Supporting Information

Superbase-Promoted Selective Carbon-Carbon Bond Cleavage Driven by Aromatization

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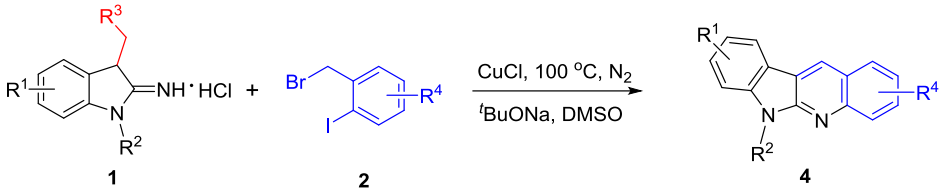
1. General Procedures

The reactions were monitored by thin layer chromatography (TLC), and the products were isolated by silica gel column chromatography. Melting points were recorded on a Beijing Tech X-4 melting point apparatus. High-resolution mass spectra (HRMS) were recorded on LCMS-IT/TOF (SHIMADZU, Japan) with an electrospray ionization source. ICP-MS was recorded on iCAP-Q (Thermo). Electron-impact mass spectra were recorded on a JEOL JMS-Q1050GC Master Quad GC/MS. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on JEOL ECS-400, JNM-ECA 600 or AV-HD-800X spectrometers. Chemical shifts were reported in ppm down field from internal Me_4Si and external $CFCl_3$, respectively. ^{1}H NMR chemical shifts were referenced to the hydrogen signal of tetramethylsilane (TMS) (δ = 0.00 ppm). In ^{13}C measurements the signal of $CDCl_3$ (δ = 77.06) was used as a reference. The following abbreviations (or combinations thereof) were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, h = heptet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, td = triplet of doublets. CuCl (CAS: 7758-89-6) and ^{t}BuONa (CAS: 865-48-5) was purchased from Energy Chemical and J & K Scientific Ltd., respectively.

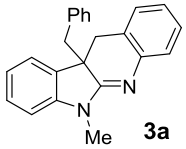
2. Synthesis and Characterization of 3a, 4a-s

2.1. General Procedures for synthesis of 4



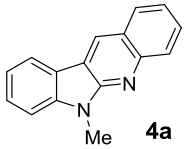
To a dried Schlenk tube were added CuCl (20 μmol, 10 mol%), **1** (*see Ref. 1 for their synthesis*) (0.22 mmol, 1.1 equiv), **2** (0.2 mmol, 1.0 equiv) and ^{t}BuONa (0.8 mmol, 4.0 equiv) under N_2, 2.0 mL of dimethylsulfoxide (DMSO) was then introduced via syringe. After stirring for 10 min at room temperature, the mixture was stirred in a pre-warmed oil bath at 100 ℃ for 20 h. The solvent was then removed under vacuum, and the residue was purified by column chromatography on silica to give the desired product **4**.

2.2. Characterization of 3a and 4a-s



3a

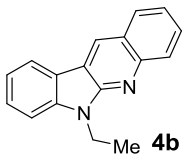
10b-Benzyl-6-methyl-10b,11-dihydro-6*H*-indolo[2,3-*b*]quinoline (3a)[2]: Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.31 (m, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.24 – 7.16 (m, 2H), 7.14 – 7.04 (m, 4H), 6.94 – 6.87 (m, 2H), 6.65 (dd, *J* = 7.7, 1.4 Hz, 2H), 6.58 (d, *J* = 7.8 Hz, 1H), 3.11 (m, 4H), 2.98 (d, *J* = 15.7 Hz, 1H), 2.77 (d, *J* = 12.8 Hz, 1H), 2.69 (d, *J* = 12.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.6, 146.4, 145. 9, 135.7, 132.3, 130.2, 128.9, 128.4, 128.1, 127.4, 126.6, 124.6, 123.7, 123.7, 123.0, 120.6, 107.3, 46.4, 40.0, 33.4, 27.3.



