Supplementary information

Assembly of substituted phenanthridines via a cascade palladium-catalyzed coupling reaction, deprotection and intramolecular cyclization

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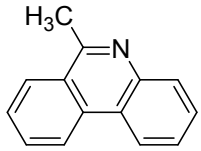
1. General details

All the reactions were monitored by thin-layer chromatography (TLC) and were visualized using UV light (254 nm). ^{1}H NMR spectra were recorded on Mercury-400 spectrometer (400 MHz). ^{13}C NMR spectra were recorded on Mercury-400 spectrometer (100 MHz) and BRUKER AV-III-500 spectrometer (125MHz). ^{1}H NMR spectra Chemical shifts (δ ppm) and coupling constants (Hz) are reported in standard fashion with reference to either internal standard tetramethylsilane (TMS) (δH=0.00 ppm) or $CDCl_3$ (δH=7.25 ppm), DMSO (δH=2.50 ppm). ^{13}C NMR spectra chemical shifts (δ ppm) and coupling constants (Hz) are reported relative to $CDCl_3$ [δC=77.36 ppm (central line of triplet)] and DMSO [δC=40.45 ppm (central line of heptet)]. HRMS (ESI) data were measured on Thermo Exactive Orbitrap plus spectrometer. Flash column chromatography was performed on Biotage Isolera one. Column chromatography characterization was performed with silica gel (300-400mesh). Melting points were measured with Yanaco MP-J3 microscope melting point apparatus.

2. General procedure for the preparation of substituted phenanthridines

2-acetyl/benzoylphenyl triflates/halide (1.0 mmol) or substituted 2-bromobenzaldehyde (1.0 mmol), 2-(Boc-amino)benzeneboronic acid pinacol ester (1.2 mmol), $Pd(PPh_3)_4$ (3 mmol%) and Na_2CO_3 (2.0 mmol) were combined in a 25 mL round bottomed flask. Glycol (3 mL) was added and the resulted reaction mixture was stirred at 120°C for 2 h under argon atmosphere. Progress of the reaction was monitored by TLC till the reaction was completed. The reaction was quenched by addition of H_2O (10 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine (3 × 20 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Purification of the residue on a silica gel column chromatography (15:1 hexanes/EtOAc) afforded the desired product.

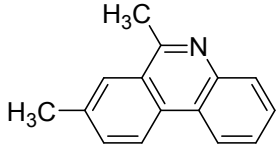
6-methylphenanthridine (3a)



3a

Yield 80%; white solid; m.p. 81-83 °C; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.58 (t, J = 9.2 Hz, 1H), 8.50 (t, J = 8.6 Hz, 1H), 8.18 (t, J = 9.2 Hz, 1H), 8.11 (d, J = 8.2 Hz, 1H), 7.80 (q, J = 8.6, 8.2 Hz, 1H), 7.74 – 7.64 (m, 1H), 7.64 – 7.52 (m, 2H), 3.04 (s, 2H); ^{13}C NMR (100 MHz, Chloroform-d) δ 159.1 , 143.9 , 132.8 , 130.7 , 129.6 , 128.8 , 127.5 , 126.7 , 126.5 , 126.1 , 124.0 , 122.5 , 122.2 , 23.6; HRMS (ESI): m/z calcd for $C_{14}H_{12}N$ $[M+H]^+$ 194.0964, found 194.0956.

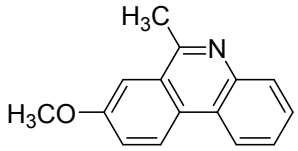
6, 8-dimethylphenanthridine (3b)



3b

Yield 75%; white solid; m.p. 83-85 °C; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.52 (t, J = 7.3 Hz, 2H), 8.11 (d, J = 8.1 Hz, 1H), 8.00 (s, 1H), 7.68 (d, J = 7.8 Hz, 2H), 7.61 (t, J = 7.6 Hz, 1H), 3.04 (s, 3H), 2.62 (s, 3H); ^{13}C NMR (125 MHz, Chloroform-d) δ 158.7 , 143.1 , 137.3 , 132.4 , 130.5 , 129.1 , 128.3 , 126.4 , 126.2 , 126.0 , 123.9 , 122.3 , 121.8 , 23.3 , 21.9; HRMS (ESI): m/z calcd for $C_{15}H_{14}N$ $[M+H]^+$ 208.1121, found 208.1122.

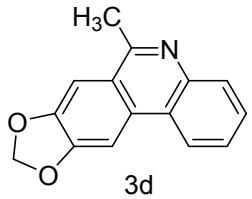
8-methoxy-6-methylphenanthridine (3c)



3c

Yield 74%; white solid; m.p. 55-57 °C; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.54 (d, J = 9.0 Hz, 1H), 8.45 (d, J = 7.9 Hz, 1H), 8.09 (d, J = 8.0 Hz, 1H), 7.65 (t, J = 7.5 Hz, 1H), 7.59 (t, J = 7.5 Hz, 1H), 7.51 (s, 1H), 7.48 (d, J = 9.1 Hz, 1H), 4.00 (s, 3H), 3.02 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 158.8 , 158.1 , 142.9 , 129.4 , 127.8 , 127.3 , 127.0 , 126.6 , 124.1 , 124.0 , 121.6 , 120.9 , 106.9 , 55.7 , 23.6; HRMS (ESI): m/z calcd for $C_{15}H_{14}ON$ $[M+H]^+$ 224.1070, found 224.1060.

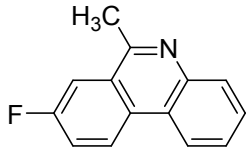
6-methyl-[1,3]dioxolo[4,5-j]phenanthridine (3d)



3d

Yield 81%; white solid; m.p. 193-195 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 (d, *J* = 8.1 Hz, 1H), 8.06 (d, *J* = 8.1 Hz, 1H), 7.89 (s, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.48 (s, 1H), 6.15 (s, 2H), 2.95 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 157.4 , 151.1 , 148.3 , 133.3 , 130.5 , 129.4 , 128.2 , 126.2 , 124.1 , 122.6 , 121.9 , 104.0 , 102.1 , 100.4 , 23.9; HRMS (ESI): m/z calcd for $C_{15}H_{12}O_2N$ $[M+H]^+$ 238.0863, found 238.0860.

8-fluoro-6-methylphenanthridine (3e)

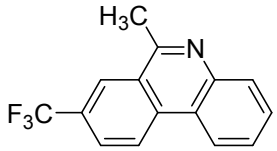


3e

Yield 69%; white solid; m.p. 92-94 °C; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.60 (s, 1H), 8.46 (d, J = 8.1 Hz, 1H), 8.10 (d, J = 8.1 Hz, 1H), 7.81 (d, J = 9.7 Hz, 1H), 7.70 (t, J = 7.6 Hz, 1H), 7.63 (d, J = 7.5 Hz, 1H), 7.58 (t, J = 9.7 Hz, 1H), 3.00 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 161.6 (d, *J* = 247.5 Hz), 158.1 , 143.5 , 136.4 , 129.7 , 128.8 , 127.3 , 127.0 , 125.1 (d, *J* =

7.4 Hz), 123.5 , 121.9 , 119.8 (d, *J* = 23.8 Hz), 111.4 (d, *J* = 21.2 Hz), 23.6; HRMS (ESI): m/z calcd for $C_{14}H_{11}NF$ $[M+H]^+$ 212.0870, found 212.0870.

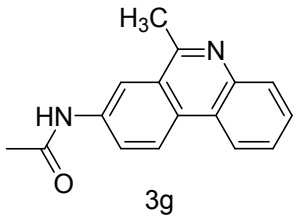
6-methyl-8-(trifluoromethyl)phenanthridine (3f)



3f

Yield 68%; white solid; m.p. 108-110 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.68 (d, *J* = 8.6 Hz, 1H), 8.51 (d, *J* = 8.3 Hz, 1H), 8.45 (s, 1H), 8.12 (d, *J* = 8.2 Hz, 1H), 8.00 (d, *J* = 8.7 Hz, 1H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 3.06 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 158.6 , 144.5 , 134.8 , 130.0 , 129.8 , 129.1 (q, *J* = 32.6 Hz), 127.0 , 126.3 (q, *J* = 3.3 Hz), 125.2 ,124.2 (q, *J* = 271 Hz), 124.0 (q, *J* = 4.3 Hz), 123.4 , 122.8 (d, *J* = 6.6 Hz), 122.4, 23.4; HRMS (ESI): m/z calcd for $C_{15}H_{11}NF_3$ $[M+H]^+$ 262.0838, found 262.0831.

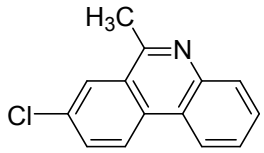
N-(6-methylphenanthridin-8-yl)acetamide (3g)



3g

Yield 64%; white solid; m.p. 248-250 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.41 (s, 1H), 8.77 (d, *J* = 8.9 Hz, 1H), 8.65 (d, *J* = 8.0 Hz, 1H), 8.60 (s, 1H), 8.08 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.4 Hz, 1H), 2.91 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 169.5 , 158.7 , 143.3 , 139.4 , 129.6 , 128.6 , 128.1 , 127.1 , 126.5 , 124.2 , 123.9 , 123.7 , 122.8 , 115.0 , 24.8 , 23.7; HRMS (ESI): m/z calcd for $C_{16}H_{15}ON_2$ $[M+H]^+$ 251.1179, found 251.1169.

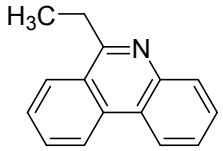
8-chloro-6-methylphenanthridine (3h)



3h

Yield 52%; white solid; m.p. 117-119 °C; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.50 (d, J = 8.8 Hz, 1H), 8.44 (d, J = 8.2 Hz, 1H), 8.14 (s, 1H), 8.09 (d, J = 8.2 Hz, 1H), 7.75 (d, J = 9.7 Hz, 1H), 7.70 (d, J = 7.7 Hz, 1H), 7.61 (t, J = 7.5 Hz, 1H), 2.99 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 157.9 , 143.8 , 133.4 , 131.2 , 131.2 , 129.7 , 129.2 , 127.0 , 127.0 , 126.1 , 124.3 , 123.3 , 122.0 , 23.5; HRMS (ESI): m/z calcd for $C_{14}H_{11}NCl$ $[M+H]^+$ 228.0575, found 228.0566.

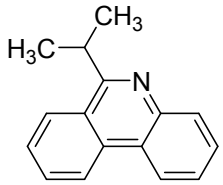
6-ethylphenanthridine (3i)



3i

Yield 77%; white solid; m.p. 51-53 °C; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.61 (d, J = 7.8 Hz, 2H), 8.52 (d, J = 8.0 Hz, 1H), 8.24 (d, J = 8.1 Hz, 1H), 8.14 (d, J = 8.2 Hz, 1H), 7.80 (t, J = 7.7 Hz, 1H), 7.76 – 7.62 (m, 1H), 7.60 (t, J = 7.6 Hz, 1H), 3.41 (q, J = 7.6 Hz, 2H), 1.52 (t, J = 7.6 Hz, 3H);^{13}C NMR (100 MHz, Chloroform-d) δ 163.4 , 144.0 , 133.1 , 130.5 , 129.8 , 128.8 , 127.4 , 126.5 , 126.4 , 125.2 , 123.9 , 122.7 , 122.1 , 29.6 , 13.8; HRMS (ESI): m/z calcd for $C_{15}H_{14}N$ $[M+H]^+$ 208.1121, found 208.1112.

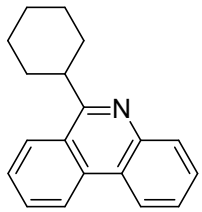
6-isopropylphenanthridine (3j)



3j

Yield 66%; yellow oil; ^{1}H NMR (400 MHz,) δ 8.66 (d, *J* = 8.3 Hz, 1H), 8.54 (d, *J* = 8.2 Hz, 1H), 8.33 (d, *J* = 8.3 Hz, 1H), 8.17 (d, *J* = 8.2 Hz, 1H), 7.82 (t, *J* = 7.7 Hz, 1H), 7.70 (q, *J* = 8.2 Hz, 2H), 7.61 (t, *J* = 7.6 Hz, 1H), 4.01 (hept, *J* = 6.6 Hz, 1H), 1.54 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, Chloroform-d) δ 166.1 , 144.0 , 136.4 , 133.3 , 130.2 , 128.6 , 127.3 , 126.4 , 125.9 , 125.0 , 123.7 , 122.8 , 122.0 , 31.7 , 22.2; HRMS (ESI): m/z calcd for $C_{16}H_{16}N$ $[M+H]^+$ 222.1277, found 222.1268.

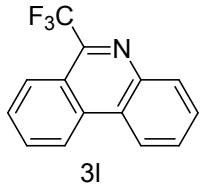
6-cyclohexylphenanthridine (3k)



3k

Yield 58%; yellow oil; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.83 (d, *J* = 8.3 Hz, 1H), 8.72 (d, *J* = 8.1 Hz, 1H), 8.41 (d, *J* = 8.2 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.90 (t, *J* = 7.7 Hz, 1H), 7.77 (t, *J* = 7.7 Hz, 1H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.64 (t, *J* = 7.7 Hz, 1H), 3.67 (s, 1H), 1.95 (d, *J* = 13.0 Hz, 2H), 1.84 (d, *J* = 12.6 Hz, 2H), 1.77 (t, *J* = 12.0 Hz, 3H), 1.55 (q, *J* = 13.2 Hz, 2H), 1.30 (q, *J* = 13.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.7 , 143.6 , 133.1 , 131.4 , 129.9 , 129.9 , 129.4 , 128.5 , 127.2 , 126.4 , 124.6 , 123.6 , 123.2 , 41.5 , 32.8 , 26.8 , 26.6; HRMS (ESI): m/z calcd for $C_{19}H_{20}N$ $[M+H]^+$ 262.1590, found 262.1579.

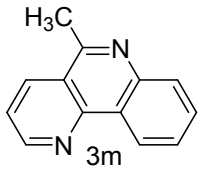
6-(trifluoromethyl)phenanthridine (3l)



3l

Yield 67%; white solid; m.p. 71-73 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.62 (d, *J* = 8.4 Hz, 1H), 8.53 (d, *J* = 7.8 Hz, 1H), 8.35 (d, *J* = 8.6 Hz, 1H), 8.26 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.83 – 7.67 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 146.7 (q, *J* = 32.8 Hz), 141.9 , 134.1 , 131.5 , 131.3 , 129.5 , 129.4 , 128.2 , 126.1 (d, *J* = 3.4 Hz), 125.3 , 122.7 , 122.2, 122.1 (d, *J* = 270.0 Hz) , 121.9 ; HRMS (ESI): m/z calcd for $C_{14}H_9NF_3$ $[M+H]^+$ 248.0682, found 248.0673.

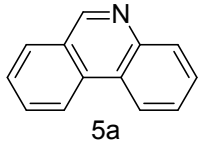
5-methylbenzo[h] [1, 6]naphthyridine (3m)



3m

Yield 55%; yellow solid; m.p. 110-112 °C; ^{1}H NMR (400 MHz,) δ 9.14 (d, *J* = 4.5 Hz, 1H), 9.09 (d, *J* = 8.1 Hz, 1H), 8.47 (d, *J* = 8.2 Hz, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 7.81 (t, *J* = 7.6 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.61 (dd, *J* = 8.3, 4.4 Hz, 1H), 3.04 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 158.7 , 152.9 , 148.8 , 145.9 , 134.2 , 130.5 , 128.8 , 127.0 , 125.0 , 123.9 , 122.5 , 120.7 , 22.9; HRMS (ESI): m/z calcd for $C_{13}H_{11}N_2$ $[M+H]^+$ 195.0917, found 195.0913.

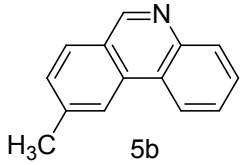
Phenanthridine (5a)



5a

Yield 66%; white solid; m.p. 105-107 °C; ^{1}H NMR (400 MHz,) δ 9.32 (s, 1H), 8.65 (d, *J* = 8.3 Hz, 1H), 8.61 (d, *J* = 8.1 Hz, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 7.9 Hz, 1H), 7.93 (t, *J* = 7.7 Hz, 1H), 7.84 – 7.63 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 153.8 , 144.7 , 132.8 , 131.2 , 130.4 , 129.0 , 128.9 , 127.7 , 127.3 , 126.6 , 124.3 , 122.4 , 122.1; HRMS (ESI): m/z calcd for $C_{13}H_{10}N$ $[M+H]^+$ 180.0808, found 180.0801.

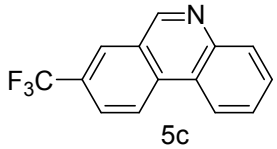
9-methylphenanthridine (5b)



5b

Yield 75%; yellow oil; ^{1}H NMR (400 MHz,) δ 9.20 (s, 1H), 8.52 (d, *J* = 8.1 Hz, 1H), 8.34 (s, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 2.62 (s, 3H).; ^{13}C NMR (100 MHz, Chloroform-d) δ 153.2 , 144.3 , 142.0 , 133.0 , 130.0 , 129.5 , 128.9 , 128.8 , 127.2 , 124.7 , 124.2 , 122.4 , 121.7 , 22.7; HRMS (ESI): m/z calcd for $C_{14}H_{12}N$ $[M+H]^+$ 194.0964, found 194.0957.

8-(trifluoromethyl)phenanthridine (5c)

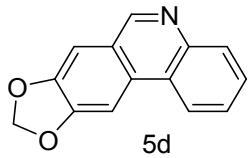


5c

Yield 63%; white solid; m.p. 103-105 °C;^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.34 (s, 1H),

8.71 (d, *J* = 8.7 Hz, 1H), 8.59 (d, *J* = 8.2 Hz, 1H), 8.34 (s, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 8.04 (d, *J* = 8.7 Hz, 1H), 7.83 (t, *J* = 7.6 Hz, 1H), 7.75 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-d) δ 153.3 , 145.3 , 134.9 , 130.6 , 130.2 , 129.7 (d, *J* = 33.0 Hz), 128.0 , 127.1 (q, *J* = 2.8 Hz), 126.4 (q, *J* = 4.1 Hz), 125.7 , 125.5 , 123.4 , 123.3 , 122.8; HRMS (ESI): m/z calcd for $C_{14}H_9NF_3$ $[M+H]^+$ 248.0682, found 248.0670.

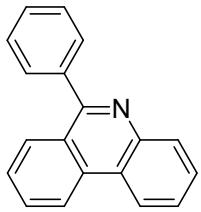
Trisphaeridine (5d)



5d

Yield 85%; white solid; m.p. 138-140 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.07 (s, 1H), 8.35 (d, *J* = 8.2 Hz, 1H), 8.15 (d, *J* = 8.1 Hz, 1H), 7.87 (s, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.31 (s, 1H), 6.15 (s, 2H); ^{13}C NMR (100 MHz, Chloroform-d) δ 151.8 , 148.4 , 144.1 , 130.5 , 130.1 , 128.3 , 126.9 , 124.5 , 123.2 , 122.2 , 110.0 , 105.7 , 102.2 , 100.1; HRMS (ESI): m/z calcd for $C_{14}H_{10}O_2N$ $[M+H]^+$ 224.0706, found 224.0697.

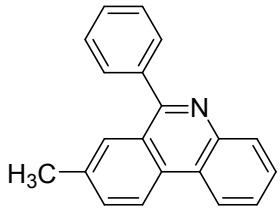
6-phenylphenanthridine (7a)



7a

Yield 89%; white solid; m.p. 103-105 °C; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.70 (d, J = 8.3 Hz, 1H), 8.62 (d, J = 8.1 Hz, 1H), 8.27 (d, J = 8.1 Hz, 1H), 8.11 (d, J = 8.3 Hz, 1H), 7.85 (t, J = 7.7 Hz, 1H), 7.75 (d, J = 7.9 Hz, 3H), 7.69 (t, J = 7.6 Hz, 1H), 7.66 – 7.48 (m, 4H); ^{13}C NMR (100 MHz, Chloroform-d) δ 161.5 , 144.0 , 140.0 , 133.7 , 130.8 , 130.6 , 130.0 , 129.2 , 129.1 , 129.0 , 128.7 , 127.4 , 127.2 , 125.5 , 124.0 , 122.4 , 122.2; HRMS (ESI): m/z calcd for $C_{19}H_{14}N$ $[M+H]^+$ 256.1121, found 256.1120.

