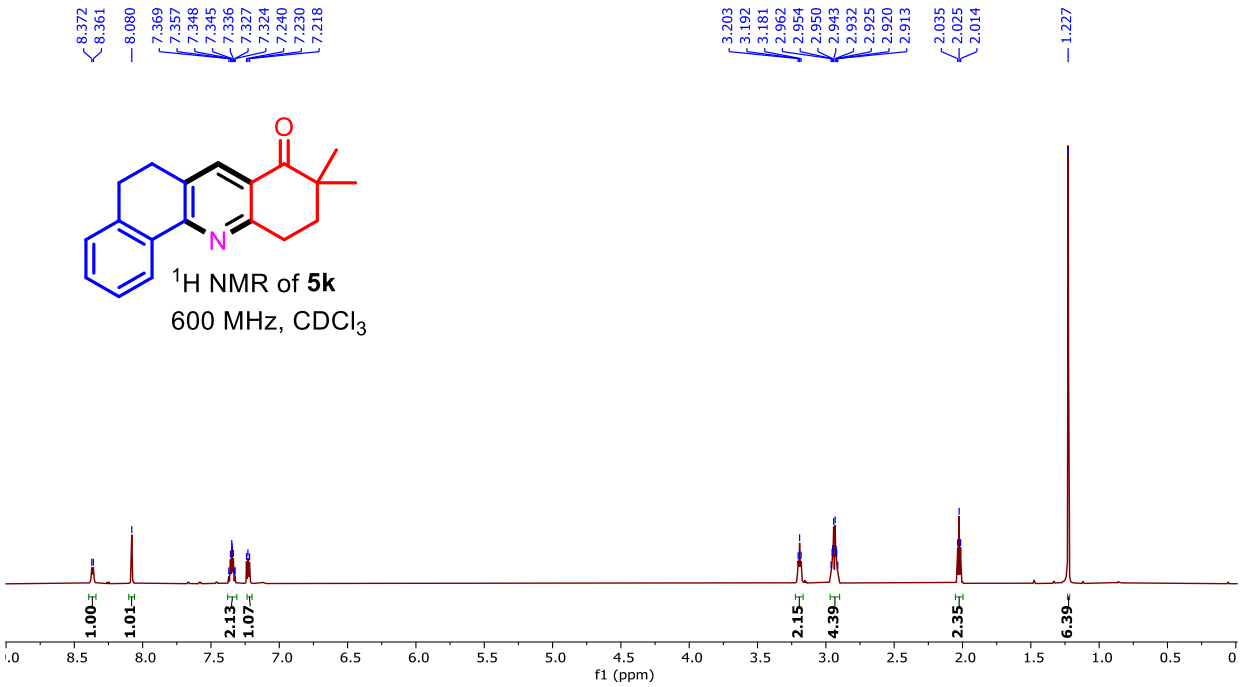
600 MHz, $CDCl_3$

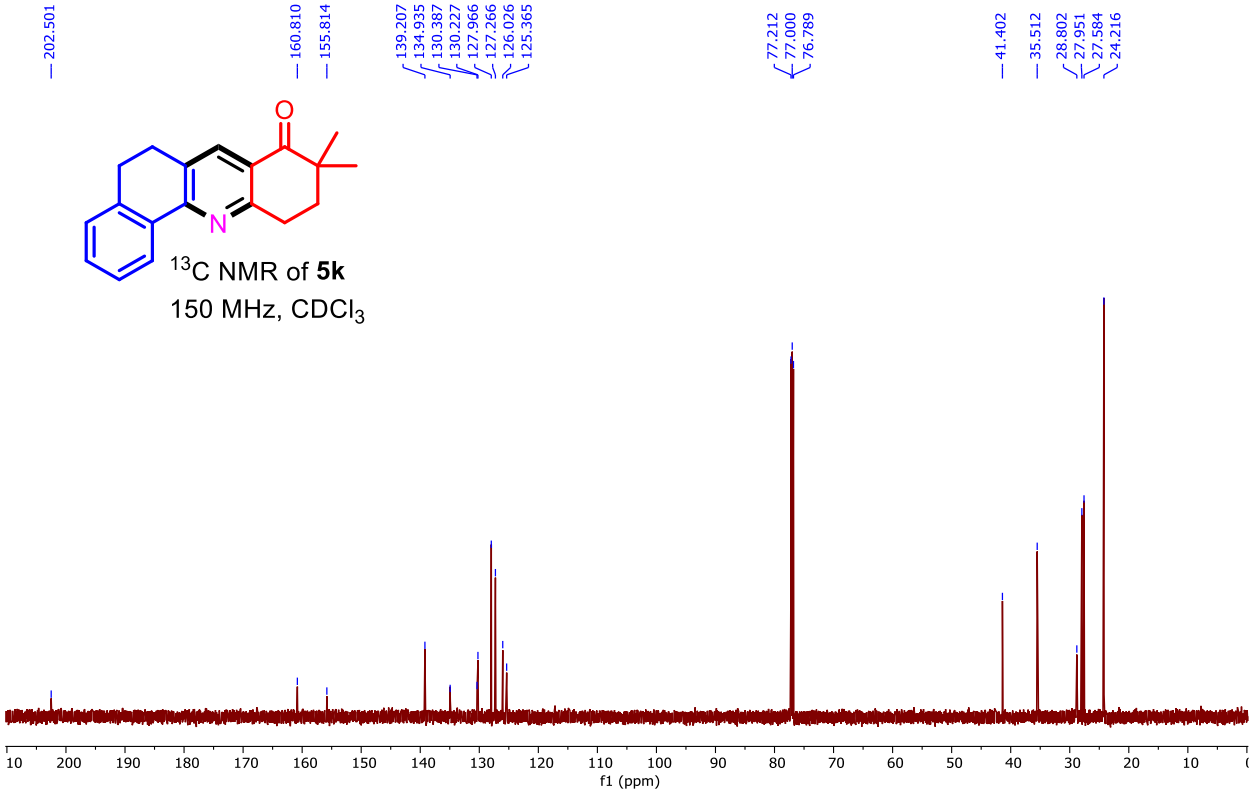


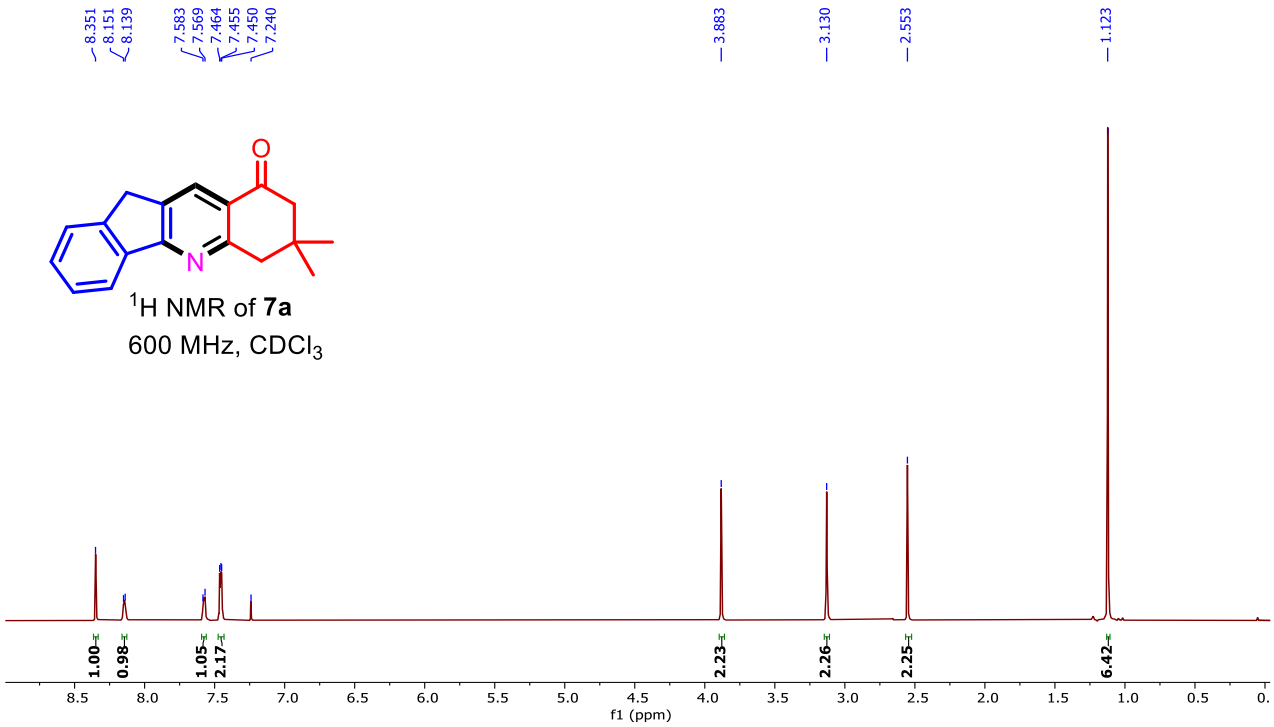


^{13}C NMR of **5j**

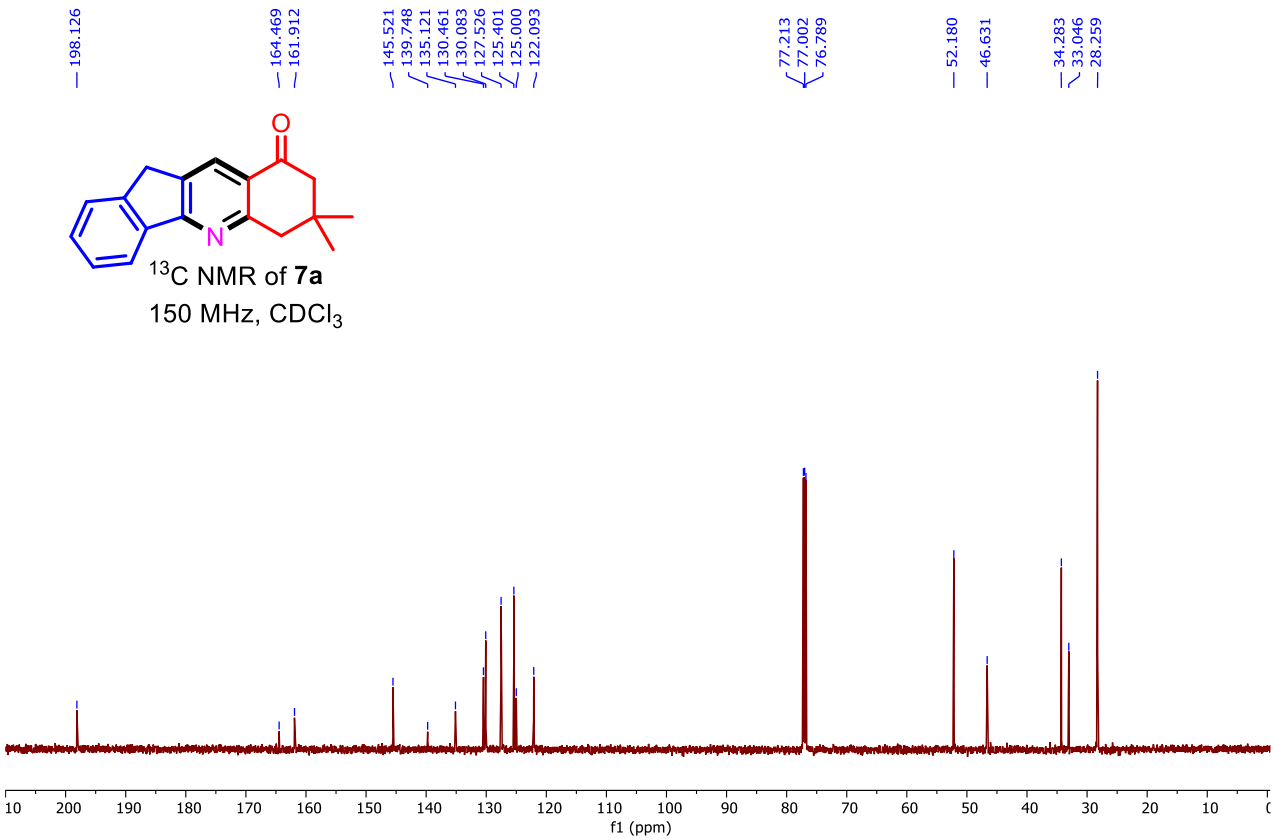
150 MHz, $CDCl_3$


8.372
8.361
8.080
7.369
7.357
7.348
7.345
7.336
7.327
7.324
7.240
7.230
7.218
3.203
3.192
3.181
2.962
2.954
2.950
2.943
2.932
2.925
2.920
2.913
2.035
2.025
2.014
1.227
O
N
1H NMR of 5k
600 MHz, CDCl3
1.00
1.01
2.13
1.07
2.15
4.39
2.35
6.39
f1 (ppm)

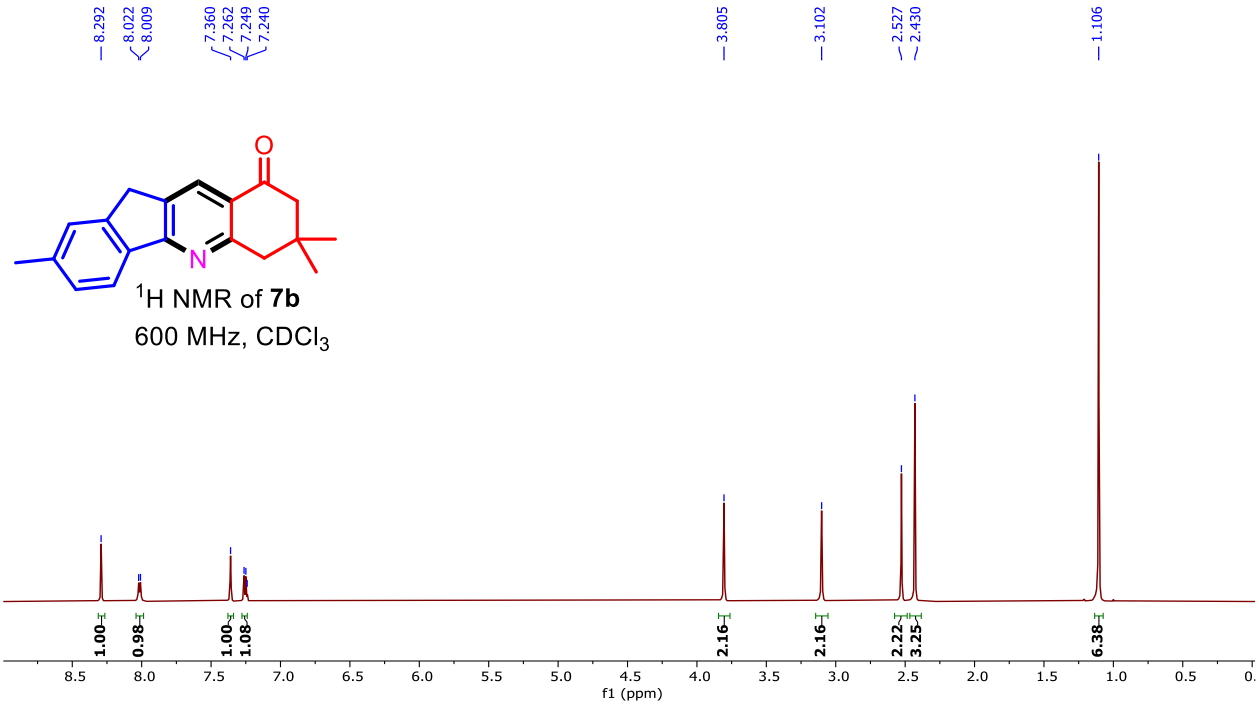

202.501
160.810
155.814
139.207
134.935
130.387
130.227
127.966
127.266
126.026
125.365
77.212
77.000
76.789
41.402
35.512
28.802
27.951
27.584
24.216
O
N
13C NMR of 5k
150 MHz, CDCl3
f1 (ppm)

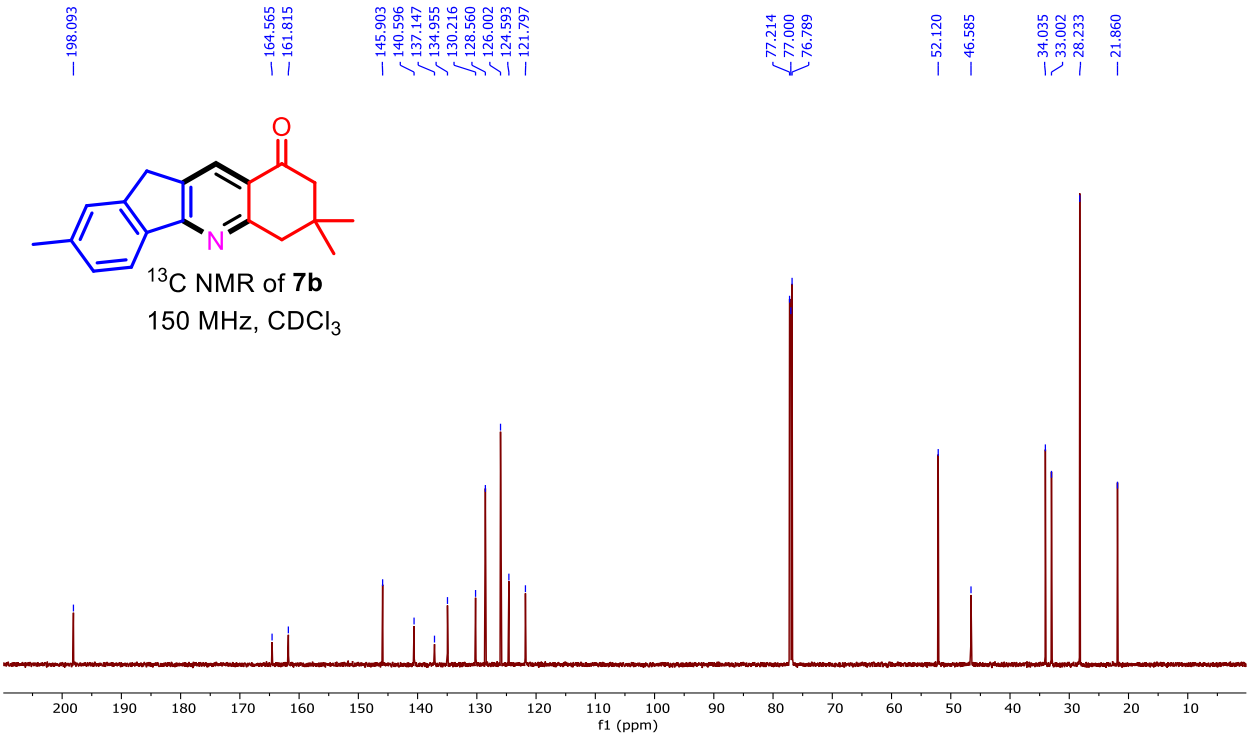


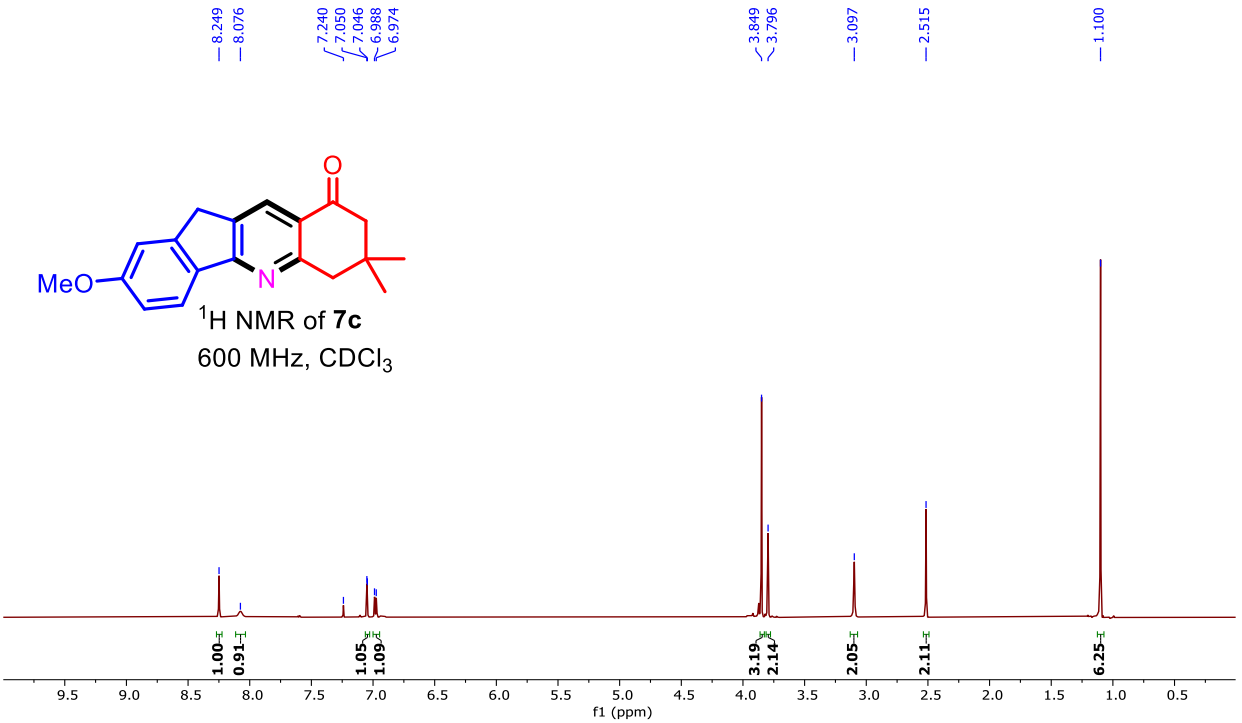
^{1}H NMR of **7a**
600 MHz, $CDCl_3$

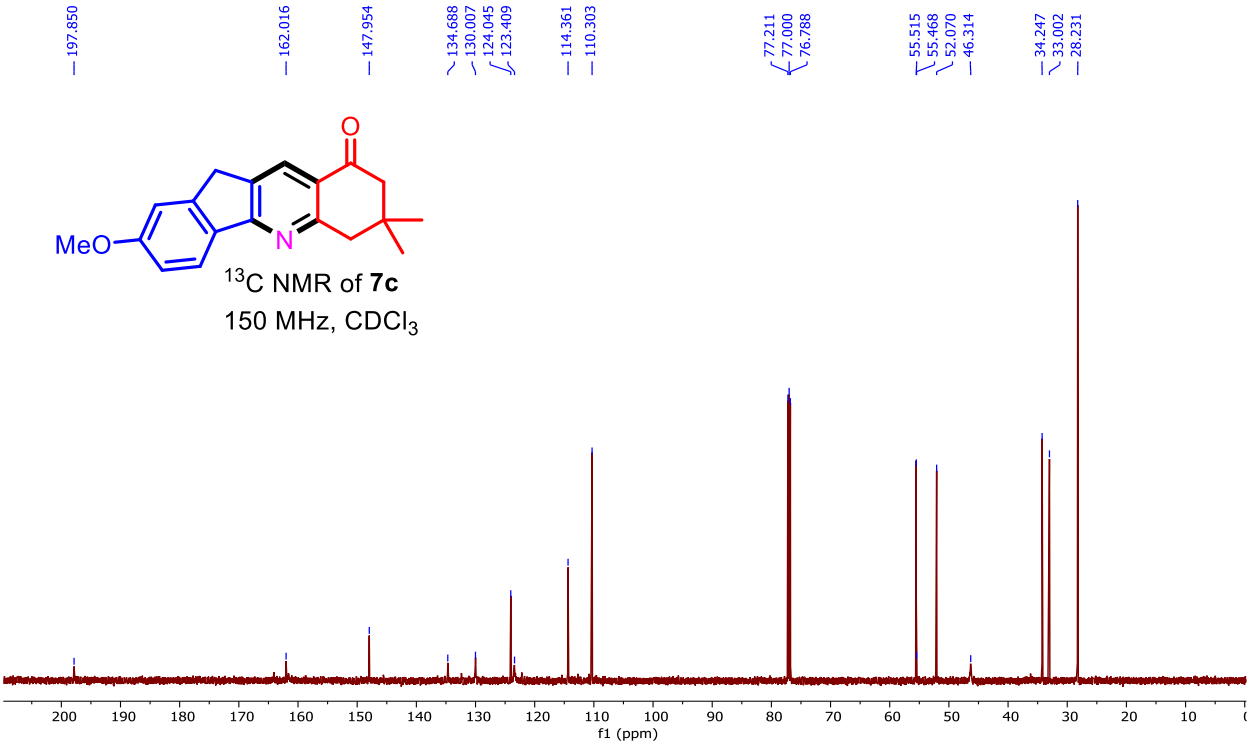


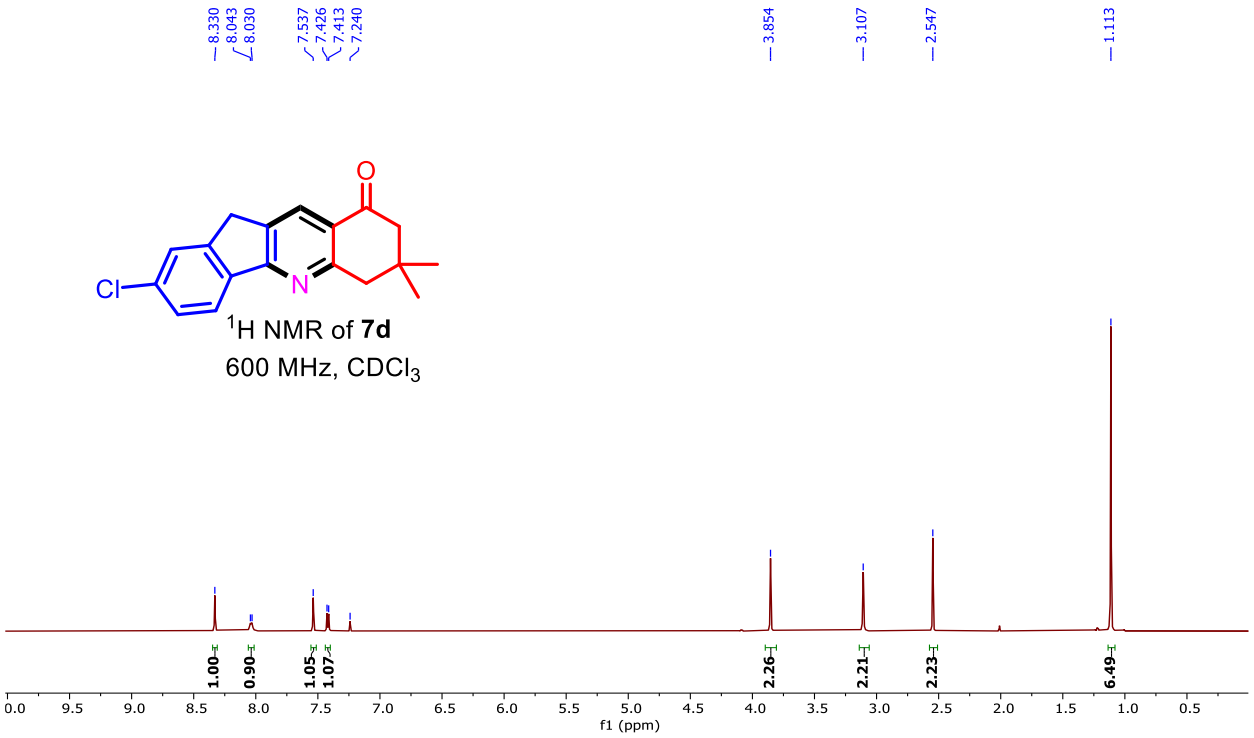
^{13}C NMR of **7a**
150 MHz, $CDCl_3$

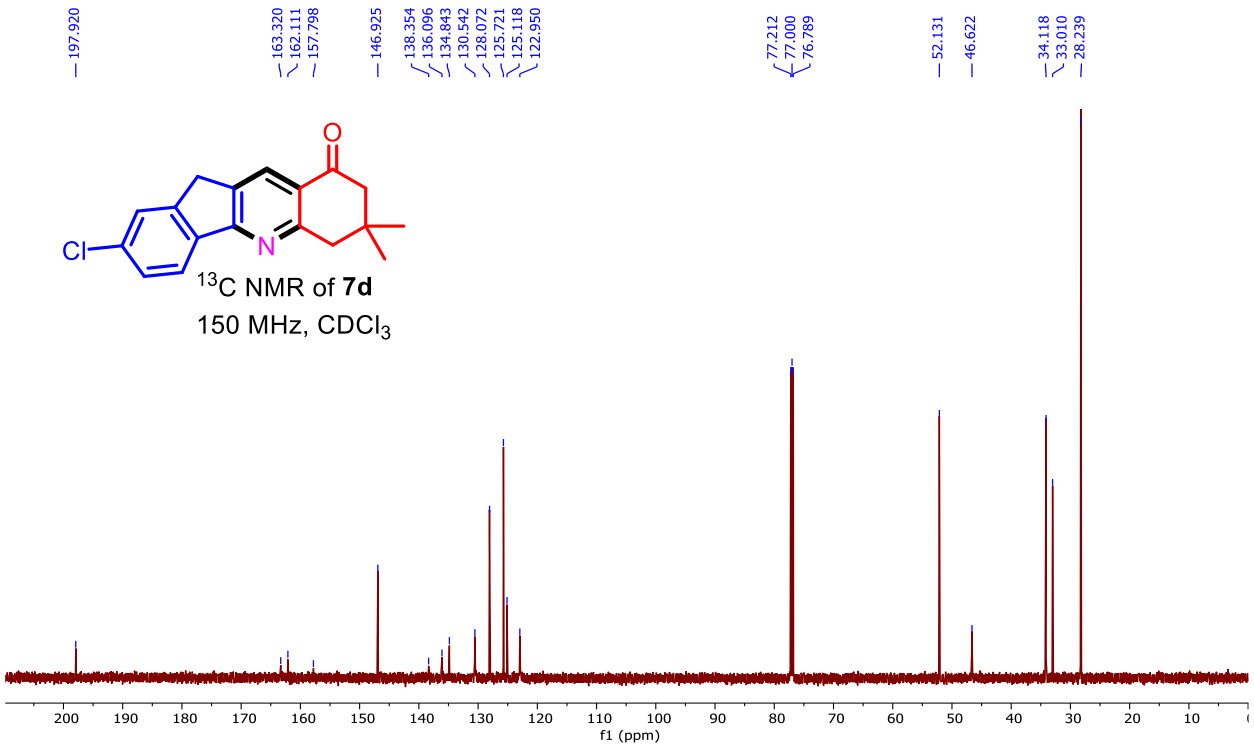

8.292
8.022
8.009
7.360
7.262
7.249
7.240
3.805
3.102
2.527
2.430
1.106
O
N
1H NMR of 7b
600 MHz, CDCl3
1.00
0.98
1.00
1.08
2.16
2.16
2.22
3.25
6.38
f1 (ppm)