4a

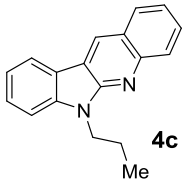
6-Methyl-6*H*-indolo[2,3-*b*]quinoline (4a)[3]: Pale yellow solid; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.11 (m, 2H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.74 – 7.66 (m, 1H), 7.55 (t, *J* = 8.2 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.28 (t, *J*

= 7.5 Hz, 1H), 3.93 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.9, 146.9, 142.9, 128.9, 128.6, 128.2, 127.6, 127.4, 124.2, 123.0, 121.5, 120.5, 120.0, 118.3, 108.8, 27.8.



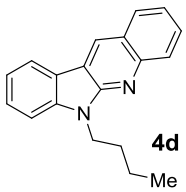
4b

6-Ethyl-6*H*-indolo[2,3-*b*]quinoline (4b)[3]: Pale yellow solid; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.14 (t, *J* = 8.3 Hz, 2H), 7.99 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.74 – 7.67 (m, 1H), 7.60 – 7.53 (m, 1H), 7.48 – 7.41 (m, 2H), 7.29 (t, *J* = 7.3 Hz, 1H), 4.59 (q, *J* = 7.2 Hz, 2H), 1.51 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2, 146.8, 141.9, 128.7, 128.5, 128.0, 127.6, 127.2, 124.1, 122.8, 121.5, 120.6, 119.7, 118.3, 108.9, 36.1, 13.7.



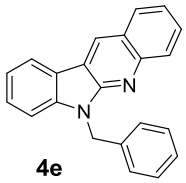
4c

6-Propyl-6*H*-indolo[2,3-*b*]quinoline (4c): Light yellow oil; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (s, 1H), 8.12 (d, *J* = 8.0 Hz, 2H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.73 – 7.66 (m, 1H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.45 – 7.39 (m, 2H), 7.26 (t, *J* = 7.5 Hz, 1H), 4.49 – 4.44 (m, 2H), 2.02 – 1.92 (m, 2H), 1.00 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.6, 146.9, 142.4, 128.7, 128.5, 127.9, 127.7, 127.2, 124.1, 122.8, 121.5, 120.5, 119.7, 118.1, 109.1, 43.0, 21.9, 11.7. HRMS (ESI^+): Calcd for $C_{18}H_{17}N_2$, $[M+H]^+$ *m*/*z* 261.1386. Found 261.1388.



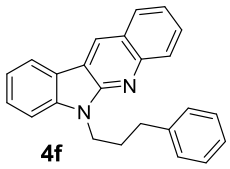
4d

6-Butyl-6*H*-indolo[2,3-*b*]quinoline (4d)[4]: Pale yellow solid; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 2H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.70 (t, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.27 (t, *J* = 7.5 Hz, 1H), 4.50 (t, *J* = 7.3 Hz, 2H), 1.92 (quint, *J* = 7.1 Hz, 2H), 1.43 (sext, *J* = 7.2 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.7, 147.0, 142.4, 128.8, 128.6, 128.0, 127.8, 127.3, 124.2, 122.9, 121.6, 120.6, 119.8, 118.2, 109.2, 41.3, 30.8, 20.5, 14.0.



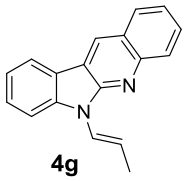
4e

6-Benzyl-6*H*-indolo[2,3-*b*]quinoline (4e)[5]: Pale yellow solid; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.72 (s, 1H), 8.13 (dd, *J* = 7.9, 5.0 Hz, 2H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.71 (t, *J* = 8.2 Hz, 1H), 7.45 (t, *J* = 8.4 Hz, 2H), 7.31 – 7.20 (m, 7H), 5.74 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.8, 147.0, 142.2, 137.4, 128.9, 128.8, 128.6, 128.2, 127.9, 127.5, 127.5, 127.3, 124.5, 123.1, 121.6, 120.8, 120.3, 118.3, 109.8, 45.1.