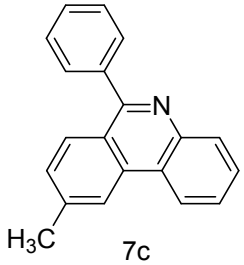
8-methyl-6-phenylphenanthridine (7b)



7b

Yield 94%; white solid; m.p. 84-86 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.56 (d, *J* = 8.5 Hz, 2H), 8.23 (d, *J* = 8.1 Hz, 1H), 7.85 (s, 1H), 7.72 (d, *J* = 7.4 Hz, 3H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.61 – 7.46 (m, 3H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 161.2 , 143.7 , 140.2 , 137.4 , 132.6 , 131.6 , 130.5 , 130.0 , 128.9 , 128.7 , 128.6 , 128.4 , 127.1 , 125.6 , 124.1 , 122.4 , 122.0 , 22.0; HRMS (ESI): m/z calcd for $C_{20}H_{16}N$ $[M+H]^+$ 270.1277, found 270.1265.

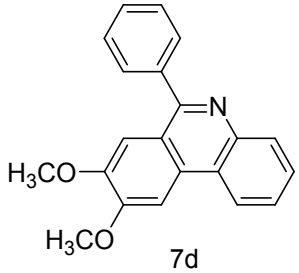
9-methyl-6-phenylphenanthridine (7c)



7c

Yield 86%; white solid; m.p. 77-79 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.61 (d, *J* = 8.1 Hz, 1H), 8.49 (s, 1H), 8.25 (d, *J* = 8.1 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 7.4 Hz, 3H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.59 – 7.50 (m, 3H), 7.44 (d, *J* = 8.5 Hz, 1H), 2.66 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 161.3 , 144.2 , 141.2 , 140.1 , 133.8 , 130.5 , 130.0 , 129.1 , 129.0 , 128.9 , 128.9 , 128.6 , 126.9 , 123.9 , 123.6 , 122.2 , 122.1 , 22.5; HRMS (ESI): m/z calcd for $C_{20}H_{16}N$ $[M+H]^+$ 270.1277, found 270.1267.

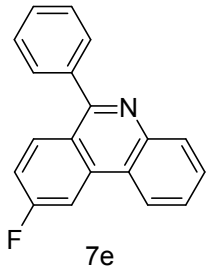
8, 9-dimethoxy-6-phenylphenanthridine (7d)



7d

Yield 60%; white solid; m.p. 137-139 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (d, *J* = 8.1 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 7.98 (s, 1H), 7.76 (d, *J* = 7.3 Hz, 2H), 7.71 (t, *J* = 7.5 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.60 – 7.49 (m, 3H), 7.45 (s, 1H), 4.16 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 159.8 , 152.7 , 149.5 , 143.7 , 140.4 , 130.6 , 129.7 , 128.9 , 128.7 , 128.2 , 126.7 , 123.7 , 121.7 , 120.7 , 108.6 , 108.5 , 102.3 , 56.4 , 56.1; HRMS (ESI): m/z calcd for $C_{21}H_{18}O_2N$ $[M+H]^+$ 316.1259, found 316.1322.

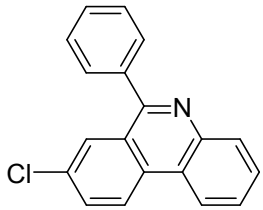
9-fluoro-6-phenylphenanthridine (7e)



7e

Yield 68%; white solid; m.p. 144-146 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 8.2 Hz, 1H), 8.25 (d, *J* = 8.6 Hz, 2H), 8.11 (dd, *J* = 9.1, 5.8 Hz, 1H), 7.78 (t, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 7.1 Hz, 2H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.65 – 7.43 (m, 3H), 7.32 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-d) δ 164.0 (d, *J* = 252.3 Hz), 160.8 , 144.3 , 139.8 , 136.1 (d, *J* = 9.3 Hz), 132.1 (d, *J* = 9.3 Hz), 130.6 , 129.9 , 129.8 , 129.1 , 128.8 , 127.2 , 123.5 (d, *J* = 4.0 Hz), 122.5 , 122.3 , 116.4 (d, *J* = 23.6 Hz), 107.6 (d, *J* = 22.2 Hz); HRMS (ESI): m/z calcd for $C_{19}H_{13}NF$ $[M+H]^+$ 274.1027, found 274.1017.

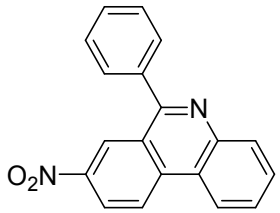
8-chloro-6-phenylphenanthridine (7f)



7f

Yield 55%; white solid; m.p. 120-122 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.64 (d, *J* = 8.8 Hz, 1H), 8.56 (d, *J* = 8.1 Hz, 1H), 8.28 (d, *J* = 8.1 Hz, 1H), 8.08 (s, 1H), 7.81 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.77 – 7.66 (m, 2H), 7.63 – 7.52 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 160.3 , 143.8 , 139.2 , 133.4 , 132.1 , 131.4 , 130.6 , 129.9 , 129.4 , 129.3 , 128.9 , 128.2 , 127.6 , 126.4 , 124.3 , 123.3 , 122.1; HRMS (ESI): m/z calcd for $C_{19}H_{13}NCl$ $[M+H]^+$ 290.0731, found 290.0722.

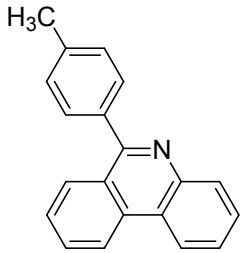
8-nitro-6-phenylphenanthridine (7g)



7g

Yield 80%; yellow solid; m.p. 230-232 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.04 (s, 1H), 8.84 (d, *J* = 9.0 Hz, 1H), 8.69 – 8.56 (m, 2H), 8.33 (d, *J* = 8.2 Hz, 1H), 7.89 (t, *J* = 7.6 Hz, 1H), 7.83 – 7.73 (m, 3H), 7.68 – 7.53 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.7 , 141.6 , 140.4 , 133.8 , 133.0 , 126.5 , 126.2 , 125.3 , 125.1 , 124.4 , 123.4 , 120.5 , 120.1 , 119.7 , 119.6 , 118.3 , 117.9; HRMS (ESI): m/z calcd for $C_{19}H_{13}O_2N_2$ $[M+H]^+$ 301.0972, found 301.0958.

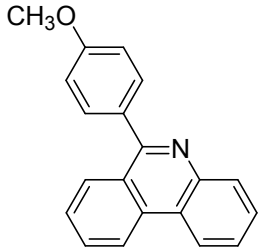
6-(p-tolyl)phenanthridine (7h)



7h

Yield 87%; white solid; m.p. 78-80 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 8.3 Hz, 1H), 8.62 (d, *J* = 8.1 Hz, 1H), 8.26 (d, *J* = 8.1 Hz, 1H), 8.15 (d, *J* = 8.3 Hz, 1H), 7.86 (t, *J* = 7.7 Hz, 1H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.38 (d, *J* = 7.7 Hz, 2H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 161.5 , 144.1 , 138.8 , 137.1 , 133.7 , 130.7 , 130.6 , 130.0 , 129.3 , 129.2 , 129.0 , 127.3 , 127.0 , 125.5 , 123.9 , 122.4 , 122.2 , 21.7; HRMS (ESI): m/z calcd for $C_{20}H_{16}N$ $[M+H]^+$ 270.1277, found 270.1269.

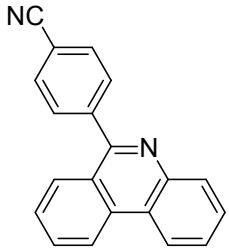
6-(4-methoxyphenyl)phenanthridine (7i)



7i

Yield59%; white solid; m.p. 146-148 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 8.3 Hz, 1H), 8.61 (d, *J* = 8.1 Hz, 1H), 8.28 (s, 1H), 8.18 (d, *J* = 8.3 Hz, 1H), 7.87 (t, *J* = 7.7 Hz, 1H), 7.80 – 7.66 (m, 4H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.10 (d, *J* = 8.2 Hz, 2H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-d) δ 161.1 , 160.4 , 144.1 , 133.7 , 132.5 , 131.5 , 130.7 , 130.5 , 129.1 , 129.0 , 127.3 , 127.0 , 125.5 , 123.8 , 122.4 , 122.2 , 114.1 , 55.7; HRMS (ESI): m/z calcd for $C_{20}H_{16}ON$ $[M+H]^+$ 286.1226, found 286.1218.

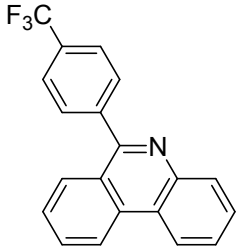
6-(4-cyano-phenyl)phenanthridine (7j)



7j

Yield 86%; white solid; m.p. 179-181 °C; ^{1}H NMR (400 MHz,) δ 8.96 (d, *J* = 8.3 Hz, 1H), 8.86 (d, *J* = 7.9 Hz, 1H), 8.12 (d, *J* = 7.9 Hz, 1H), 8.06 (d, *J* = 7.9 Hz, 2H), 7.99 (t, *J* = 7.8 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.91 (d, *J* = 7.9 Hz, 2H), 7.82 (t, *J* = 7.4 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.75 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (100MHz, DMSO-d_6) δ 159.5 , 144.3 , 143.6 , 133.5 , 133.0 , 132.1 , 131.3 , 130.5 , 130.0 , 128.8 , 128.7 , 128.4 , 124.6 , 124.1 , 123.7 , 123.5 , 119.4 , 112.2; HRMS (ESI): m/z calcd for $C_{20}H_{13}N_2$ $[M+H]^+$ 281.1073, found 281.1063.

6-(4-(trifluoromethyl)phenyl)phenanthridine (7k)

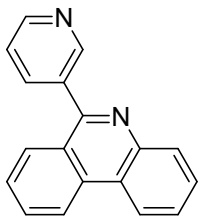


7k

Yield 89%; white solid; m.p. 171-173 °C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.75 (d, *J* = 8.4 Hz, 1H), 8.65 (d, *J* = 8.1 Hz, 1H), 8.26 (d, *J* = 8.1 Hz, 1H), 8.04 (d, *J* = 8.2 Hz, 1H), 7.95 – 7.83 (m, 5H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 159.9 , 143.9 , 143.6 , 133.7 , 131.1 , 131.0 (d, *J* = 32.3 Hz),

130.6 , 130.4 , 129.3 , 128.5 , 127.6 , 125.7 (d, J = 3.8 Hz), 125.1 , 124.5 (d, J = 270.0 Hz) 124.1 , 122.6 , 122.2 ; HRMS (ESI): m/z calcd for $C_{20}H_{13}NF_3$ $[M+H]^+$ 324.0995, found 324.0984.

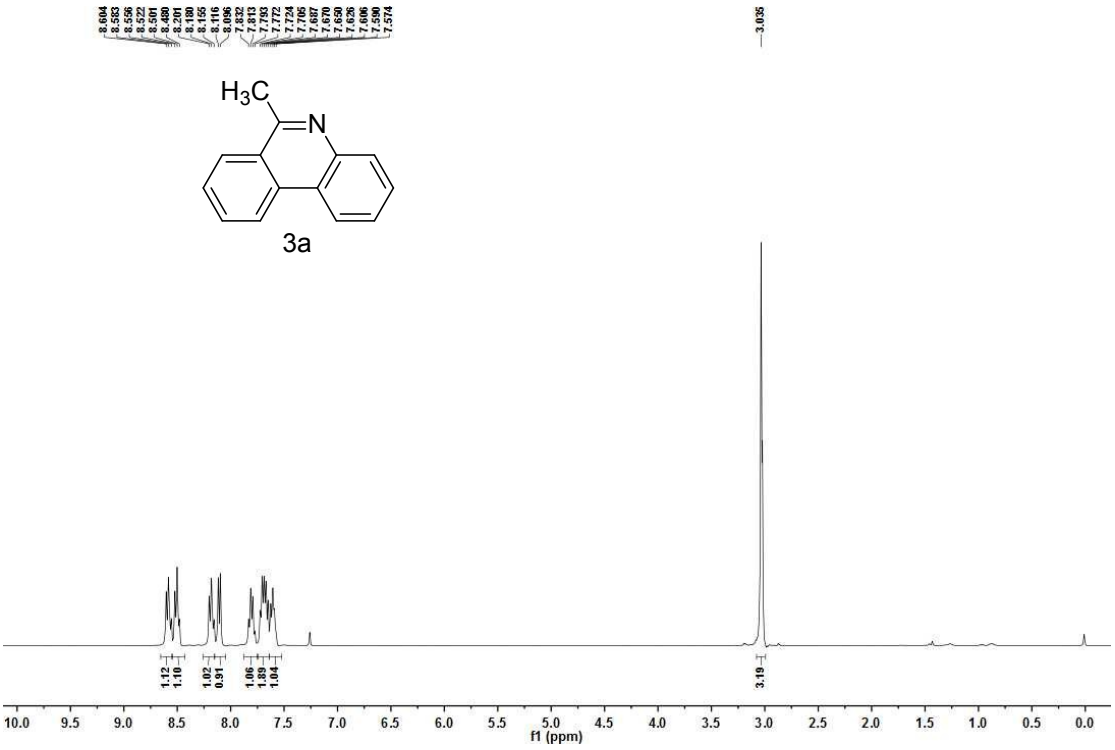
6-(pyridin-3-yl)phenanthridine (7l)

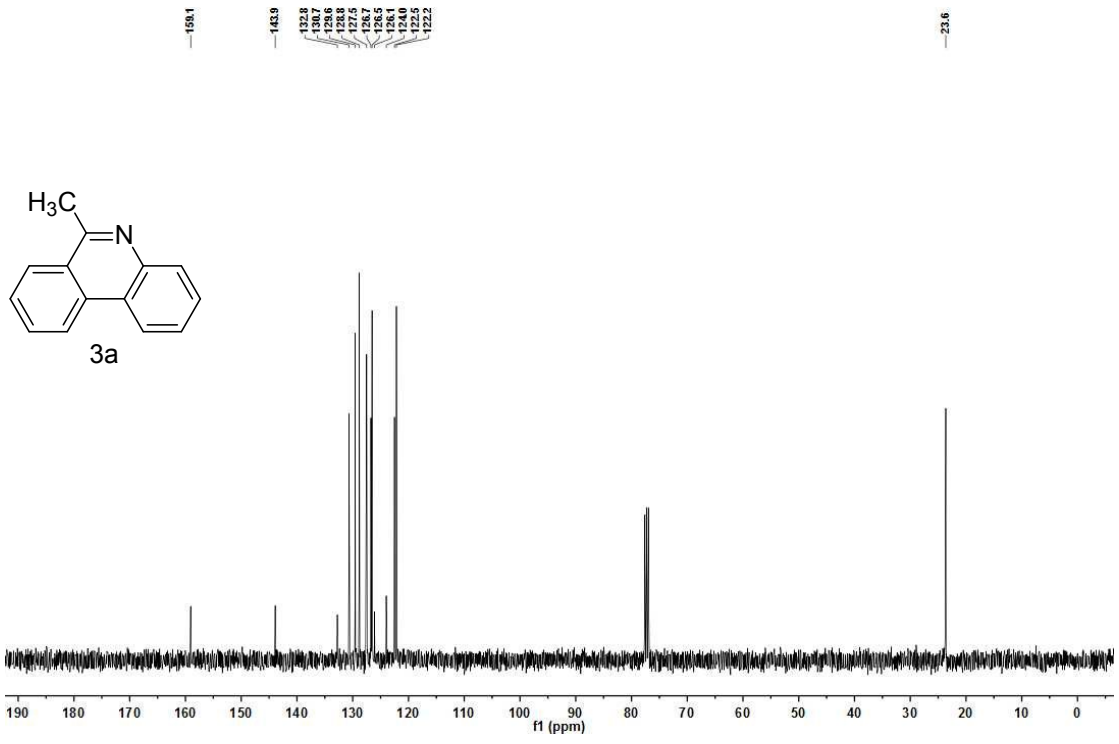


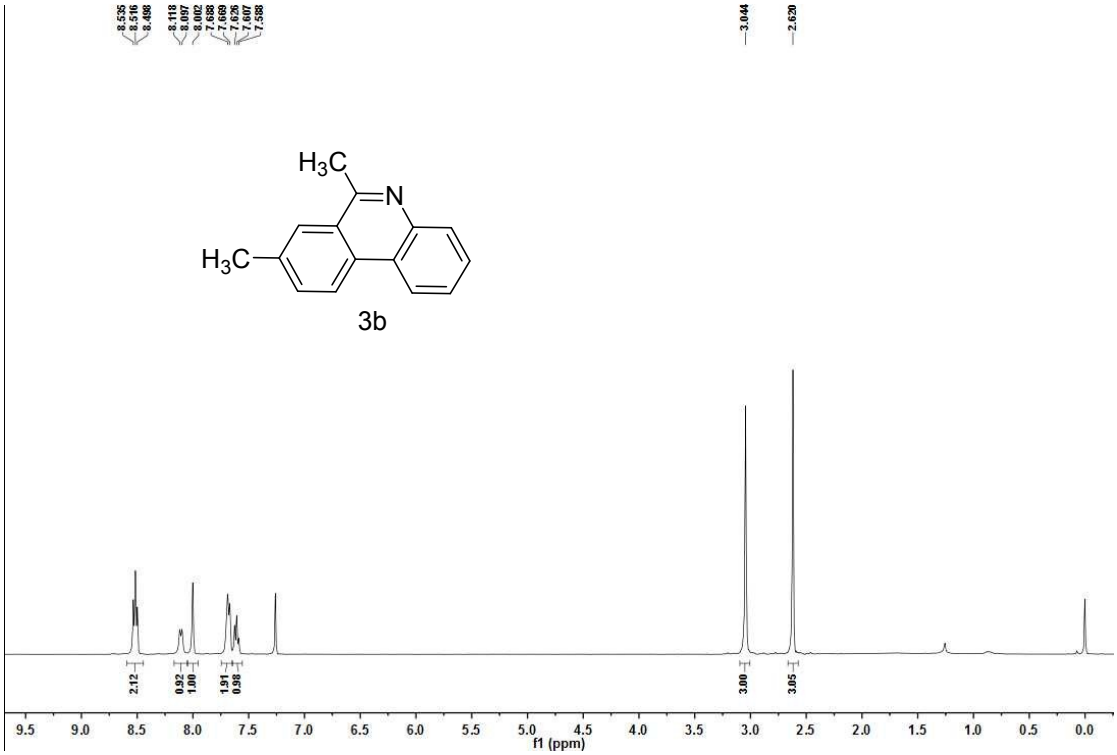
7l

Yield 51%; white solid; m.p. 102-104 °C; ^{1}H NMR (400 MHz,) δ 9.03 (s, 1H), 8.80 (d, J = 4.8 Hz, 1H), 8.74 (d, J = 8.3 Hz, 1H), 8.64 (d, J = 8.0 Hz, 1H), 8.25 (d, J = 8.0 Hz, 1H), 8.14 (d, J = 7.6 Hz, 1H), 8.05 (d, J = 8.2 Hz, 1H), 7.90 (t, J = 7.5 Hz, 1H), 7.79 (t, J = 7.5 Hz, 1H), 7.73 (t, J = 7.5 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.59 – 7.49 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-d) δ 158.2 , 150.7 , 150.1 , 144.0 , 137.5 , 135.8 , 133.7 , 131.1 , 130.6 , 129.3 , 128.3 , 127.7 , 127.6 , 125.2 , 124.1 , 123.6 , 122.7 , 122.3; HRMS (ESI): m/z calcd for $C_{18}H_{13}N_2$ $[M+H]^+$ 257.1073, found 257.1067.