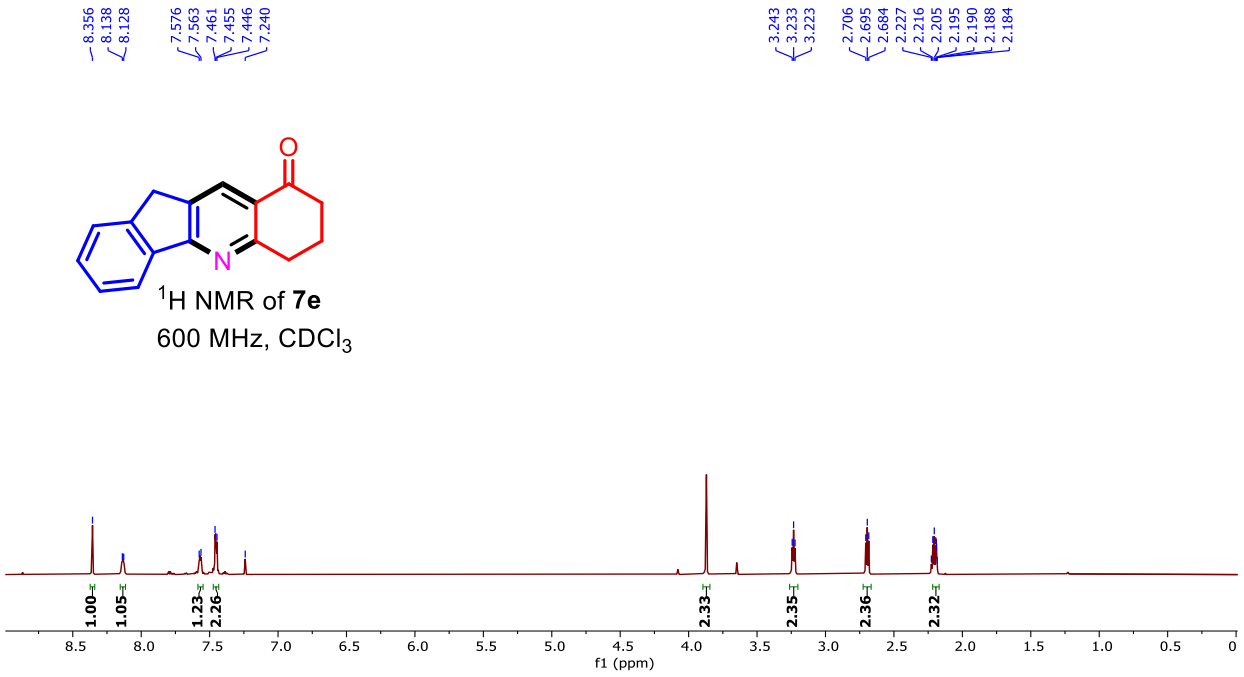

198.093
164.565
161.815
145.903
140.596
137.147
134.955
130.216
128.560
126.002
124.593
121.797
77.214
77.000
76.789
52.120
46.585
34.035
33.002
28.233
21.860
O
N
13C NMR of 7b
150 MHz, CDCl3
f1 (ppm)


8.249
8.076
7.240
7.050
7.046
6.988
6.974
3.849
3.796
3.097
2.515
1.100
O
MeO
N
1H NMR of 7c
600 MHz, CDCl3
1.00
0.91
1.05
1.09
3.19
2.14
2.05
2.11
6.25
f1 (ppm)

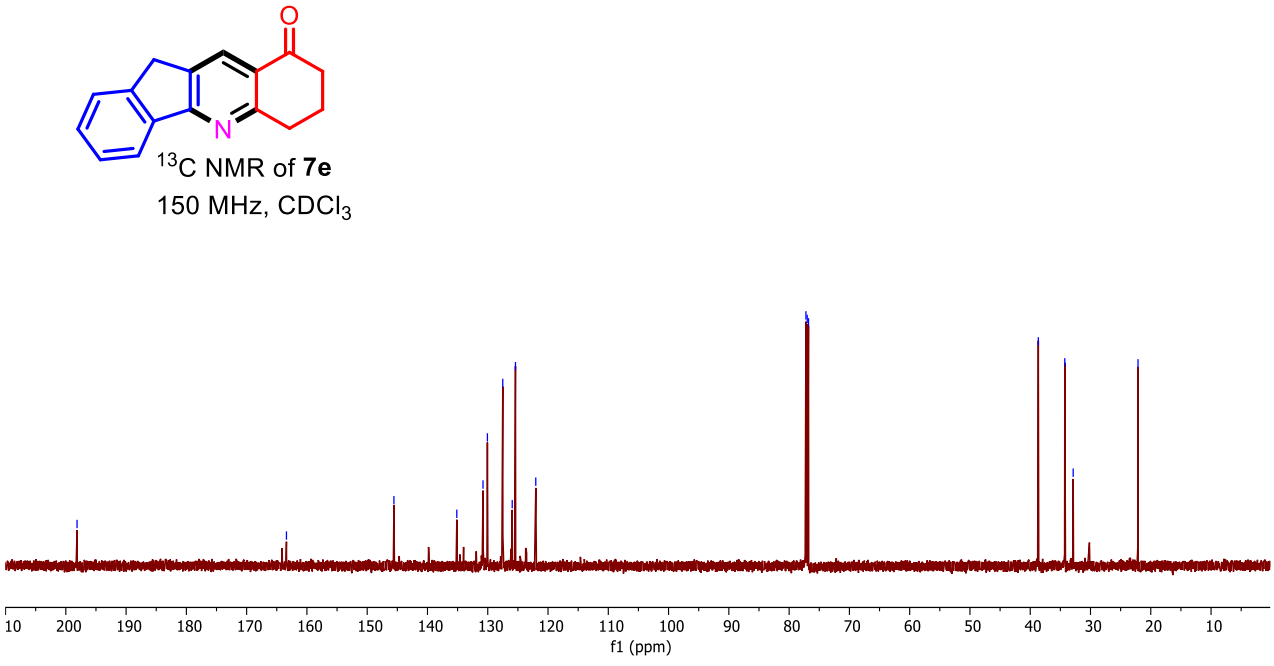

197.850
162.016
147.954
134.688
130.007
124.045
123.409
114.361
110.303
77.211
77.000
76.788
55.515
55.468
52.070
46.314
34.247
33.002
28.231
O
MeO
N
13C NMR of 7c
150 MHz, CDCl3
f1 (ppm)


8.330
8.043
8.030
7.537
7.426
7.413
7.240
3.854
3.107
2.547
1.113
O
Cl
N
1H NMR of 7d
600 MHz, CDCl3
1.00
0.90
1.05
1.07
2.26
2.21
2.23
6.49
f1 (ppm)

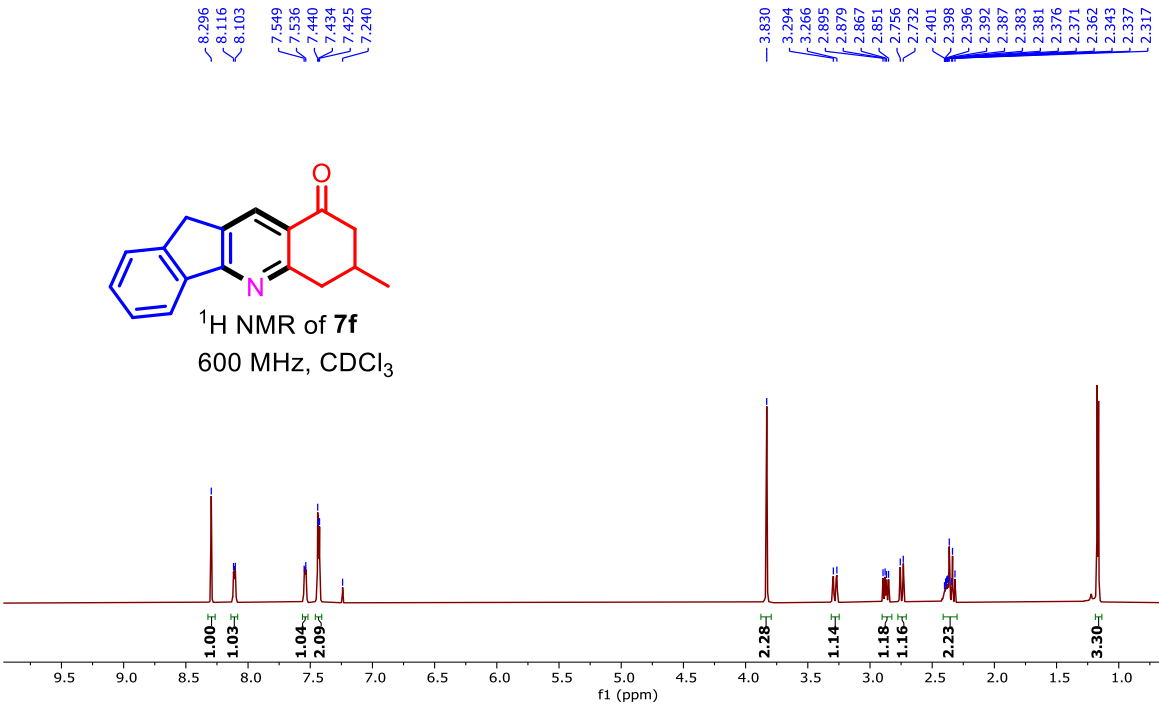

197.920
163.320
162.111
157.798
146.925
138.354
136.096
134.843
130.542
128.072
125.721
125.118
122.950
77.212
77.000
76.789
52.131
46.622
34.118
33.010
28.239
O
Cl
N
13C NMR of 7d
150 MHz, CDCl3
f1 (ppm)

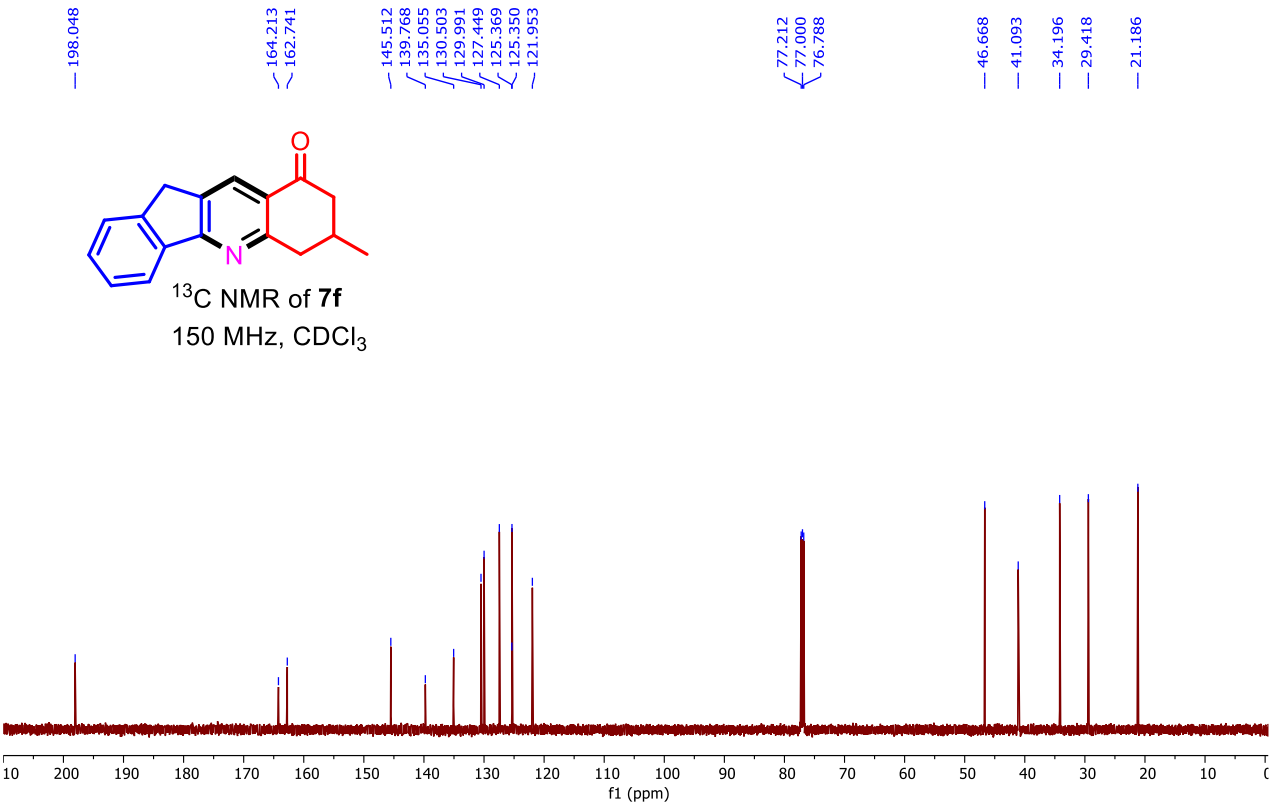


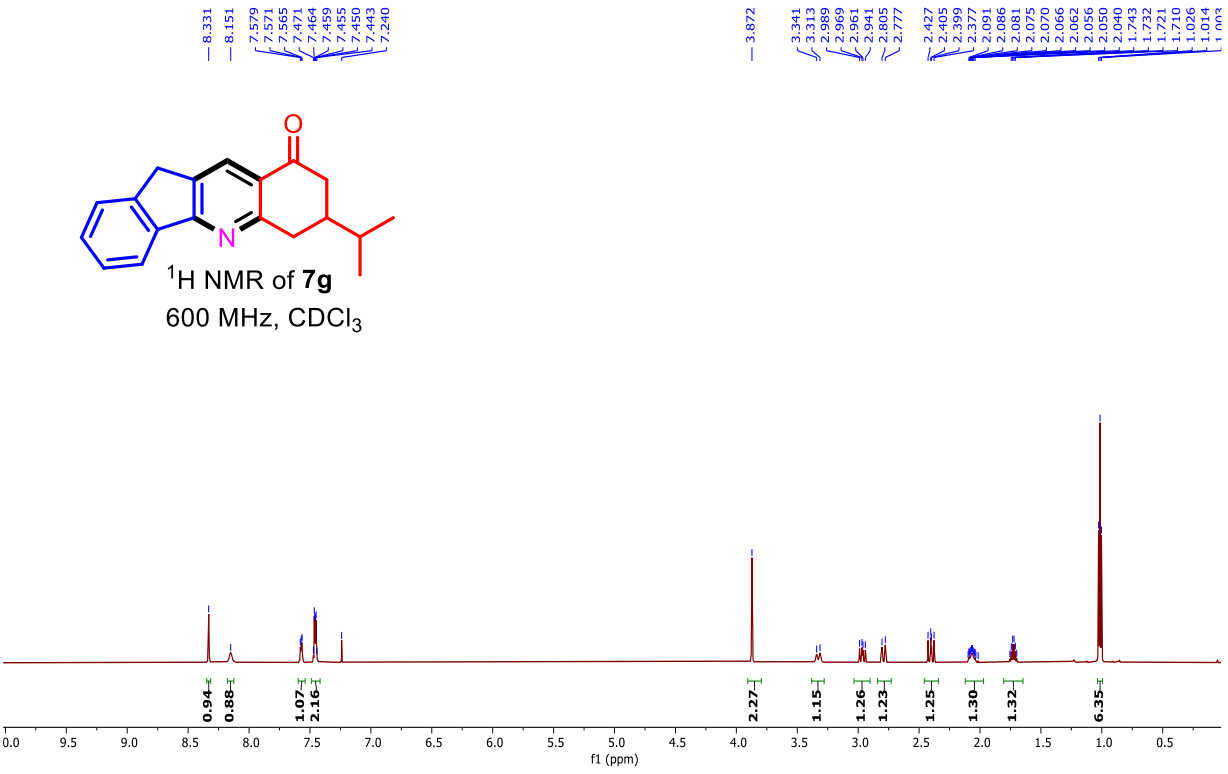
^{1}H NMR of **7e**
600 MHz, $CDCl_3$



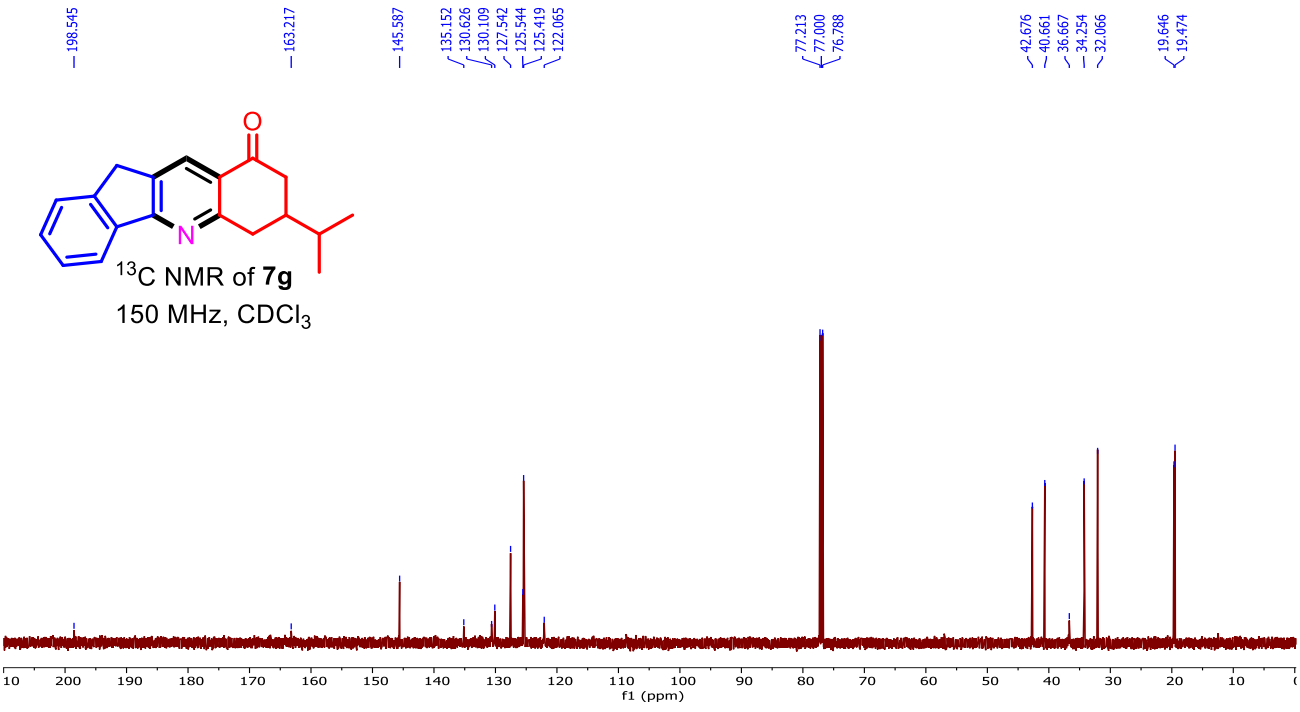
^{13}C NMR of **7e**
150 MHz, $CDCl_3$


8.296
8.116
8.103
7.549
7.536
7.440
7.434
7.425
7.240
3.830
3.294
3.266
2.895
2.879
2.867
2.851
2.756
2.732
2.401
2.398
2.396
2.392
2.387
2.383
2.381
2.376
2.371
2.362
2.343
2.337
2.317
O
N
1H NMR of 7f
600 MHz, CDCl3
1.00
1.03
1.04
2.09
2.28
1.14
1.18
1.16
2.23
3.30
f1 (ppm)

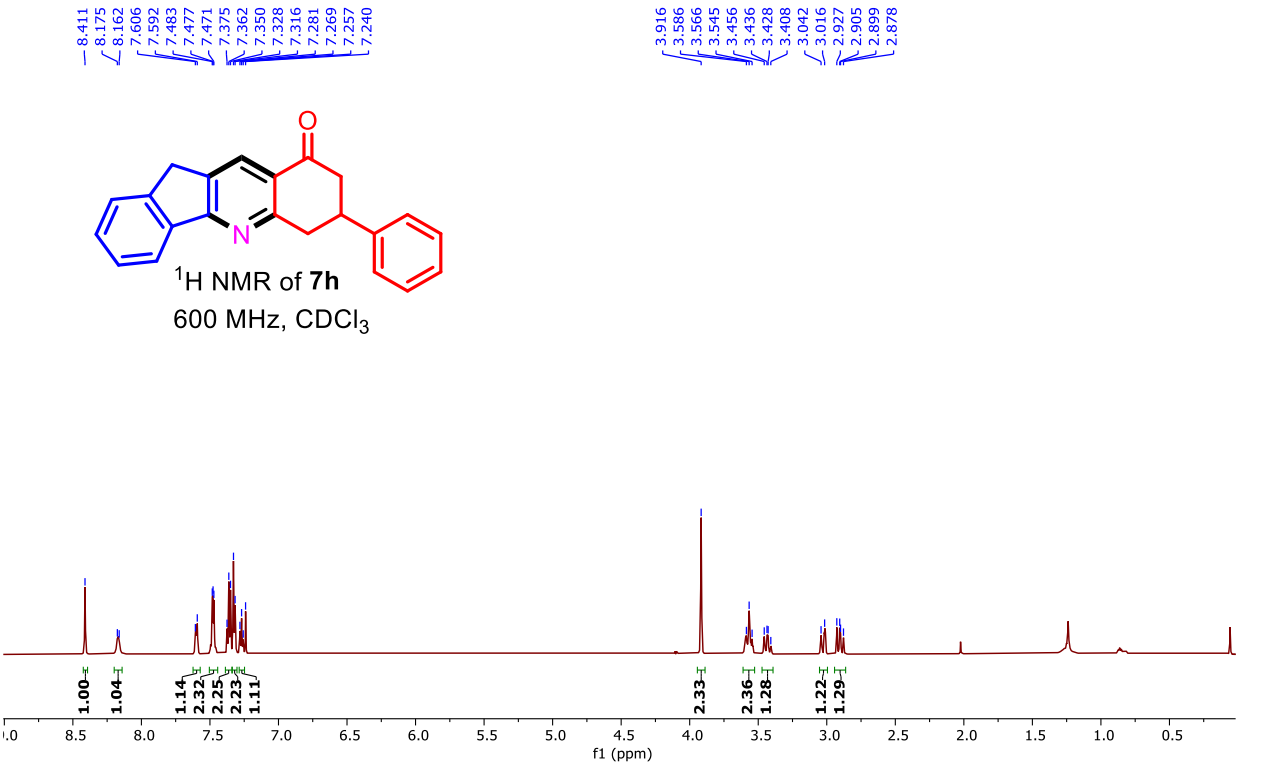

198.048
164.213
162.741
145.512
139.768
135.055
130.503
129.991
127.449
125.369
125.350
121.953
77.212
77.000
76.788
46.668
41.093
34.196
29.418
21.186
O
N
13C NMR of 7f
150 MHz, CDCl3
f1 (ppm)

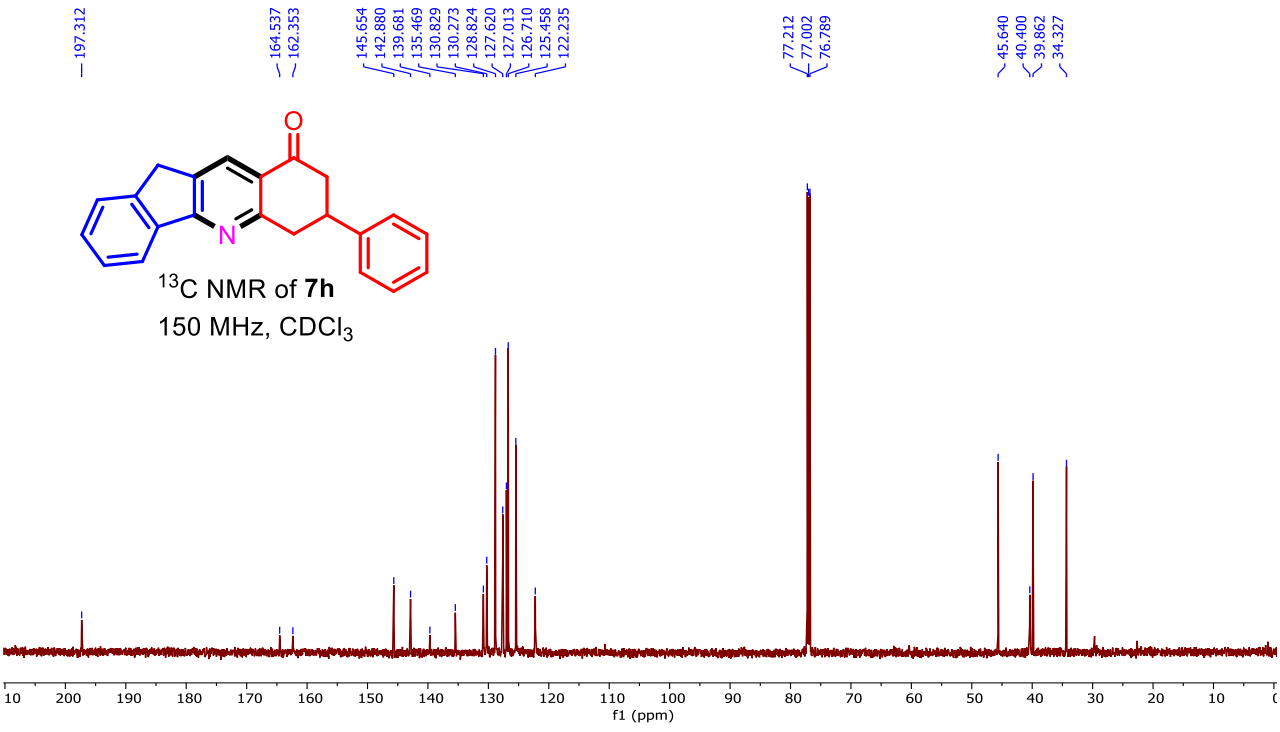


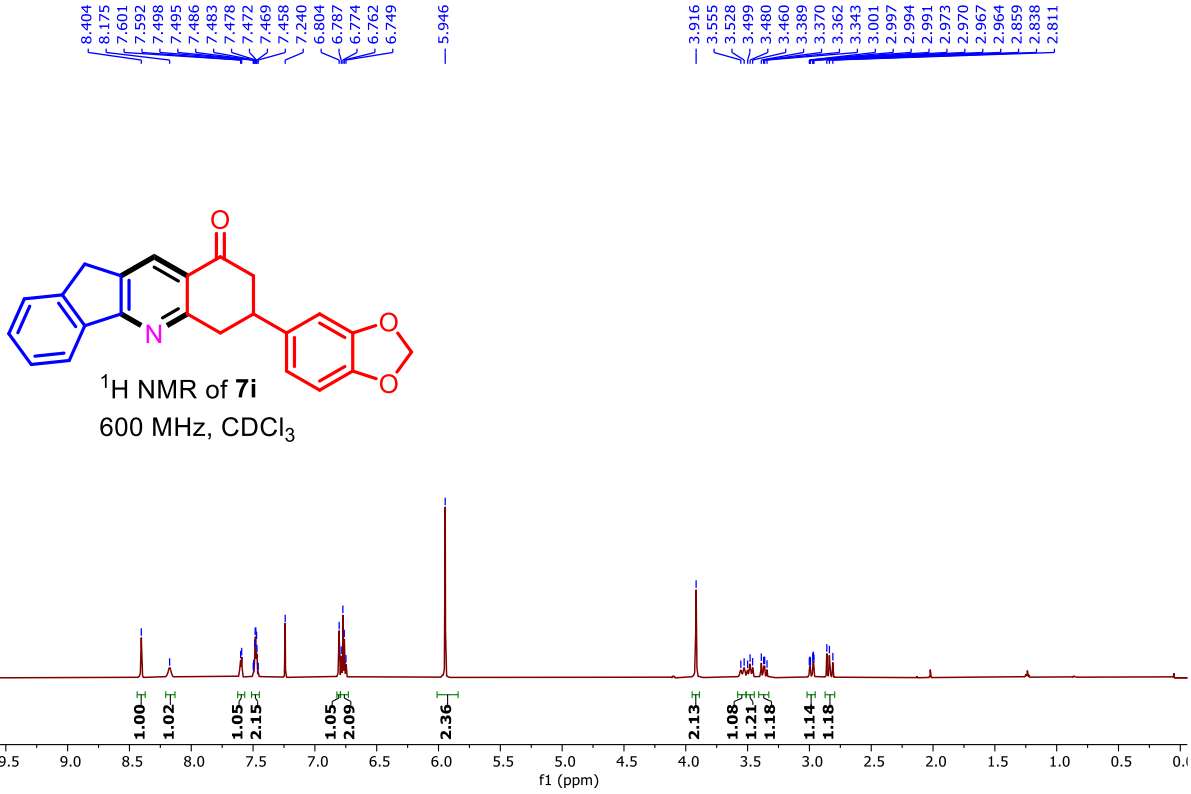
^{1}H NMR of **7g**
600 MHz, $CDCl_3$

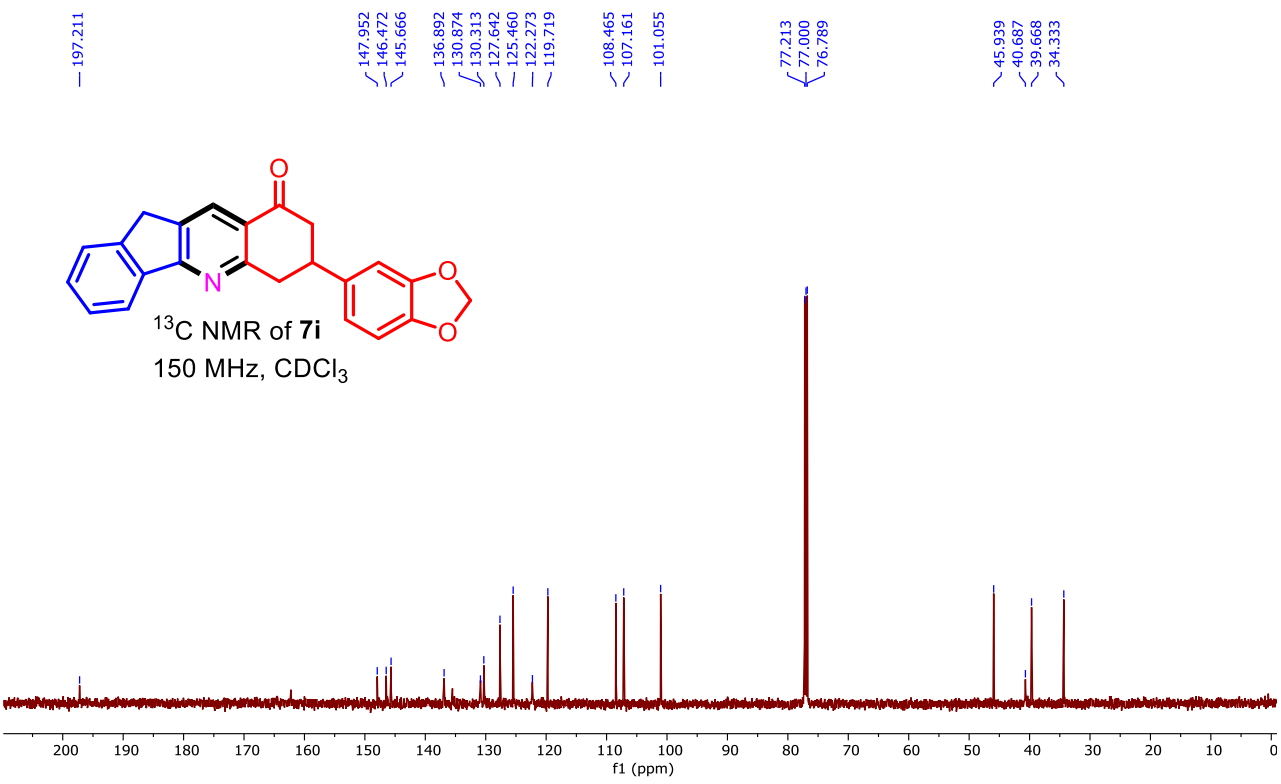


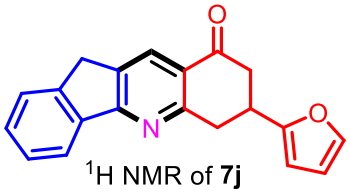
^{13}C NMR of **7g**
150 MHz, $CDCl_3$


8.411
8.175
8.162
7.606
7.592
7.483
7.477
7.471
7.375
7.362
7.350
7.328
7.316
7.281
7.269
7.257
7.240
3.916
3.586
3.566
3.545
3.456
3.436
3.428
3.408
3.042
3.016
2.927
2.905
2.899
2.878
O
N
1H NMR of 7h
600 MHz, CDCl3
1.00
1.04
1.14
2.32
2.25
2.23
1.11
2.33
2.36
1.28
1.22
1.29
f1 (ppm)


197.312
164.537
162.353
145.654
142.880
139.681
135.469
130.829
130.273
128.824
127.620
127.013
126.710
125.458
122.235
77.212
77.002
76.789
45.640
40.400
39.862
34.327
O
N
13C NMR of 7h
150 MHz, CDCl3
f1 (ppm)