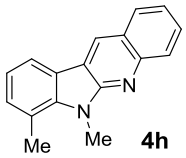
4f

6-(3-Phenylpropyl)-6*H*-indolo[2,3-*b*]quinoline (4f): Light yellow oil; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (s, 1H), 8.19 – 8.10 (m, 2H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.74 – 7.68 (m, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.29 – 7.24 (m, 3H), 7.23 – 7.20 (m, 2H), 7.18 (t, *J* = 7.3 Hz, 1H), 4.54 (t, *J* = 7.3 Hz, 2H), 2.80 – 2.73 (m, 2H), 2.29 (quint, *J* = 7.6 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.6, 146.9, 142.2, 141.5, 128.7, 128.5, 128.5, 128.4, 128.0, 127.7, 127.2, 126.0, 124.2, 122.9, 121.5, 120.6, 119.8, 118.2, 109.0, 41.0, 33.3, 29.9. HRMS (ESI$^+$): Calcd for $C_{24}H_{21}N_2$, $[M+H]^+$ *m*/*z* 337.1699. Found 337.1695.



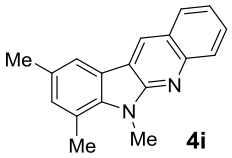
4g

6-(Prop-1-en-1-yl)-6*H*-indolo[2,3-*b*]quinoline (4g): Light yellow oil; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.14 (dd, *J* = 16.2, 8.1 Hz, 2H), 7.99 (d, *J* = 8.1 Hz, 1H), 7.74 – 7.66 (m, 2H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.35 – 7.30 (m, 2H), 6.70 – 6.61 (m, 1H), 2.06 (dd, *J* = 6.7, 1.5 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.1, 146.9, 141.2, 129.0, 128.5, 128.3, 128.2, 127.3, 124.6, 123.6, 122.9, 121.5, 121.2, 121.0, 118.4, 116.8, 110.5, 16.4. HRMS (ESI$^+$): Calcd for $C_{18}H_{15}N_2$, $[M+H]^+$ *m*/*z* 259.1230. Found 259.1232.



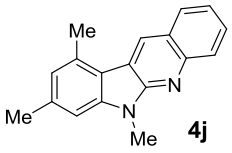
4h

6,7-Dimethyl-6*H*-indolo[2,3-*b*]quinoline (4h): Light yellow oil; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (800 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.97 (t, *J* = 6.7 Hz, 2H), 7.73 – 7.66 (m, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 7.3 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 4.27 (s, 3H), 2.86 (s, 3H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 153.3, 146.9, 141.3, 131.3, 128.7, 128.5, 127.5, 126.9, 124.2, 122.8, 121.0, 120.8, 120.0, 119.3, 118.2, 30.92, 19.9. HRMS (ESI$^+$): Calcd for $C_{17}H_{15}N_2$, $[M+H]^+$ *m*/*z* 247.1230. Found 247.1230.



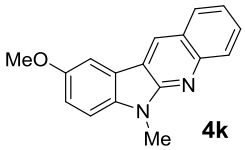
4i

6,7,9-Trimethyl-6*H*-indolo[2,3-*b*]quinoline (4i): Light yellow oil; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.09 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.70 (s, 1H), 7.67 (t, *J* = 7.1 Hz, 1H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.04 (s, 1H), 4.17 (s, 3H), 2.75 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 153.4, 146.7, 139.3, 132.4, 129.3, 128.6, 128.4, 127.4, 126.7, 124.1, 122.6, 121.0, 120.3, 119.3, 118.2, 30.8, 21.0, 19.6. HRMS (ESI$^+$): Calcd for $C_{18}H_{17}N_2$, $[M+H]^+$ *m*/*z* 261.1386. Found 261.1388.



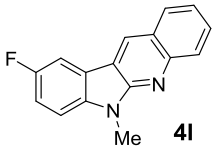
4j

6,8,10-Trimethyl-6*H*-indolo[2,3-*b*]quinoline (4j): Pale yellow solid, mp = 137-139 ℃; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.07 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.66 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.3 Hz, 1H), 6.90 (s, 1H), 6.81 (s, 1H), 3.81 (s, 3H), 2.73 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.7, 145.8, 143.1, 138.2, 134.2, 128.5, 128.4, 128.3, 127.2, 124.2, 122.9, 122.6, 118.8, 116.3, 106.6, 27.6, 22.2, 20.3. HRMS (ESI$^+$): Calcd for $C_{18}H_{17}N_2$, $[M+H]^+$ *m*/*z* 261.1386. Found 261.1386.