3. ^{1}H and ^{13}C NMR Spectra



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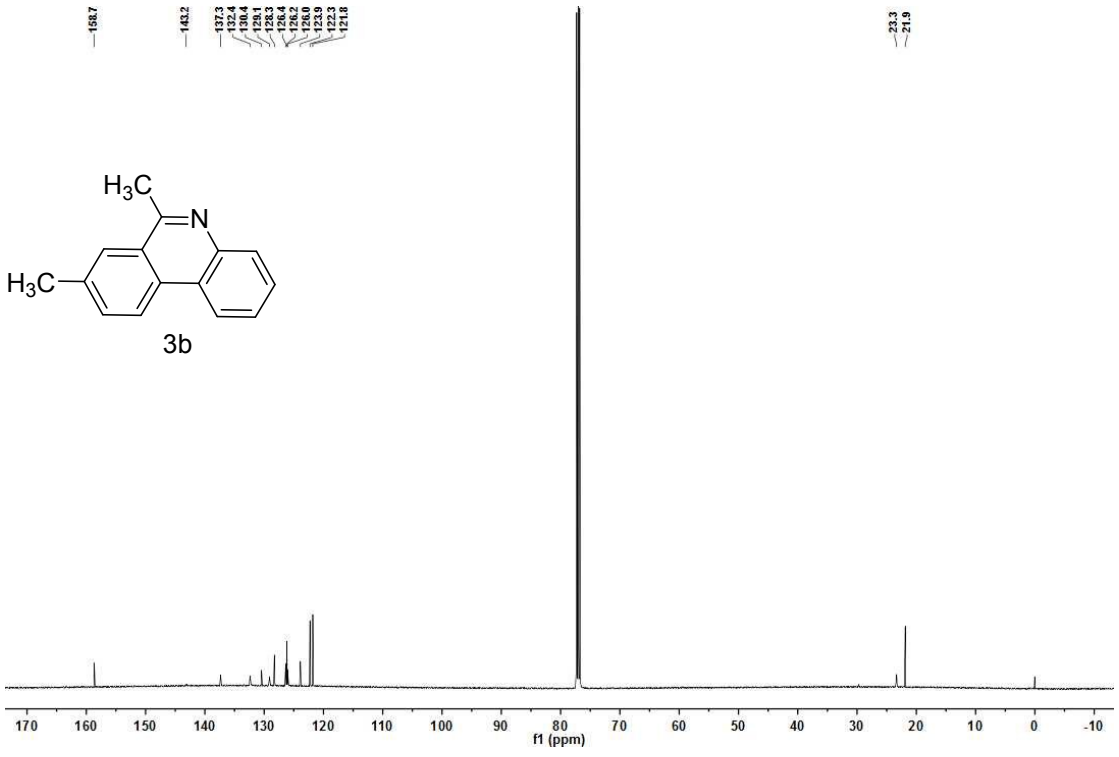
8.486
8.115
8.097
8.002
7.688
7.669
7.626
7.607
7.588
3.044
2.620
H3C
N
H3C
3b
2.12
0.92
1.00
1.91
0.98
3.00
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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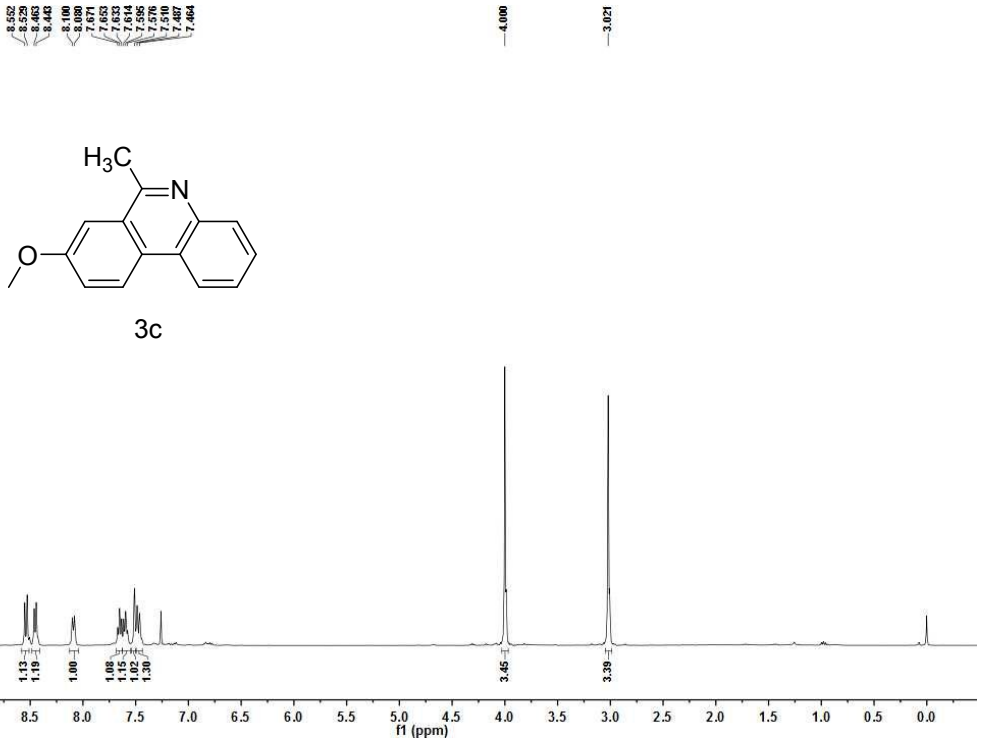
132.4
130.4
129.1
128.3
126.4
126.2
126.0
123.9
122.3
121.8
23.3
21.9
H3C
N
H3C
3b
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.614
7.595
7.576
7.510
7.487
7.464
4.000
3.021
H3C
N
O
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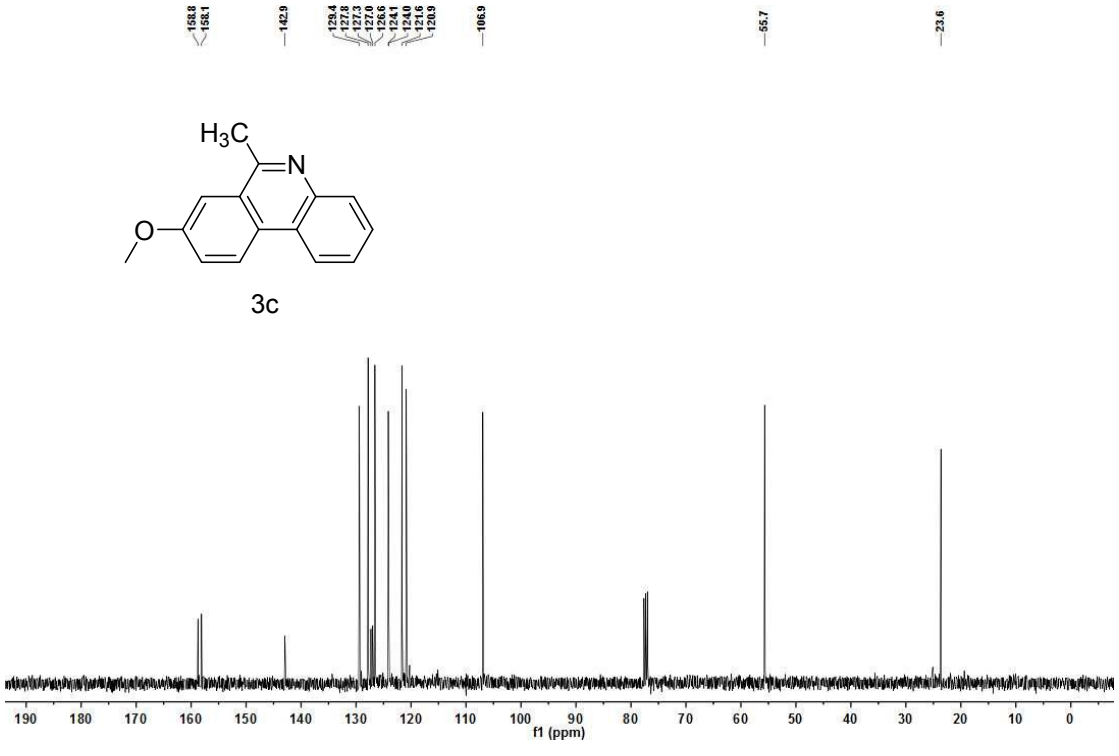
1.00
1.08
1.15
1.02
1.30
3.45
3.39
f1 (ppm)

3c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158.1
142.9
129.4
127.8
127.3
127.0
126.6
124.1
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121.6
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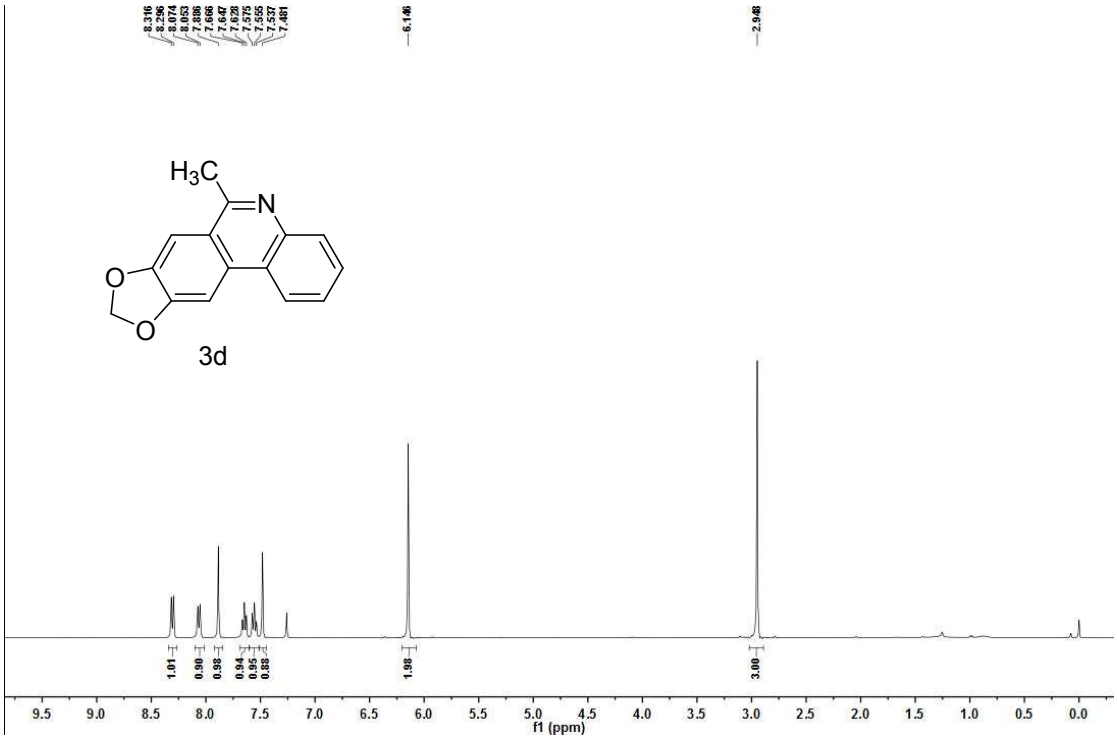
55.7
23.6
H3C
N
O
f1 (ppm)