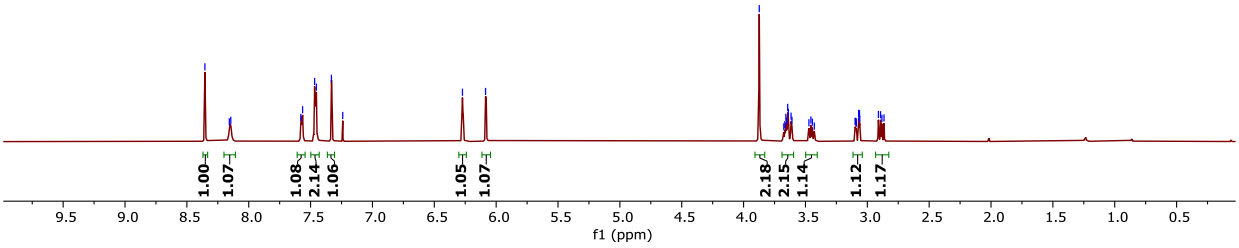

8.404
8.175
7.601
7.592
7.498
7.495
7.486
7.483
7.478
7.472
7.469
7.458
7.240
6.804
6.787
6.774
6.762
6.749
5.946
3.916
3.555
3.528
3.499
3.480
3.460
3.389
3.370
3.362
3.343
3.001
2.997
2.994
2.991
2.973
2.970
2.967
2.964
2.859
2.838
2.811
O
N
O
O
1H NMR of 7i
600 MHz, CDCl3
1.00
1.02
1.05
2.15
1.05
2.09
2.36
2.13
1.08
1.21
1.18
1.14
1.18
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

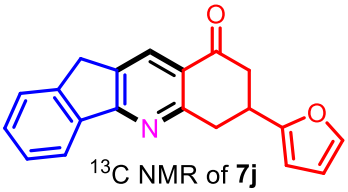

197.211
147.952
146.472
145.666
136.892
130.874
130.313
127.642
125.460
122.273
119.719
108.465
107.161
101.055
77.213
77.000
76.789
45.939
40.687
39.668
34.333
O
N
O
O
13C NMR of 7i
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



^{1}H NMR of **7j**

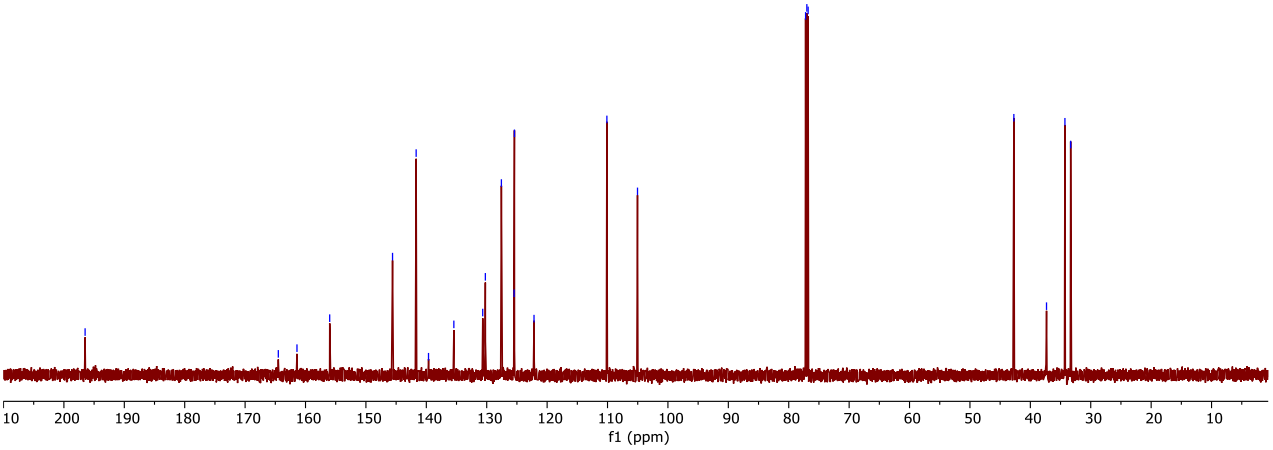
600 MHz, $CDCl_3$

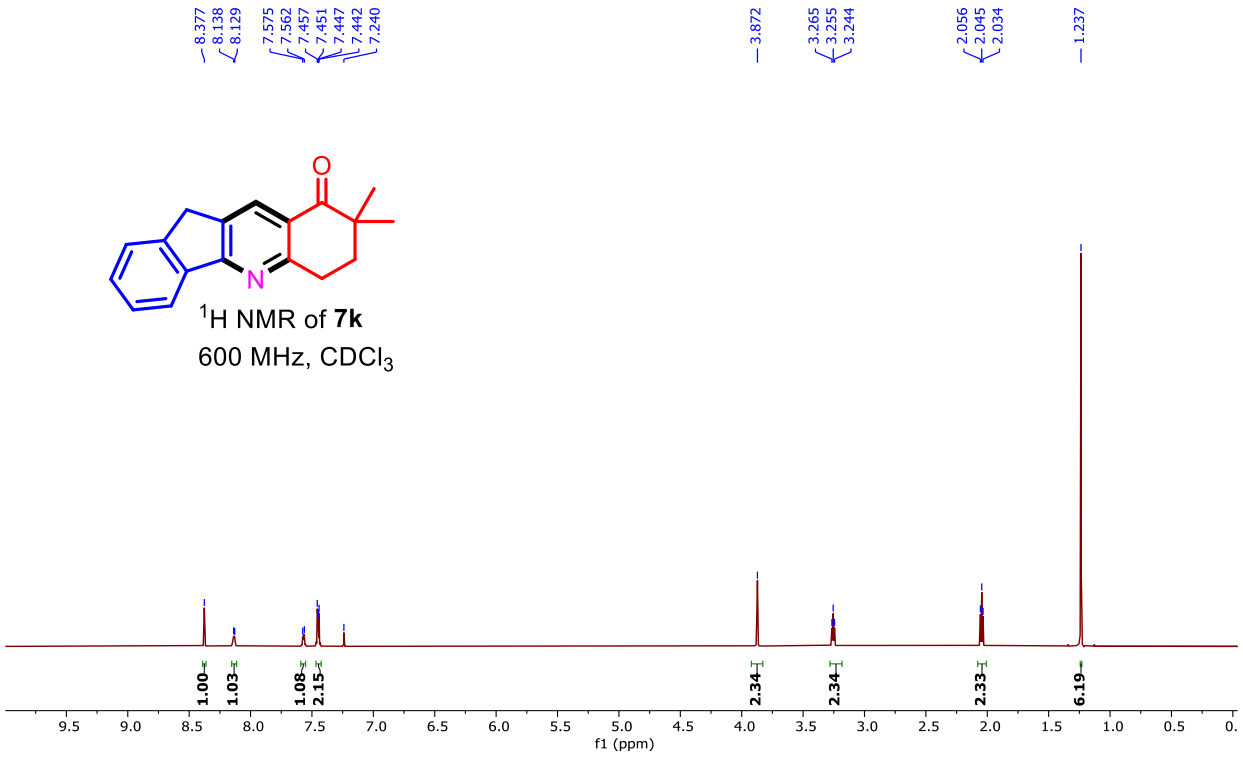




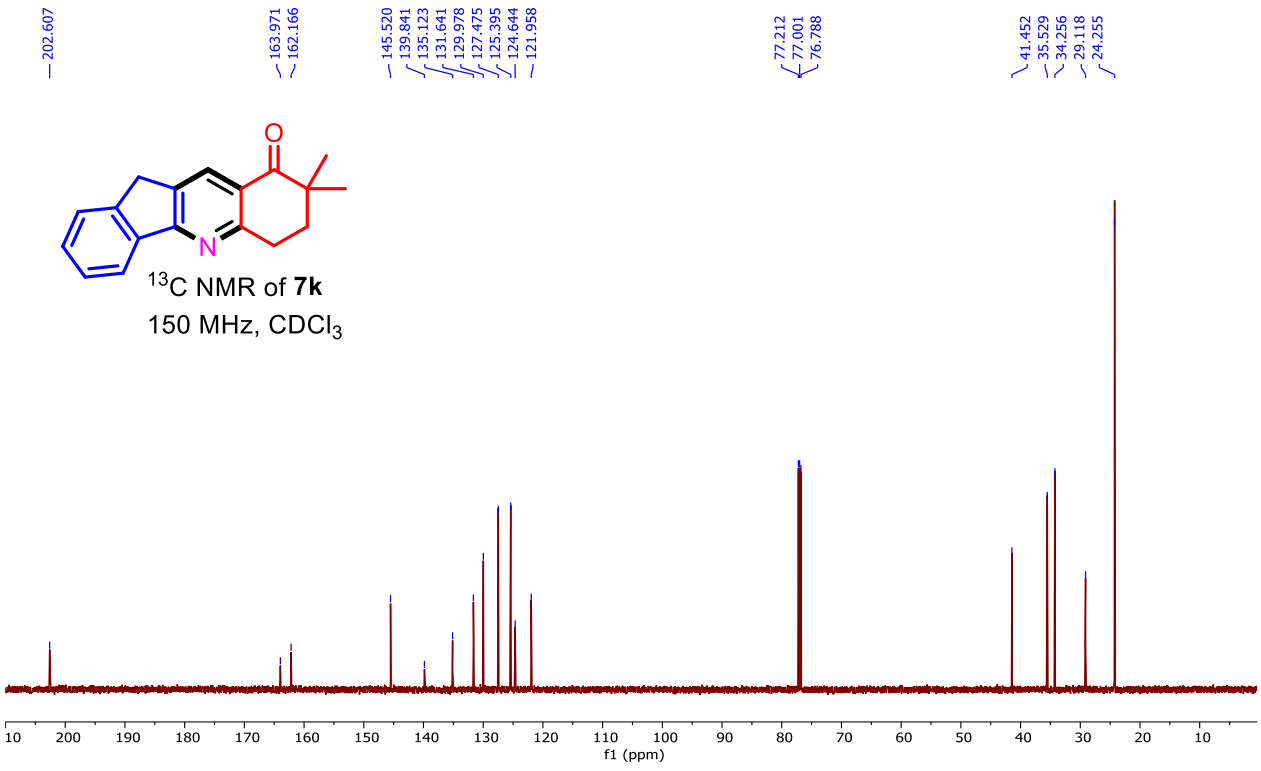
^{13}C NMR of **7j**

150 MHz, $CDCl_3$

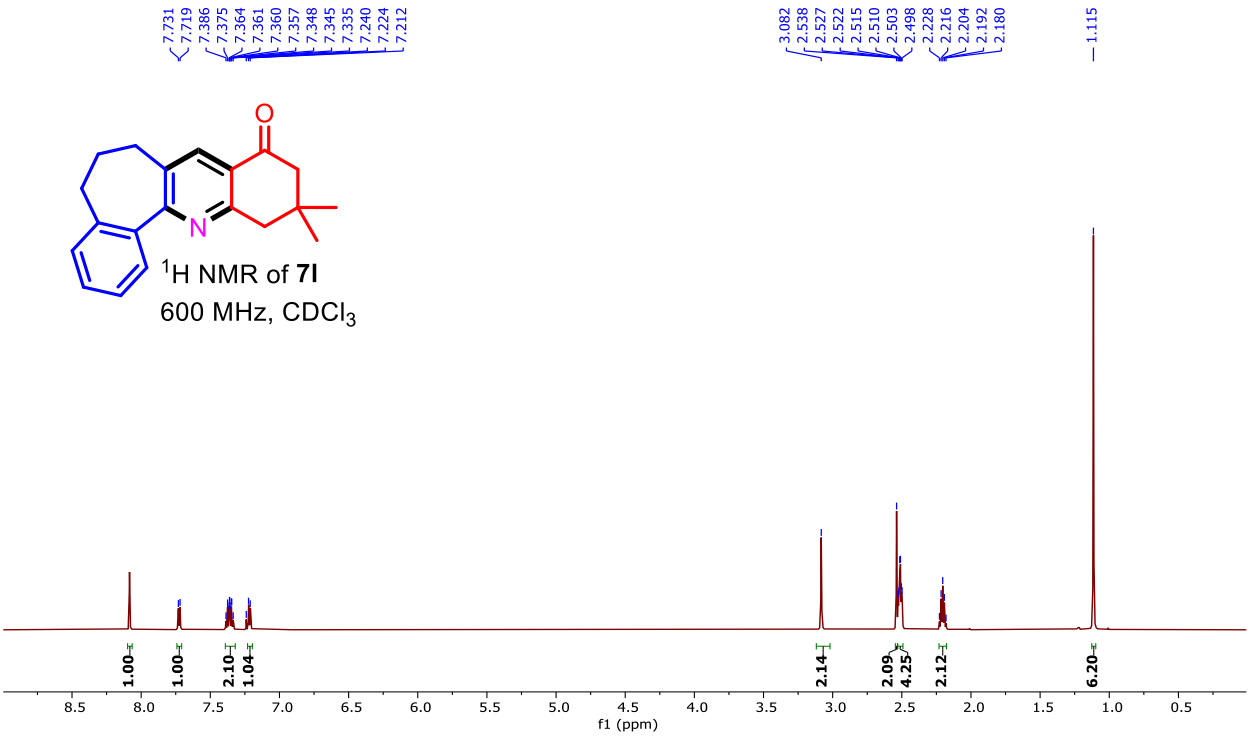


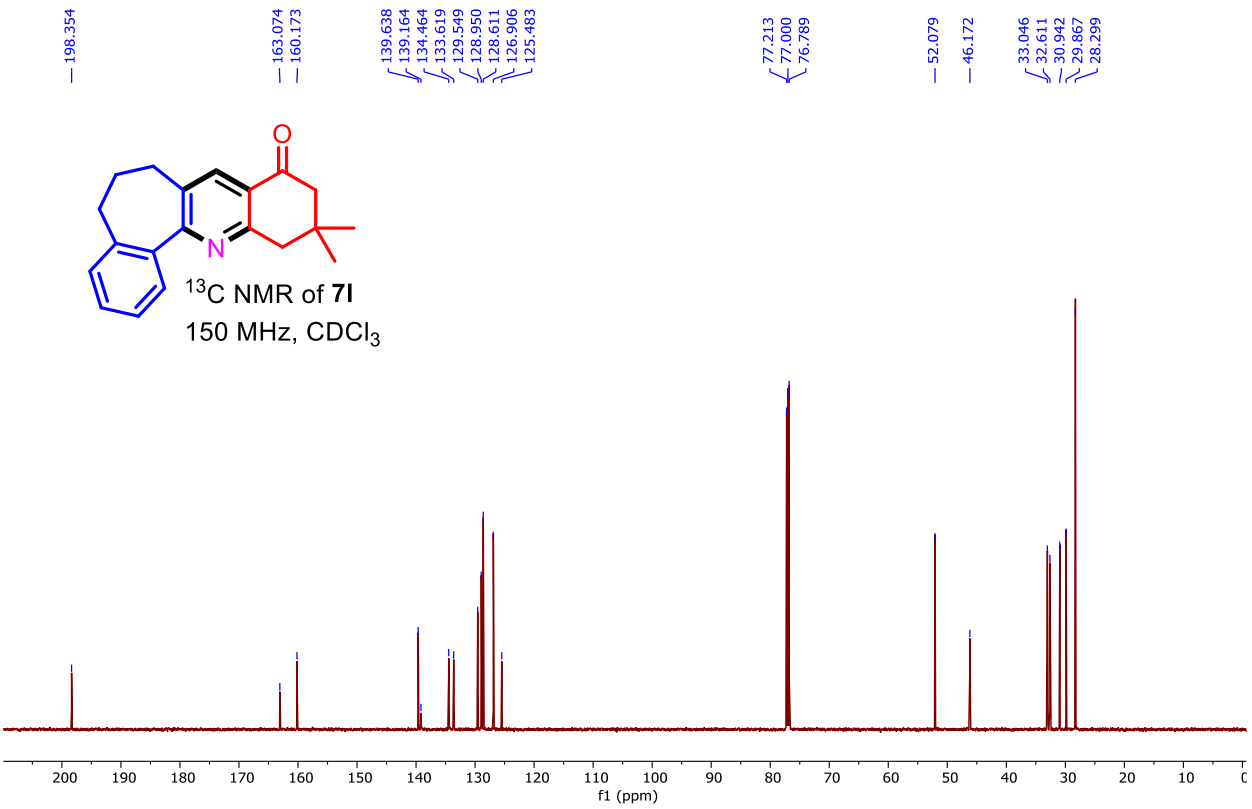


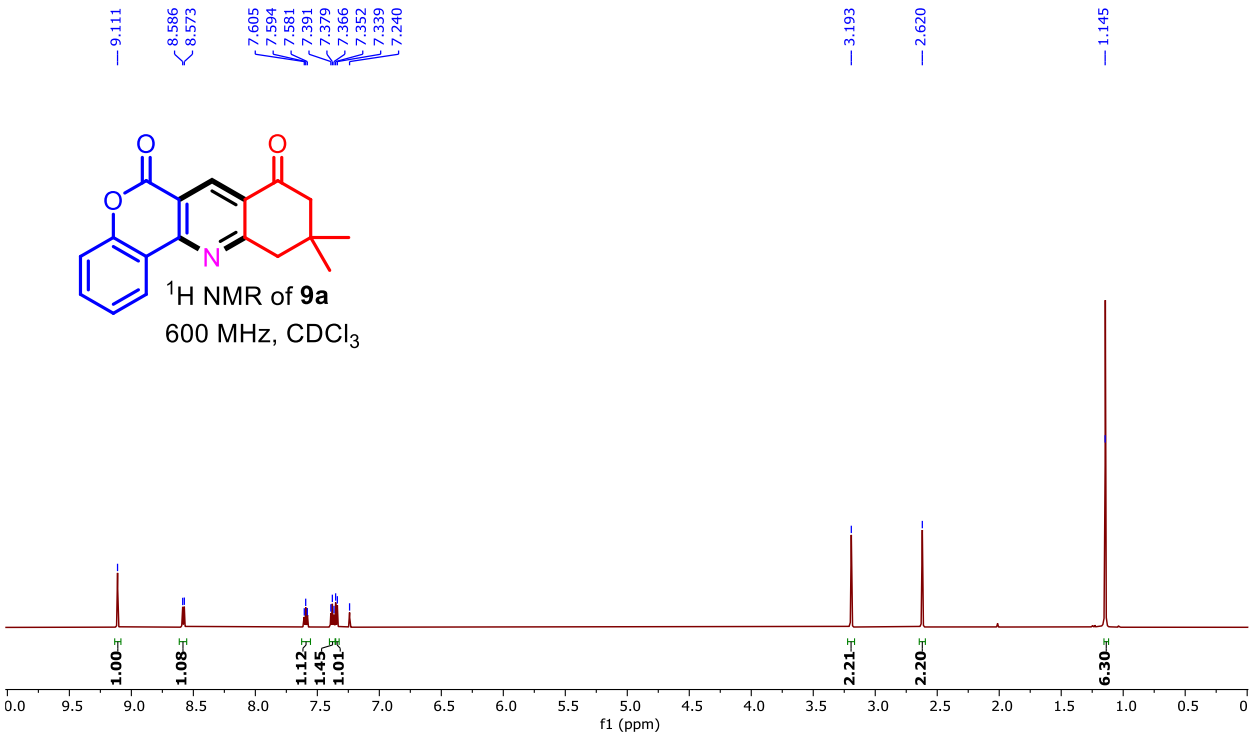
^{1}H NMR of **7k**
600 MHz, $CDCl_3$



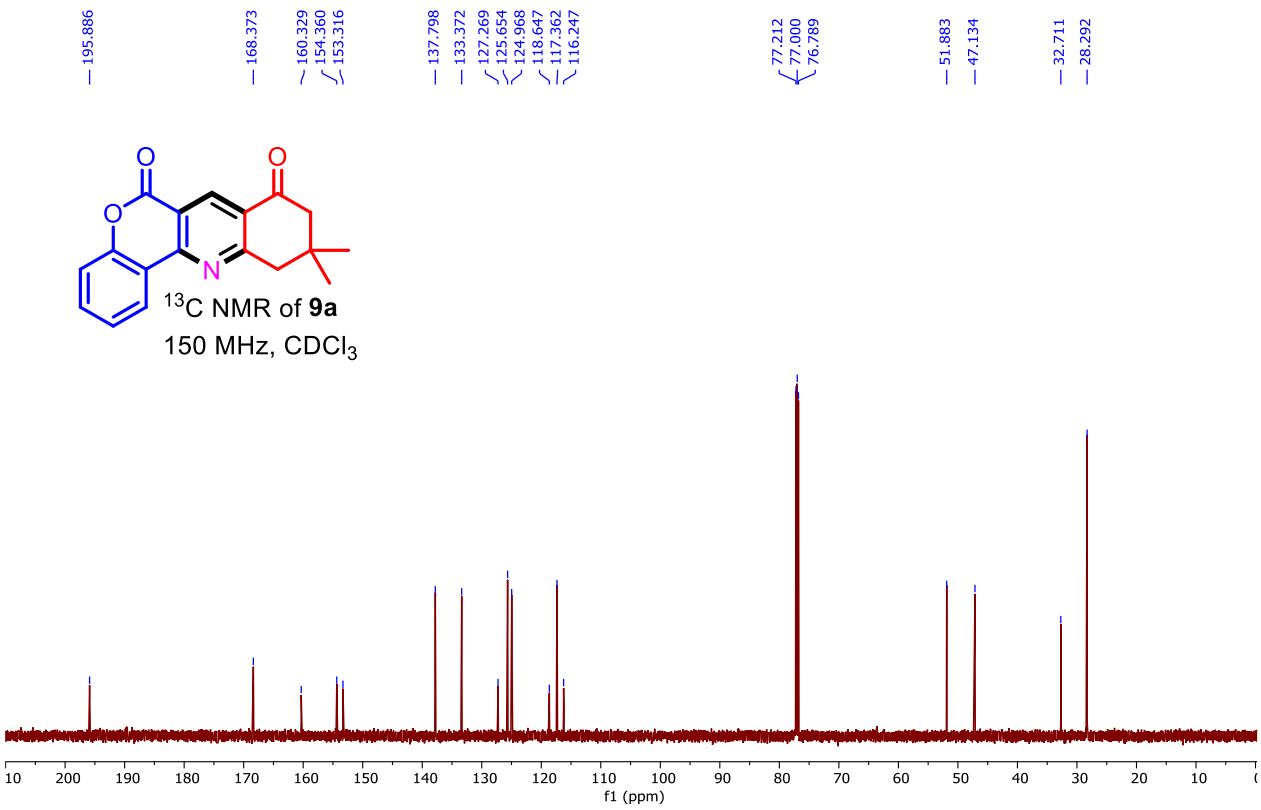
^{13}C NMR of **7k**
150 MHz, $CDCl_3$


7.731
7.719
7.386
7.375
7.364
7.361
7.360
7.357
7.348
7.345
7.335
7.240
7.224
7.212
3.082
2.538
2.527
2.522
2.515
2.510
2.503
2.498
2.228
2.216
2.204
2.192
2.180
1.115
O
N
1H NMR of 7l
600 MHz, CDCl3
1.00
1.00
2.10
1.04
2.14
2.09
4.25
2.12
6.20
f1 (ppm)

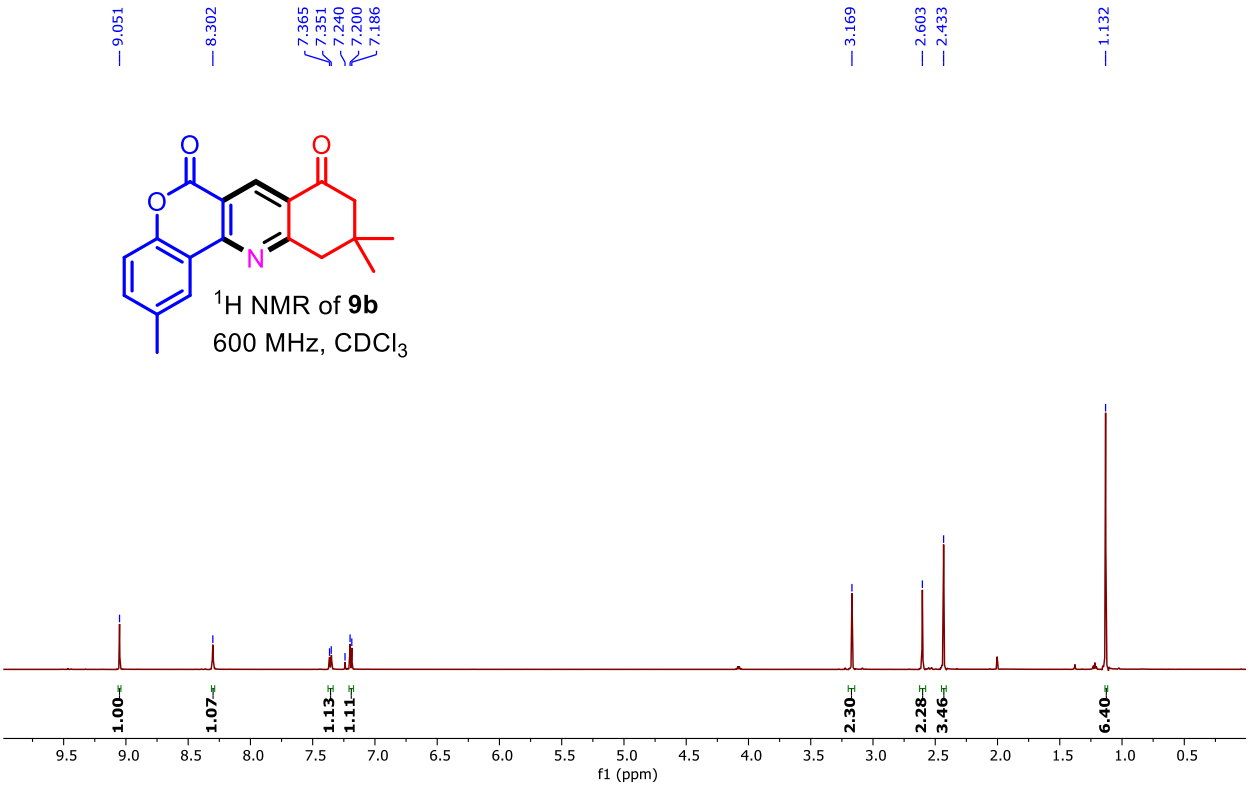

198.354
163.074
160.173
139.638
139.164
134.464
133.619
129.549
128.950
128.611
126.906
125.483
77.213
77.000
76.789
52.079
46.172
33.046
32.611
30.942
29.867
28.299
O
N
13C NMR of 7l
150 MHz, CDCl3
f1 (ppm)