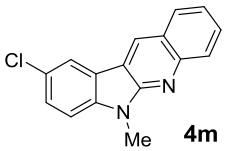
4k

9-Methoxy-6-methyl-6*H*-indolo[2,3-*b*]quinoline (4k)[3]: Pale yellow solid; Eluent: petroleum ether/EtOAc 5:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.72 – 7.66 (m, 1H), 7.57 (d, *J* = 2.3 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 8.7 Hz, 1H), 7.17 – 7.12 (m, 1H), 3.90 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 154.1, 152.9, 146.8, 137.4, 128.8, 128.5, 127.4, 127.3, 123.7, 122.6, 120.7, 118.1, 116.0, 109.2, 105.3, 56.1, 27.7.



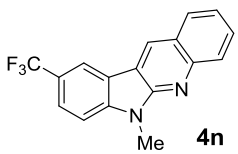
4l

9-Fluoro-6-methyl-6*H*-indolo[2,3-*b*]quinoline (4l): Light yellow oil; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (800 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 1H), 7.79 (dt, *J* = 8.3, 1.5 Hz, 1H), 7.74 – 7.68 (m, 1H), 7.48 – 7.43 (m, 1H), 7.33 – 7.26 (m, 2H), 3.95 (s, 3H); ^{13}C NMR (201 MHz, $CDCl_3$) δ 157.70 (d, *J* = 237.2 Hz), 153.1, 147.1, 139.1, 129.1, 128.7, 128.0, 127.5, 123.9, 123.0, 120.9 (d, *J* = 8.8 Hz), 117.7 (d, *J* = 3.7 Hz), 115.4 (d, *J* = 24.9 Hz), 109.2 (d, *J* = 8.8 Hz), 107.8 (d, *J* = 24.2 Hz), 27.9; ^{19}F NMR (565 MHz, $CDCl_3$) δ −124.39. HRMS (ESI^+): Calcd for $C_{16}H_{12}FN_2$, $[M+H]^+$ *m/z* 251.0979. Found 251.0978.



4m

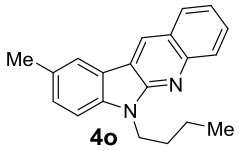
9-Chloro-6-methyl-6*H*-indolo[2,3-*b*]quinoline (4m): Pale yellow solid, mp = 129-131 ℃; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.60 (s, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 1.9 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.50 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.6, 146.9, 140.9, 129.1, 128.5, 127.8, 127.7, 127.4, 125.2, 123.9, 123.0, 121.3, 121.1, 117.0, 109.4, 27.6. HRMS (ESI^+): Calcd for $C_{16}H_{12}ClN_2$, $[M+H]^+$ *m/z* 267.0684. Found 267.0680.



4n

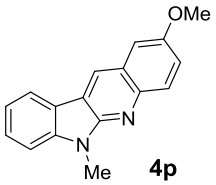
6-Methyl-9-(trifluoromethyl)-6*H*-indolo[2,3-*b*]quinoline (4n): Pale yellow solid, mp = 99-101 ℃; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (s, 1H), 8.34

(s, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 8.5 Hz, 1H), 7.77 – 7.72 (m, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.9, 147.1, 144.5, 129.5, 128.7, 128.2, 127.7, 124.9 (q, *J* = 3.8 Hz), 124.3, 123.5, 120.2, 118.7 (d, *J* = 3.8 Hz), 117.3, 108.7, 27.9; ^{19}F NMR (565 MHz, $CDCl_3$) δ −61.22. HRMS (ESI^+): Calcd for $C_{17}H_{12}F_3N_2$, $[M+H]^+$ *m*/*z* 301.0947. Found 301.0947.



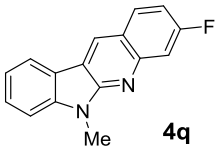
4o

6-Butyl-9-methyl-6*H*-indolo[2,3-*b*]quinoline (4o): Pale yellow solid, mp = 95-97 ℃; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.60 (s, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 7.7 Hz, 1H), 7.90 (s, 1H), 7.71 – 7.65 (m, 1H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.27 (d, *J* = 8.2 Hz, 1H), 4.46 (t, *J* = 7.3 Hz, 2H), 2.52 (s, 3H), 1.89 (quint, *J* = 7.5 Hz, 2H), 1.40 (sext, *J* = 7.4 Hz, 2H), 0.95 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.7, 146.8, 140.4, 129.0, 129.0, 128.6, 128.5, 127.6, 126.9, 124.0, 122.6, 121.7, 120.5, 118.1, 108.8, 41.2, 30.7, 21.3, 20.4, 13.9. HRMS (ESI^+): Calcd for $C_{20}H_{20}N_2$, $[M+H]^+$ *m*/*z* 289.1699. Found 289.1699.