3c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7.628
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2.948
H3C
N
O
O
3d
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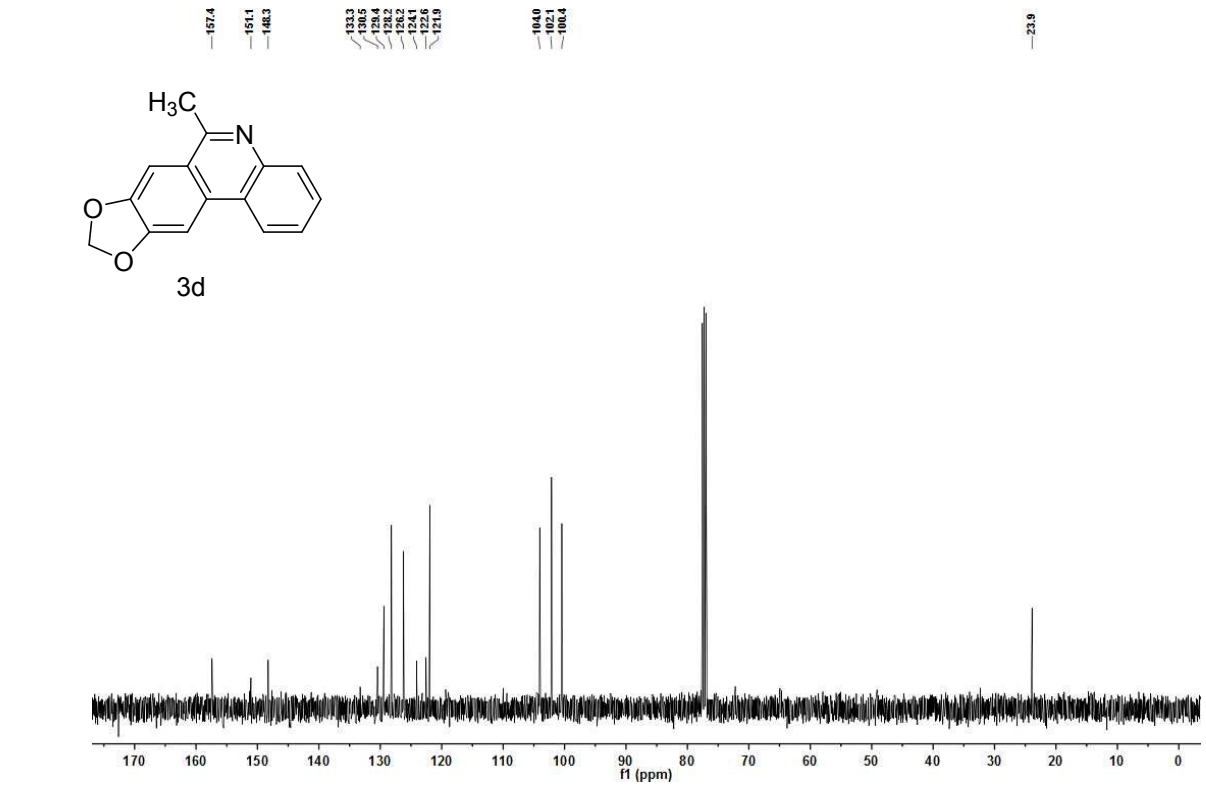
0.94
0.95
0.88
1.98
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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151.1
148.3
133.3
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128.2
126.2
124.1
121.6
121.0
104.0
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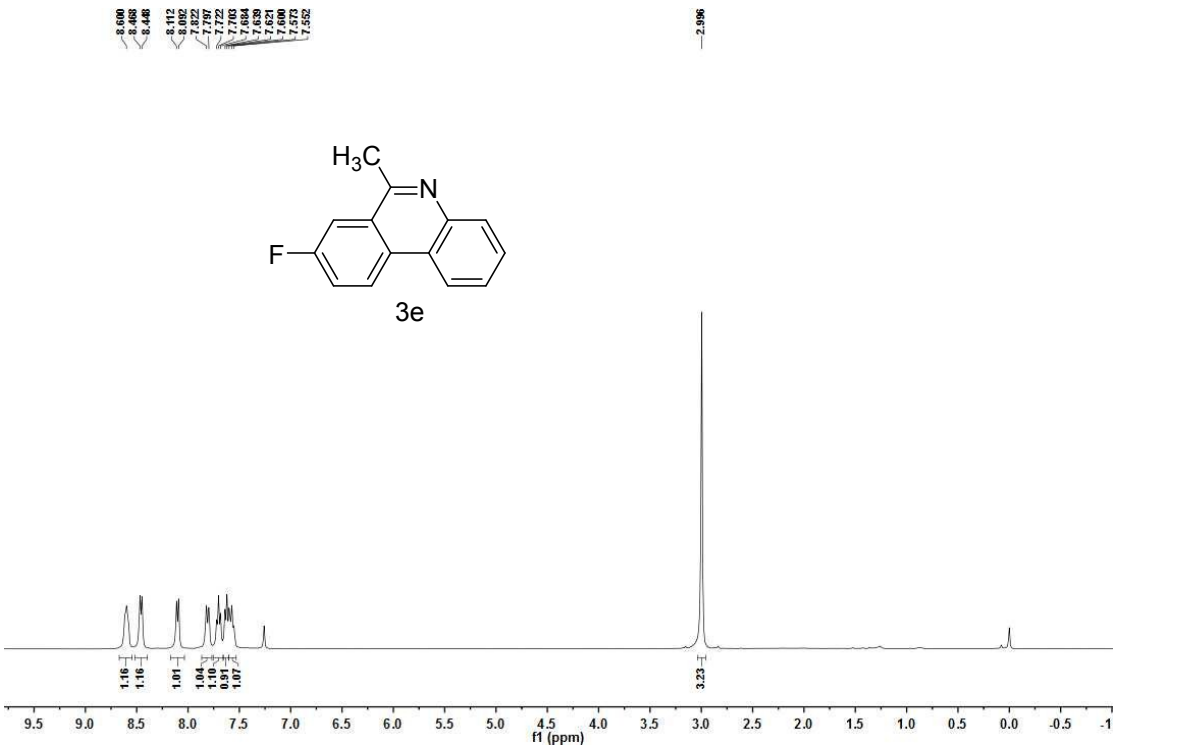
23.9
H3C
N
O
O
3d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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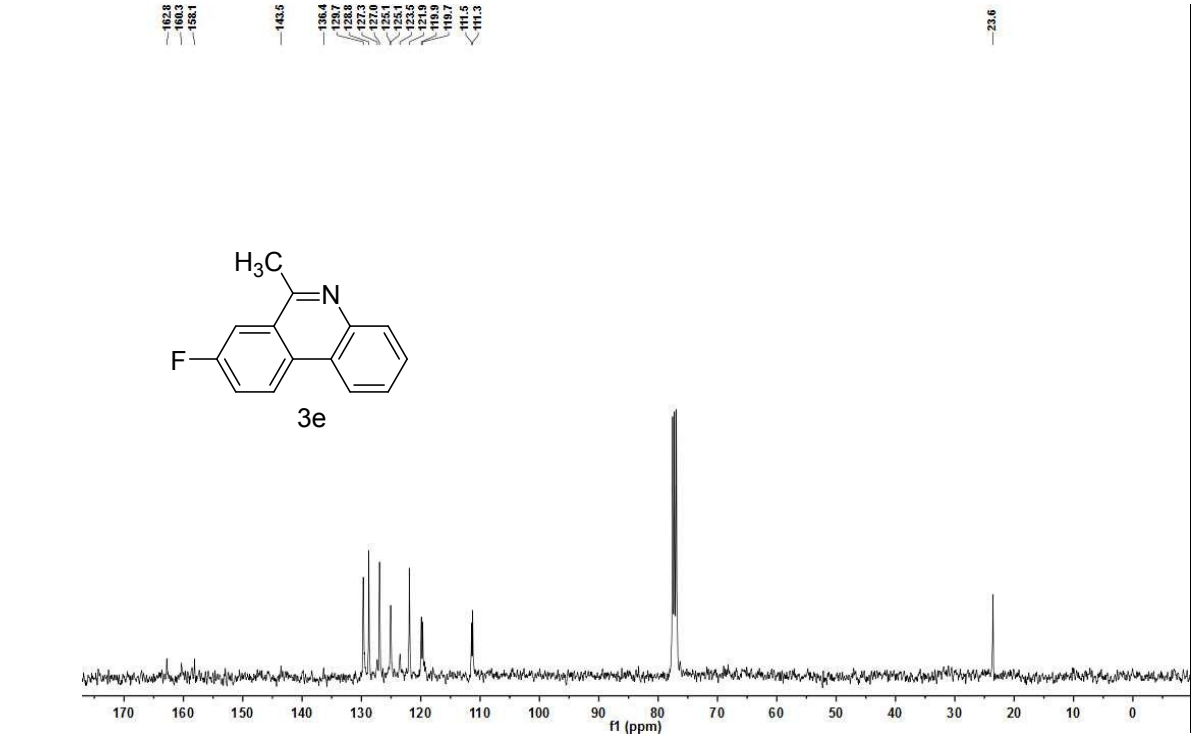
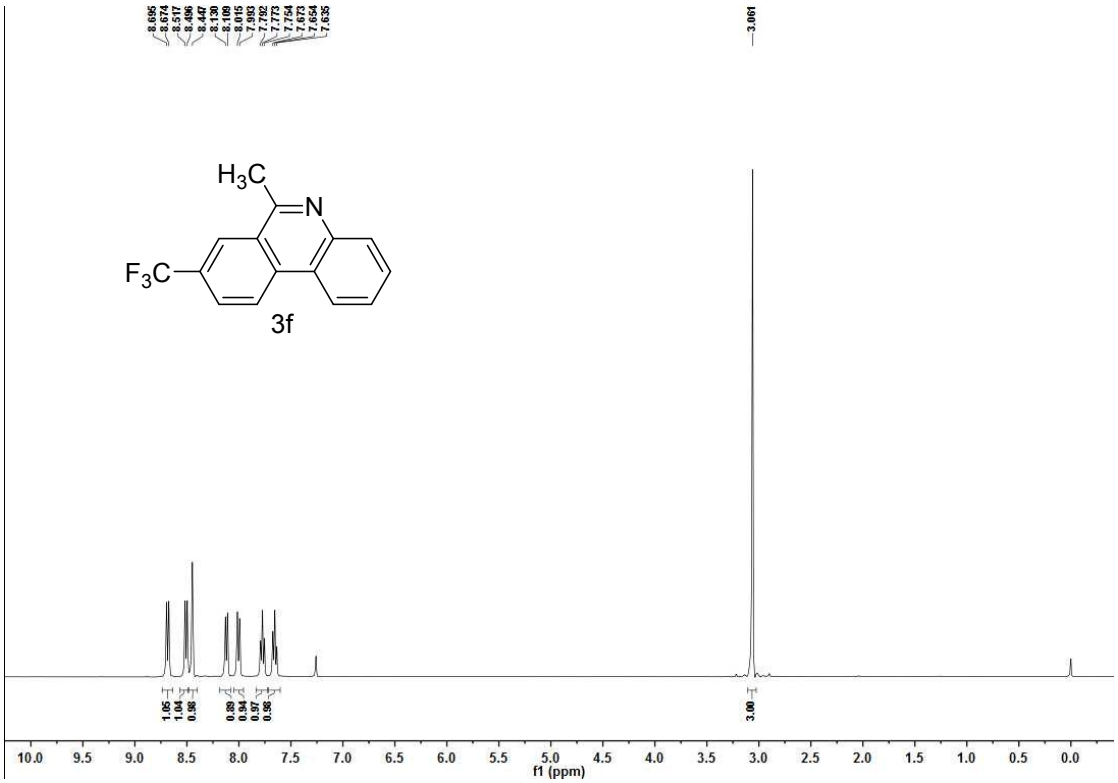
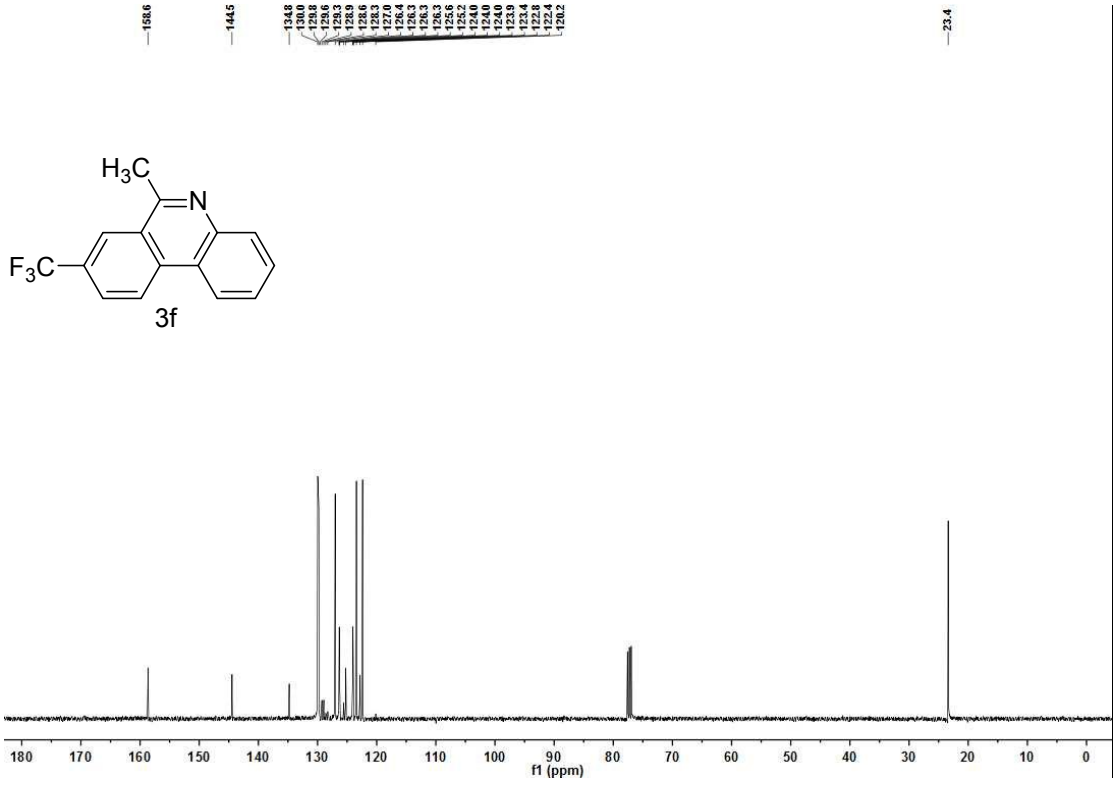
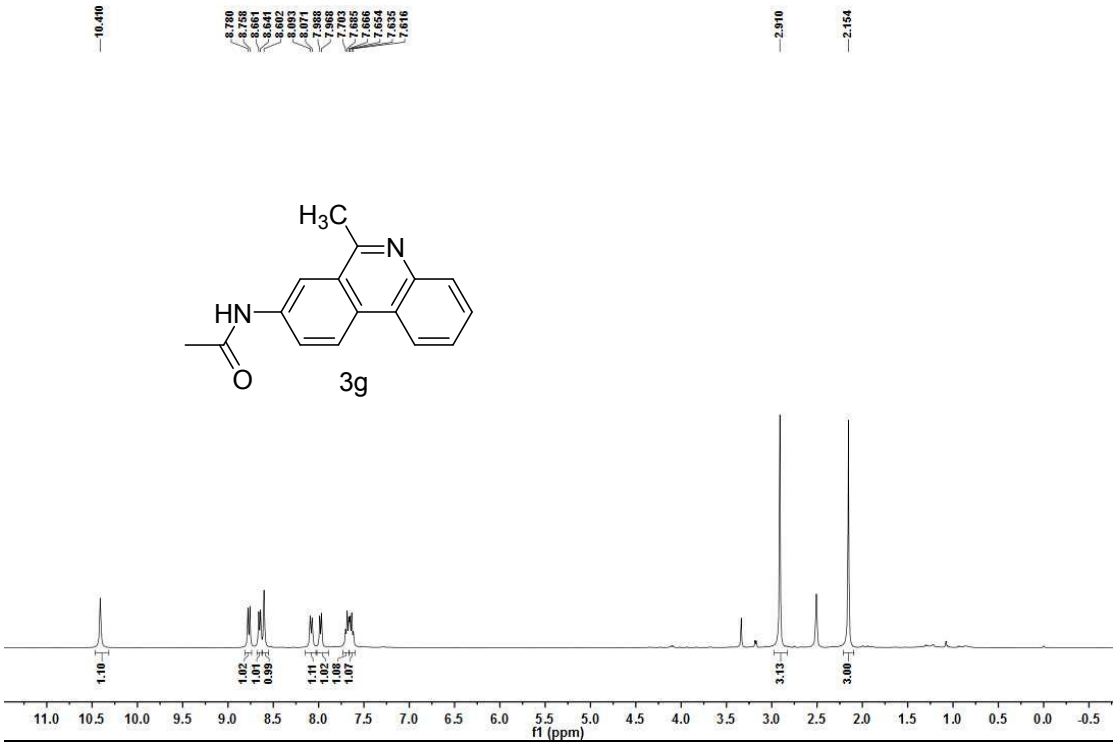
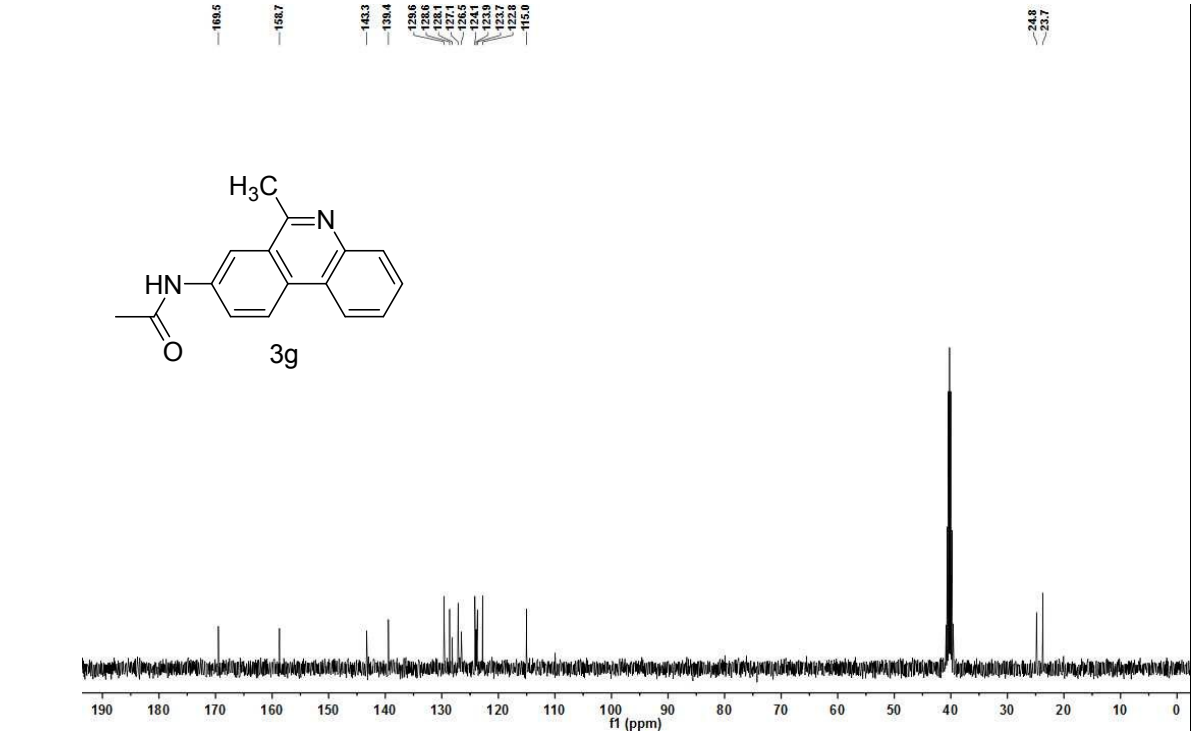
7.573
7.552
2.996
H3C
N
F
3e
1.16
1.16
1.01
1.04
1.10
0.91
1.07
3.23
f1 (ppm)

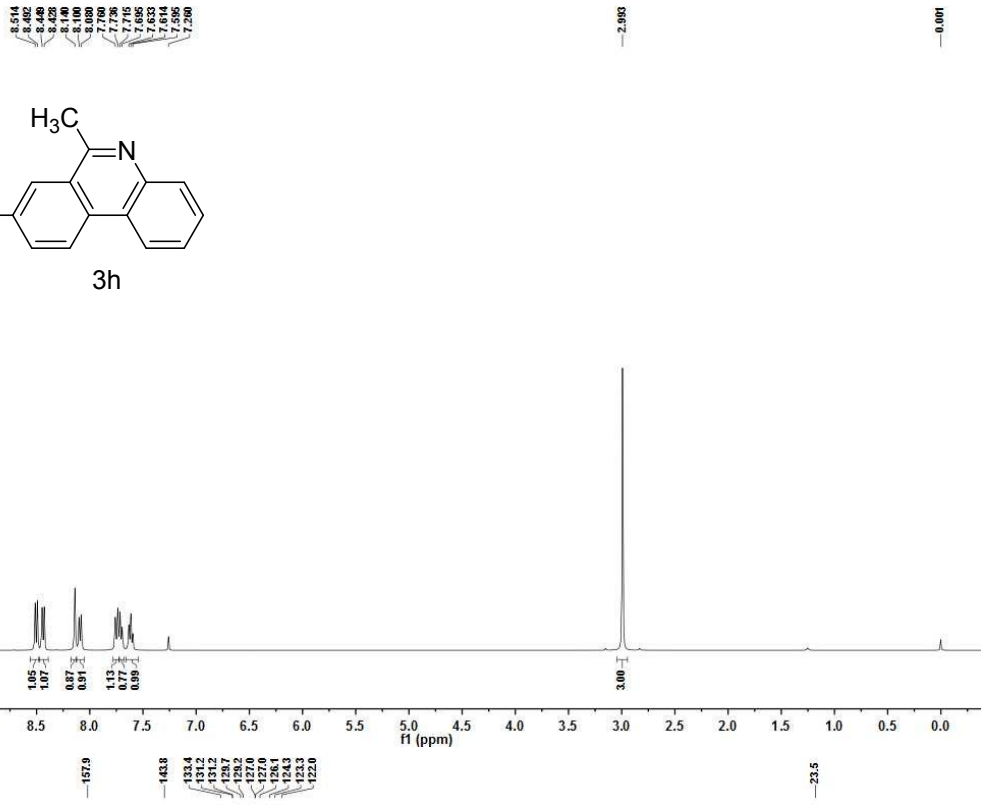

162.8
160.3
158.1
143.5
136.4
129.7
128.8
127.3
127.0
125.1
125.1
123.5
121.9
119.9
119.7
111.5
111.3
23.6
H3C
N
F
3e
f1 (ppm)

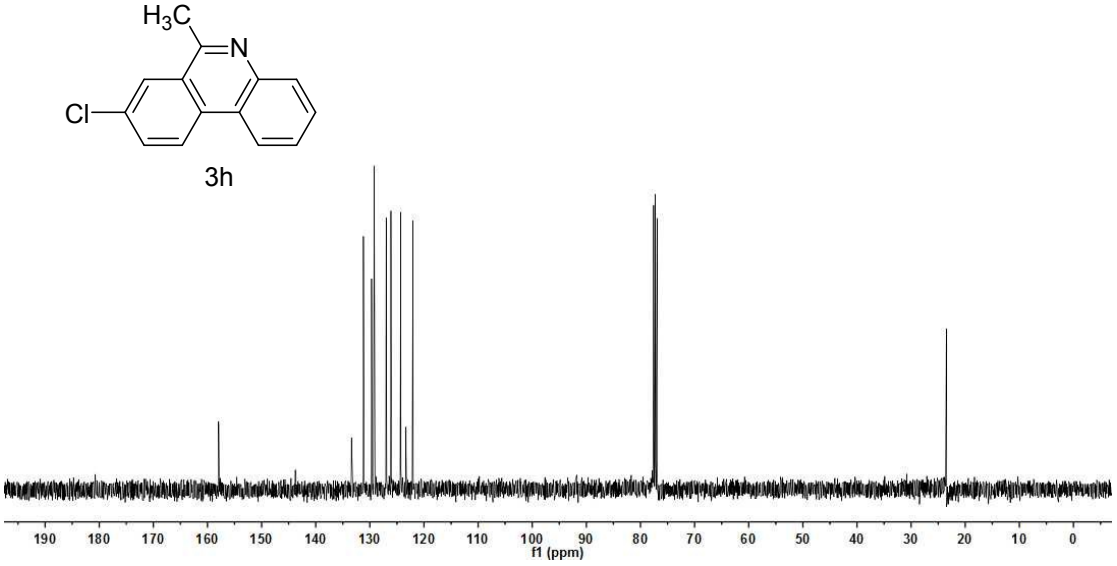

8.695
8.674
8.517
8.496
8.447
8.428
8.109
8.015
7.993
7.792
7.773
7.754
7.673
7.654
7.635
3.061
H3C
N
F3C
3f
1.05
1.04
0.98
0.89
0.94
0.97
0.98
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

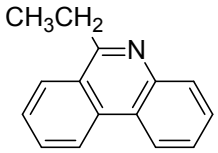

158.6
144.5
134.8
130.0
129.5
129.6
129.3
128.9
128.6
128.3
127.0
126.4
126.3
126.3
125.6
125.2
124.0
124.0
123.9
123.4
122.4
122.4
120.2
23.4
H3C
N
F3C
3f
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


10.410
8.780
8.758
8.661
8.641
8.092
8.071
7.988
7.968
7.703
7.685
7.666
7.654
7.635
7.616
2.910
2.154
H3C
N
HN
O
3g
1.10
1.02
1.01
0.99
1.11
1.02
1.00
1.07
3.13
3.00
f1 (ppm)

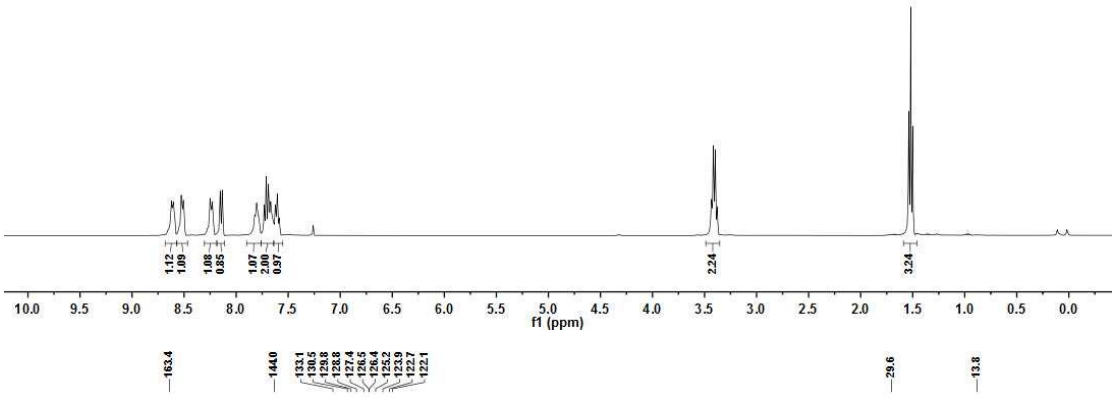

169.5
158.7
143.3
130.4
129.6
128.6
128.1
127.1
126.5
124.1
123.9
123.7
122.8
115.0
24.8
23.7
H3C
N
HN
O
3g
f1 (ppm)

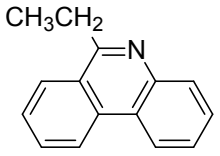

8.514
8.482
8.448
8.435
8.140
8.100
8.080
7.760
7.736
7.715
7.695
7.653
7.614
7.595
7.290
2.593
0.001
H3C
N
Cl
3h
1.05
1.07
0.87
0.91
1.13
0.77
0.99
3.00
f1 (ppm)
157.9
143.8
133.4
131.2
131.2
129.7
129.2
127.0
127.0
126.1
124.3
123.3
122.0
23.5


H3C
N
Cl
3h
f1 (ppm)