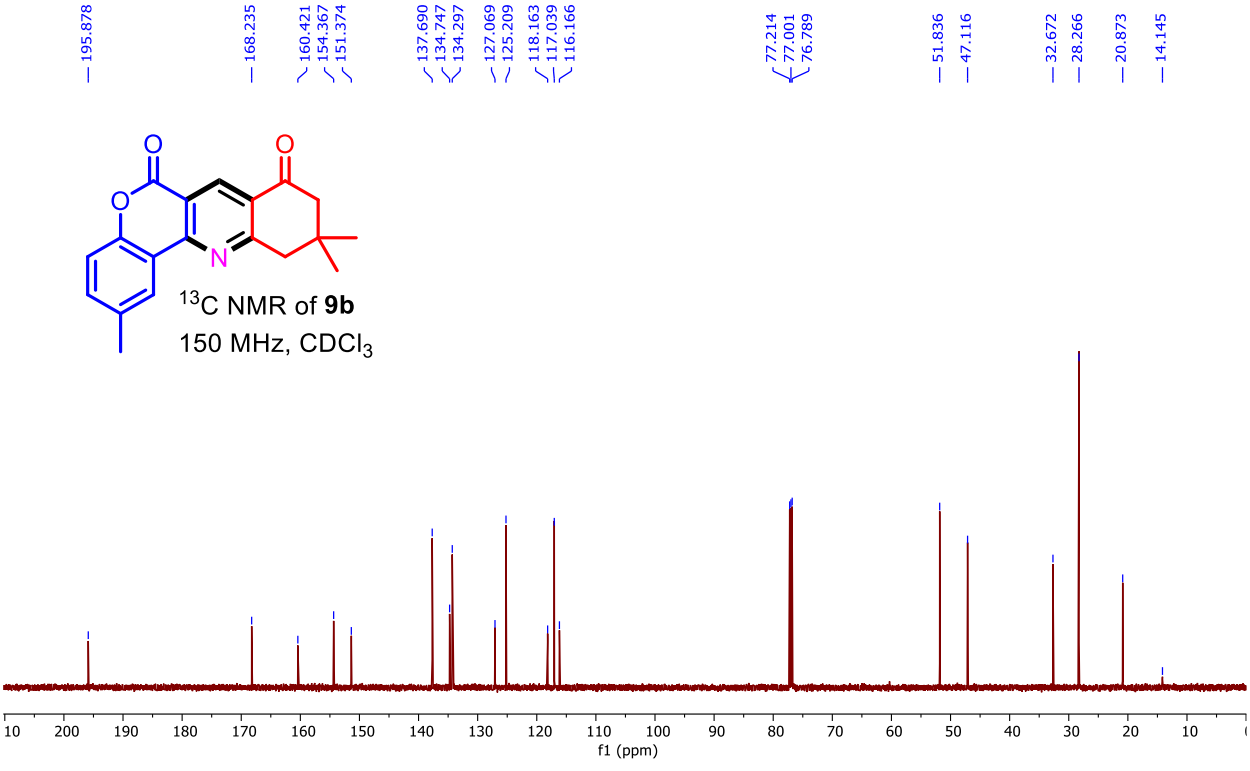


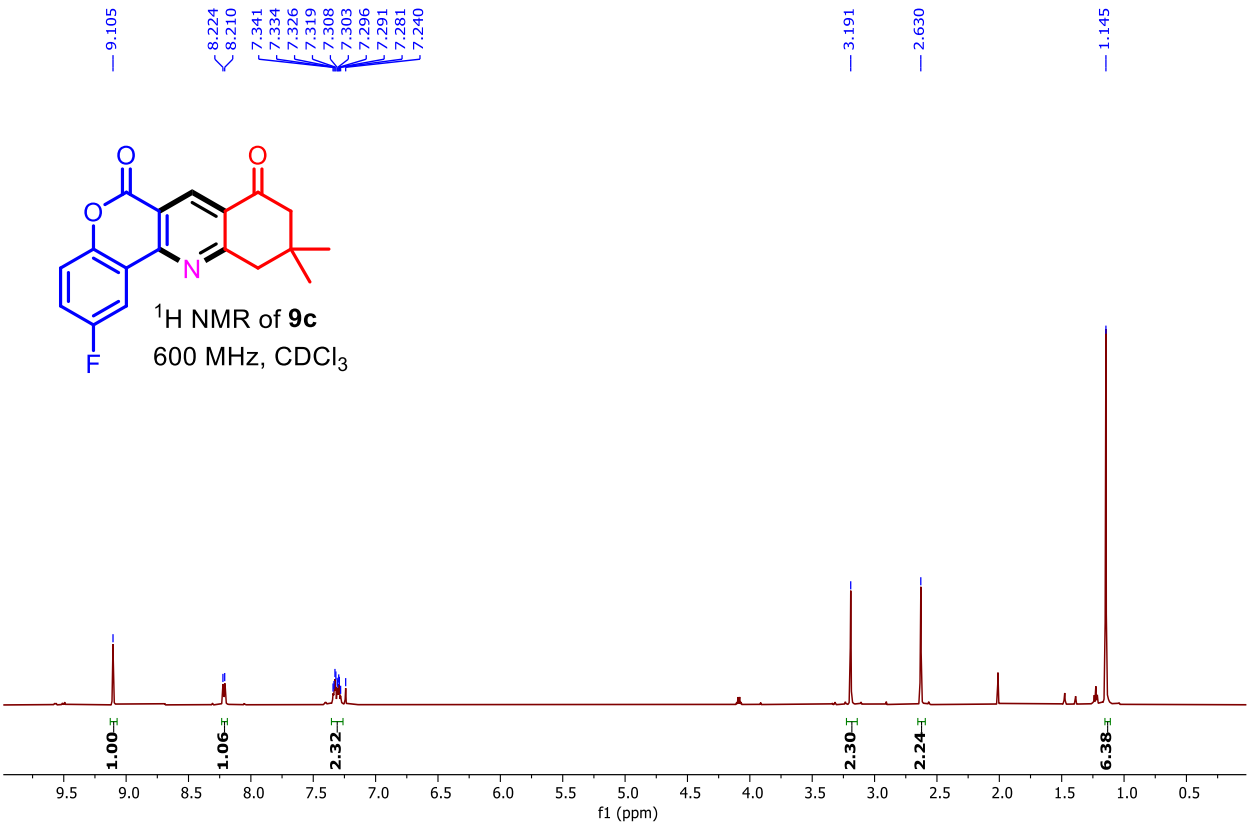
^{1}H NMR of **9a**
600 MHz, $CDCl_3$

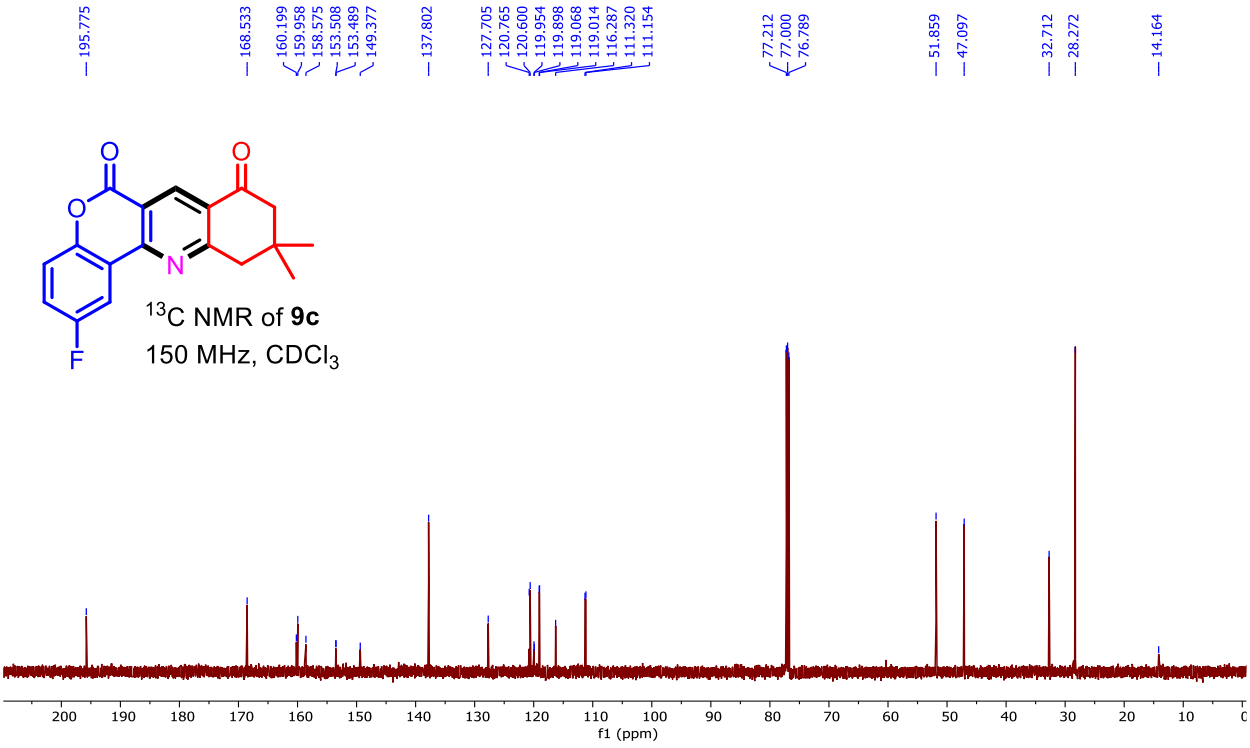


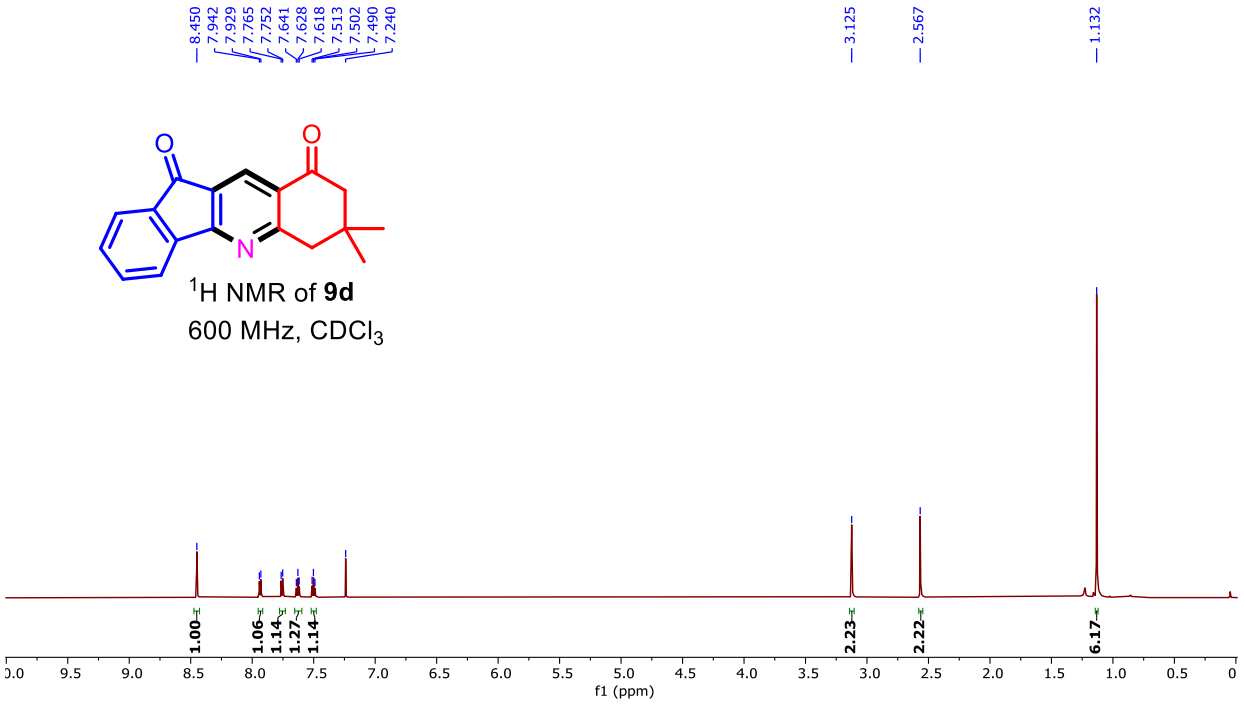
^{13}C NMR of **9a**
150 MHz, $CDCl_3$

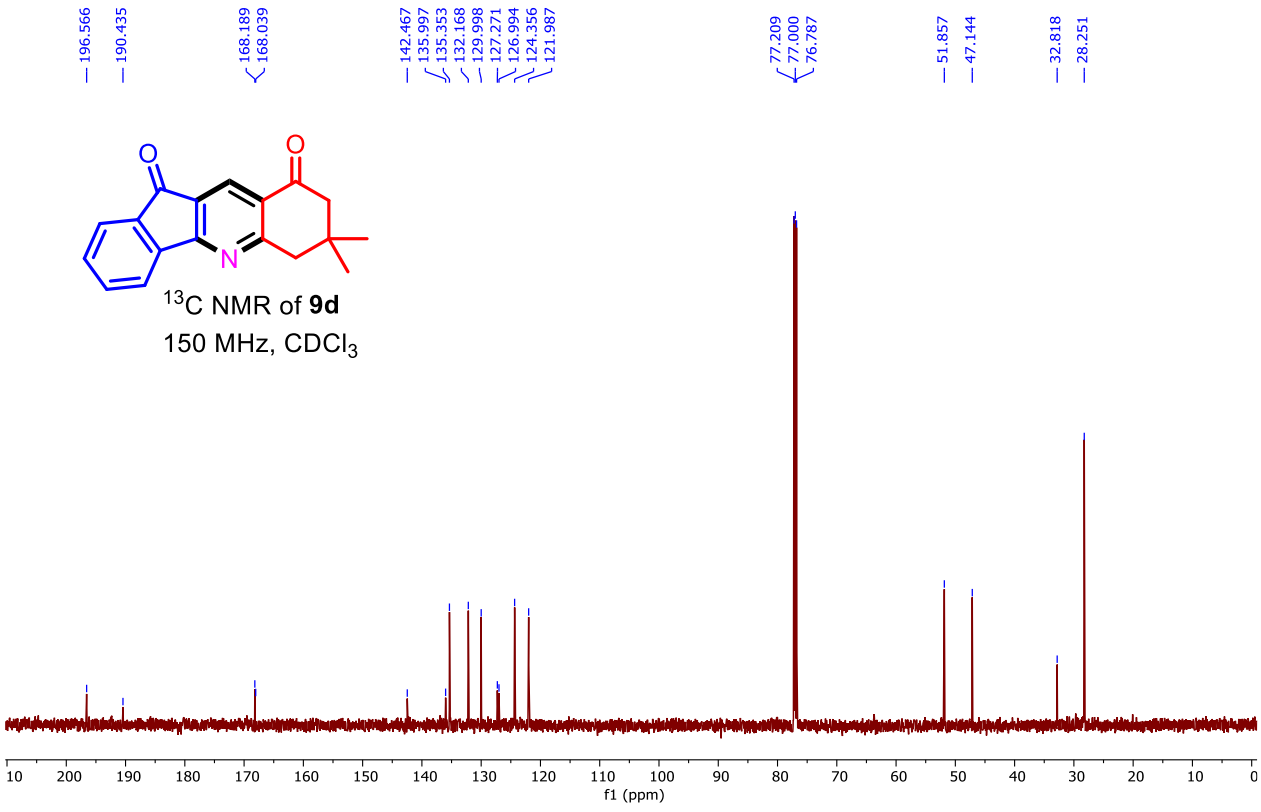

9.051
8.302
7.365
7.351
7.240
7.200
7.186
3.169
2.603
2.433
1.132
O
O
O
N
1H NMR of 9b
600 MHz, CDCl3
1.00
1.07
1.13
1.11
2.30
2.28
3.46
6.40
f1 (ppm)

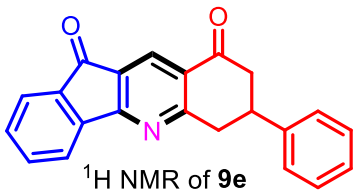

195.878
168.235
160.421
154.367
151.374
137.690
134.747
134.297
127.069
125.209
118.163
117.039
116.166
77.214
77.001
76.789
51.836
47.116
32.672
28.266
20.873
14.145
O
O
O
N
13C NMR of 9b
150 MHz, CDCl3
f1 (ppm)


9.105
8.224
8.210
7.341
7.334
7.326
7.319
7.308
7.303
7.296
7.291
7.281
7.240
3.191
2.630
1.145
O
O
O
N
F
1H NMR of 9c
600 MHz, CDCl3
1.00
1.06
2.32
2.30
2.24
6.38
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

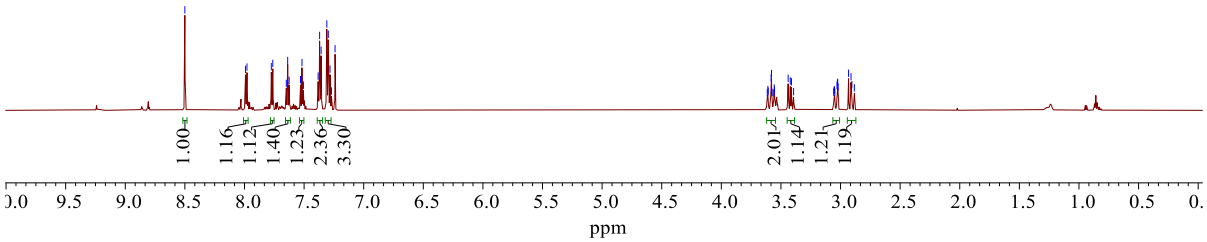

195.775
168.533
160.199
159.958
158.575
153.508
153.489
149.377
137.802
127.705
120.765
120.600
119.954
119.898
119.068
119.014
116.287
111.320
111.154
77.212
77.000
76.789
51.859
47.097
32.712
28.272
14.164
O
O
O
N
F
13C NMR of 9c
150 MHz, CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

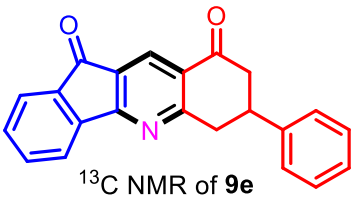

8.450
7.942
7.929
7.765
7.752
7.641
7.628
7.618
7.513
7.502
7.490
7.240
3.125
2.567
1.132
O
O
N
1H NMR of 9d
600 MHz, CDCl3
1.00
1.06
1.14
1.27
1.14
2.23
2.22
6.17
f1 (ppm)


196.566
190.435
168.189
168.039
142.467
135.997
135.353
132.168
129.998
127.271
126.994
124.356
121.987
77.209
77.000
76.787
51.857
47.144
32.818
28.251
O
O
N
13C NMR of 9d
150 MHz, CDCl3
f1 (ppm)