4p

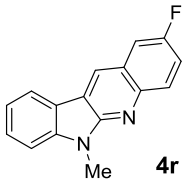
2-Methoxy-6-methyl-6*H*-indolo[2,3-*b*]quinoline (4p): Light yellow oil; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.16 – 8.09 (m, 1H), 8.03 (d, *J* = 9.2 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.41 – 7.37 (m, 2H), 7.29 – 7.25 (m, 2H), 3.95 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 151.8, 142.9, 142.8, 128.9, 128.1, 126.2, 124.7, 121.5 (2C), 120.3, 119.7, 118.3, 108.7, 106.3, 55.6, 27.8. HRMS (ESI^+): Calcd for $C_{17}H_{15}N_2O$, $[M+H]^+$ *m*/*z* 263.1179. Found 263.1178.



4q

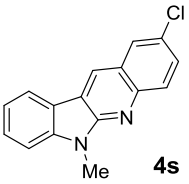
3-Fluoro-6-methyl-6*H*-indolo[2,3-*b*]quinoline (4q): Pale yellow solid, mp = 98-100 ℃; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.06 (d, *J* = 7.6 Hz, 1H),

7.89 (dd, *J* = 8.9, 6.4 Hz, 1H), 7.72 (dd, *J* = 10.9, 2.4 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.21 (td, *J* = 8.6, 2.6 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ163.0 (d, *J* = 248.0 Hz), 153.2, 147.7 (d, *J* = 13.1 Hz), 142.5, 130.3, 130.2, 128.0, 127.2, 121.3, 120.3, 120.1, 117.5 (d, *J* = 2.7 Hz), 113.1 (d, *J* = 25.3 Hz), 111.2 (d, *J* = 20.9 Hz), 108.8, 27.7; ^{19}F NMR (565 MHz, $CDCl_3$) δ −111.73. HRMS (ESI^+): Calcd for $C_{16}H_{12}FN_2$, $[M+H]^+$ *m*/*z* 251.0979. Found 251.0979.



4r

2-Fluoro-6-methyl-6*H*-indolo[2,3-*b*]quinoline (4r): Pale yellow solid, mp = 112-114 ℃; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.12 – 7.99 (m, 2H), 7.59 – 7.49 (m, 2H), 7.49 – 7.41 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.27 (t, *J* = 7.4 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3 (d, *J* = 242.7 Hz), 152.5, 143.7, 143.0, 129.5 (d, *J* = 8.9 Hz), 128.5, 126.4 (d, *J* = 5.3 Hz), 124.2 (d, *J* = 9.6 Hz), 121.7, 120.1, 119.9, 118.8, 118.8 (d, *J* = 25.5 Hz), 111.3 (d, *J* = 21.5 Hz), 108.8, 27.7. HRMS (ESI^+): Calcd for $C_{16}H_{12}N_2F$, $[M+H]^+$ m/z 251.0979. Found 251.0979.



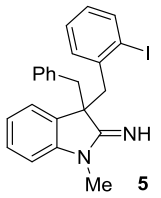
4s

2-Chloro-6-methyl-6*H*-indolo[2,3-*b*]quinoline (4s): Pale yellow solid, mp = 144-146 ℃; Eluent: petroleum ether/EtOAc 10:1; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.13 (d, *J* = 7.7 Hz, 1H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.94 (d, *J* = 2.4 Hz, 1H), 7.65 – 7.57 (m, 2H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.34 – 7.29 (m, 1H), 3.96 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.0, 145.2, 143.1, 129.6, 129.1, 128.7, 128.2, 127.1, 126.4, 124.7, 121.8, 120.3, 120.2, 119.0, 109.0, 27.9. HRMS (ESI^+): Calcd for $C_{16}H_{12}ClN_2$, $[M+H]^+$ m/z 267.0684. Found 267.0684.