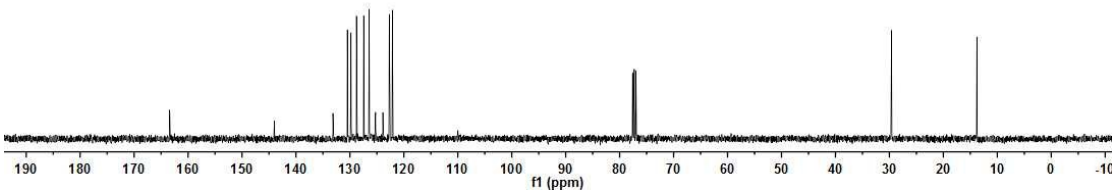


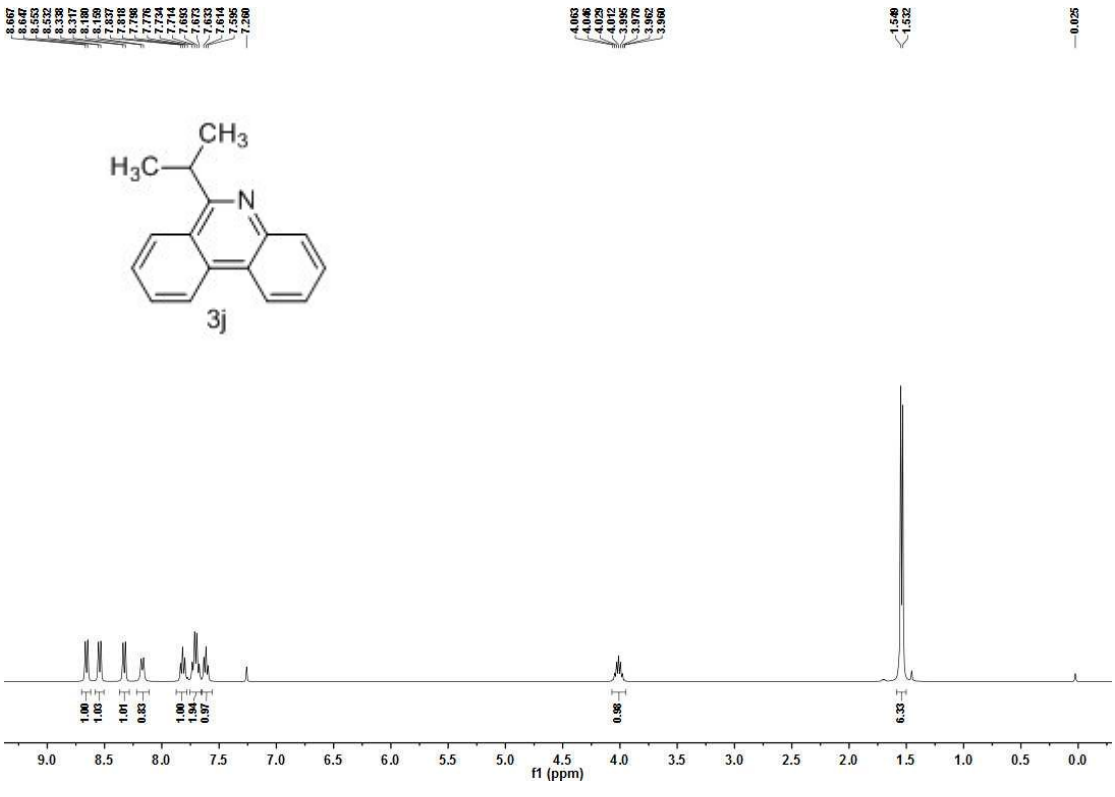
3i

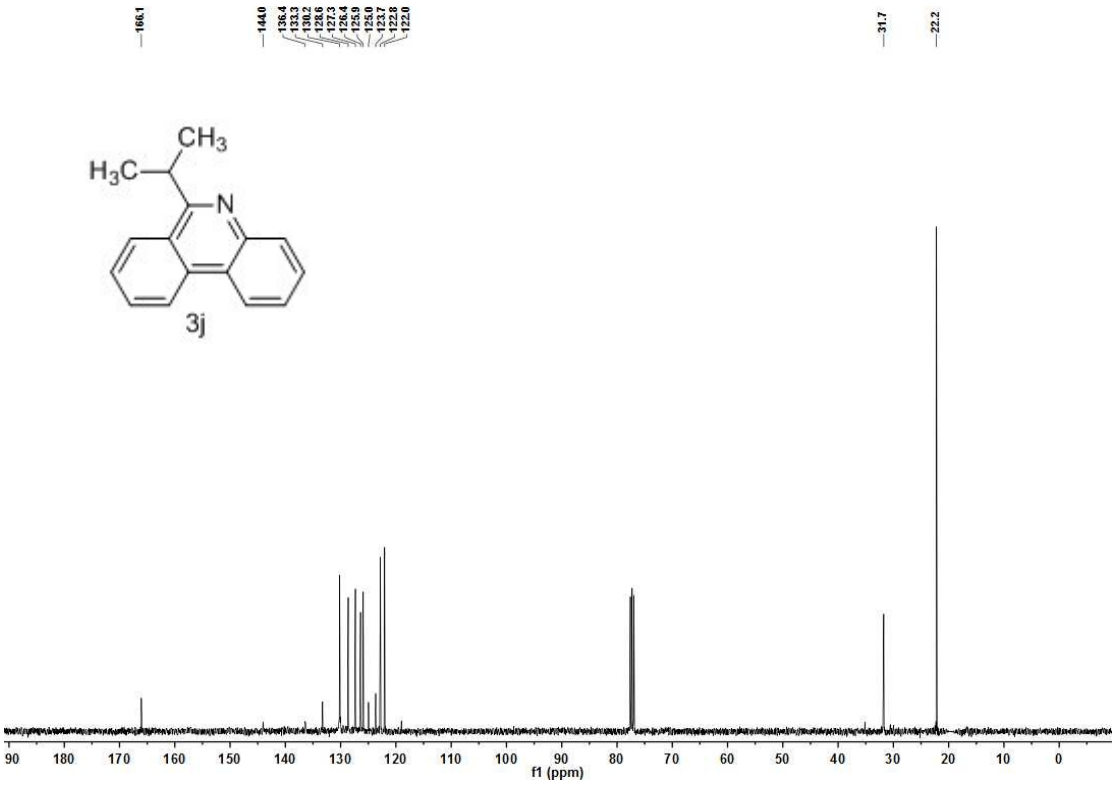


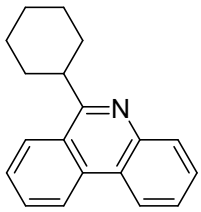


3i

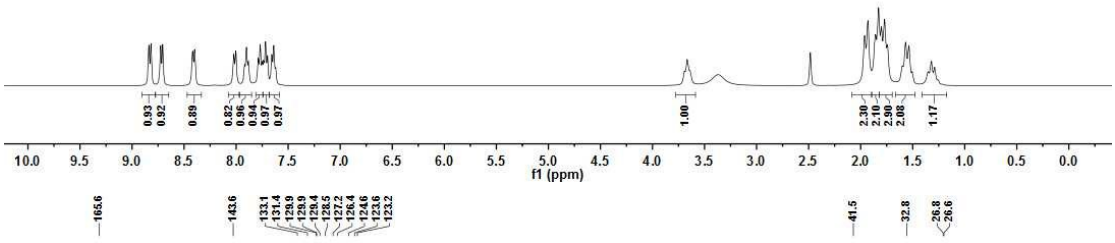


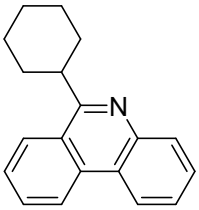

8.667
8.647
8.553
8.532
8.338
8.317
8.159
7.837
7.818
7.798
7.776
7.734
7.714
7.695
7.673
7.633
7.614
7.595
7.260
4.063
4.046
4.029
4.012
3.995
3.978
3.962
3.960
1.549
1.532
0.025
CH3
H3C
N
3j
1.00
1.03
1.01
0.83
1.00
1.94
0.97
0.98
6.33
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


166.1
144.0
136.4
133.3
130.2
128.6
127.3
126.4
125.9
125.0
123.7
123.5
122.0
31.7
22.2
CH3
H3C
N
3j
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

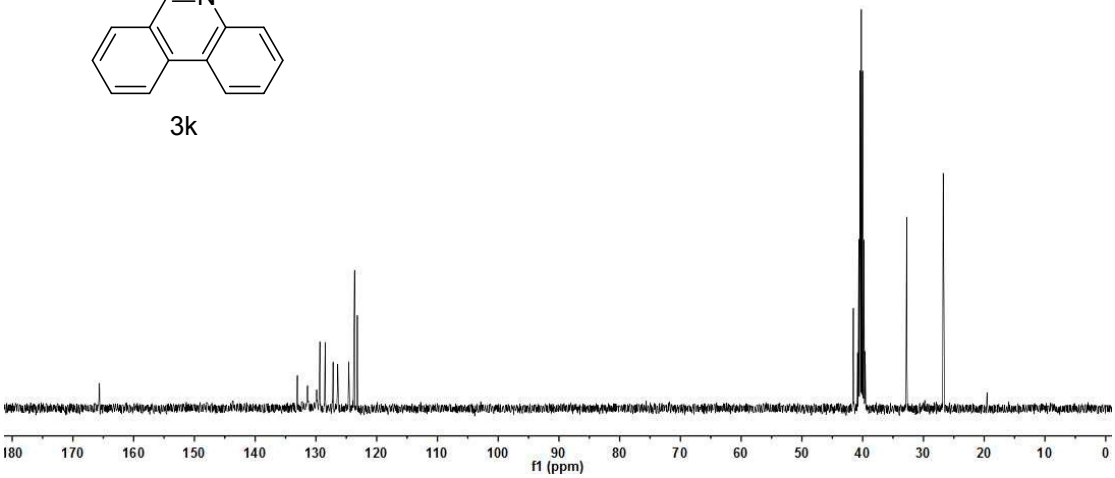


3k

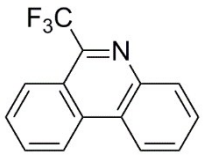




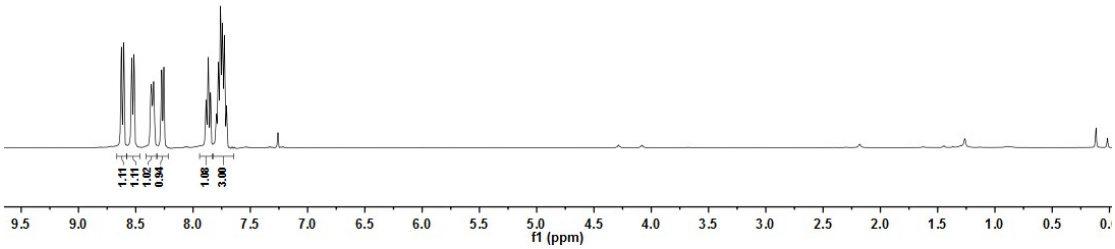
3k



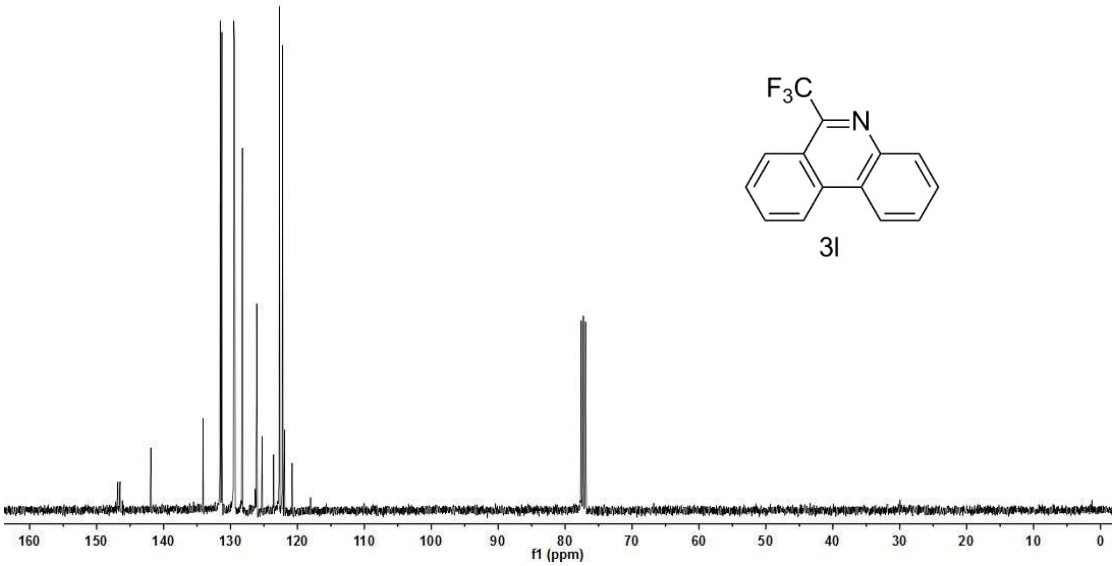

8.636
8.605
8.535
8.516
8.366
8.344
8.274
8.255
7.886
7.867
7.848
7.797
7.779
7.762
7.757
7.744
7.726
7.707


F3C
N

3l

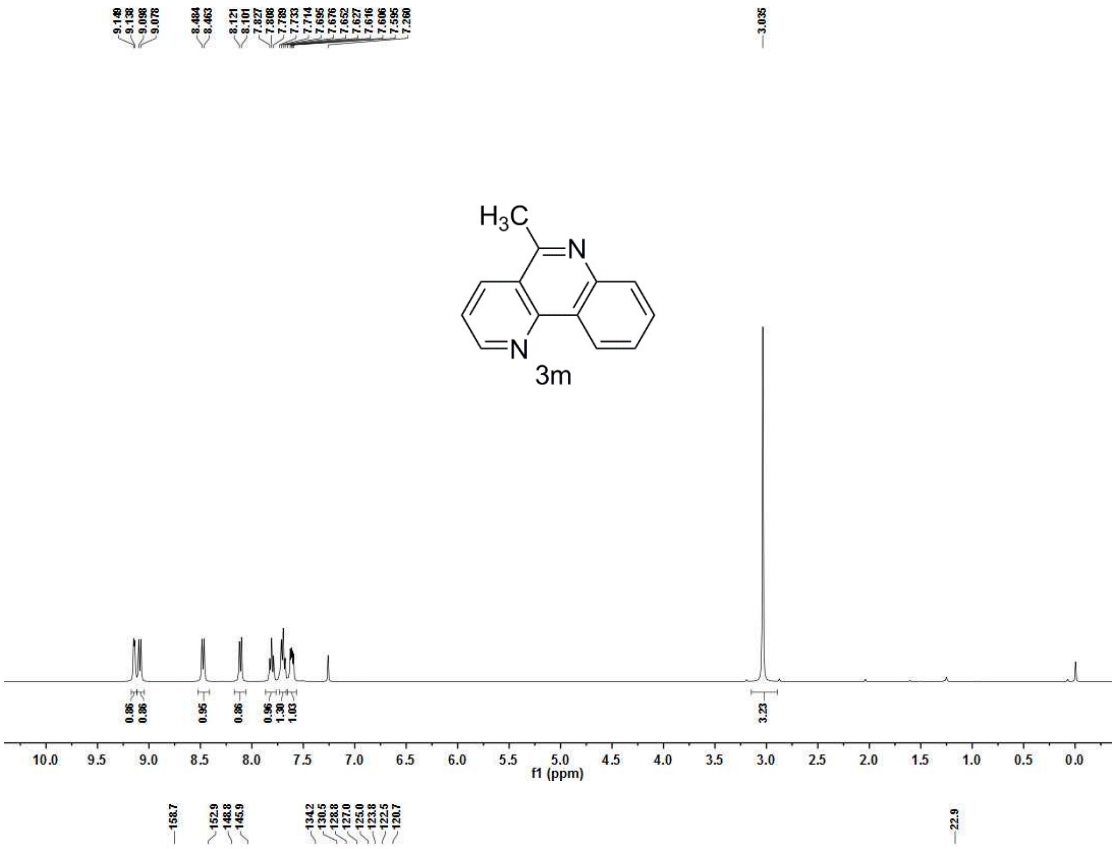

1.11
1.11
1.02
0.94
1.08
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

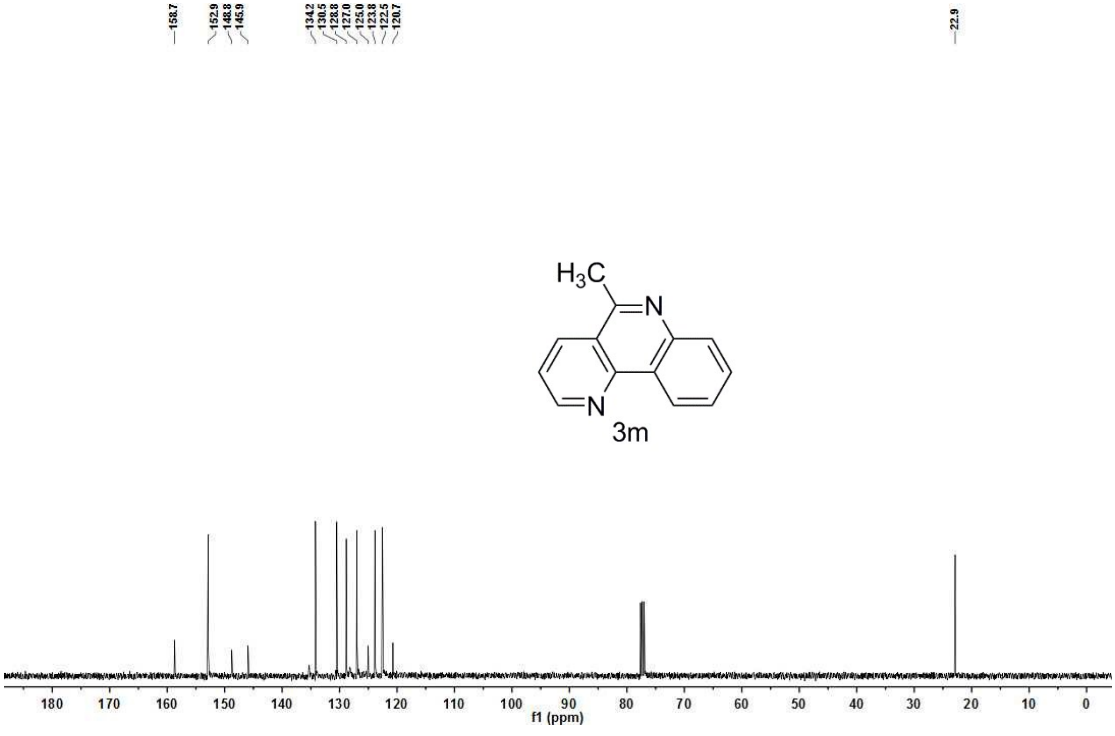

147.2
146.8
146.5
146.2
141.9
134.1
131.5
131.3
129.6
129.4
128.2
126.3
126.1
126.1
125.3
123.5
122.7
122.2
121.9
120.8
118.0


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

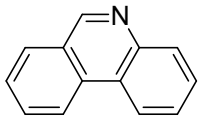
F3C
N

3l

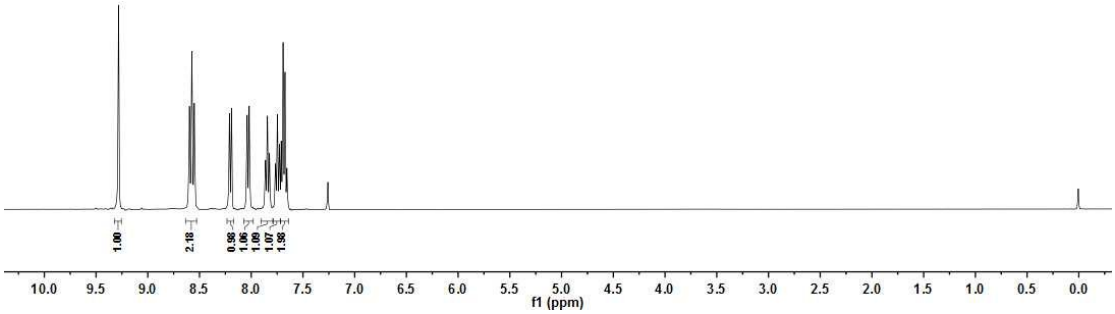

9.149
9.138
9.098
9.078
8.484
8.463
8.121
8.101
7.827
7.808
7.789
7.733
7.714
7.695
7.676
7.652
7.627
7.616
7.606
7.585
7.260
3.035
H3C
N
N
3m
0.86
0.86
0.95
0.86
0.95
1.30
1.03
3.23
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.7
152.9
148.8
145.9
134.2
130.5
128.8
127.0
125.0
123.8
122.5
120.7
22.9
H3C
N
N
3m
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

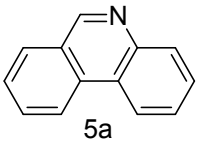

9.282
8.598
8.574
8.550
8.210
8.190
8.039
8.019
7.862
7.843
7.823
7.765
7.747
7.727
7.711
7.692
7.673
7.654