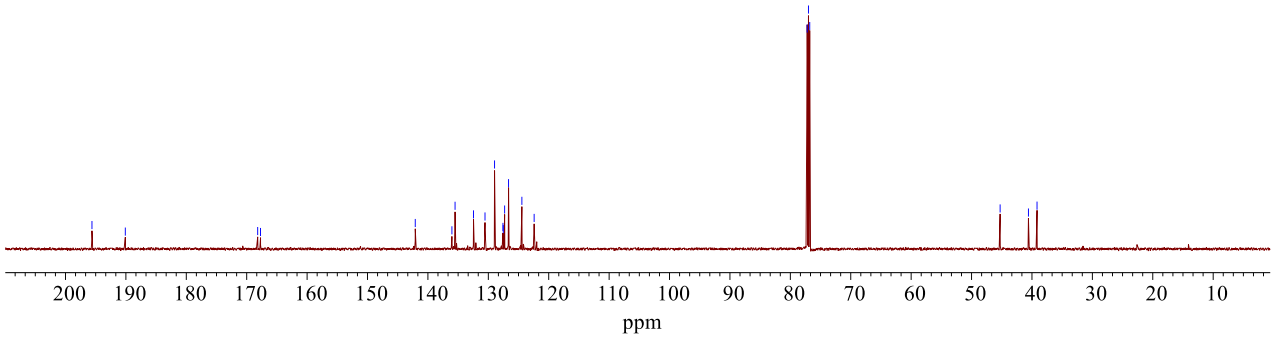


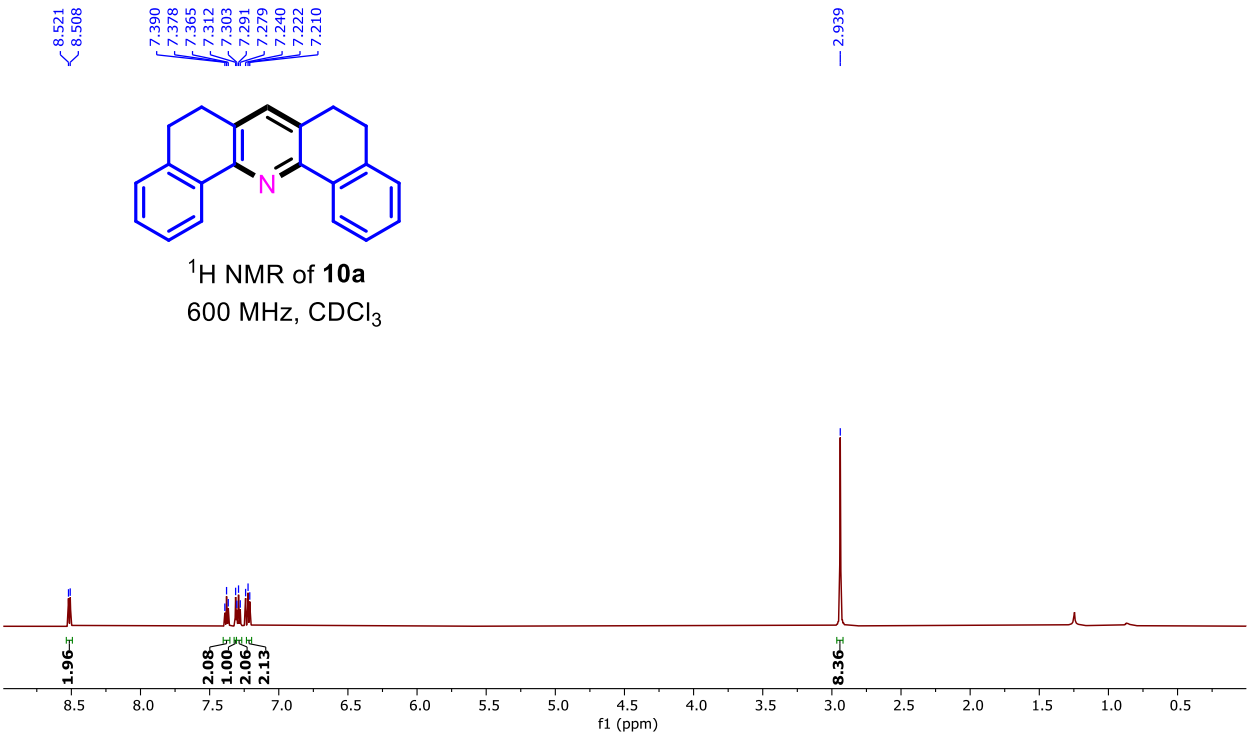
^{1}H NMR of **9e**
600 MHz, $CDCl_3$



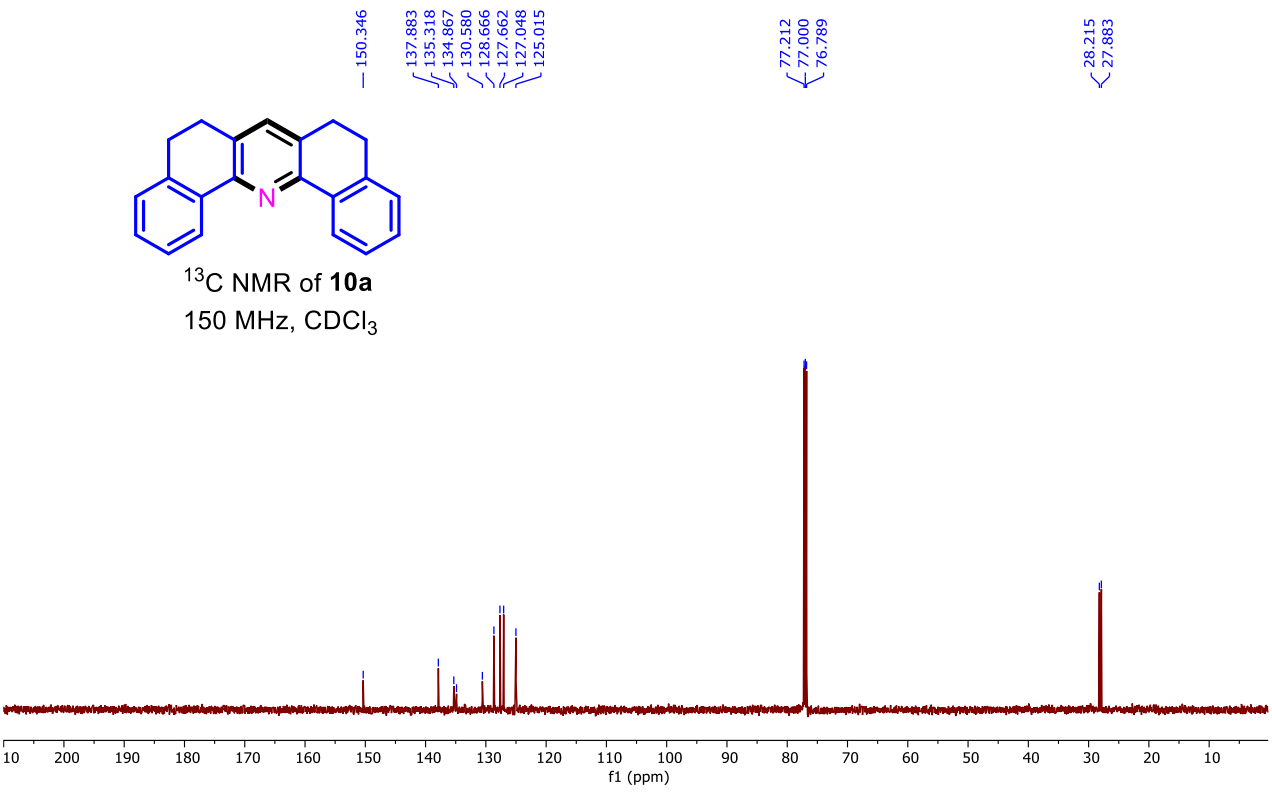


^{13}C NMR of **9e**
150 MHz, $CDCl_3$

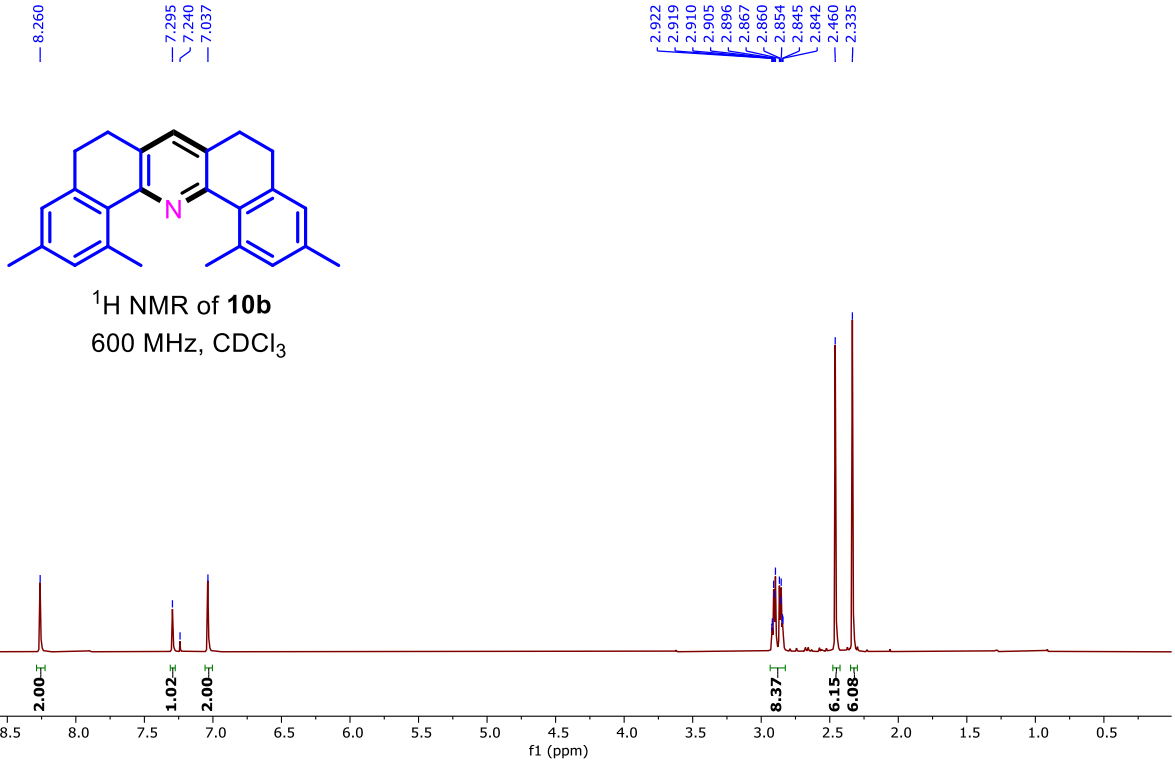




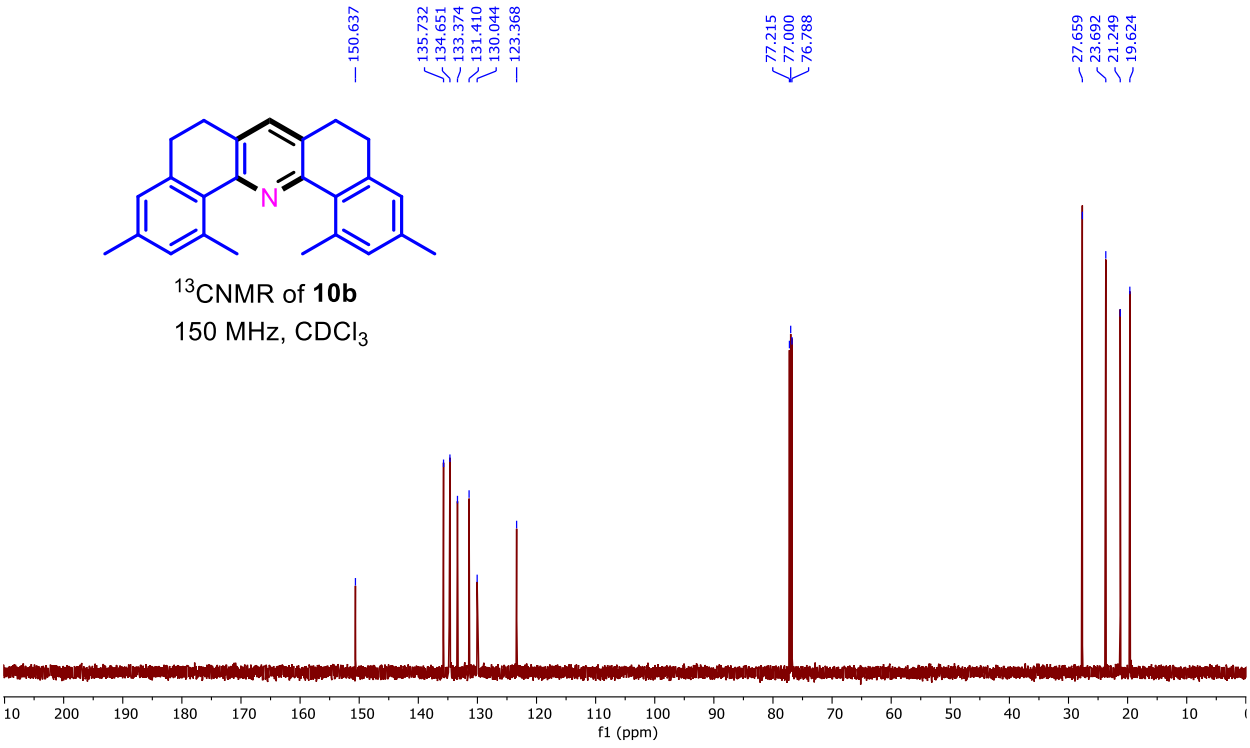
^{1}H NMR of **10a**
600 MHz, $CDCl_3$



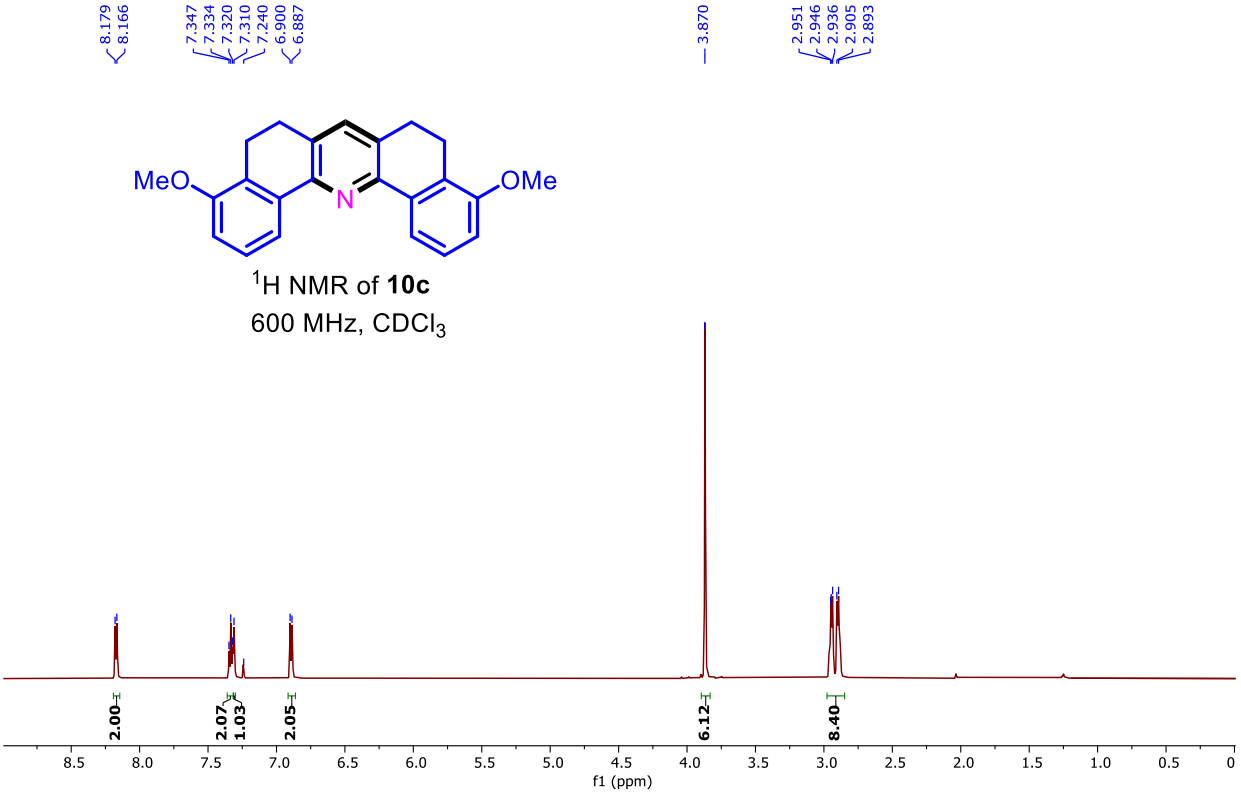
^{13}C NMR of **10a**
150 MHz, $CDCl_3$



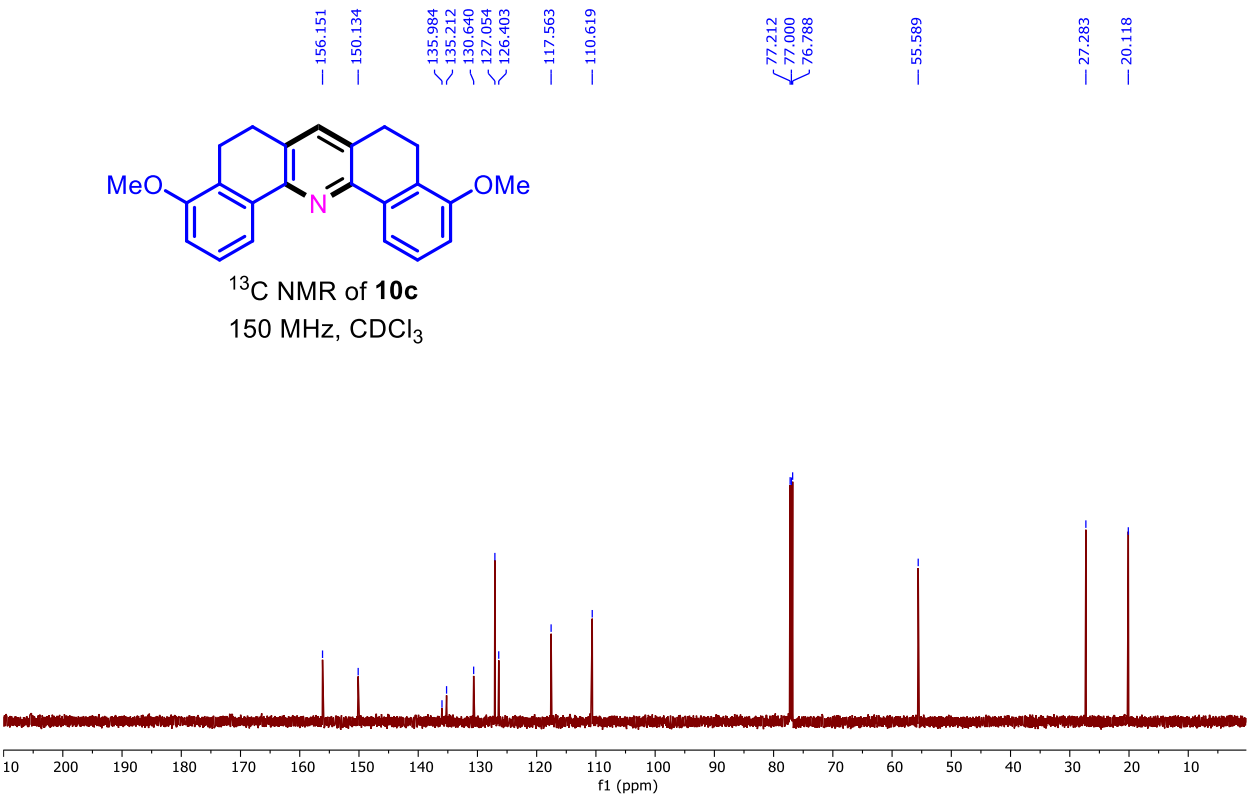
^{1}H NMR of **10b**
600 MHz, $CDCl_3$



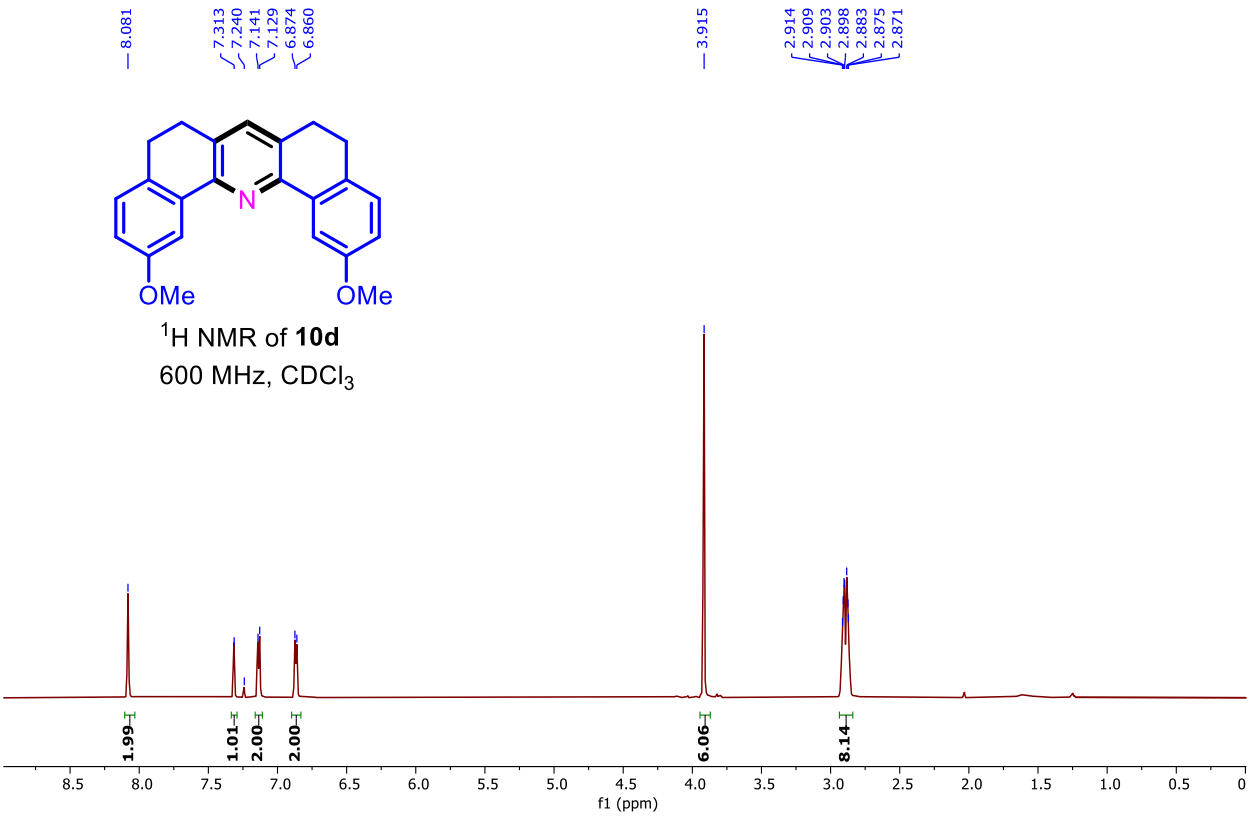
^{13}CNMR of **10b**
150 MHz, $CDCl_3$



^{1}H NMR of **10c**
600 MHz, $CDCl_3$

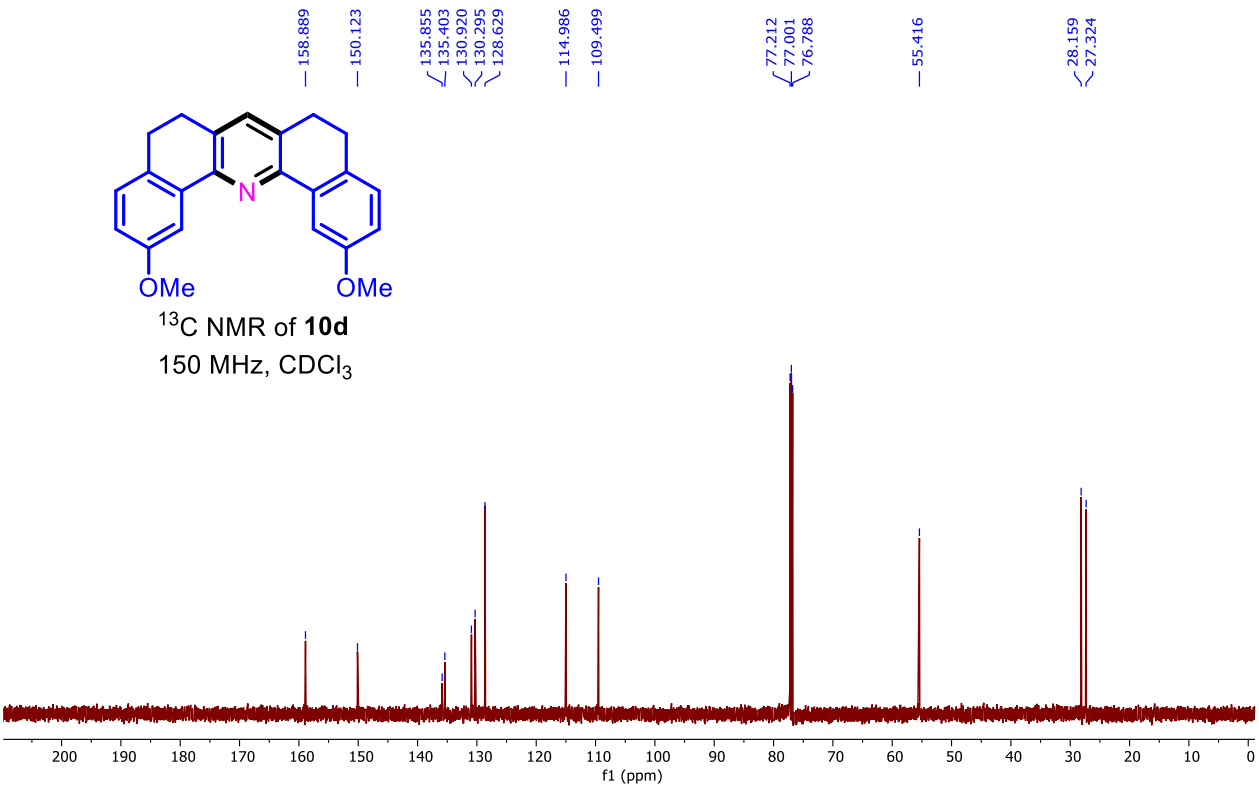


^{13}C NMR of **10c**
150 MHz, $CDCl_3$



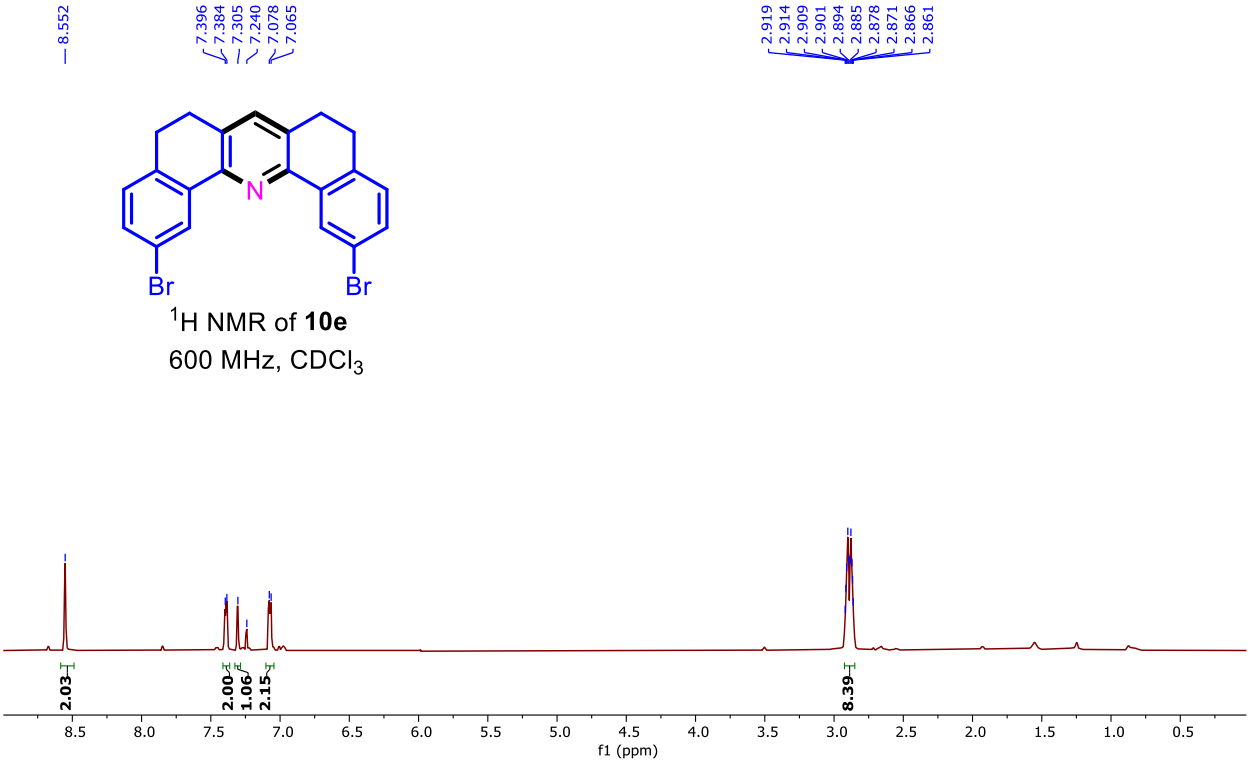
^{1}H NMR of **10d**

600 MHz, $CDCl_3$

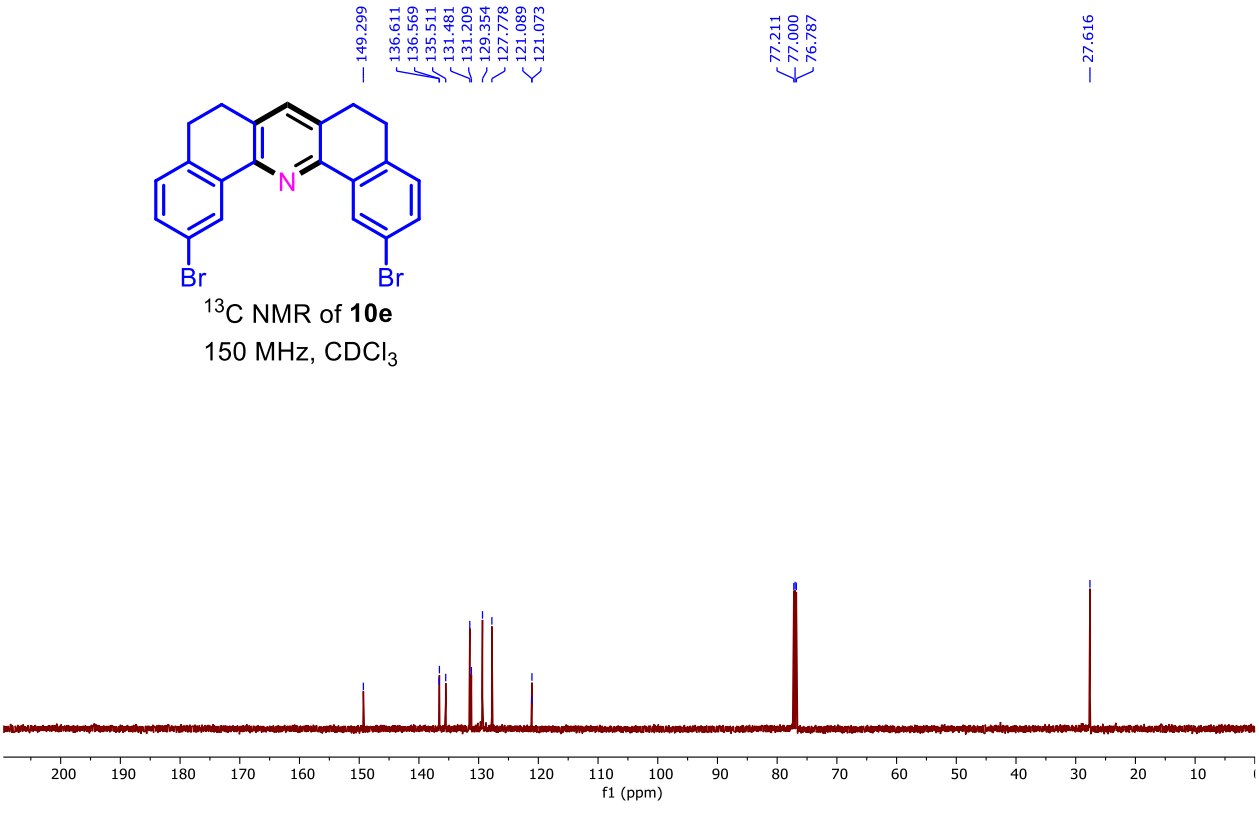


^{13}C NMR of **10d**

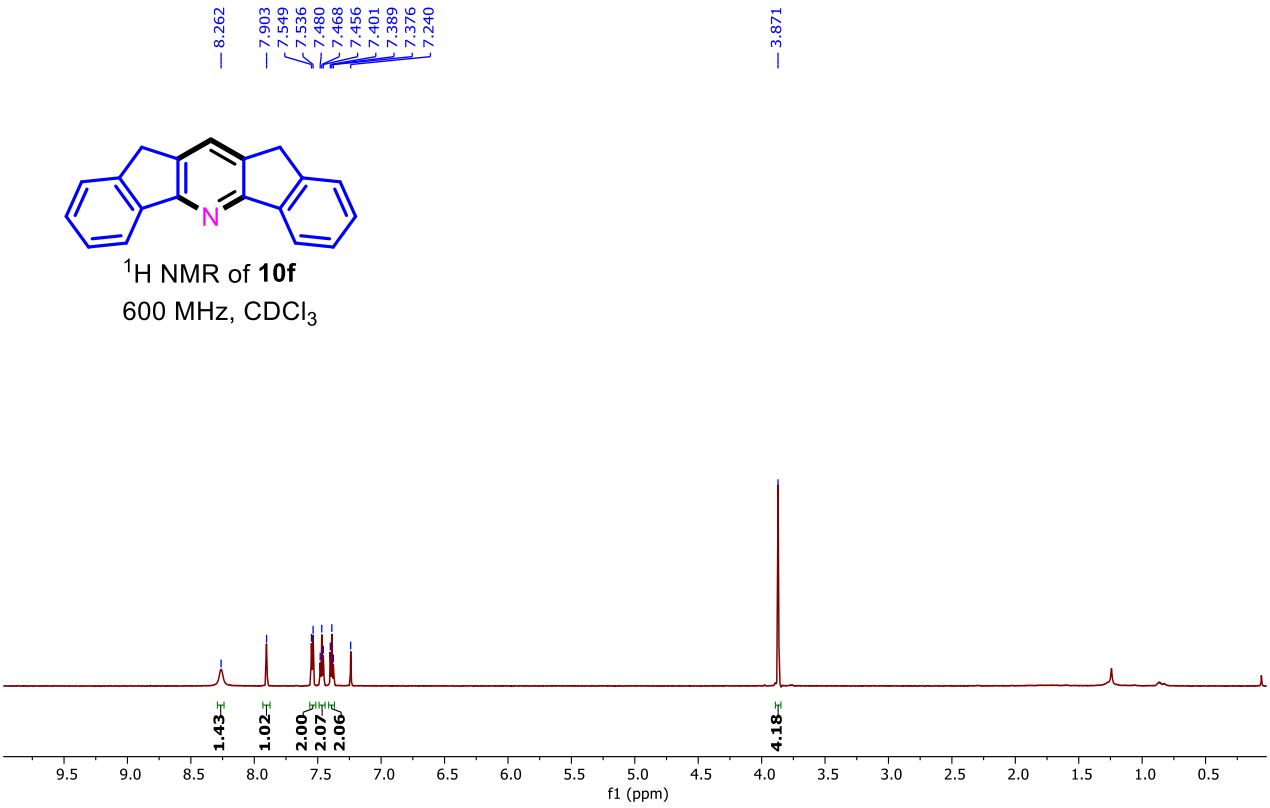
150 MHz, $CDCl_3$



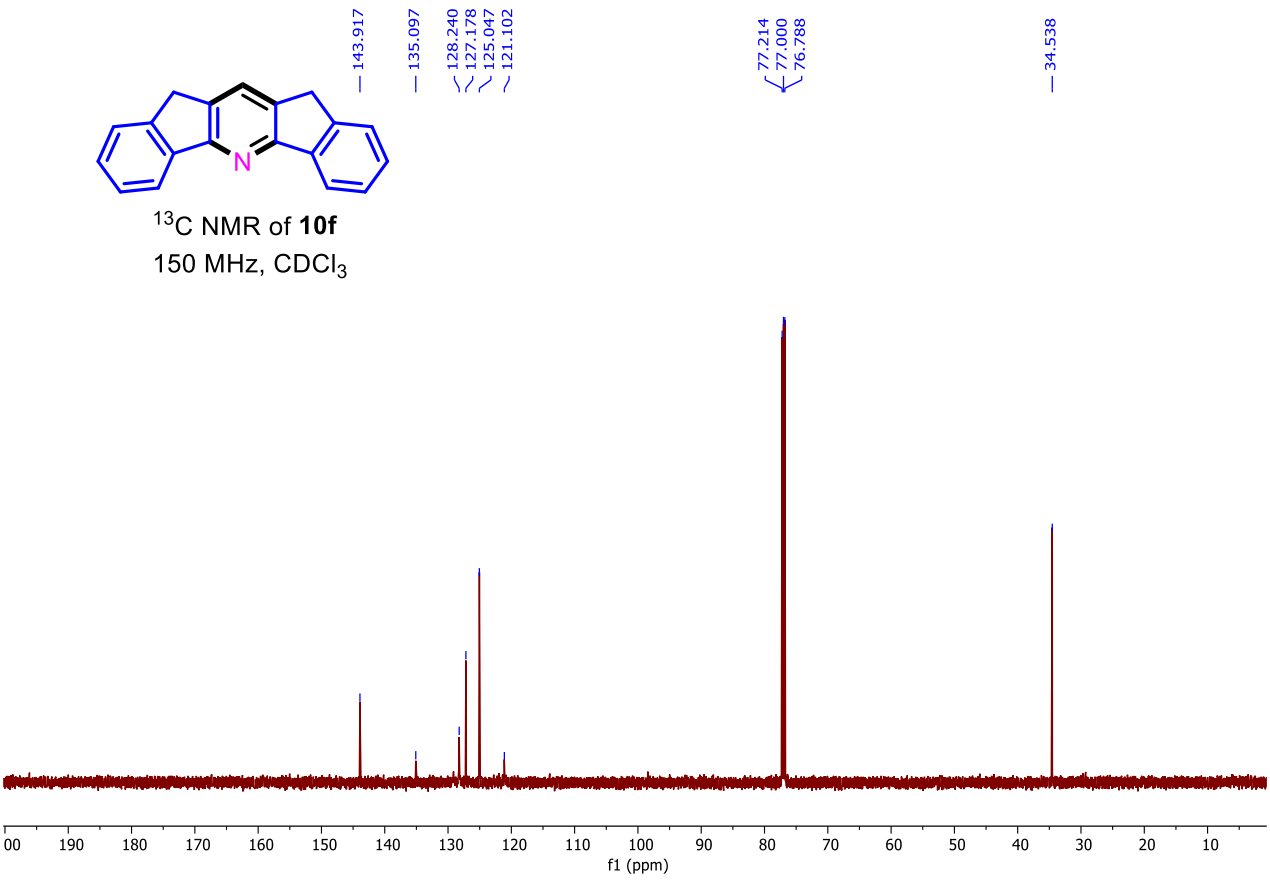
^{1}H NMR of **10e**
600 MHz, $CDCl_3$



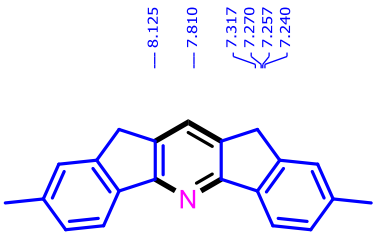
^{13}C NMR of **10e**
150 MHz, $CDCl_3$



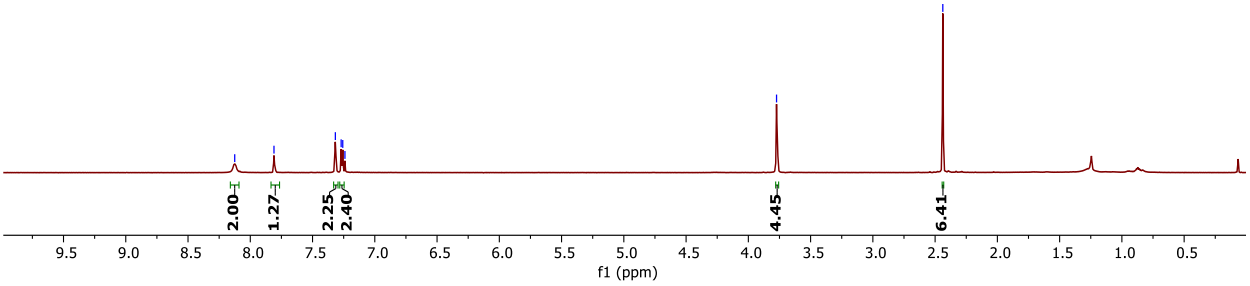
^{1}H NMR of **10f**
600 MHz, $CDCl_3$

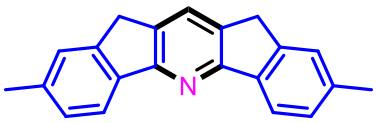


^{13}C NMR of **10f**
150 MHz, $CDCl_3$

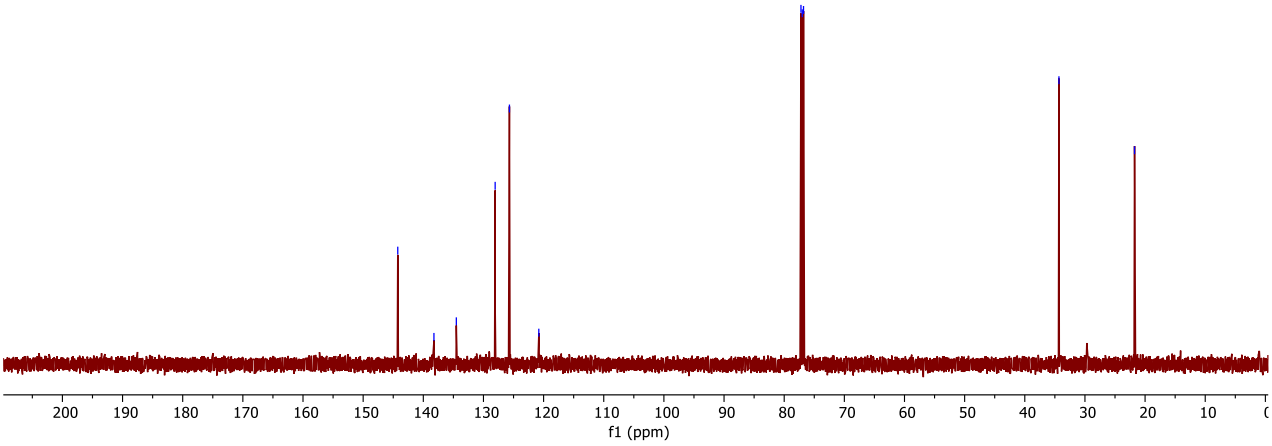


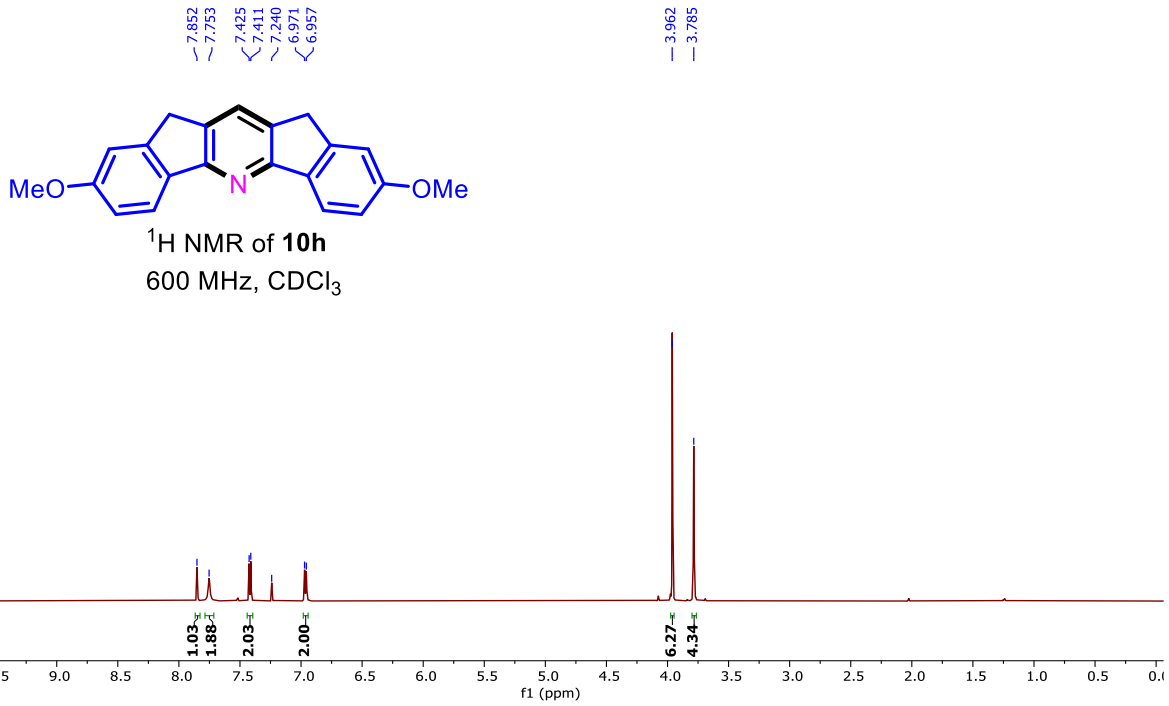
^{1}H NMR of **10g**
600 MHz, $CDCl_3$



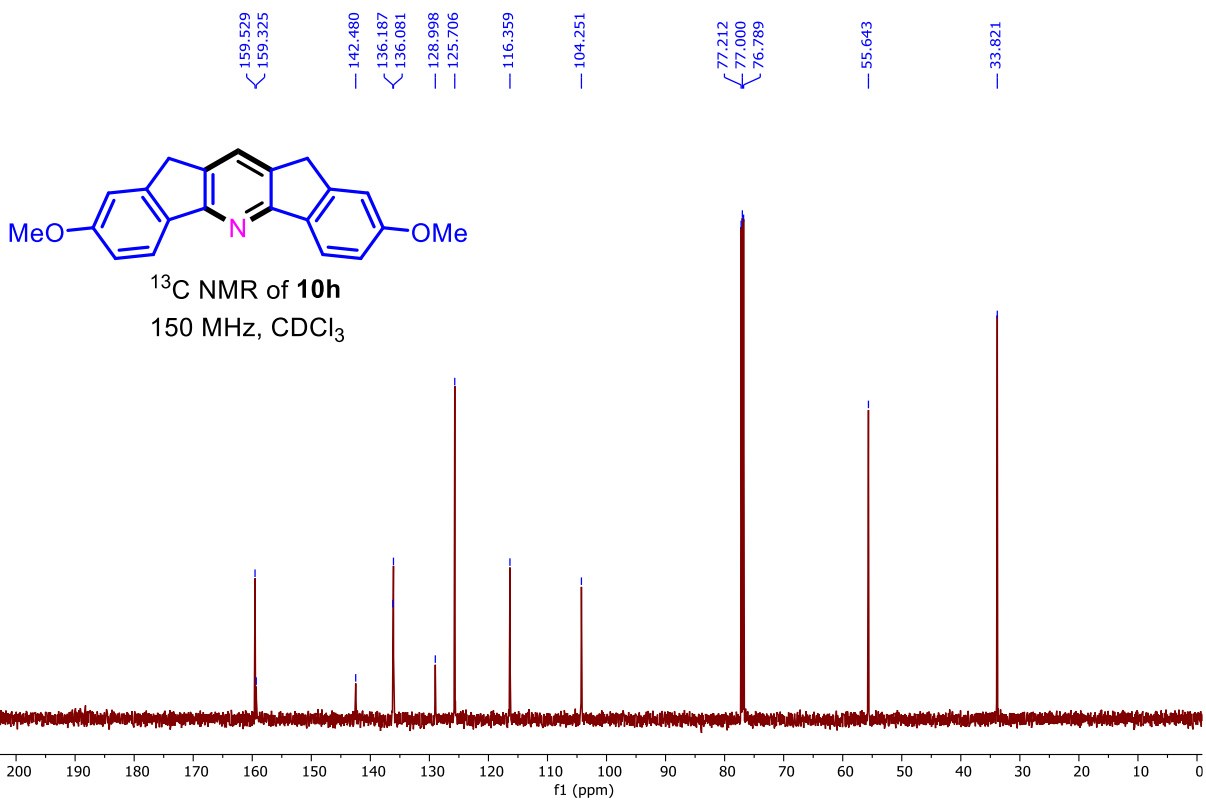


^{13}C NMR of **10g**
150 MHz, $CDCl_3$

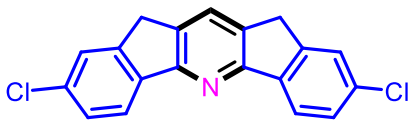




^{1}H NMR of **10h**
600 MHz, $CDCl_3$



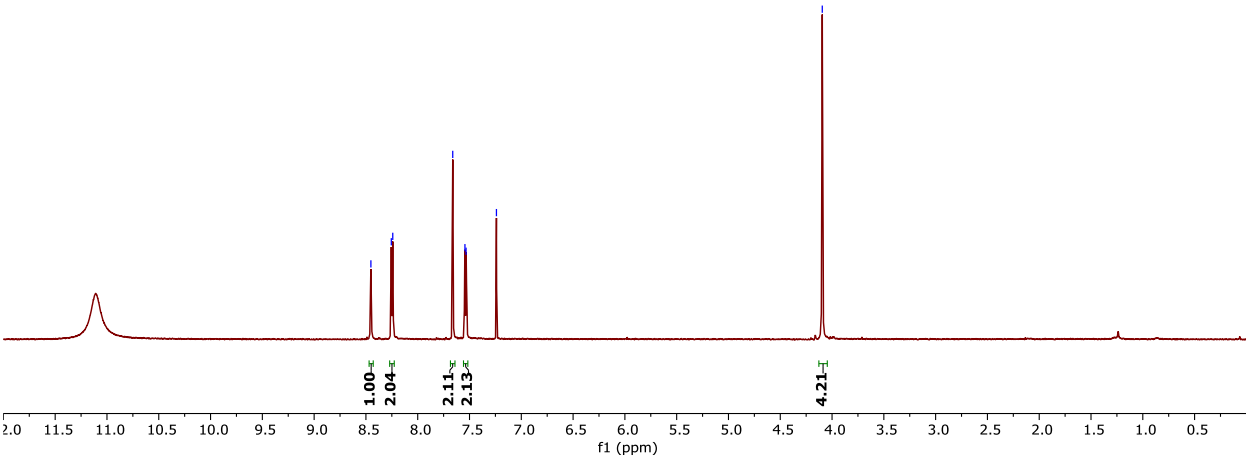
^{13}C NMR of **10h**
150 MHz, $CDCl_3$

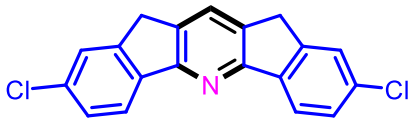


^{1}H NMR of **10i**

600 MHz, $CDCl_3$

($CDCl_3$ + 1drop of TFA(Trifluoroacetic acid))