N

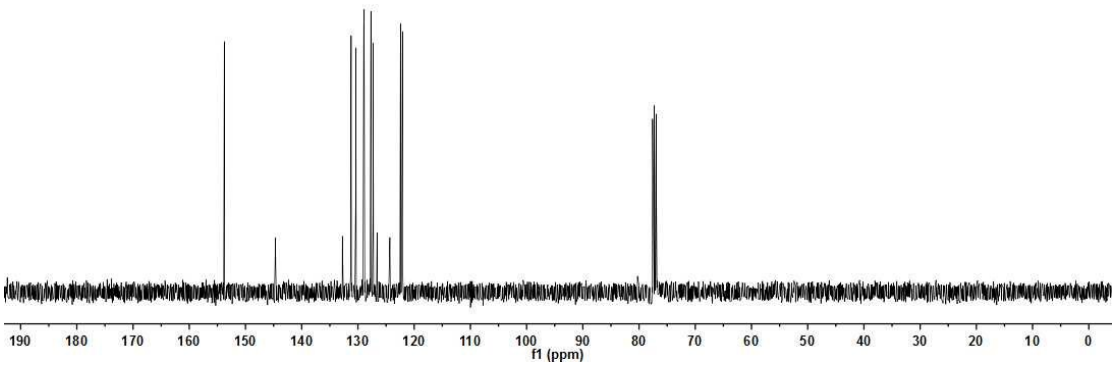
5a

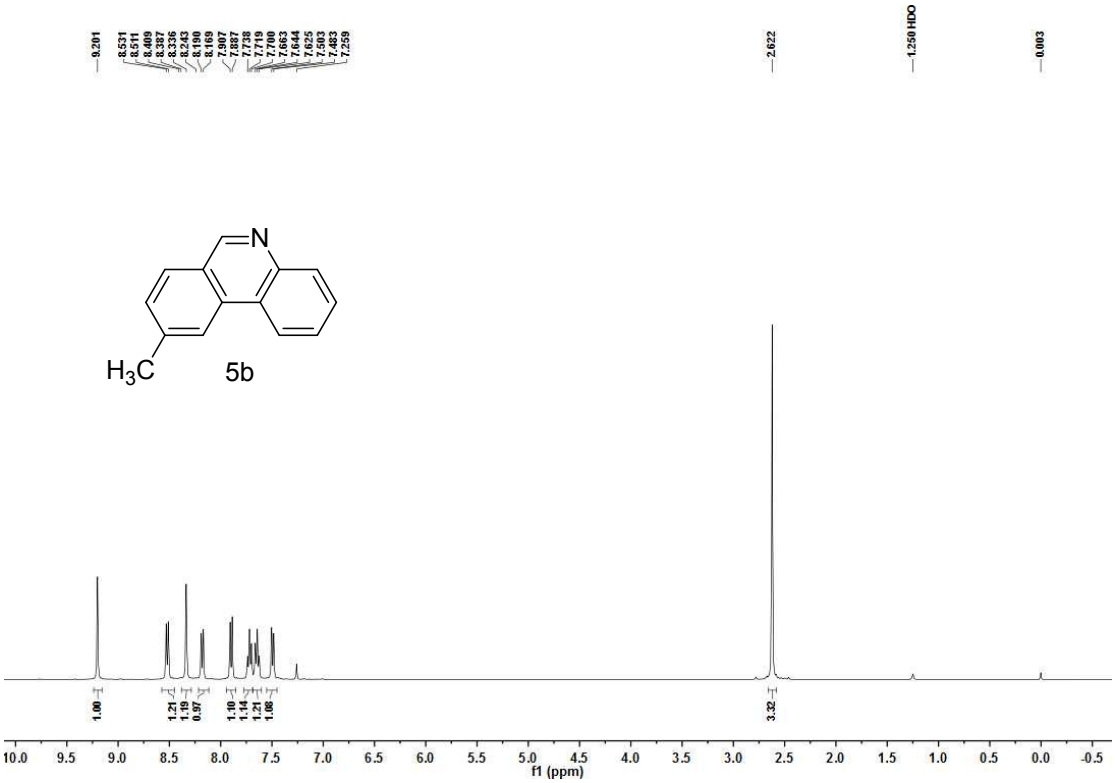

1.00
2.18
0.98
1.06
1.00
1.07
1.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

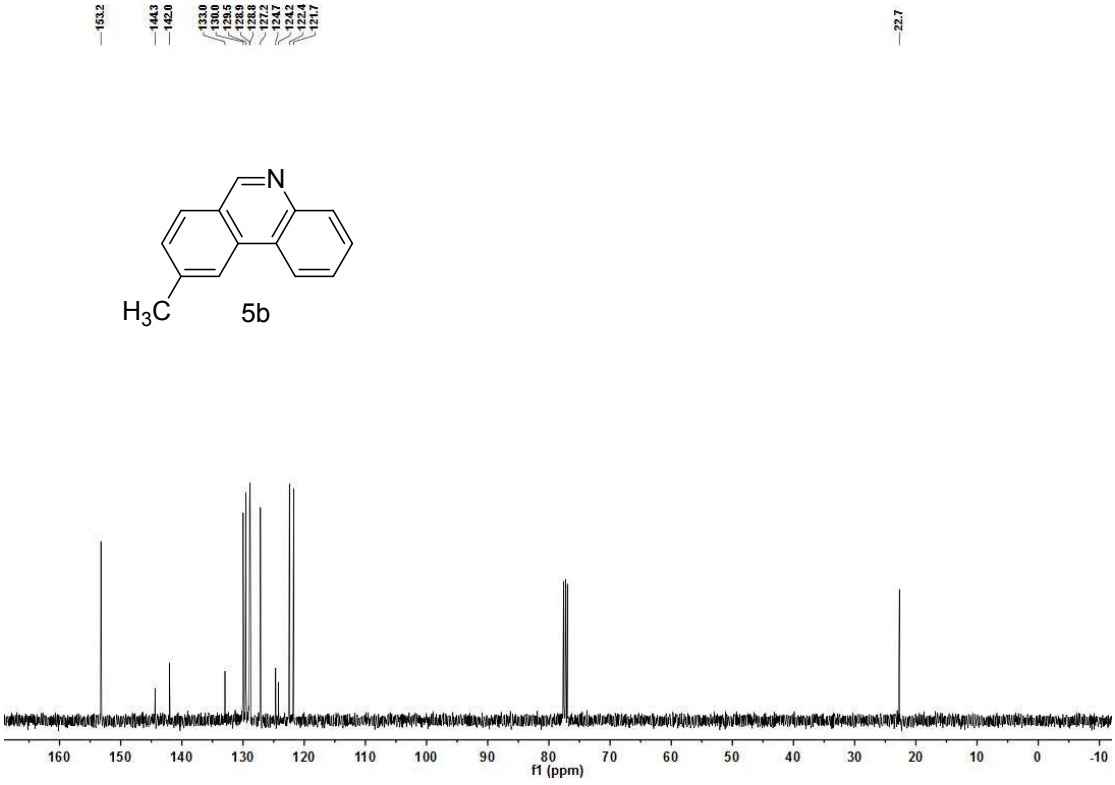

153.8
144.7
132.8
131.2
130.4
129.0
128.9
127.7
127.3
126.6
124.3
123.4
122.1

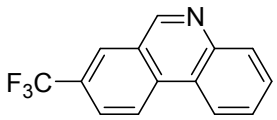

N

5a

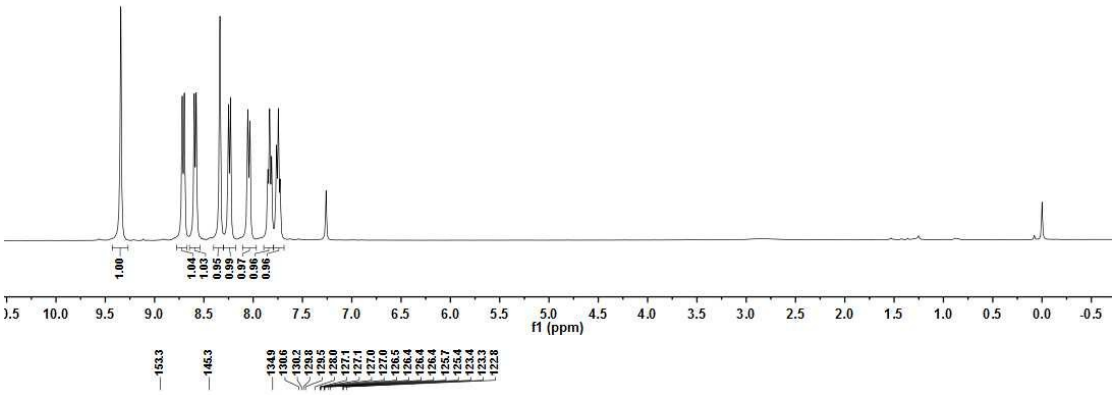

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

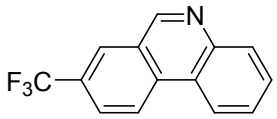

9.201
8.531
8.511
8.409
8.387
8.336
8.245
8.169
7.907
7.887
7.738
7.719
7.700
7.663
7.644
7.625
7.503
7.483
7.259
2.622
1.250 HDO
0.003
N
H3C
5b
1.00
1.21
1.19
0.97
1.10
1.14
1.21
1.00
3.32
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


153.2
144.3
142.0
133.0
130.0
128.5
128.0
126.9
127.2
124.7
124.2
122.4
121.7
22.7
N
H3C
5b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

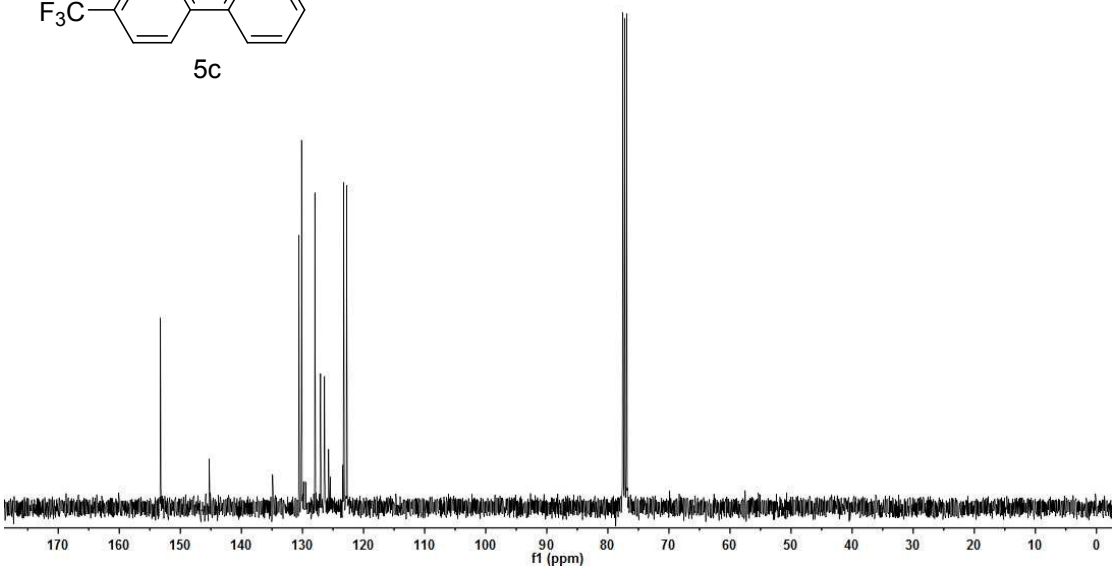


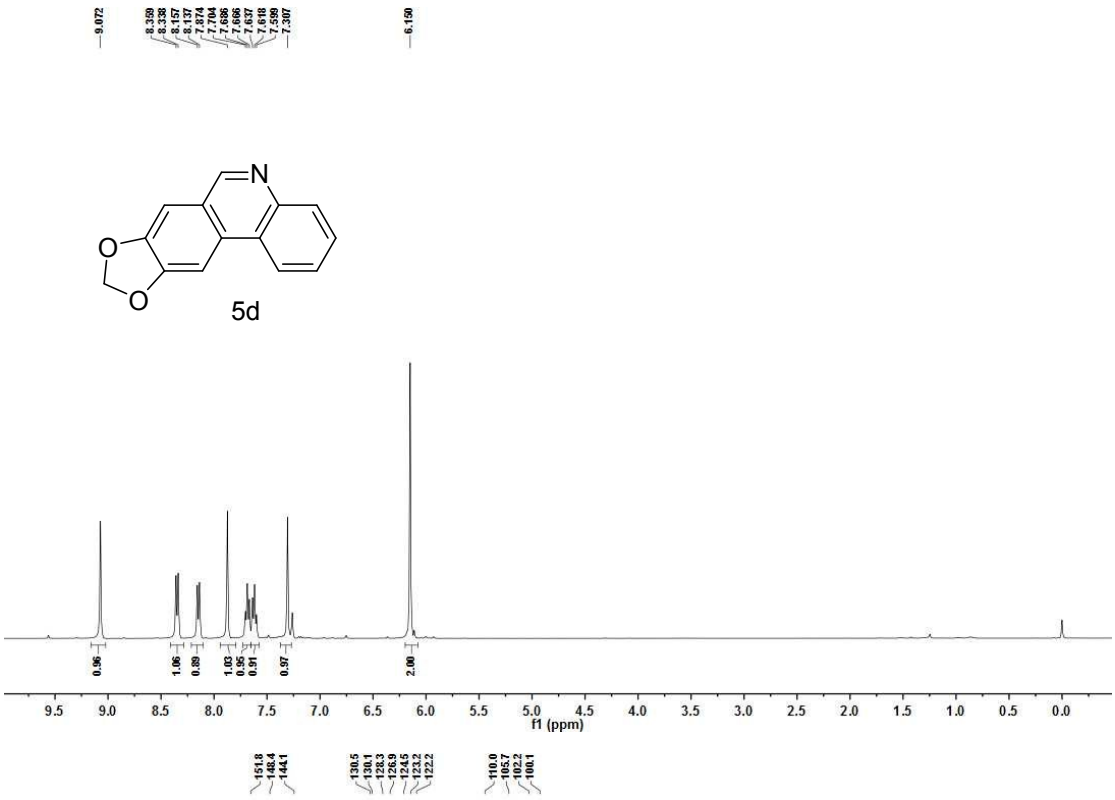
5c

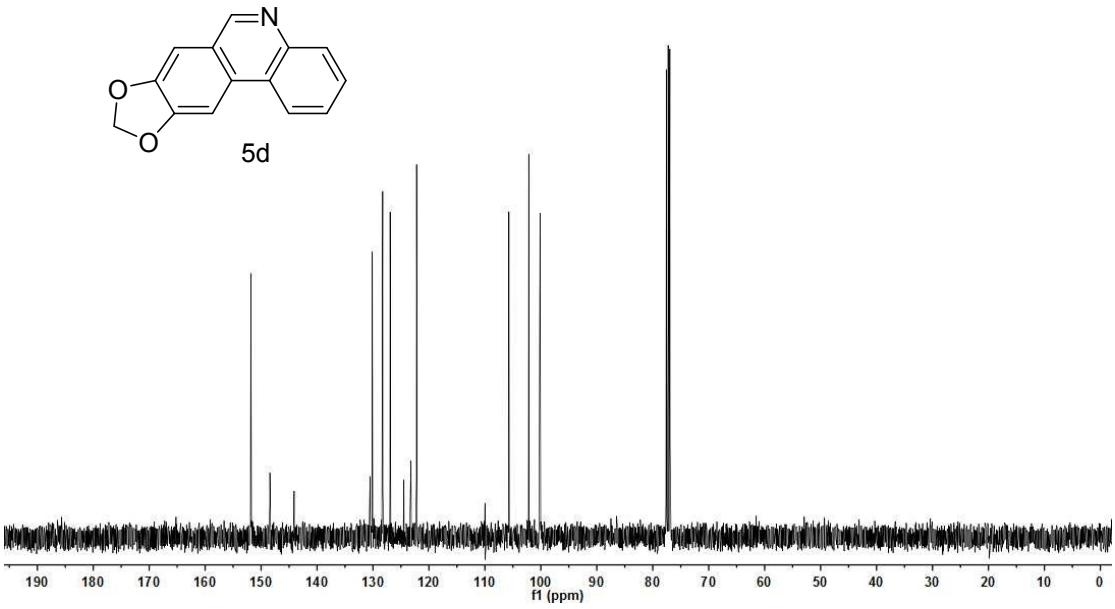




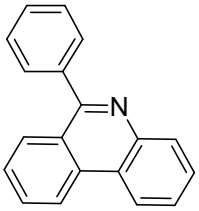
5c



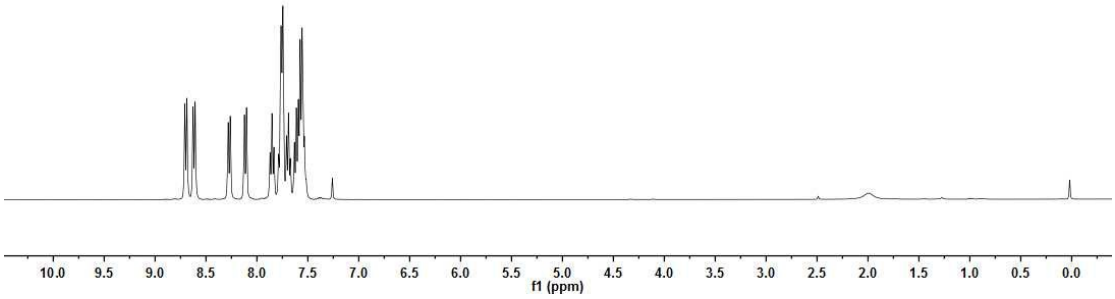

9.072
8.359
8.338
8.157
8.137
7.874
7.704
7.688
7.666
7.637
7.618
7.599
7.307
6.150
N
O
O
5d
0.96
1.06
0.89
1.03
0.95
0.91
0.97
2.00
f1 (ppm)


151.8
148.4
144.1
130.5
130.1
128.3
126.9
124.5
123.2
122.2
110.0
105.7
102.2
100.1
N
O
O
5d
f1 (ppm)

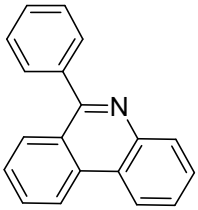

8.709
8.688
8.627
8.607
8.283
8.262
8.123
8.103
7.872
7.853
7.833
7.788
7.764
7.745
7.710
7.691
7.672
7.632
7.613
7.594
7.576
7.557
7.550
7.534
7.516


N

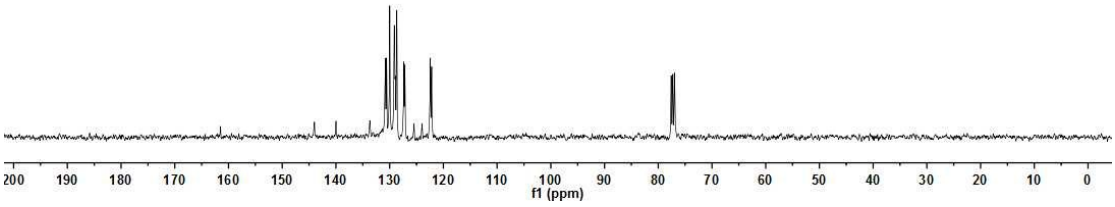
7a

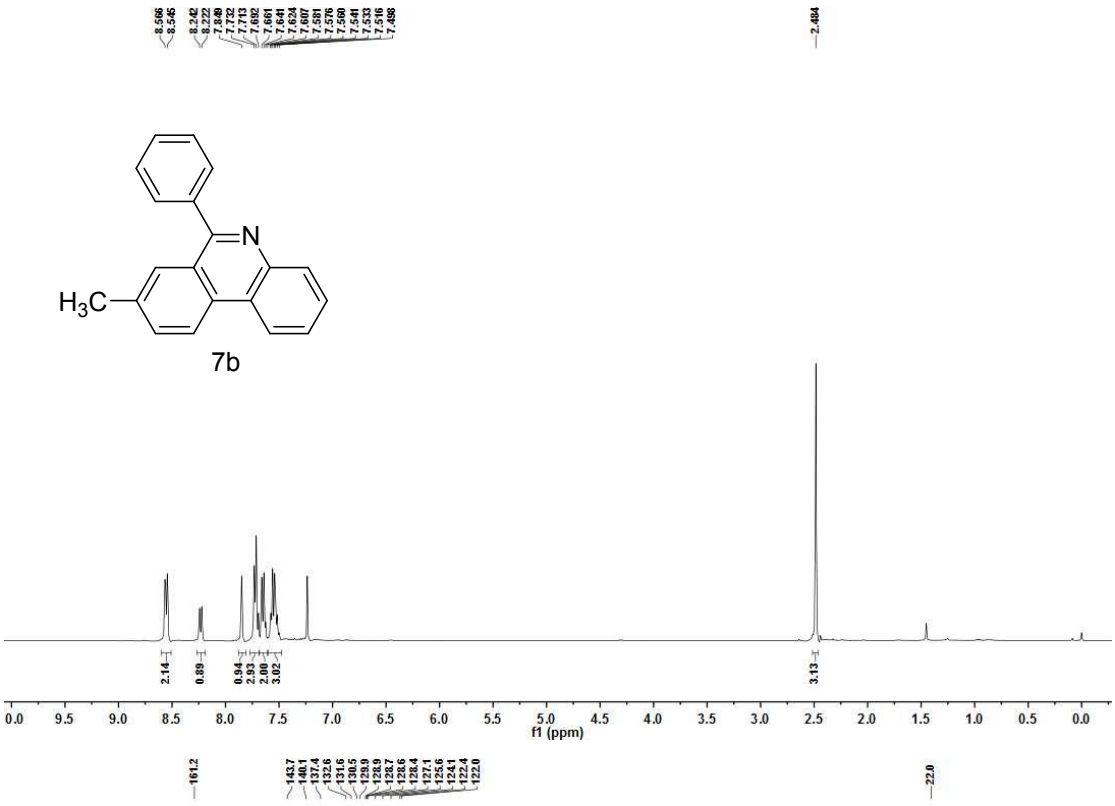

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

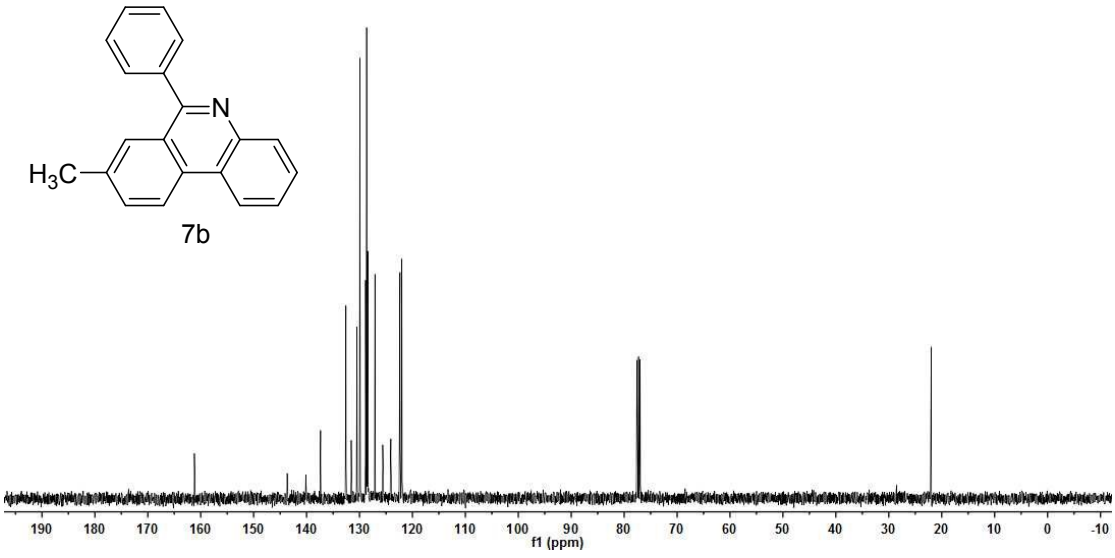

161.5
144.0
140.0
137.7
133.1
130.8
130.6
130.0
129.2
129.1
129.0
128.7
127.4
127.2
125.5
124.0
123.4
122.2

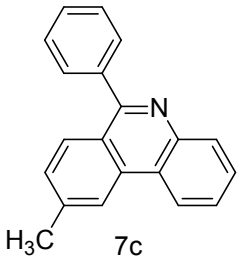

N

7a

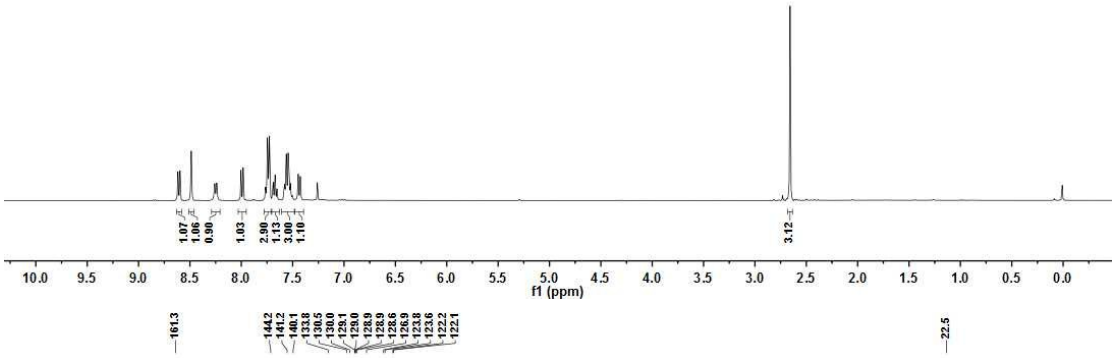

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.566
8.545
8.242
8.222
7.848
7.732
7.713
7.692
7.661
7.641
7.624
7.607
7.581
7.576
7.560
7.541
7.533
7.516
7.498
2.484
N
H3C
7b
2.14
0.89
0.94
2.93
2.00
3.02
3.13
f1 (ppm)

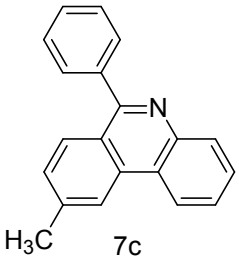

161.2
143.7
140.1
137.4
132.6
131.6
130.5
130.0
128.9
128.7
128.6
128.4
127.1
125.6
124.1
122.4
122.0
22.0
N
H3C
7b
f1 (ppm)


N
H3C

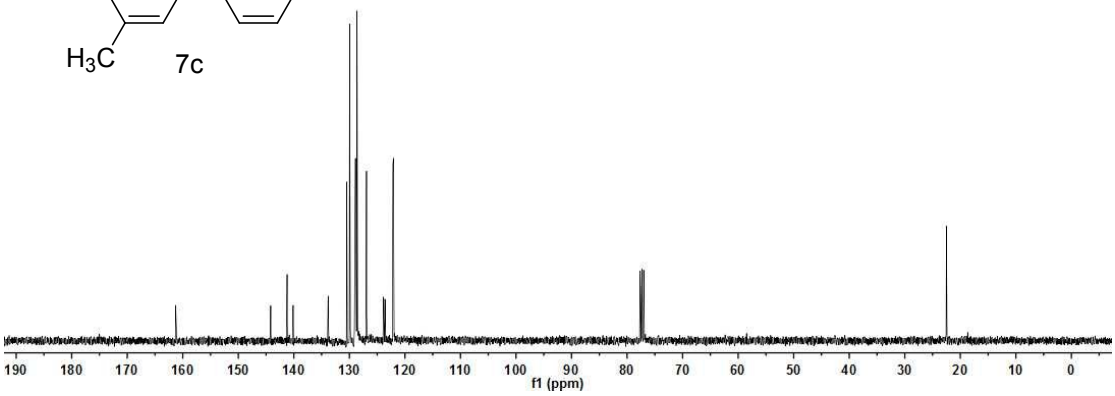
7c

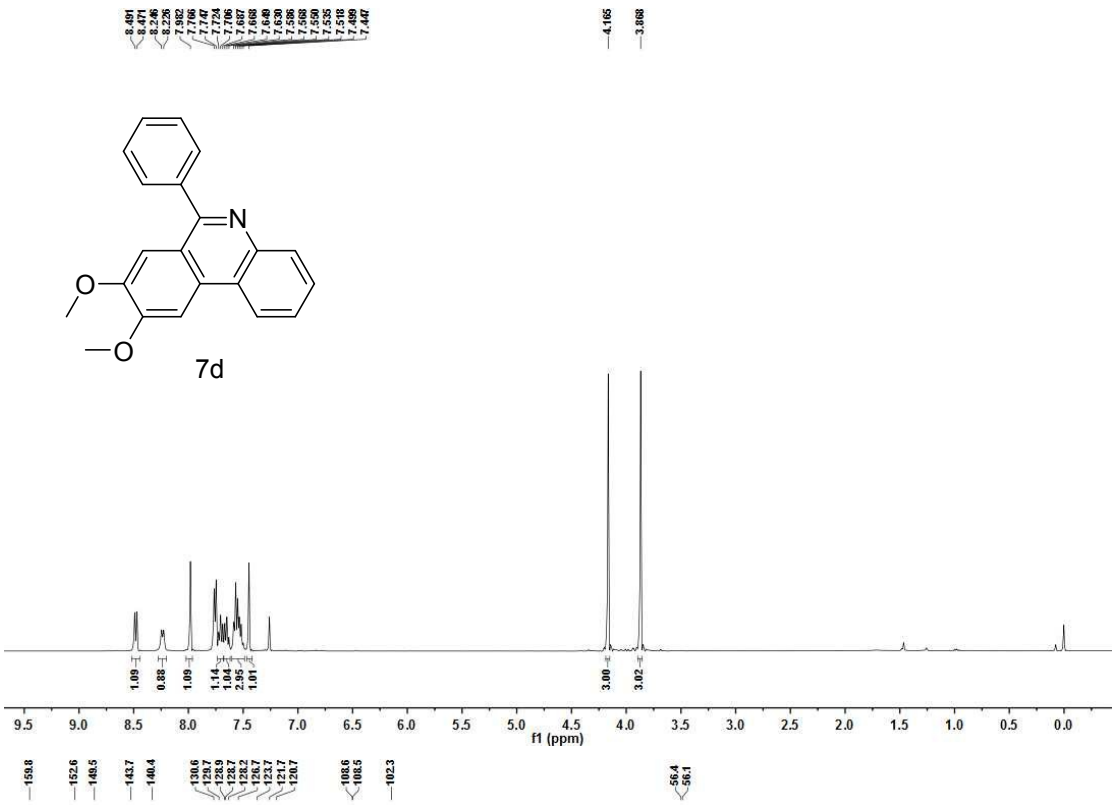

1.07
1.06
0.90
1.03
2.90
1.13
3.00
1.10
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

161.3
144.2
141.2
140.1
133.8
130.5
130.0
129.1
129.0
128.9
128.8
126.9
123.8
123.6
122.2
122.1
22.5

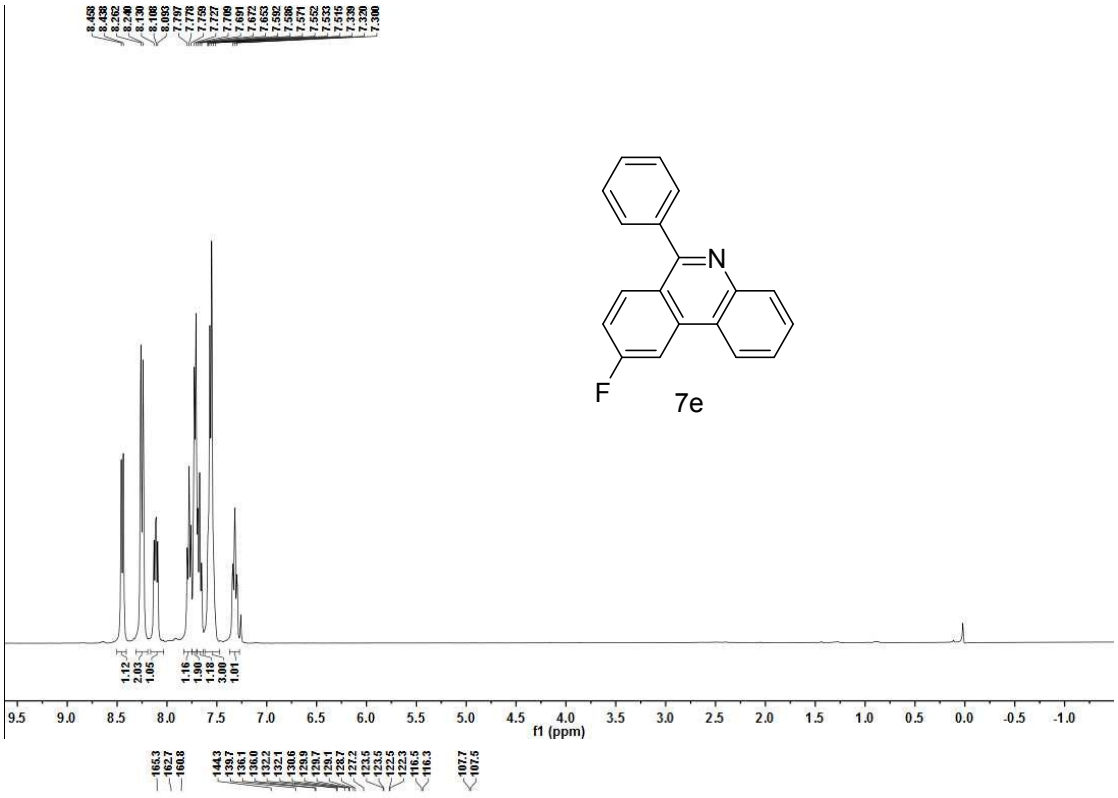

N
H3C

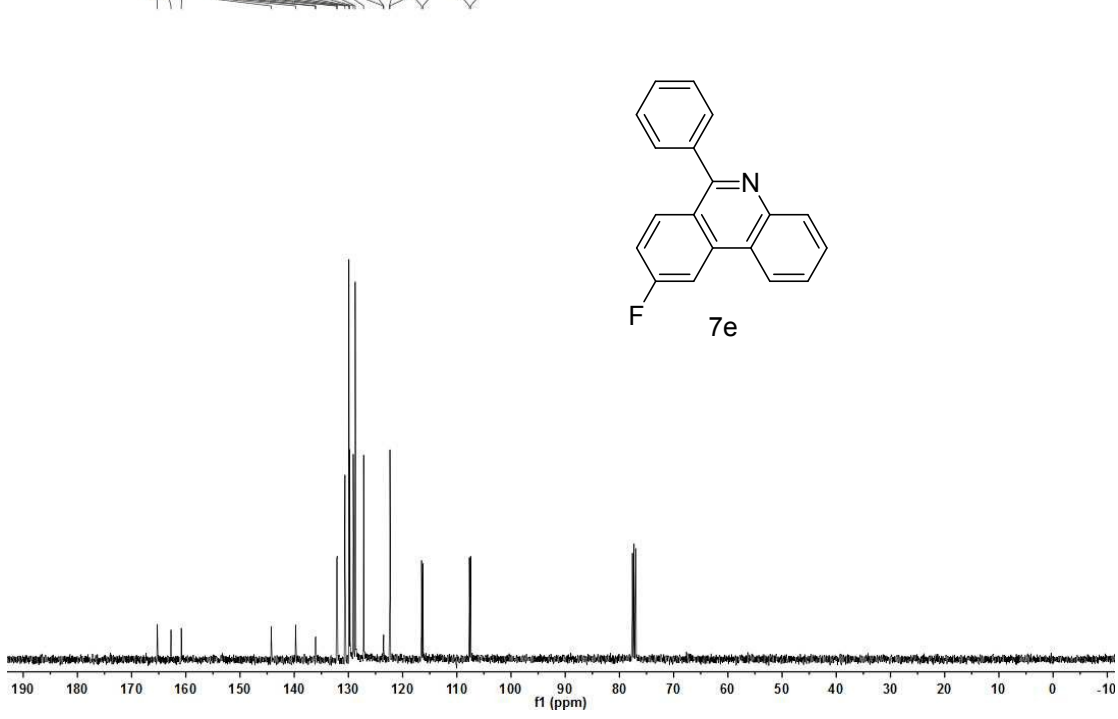
7c


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

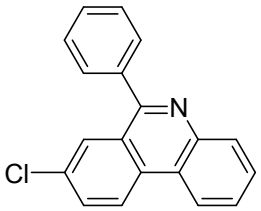

8.491
8.471
8.246
8.226
7.982
7.766
7.747
7.724
7.706
7.687
7.668
7.649
7.630
7.586
7.568
7.550
7.535
7.518
7.499
7.447
4.165
3.868
N
O
O
7d
1.09
0.88
1.09
1.14
1.04
2.05
1.01
3.00
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

159.8
152.6
149.5
143.7
140.4
130.6
129.7
128.9
128.7
128.2
126.7
123.7
121.1
120.7
108.6
108.5
102.3
56.4
56.1
N
O
O
7d
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

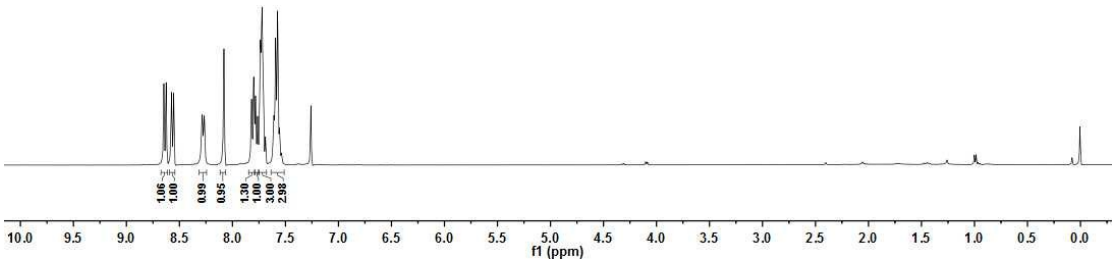

8.458
8.438
8.262
8.240
8.130
8.108
8.093
7.797
7.778
7.759
7.727
7.709
7.691
7.672
7.653
7.592
7.586
7.571
7.552
7.533
7.516
7.339
7.320
7.300
1.12
2.03
1.05
1.16
1.90
1.18
3.00
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
N
F
7e


165.3
162.7
160.8
144.3
139.7
138.1
136.0
132.2
132.1
130.6
129.9
129.7
128.1
128.1
127.2
123.5
123.5
122.5
122.3
116.5
116.3
107.7
107.5
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
N
F
7e

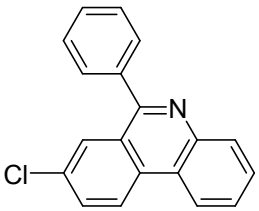

8.647
8.625
8.575
8.555
8.286
8.266
8.088
7.819
7.799
7.782
7.763
7.737
7.690
7.645
7.610
7.593
7.574
7.556
7.537


N
Cl

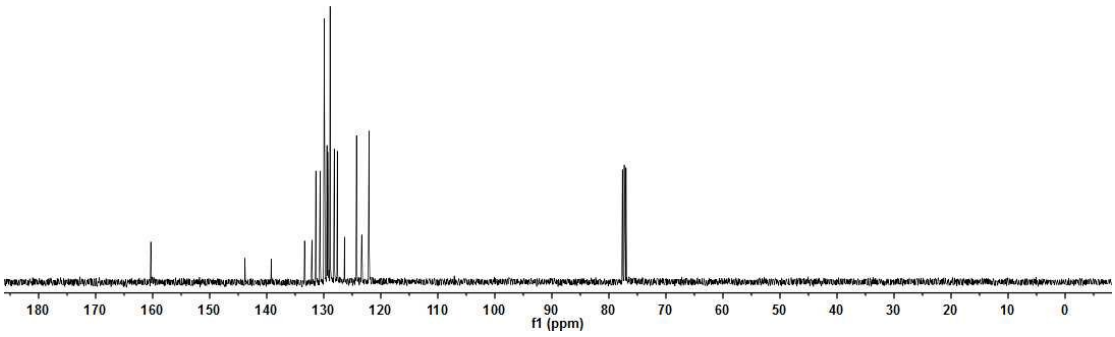
7f

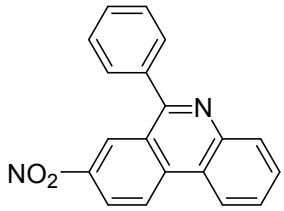

1.06
1.00
0.99
0.95
1.30
1.00
3.00
2.98
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.3
143.8
139.2
133.4
132.1
131.4
130.6
129.9
129.4
129.3
128.9
128.2
127.6
126.4
124.3
123.3
122.1