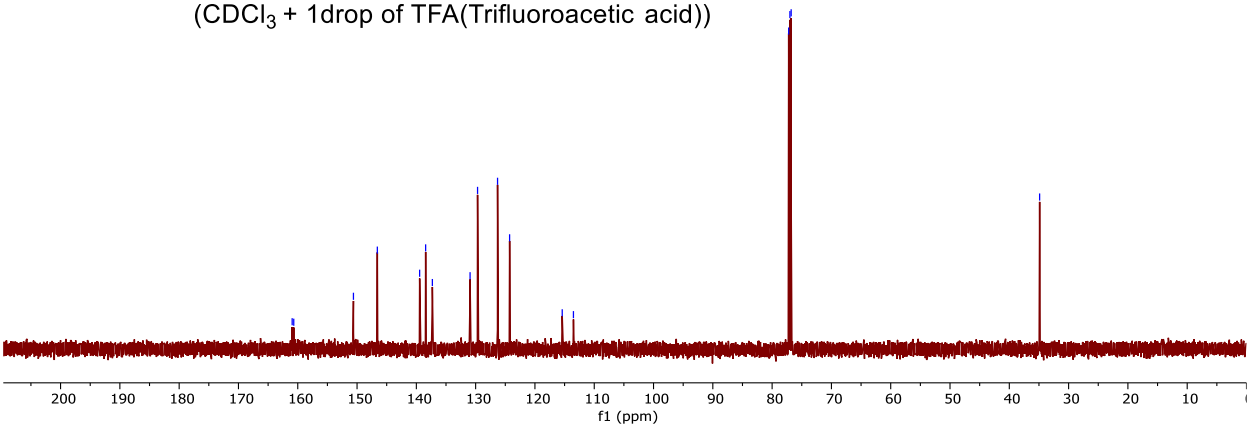


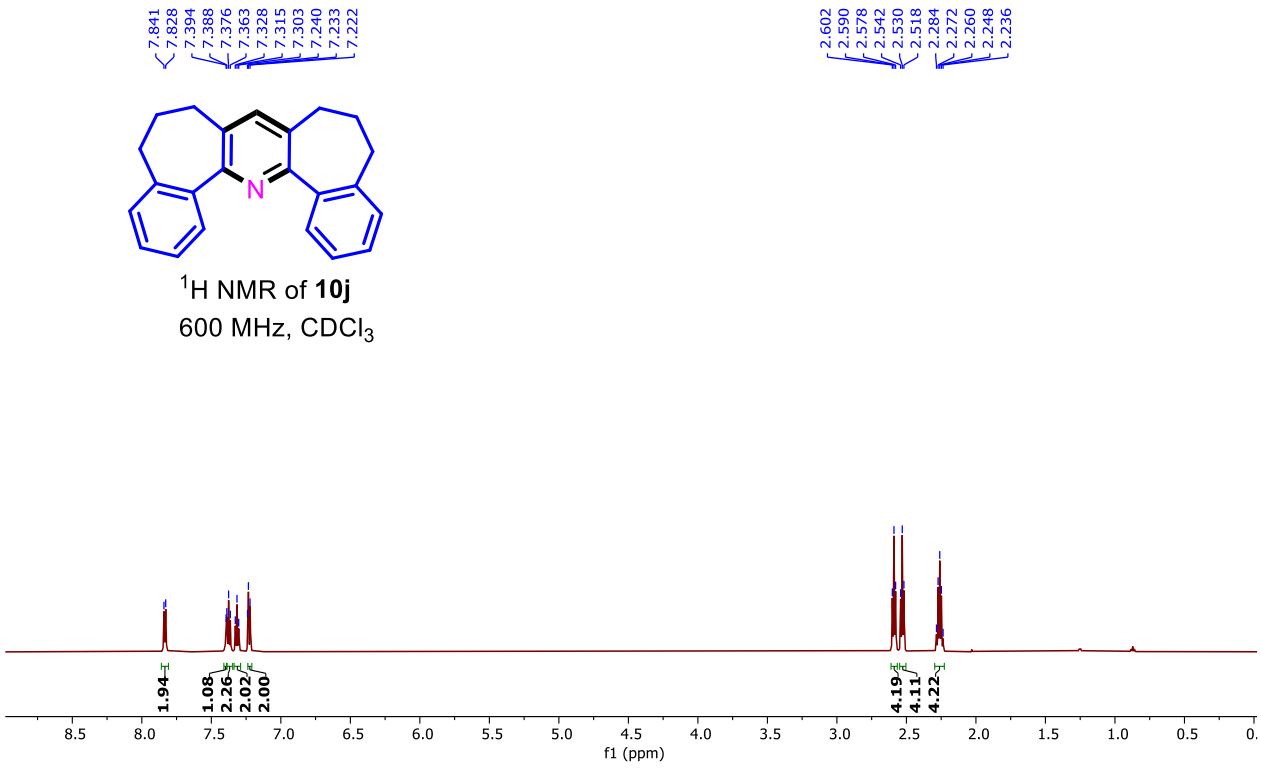


^{13}C NMR of **10i**

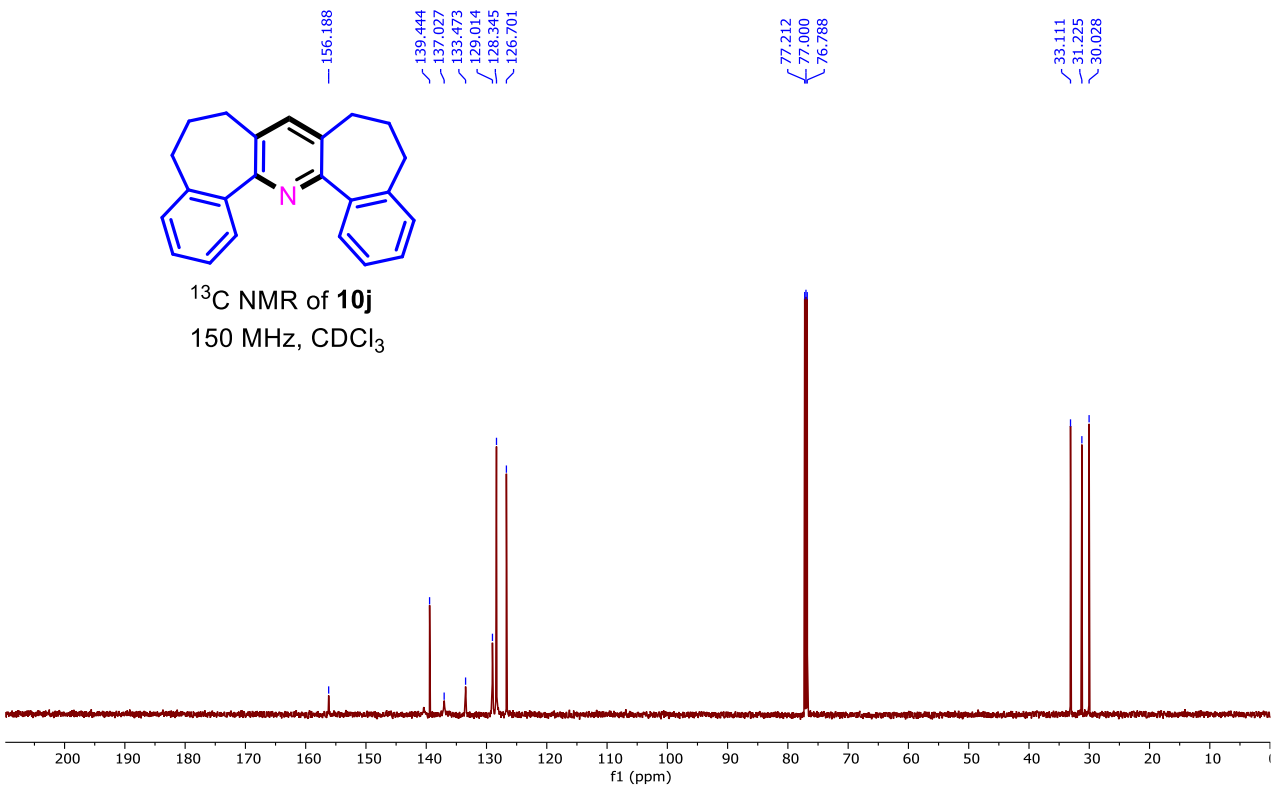
150 MHz, $CDCl_3$

($CDCl_3$ + 1drop of TFA(Trifluoroacetic acid))

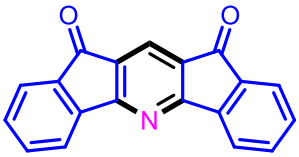




^{1}H NMR of **10j**
600 MHz, $CDCl_3$

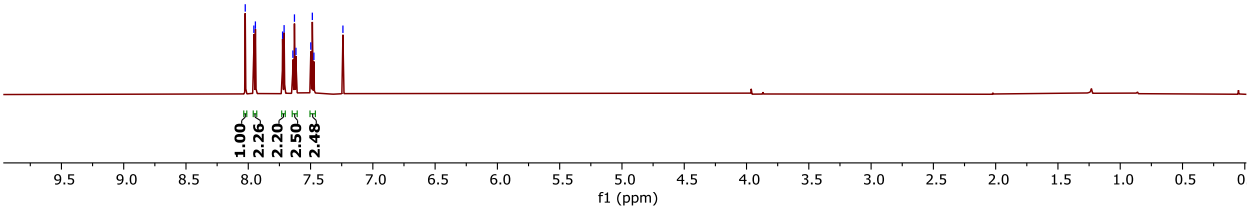


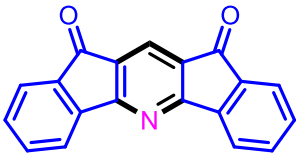
^{13}C NMR of **10j**
150 MHz, $CDCl_3$



^{1}H NMR of **10k**

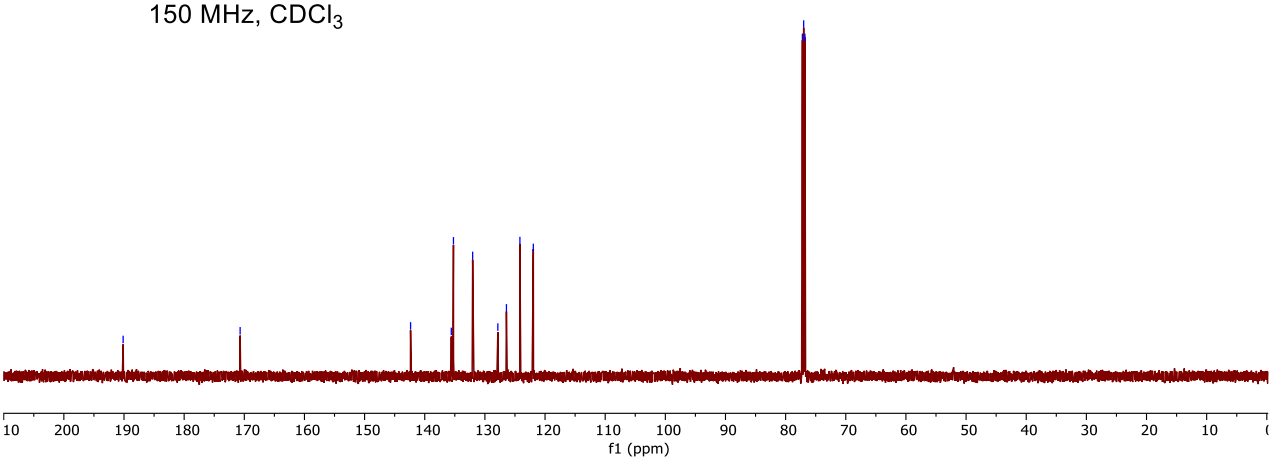
600 MHz, $CDCl_3$

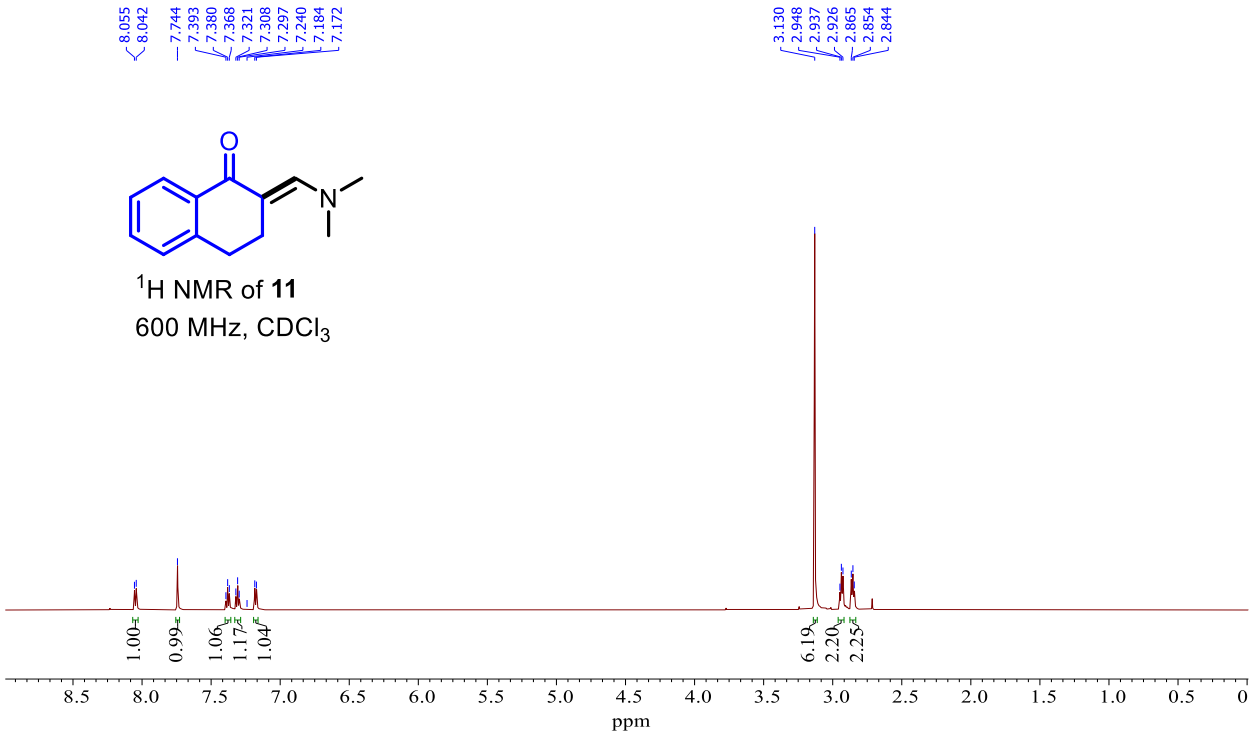




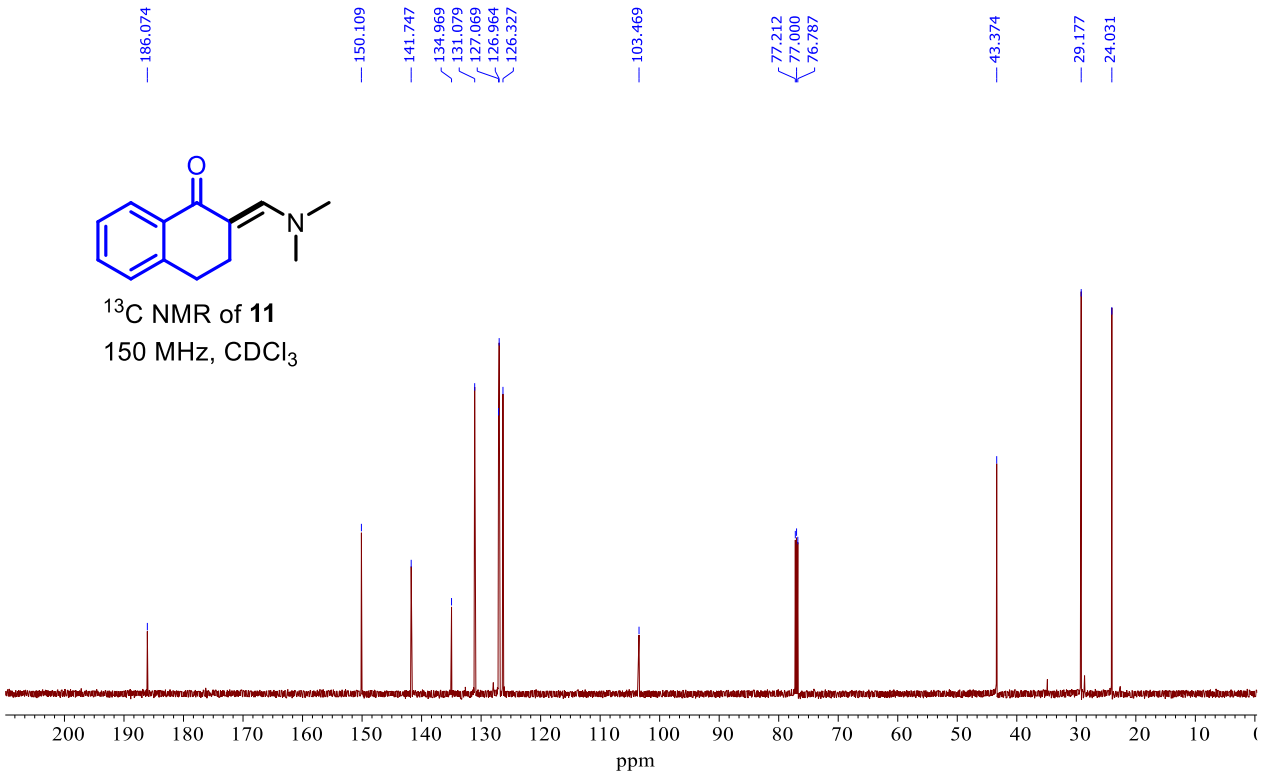
^{13}C NMR of **10k**

150 MHz, $CDCl_3$

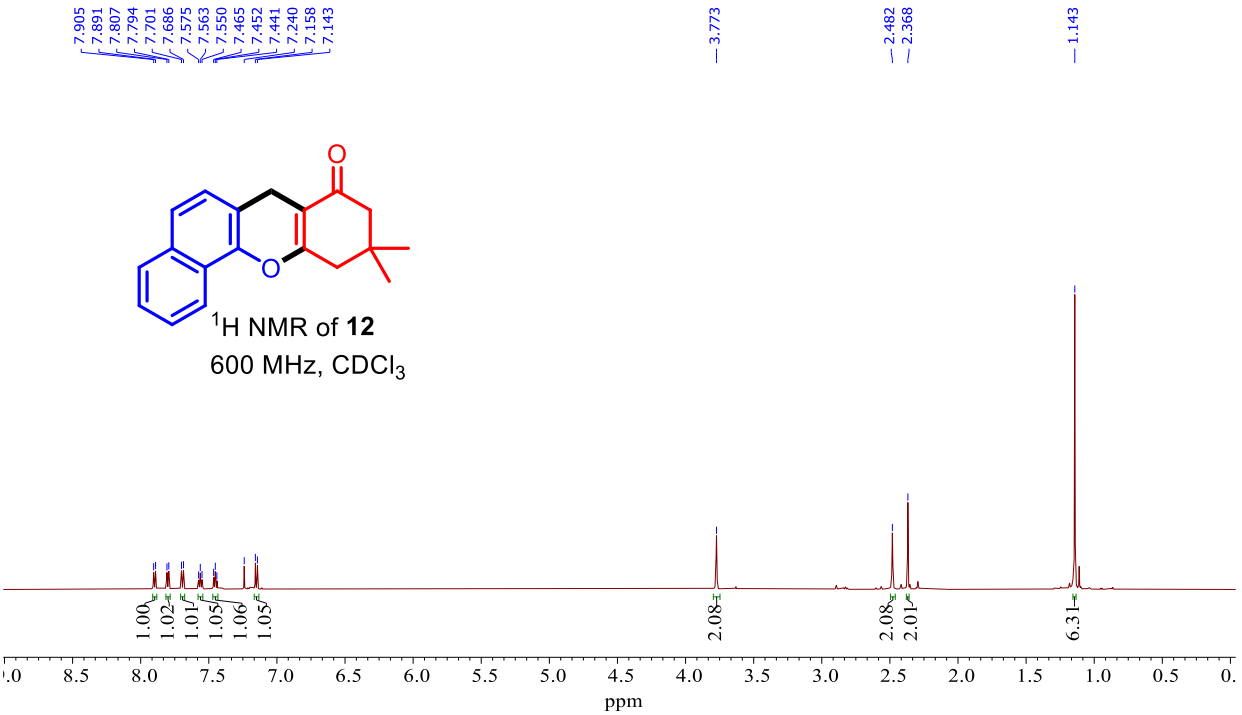




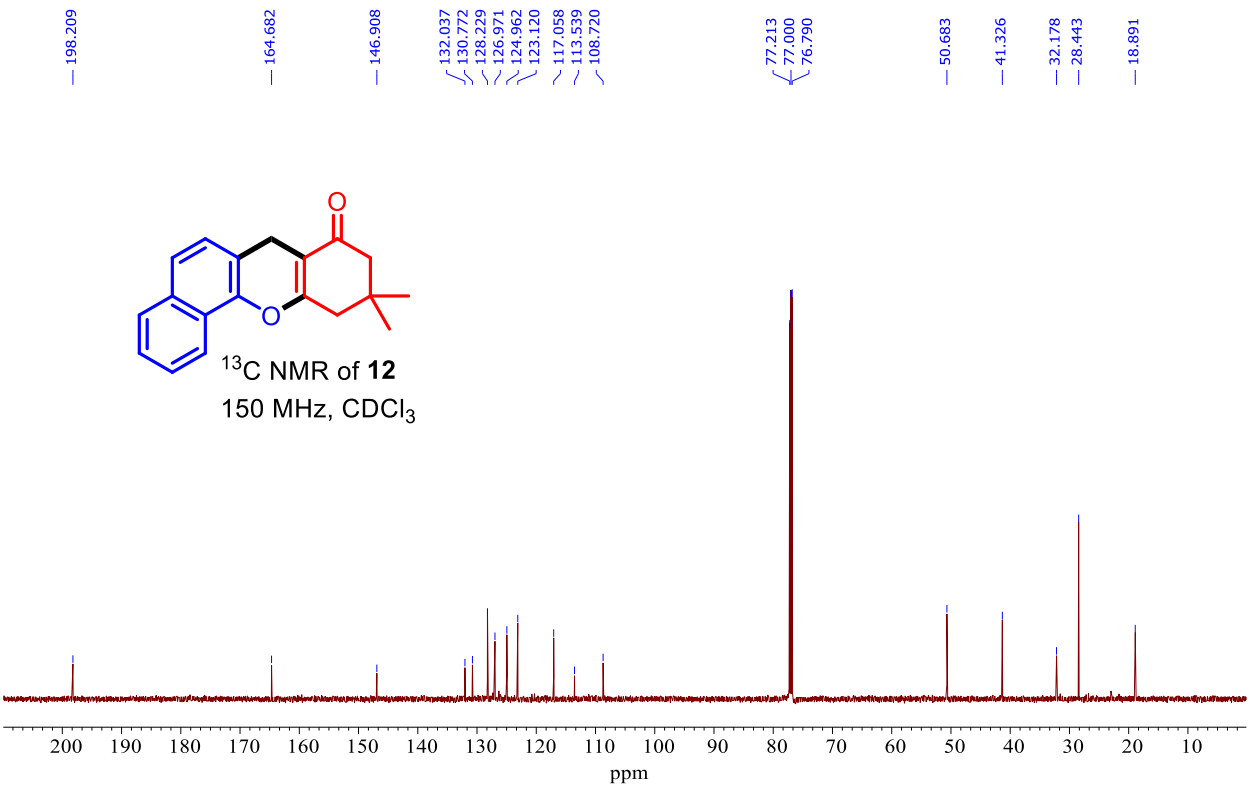
^{1}H NMR of **11**
600 MHz, $CDCl_3$



^{13}C NMR of **11**
150 MHz, $CDCl_3$



^{1}H NMR of **12**
600 MHz, $CDCl_3$



^{13}C NMR of **12**
150 MHz, $CDCl_3$

Preparation of samples for optical studies

All solutions were prepared in a standard protocol as 1mM in the solvents. For example for a comparative study of compounds **5d**, **5e**, and **7c** 1 mM solution in CH_3CN of each compound was prepared.

Procedure for Metal sensing measurements

UV-Vis and fluorescence spectra were recorded using a UV 3220 spectrometer (Optizen) and spectrofluorometer (HITACHI) F-2700 equipped with a Xe arc lamp, respectively. A stock solution of **5e** (10 mM) was prepared in ethanol:water (8:2, v/v) mixture solutions. Stock solutions of various cations (10 mM; Ag^+, Ba^{2+}, Ca^{2+}, Cd^{2+}, Ce^{3+}, Cu^{2+}, Co^{2+}, Fe^{3+}, Hg^{2+}, Mn^{2+}, Na^+, Ni^{2+}, Pb^{2+}, Sn^{2+}, Sr^{2+}, Ti^{3+}, and Zn^{2+}) were prepared in deionized water. Before spectroscopic measurements, test solutions were prepared in 1.950 μL of ethanol:water (8:2, v/v) mixture solutions mixing 25 μL stock solution of **5e** and 25 μL of each metal ions stock into cuvettes with the final volume of 2.0 mL respectively. Ag^+ and Fe^{3+} ions were detected by adding different aliquots of stock solution from 0-25 mM with **5e**. All absorption and photoluminescence emission spectra were recorded at room temperature after the addition of samples for a few seconds. The fluorescence spectra were acquired from 400 to 700 nm with the excitation wavelength set as 366 nm.

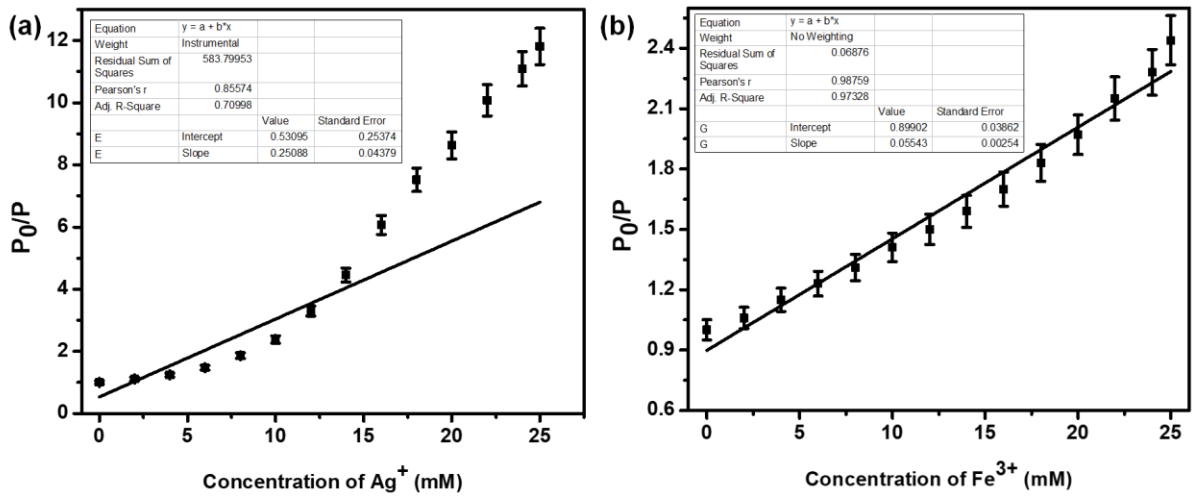


Fig. S1. Stern-Volmer plot of **5e** (10 mM) at F_0/F versus Ag^+ ions (a) and Fe^{3+} ions (b) concentrations (0-25 mM) in ethanol:water (8:2, v/v) mixture solutions.

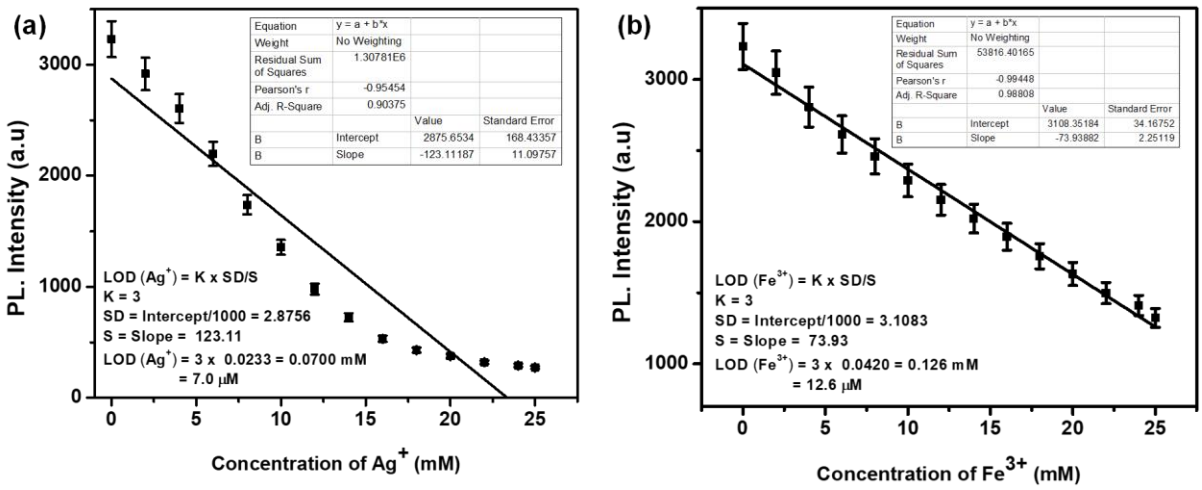


Fig. S2. Calibration curve of **5e** in the presence of Ag^{+} and Fe^{3+} ions using the monitored emission wavelength at 496 nm; (a) **5e**/Ag^{+} and (b) 5e/Fe^{3+} complex systems. The detection limit (LOD) was determined from the following equation: LOD = K × SD/S, where K = 3; SD is the standard deviation

Method of crystal growth for compounds 5d, 7k and 10j and instrumentation

In a 5 mL vial, 50 mg of the pure isolated compound was dissolved in minimum volume of ethyl acetate at room temperature. Then, 1 mL of hexane was added to the mixture. The mixture was shaken well to obtain a homogenous and clear solution. Then, the solution was covered with a porous cap and allowed to stand undisturbed at room temperature for 2 days until the crystal was formed via slow evaporation method.

The crystal structures of the compounds **5d**, **7k** and **10j** were determined by single crystal diffraction method at the Korea Basic Science Institute (KBSI, Western Seoul Center, Korea). Colorless block crystal (0.262 x 0.187 x 0.174 mm3) was picked up with paraton oil and mounted on a Bruker D8 Venture PHOTON III M14 diffractometer equipped with a graphite-monochromated Mo Kα (λ= 0.71073 Å) radiation source and a nitrogen cold stream (-50 °C). Data collection and integration were performed with SMART APEX3 (Bruker, 2016) and SAINT (Bruker, 2016) [1]. Absorption correction was performed by multi-scan method implemented in SADABS [2]. The structure was solved by direct methods and refined by full-matrix least-squares on F2 using SHELXTL [3]. All the nonhydrogen atoms were refined anisotropically, and hydrogen atoms were added to their geometrically ideal positions.

1. SMART, SAINT and SADABS, Bruker AXS Inc., Madison, Wisconsin, USA, 2016.
2. G. M. Sheldrick, SADABS v 2.03, University of Göttingen, Germany, 2002.
3. SHELXTL v 6.10; Bruker AXS, Inc: Madison, Wisconsin, USA, 2000.

Crystal refinement data for compound 5d

Empirical Formula-$C_{20}H_{21}NO_2$, M = 307.38, Triclinic, Space group P-1, a = 10.249(3) Å, b = 11.657(4) Å, c = 14.822(4) Å, V = 1608.2(8) $Å^3$, Z = 4, T = 223 (2) K, ρcalcd = 1.270 Mg/m^3, $2\Theta_{max.}$ = 28.417°. Refinement of 656 parameters on 7942 independent reflections out of 33055 collected reflections (R_{int} = 0.0986) led to R1 = 0.0755 [I >2σ(I)], wR2 = 0. 2295 (all data) and S = 1.042 with the largest difference peak and hole of 0.658 and -0.598 e.$Å^{-3}$ respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2077448). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif

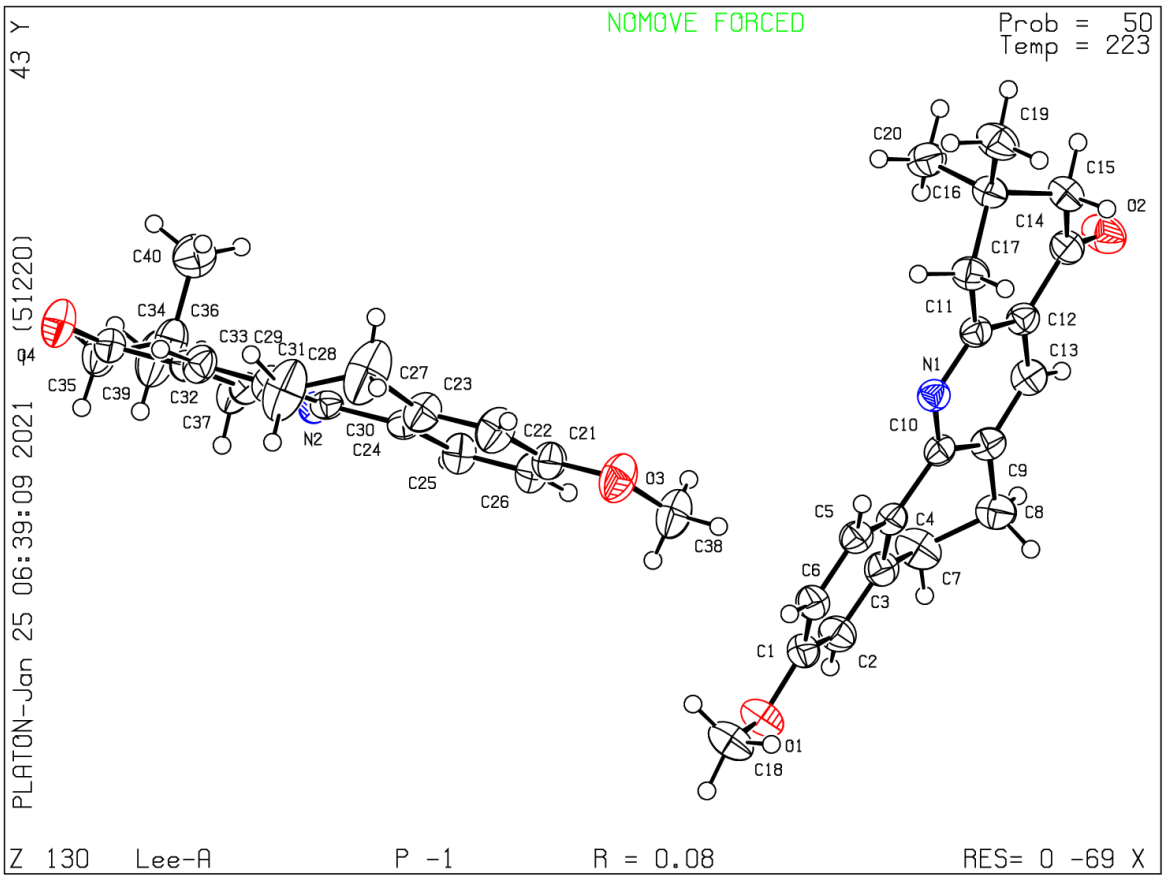


Table 1. Crystal data and structure refinement for Lee-A.

Identification code	Lee-A	
Empirical formula	C20 H21 N O2	
Formula weight	307.38	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.249(3) Å	α= 104.005(8)°.
	b = 11.657(4) Å	β= 92.306(8)°.
	c = 14.822(4) Å	γ = 109.243(7)°.
Volume	1608.2(8) $Å^3$	
Z	4	
Density (calculated)	1.270 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	656	
Crystal size	0.450 x 0.270 x 0.160 mm^3	
Theta range for data collection	1.922 to 28.417°.	
Index ranges	-13<=h<=13, -15<=k<=15, -19<=l<=19	
Reflections collected	33055	
Independent reflections	7942 [R(int) = 0.0986]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6305	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7942 / 1 / 421	
Goodness-of-fit on F2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0755, wR2 = 0.1895	
R indices (all data)	R1 = 0.1518, wR2 = 0.2295	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.658 and -0.598 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Lee-A. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6605(3)	6734(3)	-173(2)	39(1)
C(2)	5188(3)	6304(3)	-463(2)	43(1)
C(3)	4413(3)	7064(3)	-170(2)	38(1)
C(4)	5060(3)	8278(2)	434(2)	33(1)
C(5)	6485(3)	8681(3)	725(2)	36(1)
C(6)	7261(3)	7926(3)	424(2)	39(1)
C(7)	2863(3)	6605(3)	-471(3)	51(1)
C(8)	2434(3)	7690(3)	-607(2)	44(1)
C(9)	2897(3)	8770(2)	265(2)	35(1)
C(10)	4232(3)	9089(2)	740(2)	31(1)
N(1)	4797(2)	10107(2)	1478(2)	33(1)
C(11)	4041(3)	10839(2)	1774(2)	32(1)
C(12)	2682(3)	10559(2)	1371(2)	34(1)
C(13)	2130(3)	9514(3)	597(2)	38(1)
C(14)	1878(3)	11378(3)	1733(2)	38(1)
C(15)	2635(3)	12583(3)	2463(2)	42(1)
C(16)	3736(3)	12492(2)	3144(2)	36(1)
C(17)	4738(3)	12001(3)	2572(2)	39(1)
O(1)	7266(2)	5902(2)	-528(2)	51(1)
C(18)	8738(3)	6329(3)	-310(3)	57(1)
O(2)	655(2)	11086(2)	1427(2)	54(1)
C(19)	4538(3)	13797(3)	3802(2)	49(1)
C(20)	3040(3)	11589(3)	3727(2)	47(1)
C(21)	9613(3)	8177(3)	3958(2)	43(1)
C(22)	10498(3)	8549(3)	4776(2)	51(1)
C(23)	10358(3)	7772(3)	5369(2)	44(1)
C(24)	9294(3)	6602(2)	5138(2)	32(1)
C(25)	8391(3)	6256(3)	4324(2)	40(1)
C(26)	8538(3)	7022(3)	3726(2)	43(1)
C(27)	11237(4)	8238(3)	6293(3)	83(2)

C(28)	11468(3)	7179(3)	6630(3)	73(1)
C(29)	10159(3)	6098(3)	6528(2)	41(1)
C(30)	9138(3)	5781(2)	5771(2)	31(1)
N(2)	7978(2)	4741(2)	5589(2)	32(1)
C(31)	7801(3)	3997(2)	6167(2)	34(1)
C(32)	8753(3)	4247(2)	6945(2)	35(1)
C(33)	9947(3)	5326(3)	7114(2)	41(1)
C(34)	8536(3)	3403(3)	7566(2)	41(1)
C(35)	7279(3)	2218(3)	7282(2)	49(1)
C(36)	6024(3)	2361(3)	6781(2)	43(1)
C(37)	6500(3)	2844(3)	5936(2)	46(1)
O(3)	9881(2)	9010(2)	3419(2)	59(1)
C(38)	9041(4)	8632(3)	2541(3)	61(1)
O(4)	9349(2)	3653(2)	8267(2)	58(1)
C(39)	4860(4)	1080(3)	6446(3)	67(1)
C(40)	5510(4)	3285(3)	7453(3)	59(1)

Table 3. Bond lengths [Å] and angles [°] for Lee-A.

C(1)-O(1)	1.375(3)
C(1)-C(6)	1.381(4)
C(1)-C(2)	1.382(4)
C(2)-C(3)	1.382(4)
C(2)-H(2)	0.9400
C(3)-C(4)	1.402(4)
C(3)-C(7)	1.509(4)
C(4)-C(5)	1.392(4)
C(4)-C(10)	1.473(4)
C(5)-C(6)	1.381(4)
C(5)-H(5)	0.9400
C(6)-H(6)	0.9400
C(7)-C(8)	1.521(4)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(8)-C(9)	1.499(4)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(9)-C(13)	1.374(4)
C(9)-C(10)	1.402(4)
C(10)-N(1)	1.345(3)
N(1)-C(11)	1.342(3)
C(11)-C(12)	1.394(4)
C(11)-C(17)	1.504(4)
C(12)-C(13)	1.392(4)
C(12)-C(14)	1.477(4)
C(13)-H(13)	0.9400
C(14)-O(2)	1.222(3)
C(14)-C(15)	1.491(4)
C(15)-C(16)	1.530(4)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(16)-C(17)	1.524(4)

C(16)-C(19)	1.528(4)
C(16)-C(20)	1.535(4)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
O(1)-C(18)	1.420(4)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(18)-H(18C)	0.9700
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(19)-H(19C)	0.9700
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(20)-H(20C)	0.9700
C(21)-O(3)	1.369(3)
C(21)-C(22)	1.370(4)
C(21)-C(26)	1.383(4)
C(22)-C(23)	1.387(4)
C(22)-H(22)	0.9400
C(23)-C(24)	1.389(4)
C(23)-C(27)	1.484(4)
C(24)-C(25)	1.380(4)
C(24)-C(30)	1.472(3)
C(25)-C(26)	1.382(4)
C(25)-H(25)	0.9400
C(26)-H(26)	0.9400
C(27)-C(28)	1.5217(19)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(28)-C(29)	1.478(4)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(29)-C(33)	1.370(4)
C(29)-C(30)	1.393(4)
C(30)-N(2)	1.350(3)

N(2)-C(31)	1.337(3)
C(31)-C(32)	1.389(4)
C(31)-C(37)	1.504(4)
C(32)-C(33)	1.397(4)
C(32)-C(34)	1.476(4)
C(33)-H(33)	0.9400
C(34)-O(4)	1.217(3)
C(34)-C(35)	1.499(4)
C(35)-C(36)	1.535(4)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(36)-C(39)	1.523(4)
C(36)-C(40)	1.525(5)
C(36)-C(37)	1.528(4)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
O(3)-C(38)	1.418(4)
C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(38)-H(38C)	0.9700
C(39)-H(39A)	0.9700
C(39)-H(39B)	0.9700
C(39)-H(39C)	0.9700
C(40)-H(40A)	0.9700
C(40)-H(40B)	0.9700
C(40)-H(40C)	0.9700

O(1)-C(1)-C(6)	124.6(3)
O(1)-C(1)-C(2)	115.1(3)
C(6)-C(1)-C(2)	120.3(3)
C(3)-C(2)-C(1)	120.6(3)
C(3)-C(2)-H(2)	119.7
C(1)-C(2)-H(2)	119.7
C(2)-C(3)-C(4)	120.1(3)
C(2)-C(3)-C(7)	121.3(3)

C(4)-C(3)-C(7)	118.6(3)
C(5)-C(4)-C(3)	118.1(3)
C(5)-C(4)-C(10)	122.0(2)
C(3)-C(4)-C(10)	119.9(2)
C(6)-C(5)-C(4)	121.8(3)
C(6)-C(5)-H(5)	119.1
C(4)-C(5)-H(5)	119.1
C(5)-C(6)-C(1)	119.2(3)
C(5)-C(6)-H(6)	120.4
C(1)-C(6)-H(6)	120.4
C(3)-C(7)-C(8)	110.0(2)
C(3)-C(7)-H(7A)	109.7
C(8)-C(7)-H(7A)	109.7
C(3)-C(7)-H(7B)	109.7
C(8)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2
C(9)-C(8)-C(7)	110.6(2)
C(9)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
C(13)-C(9)-C(10)	117.8(3)
C(13)-C(9)-C(8)	124.2(3)
C(10)-C(9)-C(8)	118.0(3)
N(1)-C(10)-C(9)	122.8(3)
N(1)-C(10)-C(4)	117.8(2)
C(9)-C(10)-C(4)	119.4(2)
C(11)-N(1)-C(10)	118.3(2)
N(1)-C(11)-C(12)	122.7(3)
N(1)-C(11)-C(17)	116.6(2)
C(12)-C(11)-C(17)	120.7(2)
C(13)-C(12)-C(11)	117.8(3)
C(13)-C(12)-C(14)	121.3(2)
C(11)-C(12)-C(14)	120.8(3)

C(9)-C(13)-C(12)	120.5(3)
C(9)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
O(2)-C(14)-C(12)	120.9(3)
O(2)-C(14)-C(15)	121.8(3)
C(12)-C(14)-C(15)	117.2(2)
C(14)-C(15)-C(16)	114.0(2)
C(14)-C(15)-H(15A)	108.8
C(16)-C(15)-H(15A)	108.8
C(14)-C(15)-H(15B)	108.8
C(16)-C(15)-H(15B)	108.8
H(15A)-C(15)-H(15B)	107.7
C(17)-C(16)-C(19)	109.5(2)
C(17)-C(16)-C(15)	108.2(2)
C(19)-C(16)-C(15)	109.7(2)
C(17)-C(16)-C(20)	109.9(2)
C(19)-C(16)-C(20)	109.2(3)
C(15)-C(16)-C(20)	110.3(2)
C(11)-C(17)-C(16)	114.5(2)
C(11)-C(17)-H(17A)	108.6
C(16)-C(17)-H(17A)	108.6
C(11)-C(17)-H(17B)	108.6
C(16)-C(17)-H(17B)	108.6
H(17A)-C(17)-H(17B)	107.6
C(1)-O(1)-C(18)	117.5(2)
O(1)-C(18)-H(18A)	109.5
O(1)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
O(1)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5

H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(3)-C(21)-C(22)	115.7(3)
O(3)-C(21)-C(26)	124.5(3)
C(22)-C(21)-C(26)	119.8(3)
C(21)-C(22)-C(23)	121.1(3)
C(21)-C(22)-H(22)	119.4
C(23)-C(22)-H(22)	119.4
C(22)-C(23)-C(24)	119.7(3)
C(22)-C(23)-C(27)	120.3(3)
C(24)-C(23)-C(27)	119.7(3)
C(25)-C(24)-C(23)	118.4(2)
C(25)-C(24)-C(30)	121.9(2)
C(23)-C(24)-C(30)	119.7(2)
C(24)-C(25)-C(26)	122.0(3)
C(24)-C(25)-H(25)	119.0
C(26)-C(25)-H(25)	119.0
C(25)-C(26)-C(21)	118.9(3)
C(25)-C(26)-H(26)	120.5
C(21)-C(26)-H(26)	120.5
C(23)-C(27)-C(28)	112.5(3)
C(23)-C(27)-H(27A)	109.1
C(28)-C(27)-H(27A)	109.1
C(23)-C(27)-H(27B)	109.1
C(28)-C(27)-H(27B)	109.1
H(27A)-C(27)-H(27B)	107.8
C(29)-C(28)-C(27)	112.2(3)
C(29)-C(28)-H(28A)	109.2
C(27)-C(28)-H(28A)	109.2

C(29)-C(28)-H(28B)	109.2
C(27)-C(28)-H(28B)	109.2
H(28A)-C(28)-H(28B)	107.9
C(33)-C(29)-C(30)	117.8(2)
C(33)-C(29)-C(28)	122.3(3)
C(30)-C(29)-C(28)	119.7(3)
N(2)-C(30)-C(29)	122.7(2)
N(2)-C(30)-C(24)	117.4(2)
C(29)-C(30)-C(24)	120.0(2)
C(31)-N(2)-C(30)	118.4(2)
N(2)-C(31)-C(32)	123.0(2)
N(2)-C(31)-C(37)	116.7(2)
C(32)-C(31)-C(37)	120.3(2)
C(31)-C(32)-C(33)	117.4(2)
C(31)-C(32)-C(34)	121.8(2)
C(33)-C(32)-C(34)	120.7(3)
C(29)-C(33)-C(32)	120.7(3)
C(29)-C(33)-H(33)	119.6
C(32)-C(33)-H(33)	119.6
O(4)-C(34)-C(32)	121.4(3)
O(4)-C(34)-C(35)	122.0(3)
C(32)-C(34)-C(35)	116.6(3)
C(34)-C(35)-C(36)	114.0(2)
C(34)-C(35)-H(35A)	108.8
C(36)-C(35)-H(35A)	108.8
C(34)-C(35)-H(35B)	108.8
C(36)-C(35)-H(35B)	108.8
H(35A)-C(35)-H(35B)	107.7
C(39)-C(36)-C(40)	109.7(3)
C(39)-C(36)-C(37)	109.4(3)
C(40)-C(36)-C(37)	110.8(2)
C(39)-C(36)-C(35)	109.4(2)
C(40)-C(36)-C(35)	109.8(3)
C(37)-C(36)-C(35)	107.6(3)
C(31)-C(37)-C(36)	114.1(2)

C(31)-C(37)-H(37A)	108.7
C(36)-C(37)-H(37A)	108.7
C(31)-C(37)-H(37B)	108.7
C(36)-C(37)-H(37B)	108.7
H(37A)-C(37)-H(37B)	107.6
C(21)-O(3)-C(38)	117.5(2)
O(3)-C(38)-H(38A)	109.5
O(3)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
O(3)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(36)-C(39)-H(39A)	109.5
C(36)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(36)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(36)-C(40)-H(40A)	109.5
C(36)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(36)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Lee-A. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	46(2)	38(2)	41(2)	16(1)	12(1)	20(1)
C(2)	45(2)	36(2)	44(2)	7(1)	5(2)	14(1)
C(3)	40(2)	36(2)	38(2)	10(1)	6(1)	12(1)
C(4)	36(2)	34(1)	30(2)	12(1)	7(1)	12(1)
C(5)	38(2)	38(2)	31(2)	6(1)	2(1)	14(1)
C(6)	37(2)	43(2)	39(2)	11(1)	4(1)	18(1)
C(7)	40(2)	37(2)	65(2)	2(2)	2(2)	6(1)
C(8)	36(2)	49(2)	41(2)	2(1)	0(1)	15(1)
C(9)	31(1)	38(2)	34(2)	8(1)	5(1)	9(1)
C(10)	33(1)	33(1)	29(2)	12(1)	7(1)	10(1)
N(1)	32(1)	35(1)	33(1)	10(1)	6(1)	12(1)
C(11)	32(1)	36(1)	31(2)	11(1)	7(1)	12(1)
C(12)	32(1)	36(1)	33(2)	10(1)	5(1)	11(1)
C(13)	30(1)	42(2)	40(2)	10(1)	2(1)	9(1)
C(14)	34(2)	44(2)	39(2)	12(1)	6(1)	17(1)
C(15)	41(2)	41(2)	47(2)	10(1)	7(2)	21(1)
C(16)	35(2)	34(1)	37(2)	5(1)	5(1)	14(1)
C(17)	34(2)	40(2)	40(2)	6(1)	5(1)	12(1)
O(1)	48(1)	43(1)	64(2)	6(1)	10(1)	23(1)
C(18)	49(2)	53(2)	73(3)	9(2)	12(2)	29(2)
O(2)	36(1)	64(1)	58(2)	4(1)	-2(1)	24(1)
C(19)	46(2)	38(2)	54(2)	-2(1)	0(2)	16(1)
C(20)	54(2)	49(2)	41(2)	13(2)	14(2)	20(2)
C(21)	49(2)	39(2)	43(2)	18(1)	10(2)	15(1)
C(22)	53(2)	40(2)	50(2)	17(2)	1(2)	-1(1)
C(23)	47(2)	37(2)	38(2)	8(1)	-1(1)	4(1)
C(24)	30(1)	35(1)	32(2)	9(1)	9(1)	12(1)
C(25)	32(2)	42(2)	46(2)	18(1)	2(1)	7(1)
C(26)	38(2)	50(2)	45(2)	22(2)	3(1)	14(1)
C(27)	87(3)	60(2)	67(3)	24(2)	-27(2)	-22(2)

C(28)	45(2)	81(3)	70(3)	37(2)	-18(2)	-14(2)
C(29)	32(2)	47(2)	40(2)	13(1)	2(1)	10(1)
C(30)	28(1)	35(1)	29(2)	7(1)	7(1)	12(1)
N(2)	34(1)	32(1)	30(1)	9(1)	4(1)	10(1)
C(31)	34(1)	35(1)	32(2)	9(1)	5(1)	13(1)
C(32)	36(2)	39(2)	32(2)	10(1)	5(1)	17(1)
C(33)	34(2)	55(2)	36(2)	15(1)	-1(1)	15(1)
C(34)	47(2)	51(2)	36(2)	17(1)	8(2)	26(1)
C(35)	58(2)	44(2)	49(2)	23(2)	7(2)	16(2)
C(36)	44(2)	39(2)	45(2)	20(1)	4(2)	7(1)
C(37)	49(2)	42(2)	40(2)	15(1)	-2(2)	5(1)
O(3)	73(2)	46(1)	54(2)	26(1)	4(1)	8(1)
C(38)	72(2)	61(2)	55(2)	31(2)	4(2)	19(2)
O(4)	64(2)	66(2)	47(2)	25(1)	-5(1)	21(1)
C(39)	62(2)	55(2)	71(3)	35(2)	-5(2)	-6(2)
C(40)	52(2)	67(2)	65(3)	28(2)	19(2)	20(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Lee-A.

	x	y	z	U(eq)
H(2)	4748	5487	-864	51
H(5)	6930	9489	1137	43
H(6)	8224	8220	623	47
H(7A)	2363	6258	8	62
H(7B)	2616	5932	-1059	62
H(8A)	2854	7972	-1133	53
H(8B)	1419	7399	-757	53
H(13)	1226	9316	299	46
H(15A)	1955	12852	2822	50
H(15B)	3089	13234	2151	50
H(17A)	5319	12671	2317	47
H(17B)	5355	11814	2991	47
H(18A)	9155	7095	-501	85
H(18B)	9082	5683	-641	85
H(18C)	8982	6499	360	85
H(19A)	4946	14379	3435	73
H(19B)	5272	13744	4206	73
H(19C)	3906	14096	4181	73
H(20A)	3748	11543	4156	70
H(20B)	2542	10756	3312	70
H(20C)	2392	11899	4080	70
H(22)	11212	9345	4938	61
H(25)	7653	5476	4172	48
H(26)	7916	6763	3172	52
H(27A)	10788	8683	6756	100
H(27B)	12142	8844	6247	100
H(28A)	12135	6889	6270	87
H(28B)	11874	7504	7292	87
H(33)	10613	5524	7636	49

H(35A)	7004	1945	7843	58
H(35B)	7531	1554	6865	58
H(37A)	6664	2169	5468	55
H(37B)	5747	3039	5653	55
H(38A)	9088	7841	2171	92
H(38B)	9377	9274	2210	92
H(38C)	8083	8523	2642	92
H(39A)	4568	766	6982	100
H(39B)	5196	492	6027	100
H(39C)	4076	1165	6116	100
H(40A)	6262	4092	7680	89
H(40B)	5202	2955	7979	89
H(40C)	4738	3395	7127	89

Table 6. Torsion angles [°] for Lee-A.

O(1)-C(1)-C(2)-C(3)	-178.7(3)
C(6)-C(1)-C(2)-C(3)	0.8(4)
C(1)-C(2)-C(3)-C(4)	-0.6(4)
C(1)-C(2)-C(3)-C(7)	-179.3(3)
C(2)-C(3)-C(4)-C(5)	-0.2(4)
C(7)-C(3)-C(4)-C(5)	178.5(3)
C(2)-C(3)-C(4)-C(10)	179.5(3)
C(7)-C(3)-C(4)-C(10)	-1.8(4)
C(3)-C(4)-C(5)-C(6)	0.9(4)
C(10)-C(4)-C(5)-C(6)	-178.8(2)
C(4)-C(5)-C(6)-C(1)	-0.7(4)
O(1)-C(1)-C(6)-C(5)	179.3(3)
C(2)-C(1)-C(6)-C(5)	-0.1(4)
C(2)-C(3)-C(7)-C(8)	-144.7(3)
C(4)-C(3)-C(7)-C(8)	36.6(4)
C(3)-C(7)-C(8)-C(9)	-55.2(4)
C(7)-C(8)-C(9)-C(13)	-142.1(3)
C(7)-C(8)-C(9)-C(10)	41.9(4)
C(13)-C(9)-C(10)-N(1)	-2.3(4)
C(8)-C(9)-C(10)-N(1)	174.0(2)
C(13)-C(9)-C(10)-C(4)	176.9(2)
C(8)-C(9)-C(10)-C(4)	-6.8(4)
C(5)-C(4)-C(10)-N(1)	-15.7(4)
C(3)-C(4)-C(10)-N(1)	164.6(2)
C(5)-C(4)-C(10)-C(9)	165.0(2)
C(3)-C(4)-C(10)-C(9)	-14.7(4)
C(9)-C(10)-N(1)-C(11)	0.5(4)
C(4)-C(10)-N(1)-C(11)	-178.7(2)
C(10)-N(1)-C(11)-C(12)	2.5(4)
C(10)-N(1)-C(11)-C(17)	-177.2(2)
N(1)-C(11)-C(12)-C(13)	-3.7(4)
C(17)-C(11)-C(12)-C(13)	176.0(2)
N(1)-C(11)-C(12)-C(14)	178.7(2)

C(17)-C(11)-C(12)-C(14)	-1.6(4)
C(10)-C(9)-C(13)-C(12)	1.0(4)
C(8)-C(9)-C(13)-C(12)	-175.0(3)
C(11)-C(12)-C(13)-C(9)	1.8(4)
C(14)-C(12)-C(13)-C(9)	179.4(2)
C(13)-C(12)-C(14)-O(2)	7.9(4)
C(11)-C(12)-C(14)-O(2)	-174.6(3)
C(13)-C(12)-C(14)-C(15)	-170.5(3)
C(11)-C(12)-C(14)-C(15)	7.0(4)
O(2)-C(14)-C(15)-C(16)	146.5(3)
C(12)-C(14)-C(15)-C(16)	-35.1(4)
C(14)-C(15)-C(16)-C(17)	55.4(3)
C(14)-C(15)-C(16)-C(19)	174.8(3)
C(14)-C(15)-C(16)-C(20)	-64.9(3)
N(1)-C(11)-C(17)-C(16)	-155.8(2)
C(12)-C(11)-C(17)-C(16)	24.5(4)
C(19)-C(16)-C(17)-C(11)	-169.1(2)
C(15)-C(16)-C(17)-C(11)	-49.6(3)
C(20)-C(16)-C(17)-C(11)	70.9(3)
C(6)-C(1)-O(1)-C(18)	-4.0(4)
C(2)-C(1)-O(1)-C(18)	175.4(3)
O(3)-C(21)-C(22)-C(23)	-178.2(3)
C(26)-C(21)-C(22)-C(23)	1.7(5)
C(21)-C(22)-C(23)-C(24)	-0.8(5)
C(21)-C(22)-C(23)-C(27)	-174.1(4)
C(22)-C(23)-C(24)-C(25)	-0.8(5)
C(27)-C(23)-C(24)-C(25)	172.4(3)
C(22)-C(23)-C(24)-C(30)	-179.5(3)
C(27)-C(23)-C(24)-C(30)	-6.2(5)
C(23)-C(24)-C(25)-C(26)	1.7(5)
C(30)-C(24)-C(25)-C(26)	-179.7(3)
C(24)-C(25)-C(26)-C(21)	-0.8(5)
O(3)-C(21)-C(26)-C(25)	179.0(3)
C(22)-C(21)-C(26)-C(25)	-0.9(5)
C(22)-C(23)-C(27)-C(28)	-152.8(4)

C(24)-C(23)-C(27)-C(28)	34.0(5)
C(23)-C(27)-C(28)-C(29)	-46.7(5)
C(27)-C(28)-C(29)-C(33)	-150.6(4)
C(27)-C(28)-C(29)-C(30)	34.5(5)
C(33)-C(29)-C(30)-N(2)	-1.3(4)
C(28)-C(29)-C(30)-N(2)	173.8(3)
C(33)-C(29)-C(30)-C(24)	178.0(3)
C(28)-C(29)-C(30)-C(24)	-6.8(4)
C(25)-C(24)-C(30)-N(2)	-7.9(4)
C(23)-C(24)-C(30)-N(2)	170.7(3)
C(25)-C(24)-C(30)-C(29)	172.7(3)
C(23)-C(24)-C(30)-C(29)	-8.7(4)
C(29)-C(30)-N(2)-C(31)	0.8(4)
C(24)-C(30)-N(2)-C(31)	-178.5(2)
C(30)-N(2)-C(31)-C(32)	0.1(4)
C(30)-N(2)-C(31)-C(37)	-179.6(3)
N(2)-C(31)-C(32)-C(33)	-0.4(4)
C(37)-C(31)-C(32)-C(33)	179.3(3)
N(2)-C(31)-C(32)-C(34)	-179.4(3)
C(37)-C(31)-C(32)-C(34)	0.3(4)
C(30)-C(29)-C(33)-C(32)	1.0(5)
C(28)-C(29)-C(33)-C(32)	-174.0(3)
C(31)-C(32)-C(33)-C(29)	-0.2(4)
C(34)-C(32)-C(33)-C(29)	178.9(3)
C(31)-C(32)-C(34)-O(4)	-177.2(3)
C(33)-C(32)-C(34)-O(4)	3.8(5)
C(31)-C(32)-C(34)-C(35)	3.7(4)
C(33)-C(32)-C(34)-C(35)	-175.3(3)
O(4)-C(34)-C(35)-C(36)	147.7(3)
C(32)-C(34)-C(35)-C(36)	-33.1(4)
C(34)-C(35)-C(36)-C(39)	174.8(3)
C(34)-C(35)-C(36)-C(40)	-64.7(3)
C(34)-C(35)-C(36)-C(37)	56.0(4)
N(2)-C(31)-C(37)-C(36)	-154.9(3)
C(32)-C(31)-C(37)-C(36)	25.4(4)

C(39)-C(36)-C(37)-C(31)	-170.4(3)
C(40)-C(36)-C(37)-C(31)	68.5(3)
C(35)-C(36)-C(37)-C(31)	-51.6(3)
C(22)-C(21)-O(3)-C(38)	176.5(3)
C(26)-C(21)-O(3)-C(38)	-3.4(5)

Symmetry transformations used to generate equivalent atoms:

Crystal refinement data for compound 7k

Empirical Formula-$C_{18}H_{17}NO$, M = 263.32, Monoclinic, Space group $P2_1/n$, a = 5.8897(12) Å, b = 19.960(4) Å, c = 11.987(3) Å, V = 1372.6(5) $Å^3$, Z = 4, T = 223 (2) K, ρcalcd = 1.274 Mg/m^3, $2\Theta_{max.}$ = 28.576°. Refinement of 560 parameters on 3456 independent reflections out of 22261 collected reflections (R_{int} = 0.1023) led to R1 = 0.0567 [I >2σ(I)], wR2 = 0. 1594 (all data) and S = 1.042 with the largest difference peak and hole of 0.249 and -0.298 e.$Å^{-3}$ respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2077449). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif

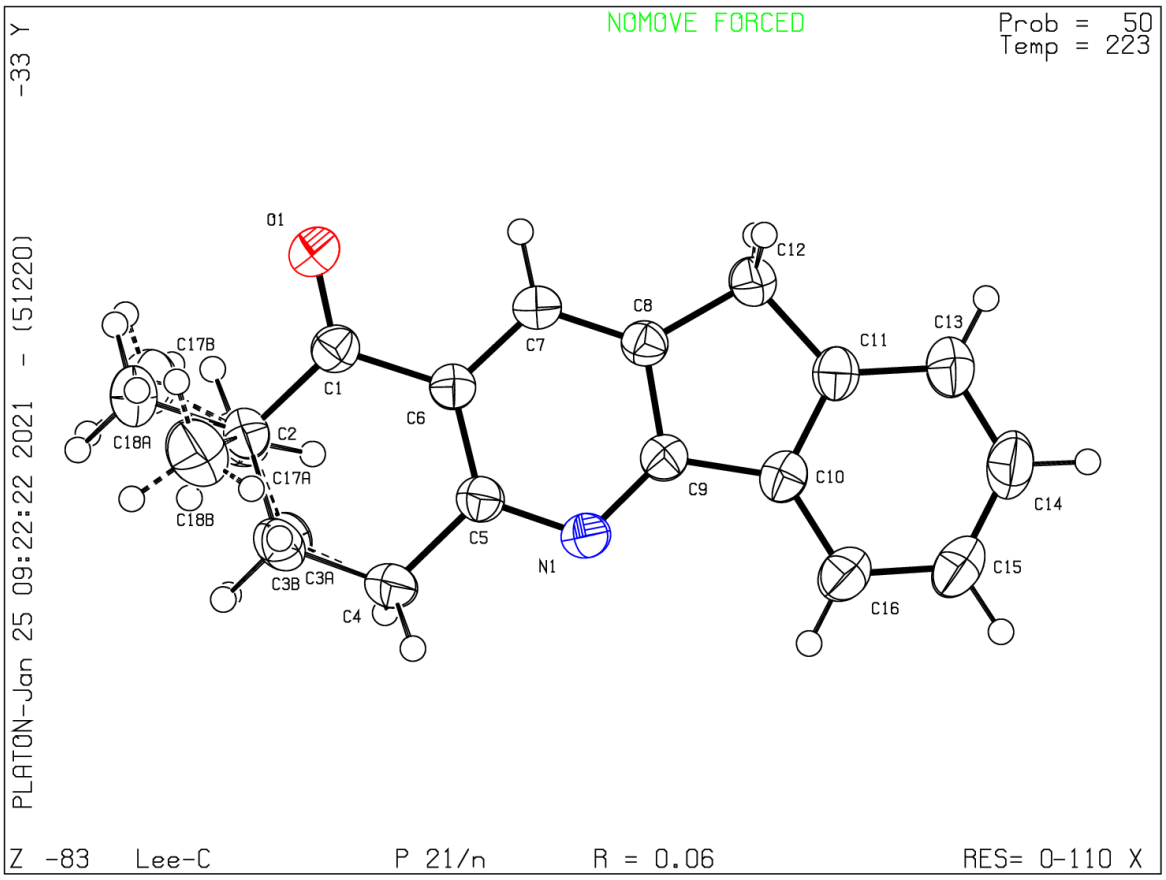


Table 1. Crystal data and structure refinement for Lee-C.