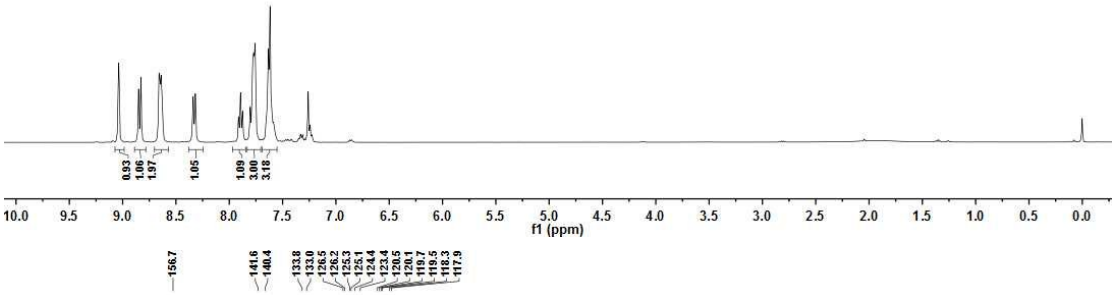

N
Cl

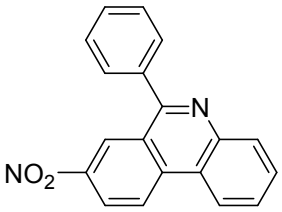
7f


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

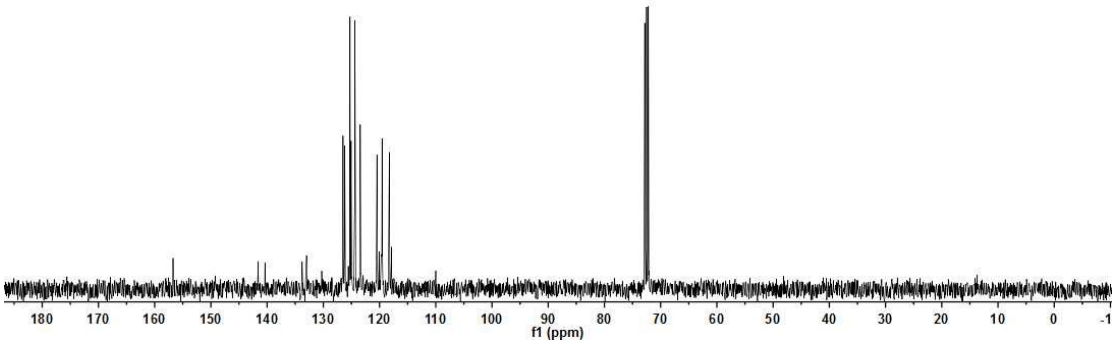


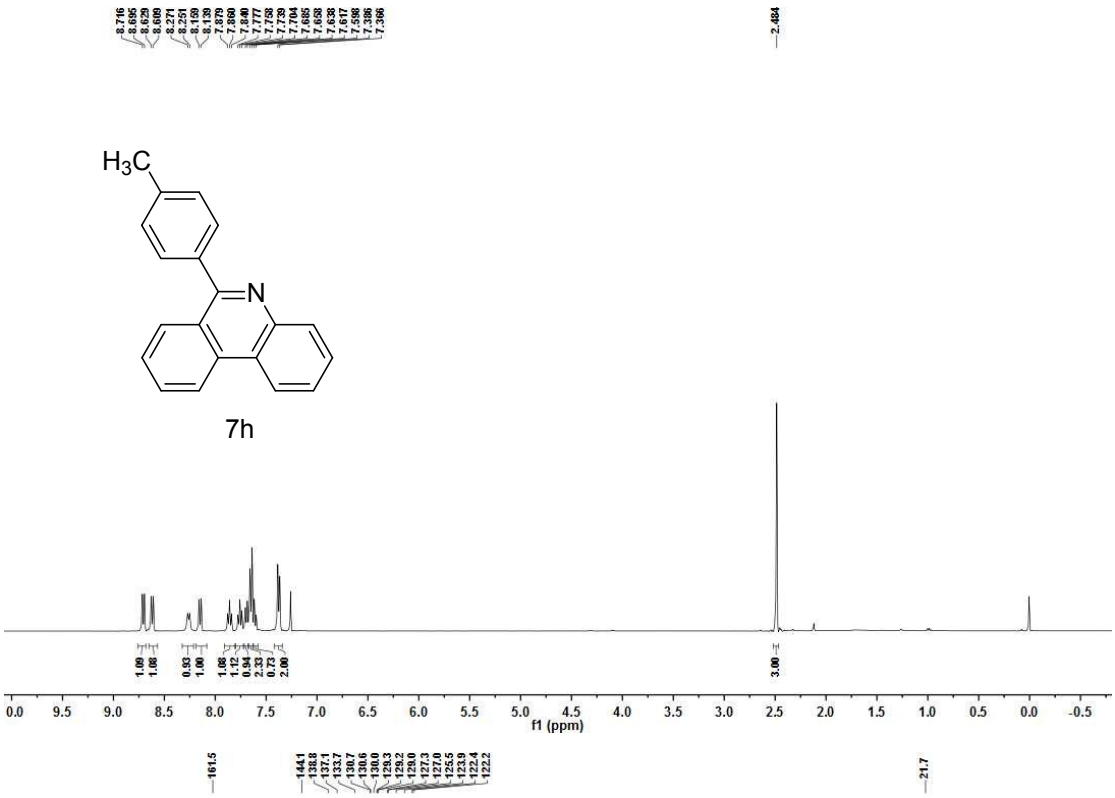
7g

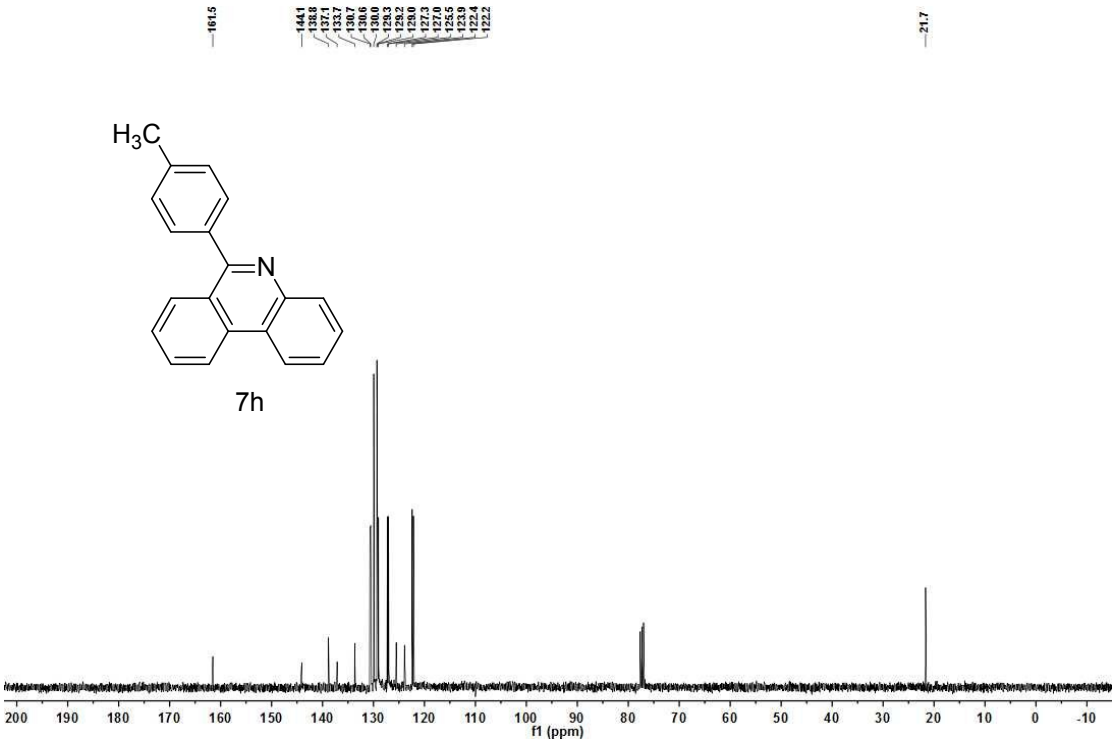


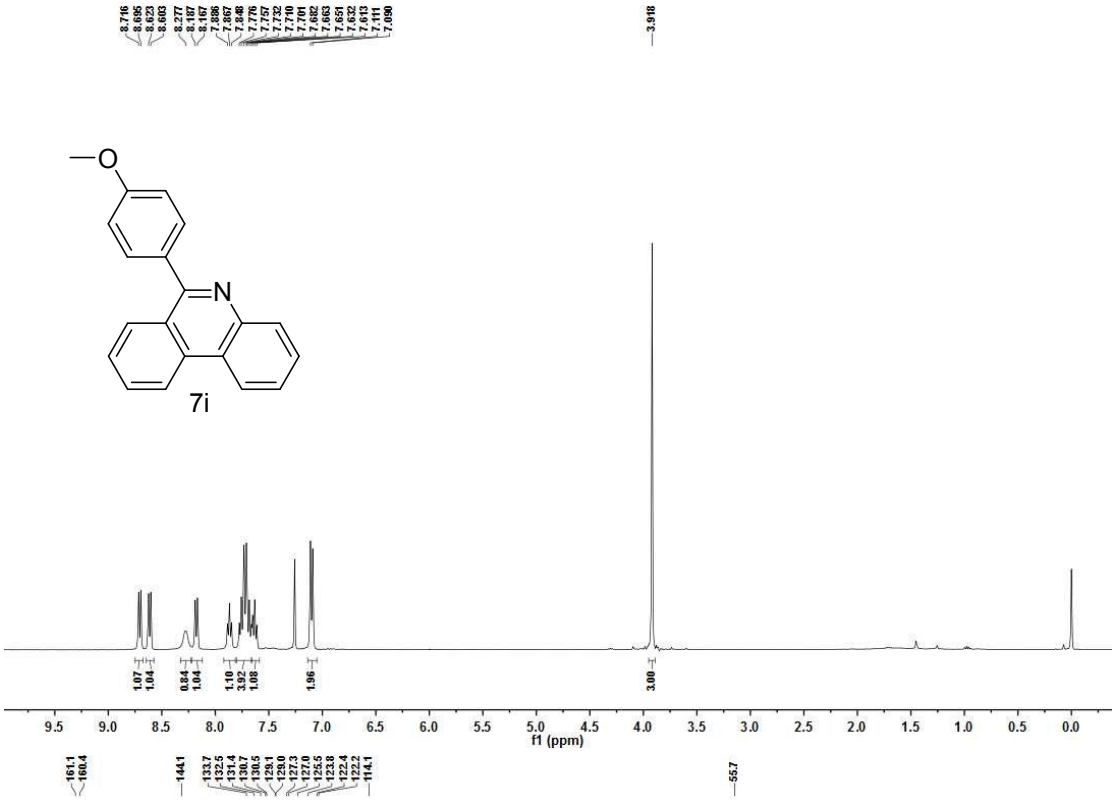


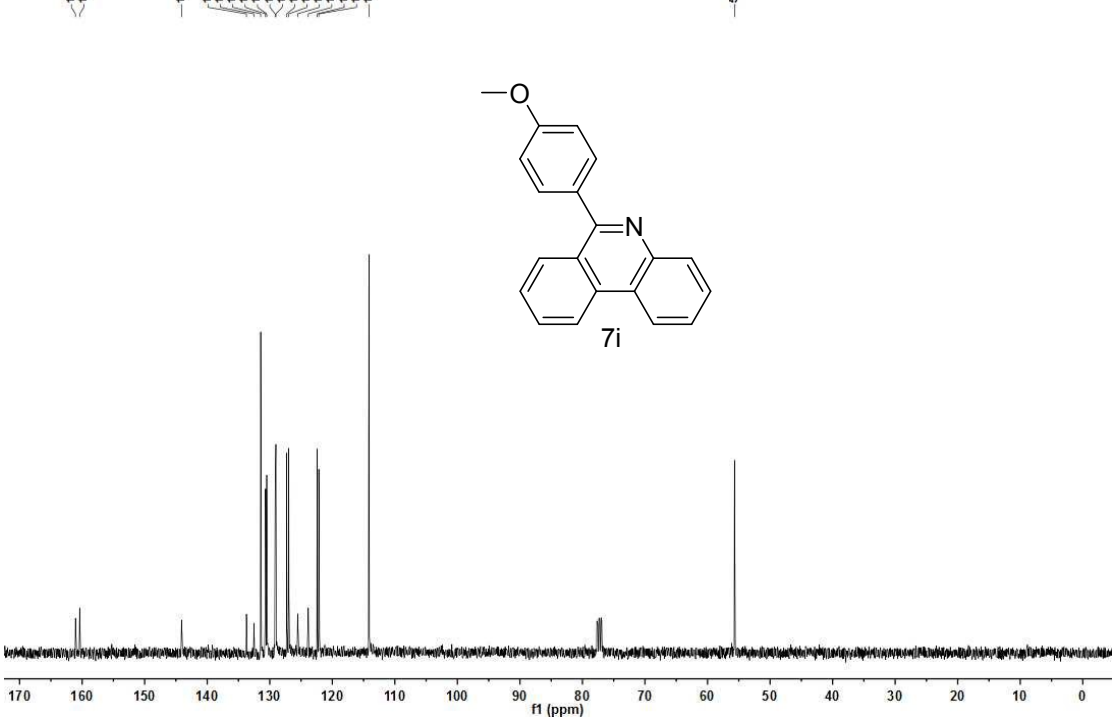
7g

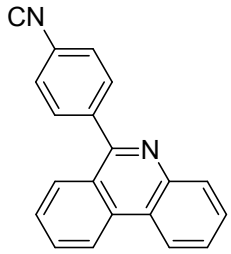



8.716
8.695
8.629
8.609
8.271
8.255
8.159
8.139
7.879
7.860
7.840
7.777
7.758
7.733
7.704
7.685
7.658
7.638
7.617
7.598
7.386
7.366
2.484
H3C
N
7h
1.09
1.08
0.93
1.00
1.08
1.12
0.94
2.33
0.73
2.00
3.00
f1 (ppm)

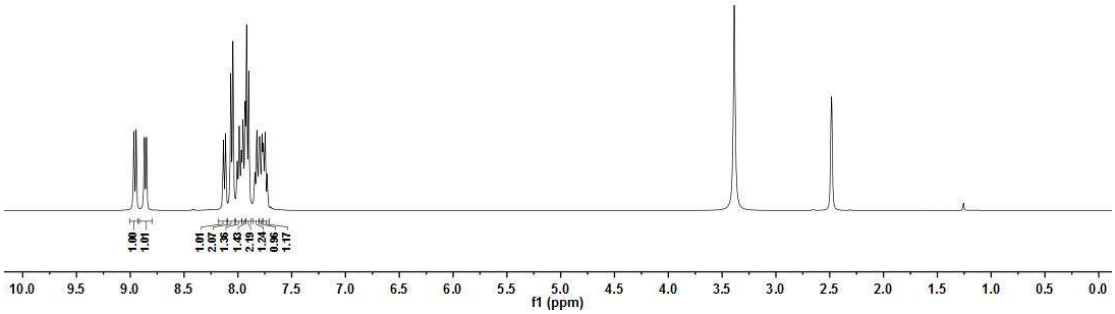

161.5
144.1
138.8
137.1
133.7
130.7
130.6
130.0
129.3
129.2
129.0
127.3
127.0
125.5
123.9
122.4
122.2
21.7
H3C
N
7h
f1 (ppm)

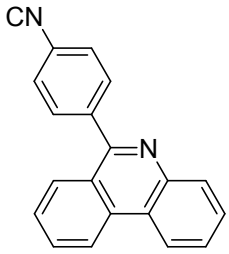

8.716
8.695
8.623
8.603
8.277
8.187
8.167
7.686
7.667
7.646
7.776
7.757
7.732
7.710
7.701
7.682
7.663
7.651
7.632
7.613
7.111
7.090
3.918
—O
N
7i
1.07
1.04
0.84
1.04
1.10
3.92
1.08
1.96
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.1
160.4
144.1
133.7
132.5
131.4
130.7
130.5
129.1
128.0
127.3
127.0
125.5
123.8
122.4
122.2
114.1
55.7
—O
N
7i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CN
N

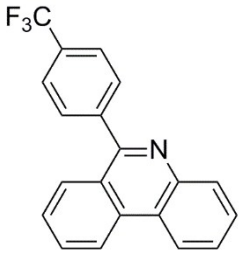
7j


1.00
1.01
1.01
2.07
1.36
1.43
2.19
1.24
0.96
1.17
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

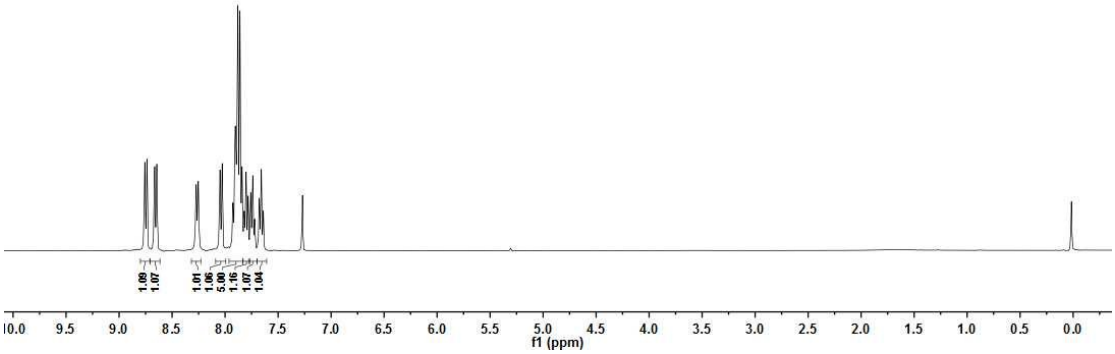

CN
N

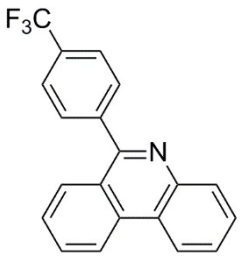
7j

70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

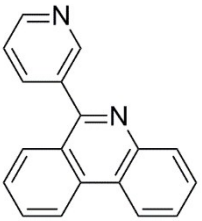


7k

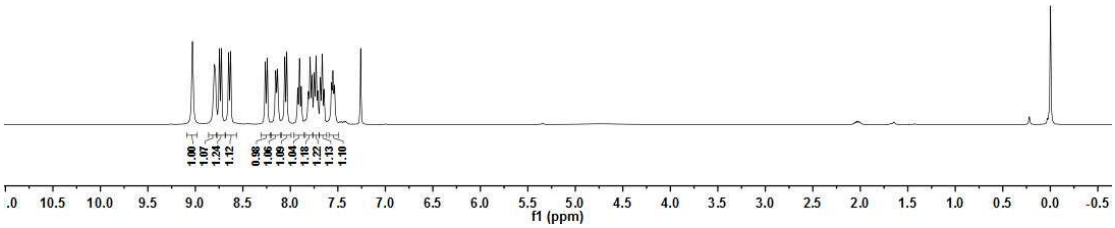


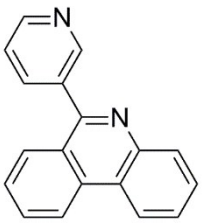


7k



7l





7l