Identification code	Lee-C	
Empirical formula	C18 H17 N O	
Formula weight	263.32	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 5.8897(12) Å	α= 90°.
	b = 19.960(4) Å	β= 103.094(7)°.
	c = 11.987(3) Å	γ = 90°.
Volume	1372.6(5) $Å^3$	
Z	4	
Density (calculated)	1.274 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	560	
Crystal size	0.230 x 0.210 x 0.160 mm^3	
Theta range for data collection	2.685 to 28.576°.	
Index ranges	-7<=h<=7, -26<=k<=26, -15<=l<=16	
Reflections collected	22261	
Independent reflections	3456 [R(int) = 0.1023]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6934 and 0.6175	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3456 / 4 / 213	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0567, wR2 = 0.1367	
R indices (all data)	R1 = 0.0915, wR2 = 0.1594	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.249 and -0.298 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Lee-C. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5653(2)	3856(1)	1604(1)	47(1)
C(1)	4464(3)	3550(1)	2141(2)	34(1)
C(2)	2867(3)	2982(1)	1621(1)	41(1)
C(3A)	718(4)	2979(1)	2121(2)	44(1)
C(3B)	1900(20)	2598(6)	2434(9)	53(3)
C(4)	1237(3)	2947(1)	3411(2)	46(1)
C(5)	3107(3)	3428(1)	3984(2)	35(1)
C(6)	4645(3)	3704(1)	3375(1)	32(1)
C(7)	6430(3)	4128(1)	3940(1)	34(1)
C(8)	6618(3)	4253(1)	5082(1)	32(1)
C(9)	4966(3)	3963(1)	5614(1)	33(1)
N(1)	3227(2)	3563(1)	5099(1)	37(1)
C(10)	5498(3)	4162(1)	6820(1)	36(1)
C(11)	7502(3)	4560(1)	7021(2)	37(1)
C(12)	8366(3)	4648(1)	5944(1)	38(1)
C(13)	8426(4)	4809(1)	8109(2)	49(1)
C(14)	7302(4)	4659(1)	8975(2)	58(1)
C(15)	5319(4)	4266(1)	8775(2)	55(1)
C(16)	4385(4)	4013(1)	7696(2)	46(1)
C(17A)	4322(4)	2336(1)	1946(2)	50(1)
C(18A)	2193(5)	3034(2)	313(2)	59(1)
C(17B)	3850(20)	2592(6)	729(9)	71(4)
C(18B)	812(16)	3369(6)	870(11)	88(5)

Table 3. Bond lengths [Å] and angles [°] for Lee-C.

O(1)-C(1)	1.216(2)
C(1)-C(6)	1.491(2)
C(1)-C(2)	1.515(2)
C(2)-C(3B)	1.454(11)
C(2)-C(3A)	1.518(3)
C(2)-C(18A)	1.5311(18)
C(2)-C(17B)	1.538(2)
C(2)-C(18B)	1.543(2)
C(2)-C(17A)	1.5482(17)
C(3A)-C(4)	1.509(3)
C(3A)-H(3A)	0.9800
C(3A)-H(3B)	0.9800
C(3B)-C(4)	1.489(10)
C(3B)-H(3B1)	0.9800
C(3B)-H(3B2)	0.9800
C(4)-C(5)	1.504(2)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(5)-N(1)	1.349(2)
C(5)-C(6)	1.400(2)
C(6)-C(7)	1.400(2)
C(7)-C(8)	1.370(2)
C(7)-H(7)	0.9400
C(8)-C(9)	1.403(2)
C(8)-C(12)	1.506(2)
C(9)-N(1)	1.335(2)
C(9)-C(10)	1.463(2)
C(10)-C(16)	1.390(2)
C(10)-C(11)	1.398(2)
C(11)-C(13)	1.386(3)
C(11)-C(12)	1.501(2)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800

C(13)-C(14)	1.384(3)
C(13)-H(13)	0.9400
C(14)-C(15)	1.382(3)
C(14)-H(14)	0.9400
C(15)-C(16)	1.382(3)
C(15)-H(15)	0.9400
C(16)-H(16)	0.9400
C(17A)-H(17A)	0.9700
C(17A)-H(17B)	0.9700
C(17A)-H(17C)	0.9700
C(18A)-H(18A)	0.9700
C(18A)-H(18B)	0.9700
C(18A)-H(18C)	0.9700
C(17B)-H(17D)	0.9700
C(17B)-H(17E)	0.9700
C(17B)-H(17F)	0.9700
C(18B)-H(18D)	0.9700
C(18B)-H(18E)	0.9700
C(18B)-H(18F)	0.9700

O(1)-C(1)-C(6)	120.05(15)
O(1)-C(1)-C(2)	122.42(15)
C(6)-C(1)-C(2)	117.43(14)
C(3B)-C(2)-C(1)	114.8(4)
C(1)-C(2)-C(3A)	109.59(15)
C(1)-C(2)-C(18A)	111.26(16)
C(3A)-C(2)-C(18A)	111.01(18)
C(3B)-C(2)-C(17B)	117.9(7)
C(1)-C(2)-C(17B)	111.5(5)
C(3B)-C(2)-C(18B)	106.3(7)
C(1)-C(2)-C(18B)	101.3(5)
C(17B)-C(2)-C(18B)	102.6(8)
C(1)-C(2)-C(17A)	105.28(15)
C(3A)-C(2)-C(17A)	111.16(18)
C(18A)-C(2)-C(17A)	108.39(19)

C(4)-C(3A)-C(2)	114.32(18)
C(4)-C(3A)-H(3A)	108.7
C(2)-C(3A)-H(3A)	108.7
C(4)-C(3A)-H(3B)	108.7
C(2)-C(3A)-H(3B)	108.7
H(3A)-C(3A)-H(3B)	107.6
C(2)-C(3B)-C(4)	119.6(7)
C(2)-C(3B)-H(3B1)	107.4
C(4)-C(3B)-H(3B1)	107.4
C(2)-C(3B)-H(3B2)	107.4
C(4)-C(3B)-H(3B2)	107.4
H(3B1)-C(3B)-H(3B2)	107.0
C(3B)-C(4)-C(5)	111.3(4)
C(5)-C(4)-C(3A)	113.50(16)
C(5)-C(4)-H(4A)	108.9
C(3A)-C(4)-H(4A)	108.9
C(5)-C(4)-H(4B)	108.9
C(3A)-C(4)-H(4B)	108.9
H(4A)-C(4)-H(4B)	107.7
N(1)-C(5)-C(6)	122.92(15)
N(1)-C(5)-C(4)	116.66(15)
C(6)-C(5)-C(4)	120.41(15)
C(7)-C(6)-C(5)	119.32(15)
C(7)-C(6)-C(1)	118.82(14)
C(5)-C(6)-C(1)	121.85(15)
C(8)-C(7)-C(6)	118.36(15)
C(8)-C(7)-H(7)	120.8
C(6)-C(7)-H(7)	120.8
C(7)-C(8)-C(9)	118.12(15)
C(7)-C(8)-C(12)	131.93(15)
C(9)-C(8)-C(12)	109.93(15)
N(1)-C(9)-C(8)	125.12(15)
N(1)-C(9)-C(10)	126.13(15)
C(8)-C(9)-C(10)	108.74(14)
C(9)-N(1)-C(5)	116.11(14)

C(16)-C(10)-C(11)	121.03(17)
C(16)-C(10)-C(9)	131.00(17)
C(11)-C(10)-C(9)	107.96(15)
C(13)-C(11)-C(10)	120.10(17)
C(13)-C(11)-C(12)	129.08(17)
C(10)-C(11)-C(12)	110.82(15)
C(11)-C(12)-C(8)	102.53(14)
C(11)-C(12)-H(12A)	111.3
C(8)-C(12)-H(12A)	111.3
C(11)-C(12)-H(12B)	111.3
C(8)-C(12)-H(12B)	111.3
H(12A)-C(12)-H(12B)	109.2
C(14)-C(13)-C(11)	118.5(2)
C(14)-C(13)-H(13)	120.8
C(11)-C(13)-H(13)	120.8
C(15)-C(14)-C(13)	121.40(19)
C(15)-C(14)-H(14)	119.3
C(13)-C(14)-H(14)	119.3
C(14)-C(15)-C(16)	120.8(2)
C(14)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6
C(15)-C(16)-C(10)	118.24(19)
C(15)-C(16)-H(16)	120.9
C(10)-C(16)-H(16)	120.9
C(2)-C(17A)-H(17A)	109.5
C(2)-C(17A)-H(17B)	109.5
H(17A)-C(17A)-H(17B)	109.5
C(2)-C(17A)-H(17C)	109.5
H(17A)-C(17A)-H(17C)	109.5
H(17B)-C(17A)-H(17C)	109.5
C(2)-C(18A)-H(18A)	109.5
C(2)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(2)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5

H(18B)-C(18A)-H(18C)	109.5
C(2)-C(17B)-H(17D)	109.5
C(2)-C(17B)-H(17E)	109.5
H(17D)-C(17B)-H(17E)	109.5
C(2)-C(17B)-H(17F)	109.5
H(17D)-C(17B)-H(17F)	109.5
H(17E)-C(17B)-H(17F)	109.5
C(2)-C(18B)-H(18D)	109.5
C(2)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(2)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Lee-C. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	52(1)	54(1)	38(1)	-3(1)	18(1)	-11(1)
C(1)	33(1)	35(1)	36(1)	0(1)	9(1)	2(1)
C(2)	40(1)	46(1)	38(1)	-9(1)	9(1)	-7(1)
C(3A)	30(1)	49(1)	50(2)	-10(1)	4(1)	-4(1)
C(3B)	62(7)	49(6)	48(6)	-15(5)	16(5)	-16(5)
C(4)	40(1)	53(1)	50(1)	-11(1)	18(1)	-15(1)
C(5)	33(1)	35(1)	37(1)	-2(1)	10(1)	-2(1)
C(6)	32(1)	31(1)	32(1)	0(1)	7(1)	0(1)
C(7)	33(1)	35(1)	35(1)	1(1)	10(1)	-3(1)
C(8)	32(1)	32(1)	33(1)	1(1)	7(1)	-1(1)
C(9)	34(1)	30(1)	33(1)	2(1)	8(1)	1(1)
N(1)	39(1)	38(1)	38(1)	-1(1)	14(1)	-5(1)
C(10)	42(1)	33(1)	33(1)	2(1)	9(1)	4(1)
C(11)	40(1)	38(1)	32(1)	0(1)	4(1)	4(1)
C(12)	38(1)	42(1)	34(1)	0(1)	5(1)	-4(1)
C(13)	52(1)	56(1)	37(1)	-6(1)	4(1)	-3(1)
C(14)	67(2)	72(1)	34(1)	-9(1)	6(1)	-1(1)
C(15)	70(1)	64(1)	36(1)	1(1)	20(1)	2(1)
C(16)	54(1)	49(1)	39(1)	2(1)	17(1)	0(1)
C(17A)	48(1)	38(1)	65(2)	-10(1)	18(1)	-3(1)
C(18A)	64(2)	74(2)	37(2)	-11(1)	7(1)	-18(2)
C(17B)	77(8)	74(8)	67(8)	-28(7)	30(7)	-13(7)
C(18B)	89(10)	107(11)	63(9)	-8(8)	6(7)	-40(9)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Lee-C.

	x	y	z	U(eq)
H(3A)	-188	3385	1869	52
H(3B)	-253	2594	1811	52
H(3B1)	3034	2250	2755	63
H(3B2)	505	2368	2000	63
H(4A)	-195	3045	3667	56
H(4B)	1721	2490	3656	56
H(7)	7473	4323	3546	41
H(12A)	9942	4466	6030	46
H(12B)	8365	5121	5725	46
H(13)	9783	5072	8255	59
H(14)	7900	4829	9715	70
H(15)	4598	4170	9380	66
H(16)	3032	3748	7557	56
H(17A)	3343	1947	1707	74
H(17B)	4923	2322	2769	74
H(17C)	5612	2333	1566	74
H(18A)	1314	3443	94	89
H(18B)	1246	2651	1	89
H(18C)	3593	3042	15	89
H(17D)	5204	2335	1115	106
H(17E)	4311	2905	200	106
H(17F)	2673	2290	310	106
H(18D)	-261	3056	406	132
H(18E)	1398	3677	374	132
H(18F)	6	3620	1357	132

Table 6. Torsion angles [°] for Lee-C.

O(1)-C(1)-C(2)-C(3B)	169.6(6)
C(6)-C(1)-C(2)-C(3B)	-6.9(6)
O(1)-C(1)-C(2)-C(3A)	-146.32(19)
C(6)-C(1)-C(2)-C(3A)	37.1(2)
O(1)-C(1)-C(2)-C(18A)	-23.2(3)
C(6)-C(1)-C(2)-C(18A)	160.25(18)
O(1)-C(1)-C(2)-C(17B)	32.2(6)
C(6)-C(1)-C(2)-C(17B)	-144.4(6)
O(1)-C(1)-C(2)-C(18B)	-76.3(6)
C(6)-C(1)-C(2)-C(18B)	107.1(6)
O(1)-C(1)-C(2)-C(17A)	94.0(2)
C(6)-C(1)-C(2)-C(17A)	-82.54(19)
C(1)-C(2)-C(3A)-C(4)	-55.1(2)
C(18A)-C(2)-C(3A)-C(4)	-178.42(19)
C(17A)-C(2)-C(3A)-C(4)	60.8(2)
C(1)-C(2)-C(3B)-C(4)	36.7(11)
C(17B)-C(2)-C(3B)-C(4)	171.3(8)
C(18B)-C(2)-C(3B)-C(4)	-74.4(10)
C(2)-C(3B)-C(4)-C(5)	-45.6(10)
C(2)-C(3A)-C(4)-C(5)	46.5(3)
C(3B)-C(4)-C(5)-N(1)	-153.6(6)
C(3A)-C(4)-C(5)-N(1)	162.38(17)
C(3B)-C(4)-C(5)-C(6)	25.4(6)
C(3A)-C(4)-C(5)-C(6)	-18.7(3)
N(1)-C(5)-C(6)-C(7)	1.4(2)
C(4)-C(5)-C(6)-C(7)	-177.41(16)
N(1)-C(5)-C(6)-C(1)	-179.57(15)
C(4)-C(5)-C(6)-C(1)	1.6(2)
O(1)-C(1)-C(6)-C(7)	-9.3(2)
C(2)-C(1)-C(6)-C(7)	167.32(14)
O(1)-C(1)-C(6)-C(5)	171.65(15)
C(2)-C(1)-C(6)-C(5)	-11.7(2)
C(5)-C(6)-C(7)-C(8)	0.7(2)

C(1)-C(6)-C(7)-C(8)	-178.33(14)
C(6)-C(7)-C(8)-C(9)	-1.9(2)
C(6)-C(7)-C(8)-C(12)	176.53(16)
C(7)-C(8)-C(9)-N(1)	1.1(2)
C(12)-C(8)-C(9)-N(1)	-177.62(15)
C(7)-C(8)-C(9)-C(10)	-179.88(14)
C(12)-C(8)-C(9)-C(10)	1.40(18)
C(8)-C(9)-N(1)-C(5)	0.9(2)
C(10)-C(9)-N(1)-C(5)	-177.91(15)
C(6)-C(5)-N(1)-C(9)	-2.2(2)
C(4)-C(5)-N(1)-C(9)	176.70(15)
N(1)-C(9)-C(10)-C(16)	-1.6(3)
C(8)-C(9)-C(10)-C(16)	179.40(17)
N(1)-C(9)-C(10)-C(11)	177.66(15)
C(8)-C(9)-C(10)-C(11)	-1.34(18)
C(16)-C(10)-C(11)-C(13)	0.6(3)
C(9)-C(10)-C(11)-C(13)	-178.75(16)
C(16)-C(10)-C(11)-C(12)	-179.89(16)
C(9)-C(10)-C(11)-C(12)	0.76(19)
C(13)-C(11)-C(12)-C(8)	179.52(18)
C(10)-C(11)-C(12)-C(8)	0.06(18)
C(7)-C(8)-C(12)-C(11)	-179.38(17)
C(9)-C(8)-C(12)-C(11)	-0.90(18)
C(10)-C(11)-C(13)-C(14)	-0.7(3)
C(12)-C(11)-C(13)-C(14)	179.84(18)
C(11)-C(13)-C(14)-C(15)	0.7(3)
C(13)-C(14)-C(15)-C(16)	-0.5(3)
C(14)-C(15)-C(16)-C(10)	0.3(3)
C(11)-C(10)-C(16)-C(15)	-0.4(3)
C(9)-C(10)-C(16)-C(15)	178.81(17)

Symmetry transformations used to generate equivalent atoms:

Crystal refinement data for compound 10j

Empirical Formula-$C_{23}H_{21}N$, M = 311.41, Orthorhombic, Space group Pbcn, a = 11.1052(10) Å, b = 16.1802(15) Å, c = 9.2208(9) Å, V = 1656.8(3) $Å^3$, Z = 4, T = 223 (2) K, ρcalcd = 1.248 Mg/m^3, $2\Theta_{max.}$ = 28.339°. Refinement of 664 parameters on 2066 independent reflections out of 21473 collected reflections (R_{int} = 0.0563) led to R1 = 0.0412 [I >2σ(I)], wR2 = 0. 1118 (all data) and S = 1.061 with the largest difference peak and hole of 0.223 and -0.183 e.$Å^{-3}$ respectively. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2077450). The data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/data_request/cif

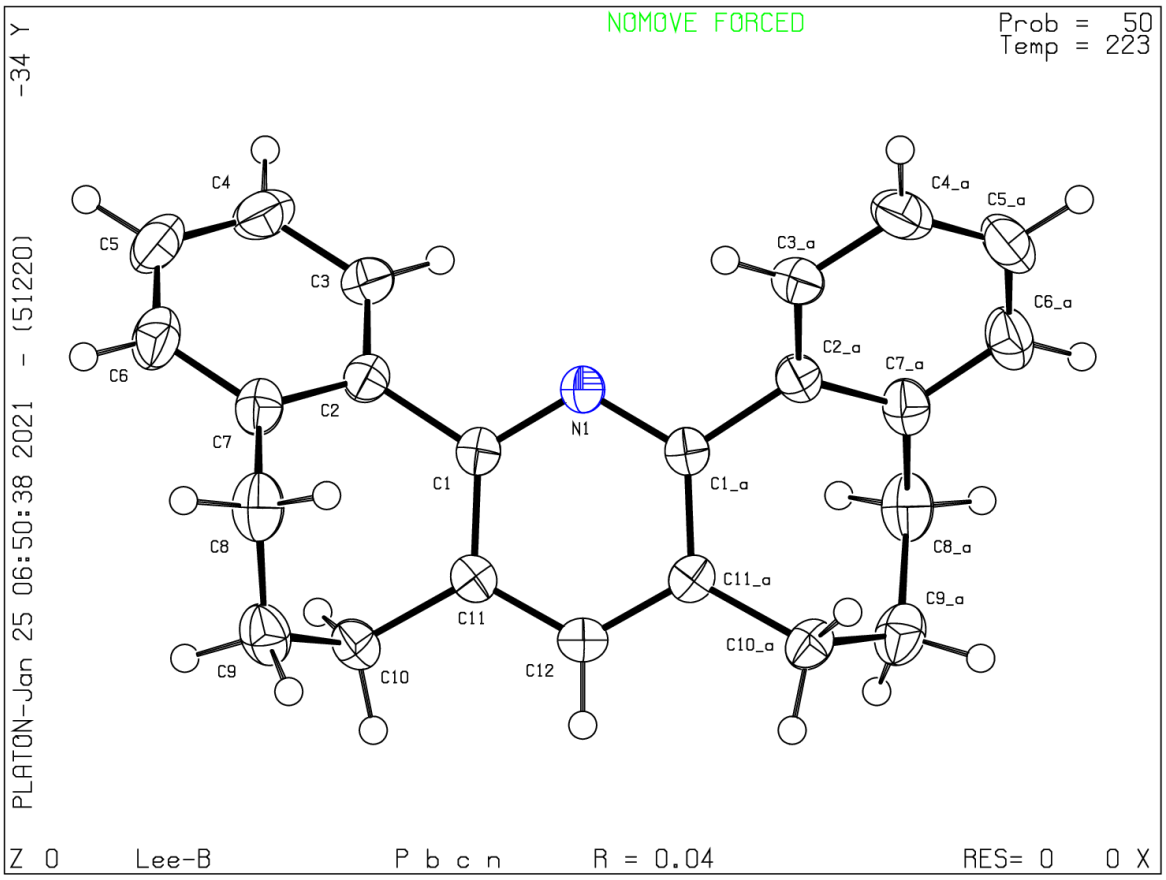


Table 1. Crystal data and structure refinement for Lee-B.

Identification code	Lee-B	
Empirical formula	C23 H21 N	
Formula weight	311.41	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 11.1052(10) Å	α= 90°.
	b = 16.1802(15) Å	β= 90°.
	c = 9.2208(9) Å	γ = 90°.
Volume	1656.8(3) $Å^3$	
Z	4	
Density (calculated)	1.248 Mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	664	
Crystal size	0.420 x 0.230 x 0.130 mm^3	
Theta range for data collection	3.135 to 28.339°.	
Index ranges	-14<=h<=14, -21<=k<=20, -11<=l<=12	
Reflections collected	21473	
Independent reflections	2066 [R(int) = 0.0563]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6458	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2066 / 0 / 110	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0412, wR2 = 0.1000	
R indices (all data)	R1 = 0.0577, wR2 = 0.1118	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.223 and -0.183 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Lee-B. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	5000	6211(1)	7500	26(1)
C(1)	4208(1)	5788(1)	6683(1)	25(1)
C(2)	3388(1)	6288(1)	5757(1)	28(1)
C(3)	3847(1)	6950(1)	4968(1)	35(1)
C(4)	3118(1)	7403(1)	4044(2)	44(1)
C(5)	1915(1)	7205(1)	3912(2)	47(1)
C(6)	1446(1)	6560(1)	4716(2)	42(1)
C(7)	2160(1)	6092(1)	5645(1)	33(1)
C(8)	1633(1)	5409(1)	6553(2)	40(1)
C(9)	1991(1)	4540(1)	6072(2)	40(1)
C(10)	3320(1)	4473(1)	5648(1)	32(1)
C(11)	4175(1)	4920(1)	6642(1)	26(1)
C(12)	5000	4503(1)	7500	27(1)

Table 3. Bond lengths [Å] and angles [°] for Lee-B.

N(1)-C(1)	1.3448(13)
N(1)-C(1)#1	1.3448(13)
C(1)-C(11)	1.4049(16)
C(1)-C(2)	1.4871(16)
C(2)-C(3)	1.3920(17)
C(2)-C(7)	1.4044(17)
C(3)-C(4)	1.3853(18)
C(3)-H(3)	0.9400
C(4)-C(5)	1.379(2)
C(4)-H(4)	0.9400
C(5)-C(6)	1.382(2)
C(5)-H(5)	0.9400
C(6)-C(7)	1.3914(18)
C(6)-H(6)	0.9400
C(7)-C(8)	1.5044(19)
C(8)-C(9)	1.5273(19)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(9)-C(10)	1.5303(18)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(10)-C(11)	1.5053(16)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(11)-C(12)	1.3868(14)
C(12)-C(11)#1	1.3868(14)
C(12)-H(12)	0.9400

C(1)-N(1)-C(1)#1	118.88(14)
N(1)-C(1)-C(11)	122.72(11)
N(1)-C(1)-C(2)	116.48(10)
C(11)-C(1)-C(2)	120.75(10)
C(3)-C(2)-C(7)	119.43(11)

C(3)-C(2)-C(1)	119.62(11)
C(7)-C(2)-C(1)	120.95(11)
C(4)-C(3)-C(2)	120.99(13)
C(4)-C(3)-H(3)	119.5
C(2)-C(3)-H(3)	119.5
C(5)-C(4)-C(3)	119.81(14)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	119.59(13)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
C(5)-C(6)-C(7)	121.77(13)
C(5)-C(6)-H(6)	119.1
C(7)-C(6)-H(6)	119.1
C(6)-C(7)-C(2)	118.40(12)
C(6)-C(7)-C(8)	121.37(12)
C(2)-C(7)-C(8)	120.20(11)
C(7)-C(8)-C(9)	114.41(11)
C(7)-C(8)-H(8A)	108.7
C(9)-C(8)-H(8A)	108.7
C(7)-C(8)-H(8B)	108.7
C(9)-C(8)-H(8B)	108.7
H(8A)-C(8)-H(8B)	107.6
C(8)-C(9)-C(10)	113.00(11)
C(8)-C(9)-H(9A)	109.0
C(10)-C(9)-H(9A)	109.0
C(8)-C(9)-H(9B)	109.0
C(10)-C(9)-H(9B)	109.0
H(9A)-C(9)-H(9B)	107.8
C(11)-C(10)-C(9)	114.73(11)
C(11)-C(10)-H(10A)	108.6
C(9)-C(10)-H(10A)	108.6
C(11)-C(10)-H(10B)	108.6
C(9)-C(10)-H(10B)	108.6
H(10A)-C(10)-H(10B)	107.6

C(12)-C(11)-C(1)	117.02(11)
C(12)-C(11)-C(10)	121.98(11)
C(1)-C(11)-C(10)	120.92(11)
C(11)#1-C(12)-C(11)	121.65(15)
C(11)#1-C(12)-H(12)	119.2
C(11)-C(12)-H(12)	119.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Lee-B. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	25(1)	28(1)	25(1)	0	0(1)	0
C(1)	24(1)	30(1)	23(1)	-1(1)	2(1)	1(1)
C(2)	30(1)	30(1)	24(1)	-3(1)	-1(1)	5(1)
C(3)	39(1)	28(1)	38(1)	0(1)	-3(1)	3(1)
C(4)	58(1)	32(1)	43(1)	5(1)	-4(1)	9(1)
C(5)	53(1)	44(1)	43(1)	0(1)	-13(1)	21(1)
C(6)	33(1)	51(1)	43(1)	-5(1)	-7(1)	13(1)
C(7)	29(1)	41(1)	29(1)	-6(1)	0(1)	7(1)
C(8)	26(1)	61(1)	34(1)	1(1)	6(1)	0(1)
C(9)	32(1)	49(1)	38(1)	5(1)	0(1)	-11(1)
C(10)	33(1)	33(1)	29(1)	-3(1)	-2(1)	-5(1)
C(11)	26(1)	29(1)	23(1)	-2(1)	3(1)	-2(1)
C(12)	31(1)	25(1)	26(1)	0	4(1)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Lee-B.

	x	y	z	U(eq)
H(3)	4664	7092	5064	42
H(4)	3442	7844	3508	53
H(5)	1418	7506	3280	56
H(6)	622	6434	4633	51
H(8A)	753	5453	6525	49
H(8B)	1887	5488	7561	49
H(9A)	1494	4378	5241	48
H(9B)	1826	4151	6863	48
H(10A)	3544	3887	5624	38
H(10B)	3419	4692	4664	38
H(12)	5000	3922	7500	33

Table 6. Torsion angles [°] for Lee-B.

C(1)#1-N(1)-C(1)-C(11)	-0.22(8)
C(1)#1-N(1)-C(1)-C(2)	-177.60(11)
N(1)-C(1)-C(2)-C(3)	44.12(15)
C(11)-C(1)-C(2)-C(3)	-133.31(12)
N(1)-C(1)-C(2)-C(7)	-137.02(11)
C(11)-C(1)-C(2)-C(7)	45.55(16)
C(7)-C(2)-C(3)-C(4)	-1.92(19)
C(1)-C(2)-C(3)-C(4)	176.96(12)
C(2)-C(3)-C(4)-C(5)	0.9(2)
C(3)-C(4)-C(5)-C(6)	0.6(2)
C(4)-C(5)-C(6)-C(7)	-1.0(2)
C(5)-C(6)-C(7)-C(2)	0.0(2)
C(5)-C(6)-C(7)-C(8)	177.97(13)
C(3)-C(2)-C(7)-C(6)	1.47(18)
C(1)-C(2)-C(7)-C(6)	-177.39(11)
C(3)-C(2)-C(7)-C(8)	-176.53(11)
C(1)-C(2)-C(7)-C(8)	4.61(18)
C(6)-C(7)-C(8)-C(9)	109.22(14)
C(2)-C(7)-C(8)-C(9)	-72.84(16)
C(7)-C(8)-C(9)-C(10)	41.60(16)
C(8)-C(9)-C(10)-C(11)	42.25(16)
N(1)-C(1)-C(11)-C(12)	0.43(15)
C(2)-C(1)-C(11)-C(12)	177.70(9)
N(1)-C(1)-C(11)-C(10)	-176.52(9)
C(2)-C(1)-C(11)-C(10)	0.76(17)
C(9)-C(10)-C(11)-C(12)	113.26(12)
C(9)-C(10)-C(11)-C(1)	-69.96(15)
C(1)-C(11)-C(12)-C(11)#1	-0.20(7)
C(10)-C(11)-C(12)-C(11)#1	176.71(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2