2.3. Synthesis and Characterization of 5

To a mixture of **1a** (0.3 mmol, 1.0 equiv), **2a** (0.3 mmol, 1.0 equiv) and K_2CO_3 (0.75 mmol, 2.5 equiv) was added 3 mL of DMSO, and the mixture was heated with stirring for 12 h at RT. After

removal of all volatiles *in vacuo*, the residue was purified by column chromatography on silica eluted with EtOAc to give the desired product **5** as a light yellow oil.

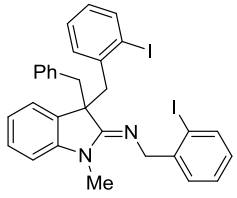


5

3-Benzyl-3-(2-iodobenzyl)-1-methylindolin-2-imine (5): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, J = 7.9, 1.2 Hz, 1H), 7.11 – 6.99 (m, 6H), 6.96 – 6.91 (m, 1H), 6.87 – 6.78 (m, 3H), 6.75 (td, J = 7.7, 1.7 Hz, 1H), 6.36 (d, J = 7.8 Hz, 1H), 3.52 – 3.45 (m, 1H), 3.43 – 3.35 (m, 1H), 3.23 – 3.17 (m, 1H), 3.17 – 3.10 (m, 1H), 2.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.7, 145.5, 139.6, 139.5, 135.4, 130.3, 130.2, 129.8, 128.3, 128.1, 127.8, 127.5, 126.5, 124.4, 120.0, 106.4, 103.6, 55.3, 47.7, 45.9 26.8. HRMS (ESI^+): Calcd for $C_{23}H_{22}IN_2$, $[M+H]^+$ m/z 453.0828. Found 453.0826.

2.4. Synthesis and Characterization of 6

To a mixture of **1a** (0.3 mmol, 1.0 equiv), **2a** (0.66 mmol, 2.2 equiv) and K_2CO_3 (1.05 mmol, 3.5 equiv) was added 3 mL of DMSO, and the mixture was heated with stirring for 12 h at RT. After removal of all volatiles *in vacuo*, the residue was purified by column chromatography on silica eluted with petroleum ether/EtOAc (15:1 in volume) to give the desired product **6** as a light yellow oil.

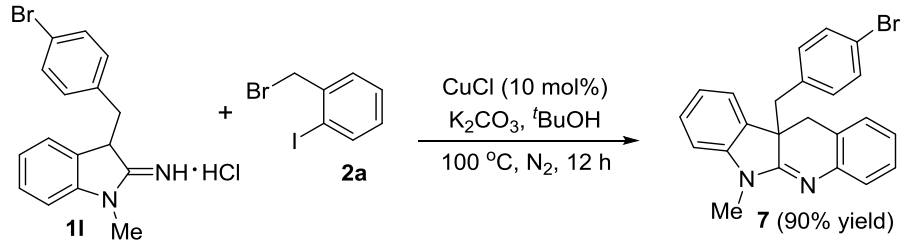


6

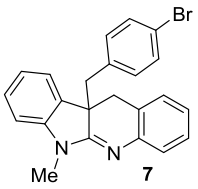
3-Benzyl-*N*,3-bis(2-iodobenzyl)-1-methylindolin-2-imine (6): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.8 Hz, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.12 – 6.91 (m, 8H), 6.80 – 6.69 (m, 4H), 6.38 (d, *J* = 7.8 Hz, 1H), 5.08 (d, *J* = 17.4 Hz, 1H), 4.91 (d, *J* = 17.4 Hz, 1H), 3.81 (d, *J* = 15.8 Hz, 1H), 3.75 – 3.66 (m, 2H), 3.28 (d, *J* = 13.4 Hz, 1H), 2.98 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.8, 145.8, 143.5, 139.8, 139.7, 138.7, 135.8, 130.9, 129.9, 129.1, 128.7, 128.3, 128.3, 128.2, 128.0, 127.6, 126.6, 123.3, 119.5, 106.1, 103.3, 99.1,

56.4, 55.2, 46.7, 44.4, 27.4. HRMS (ESI$^+$): Calcd for $C_{30}H_{27}I_2N_2$, $[M+H]^+$ m/z 669.0264. Found 669.0263.

2.5. Synthesis and Characterization of 7[1]

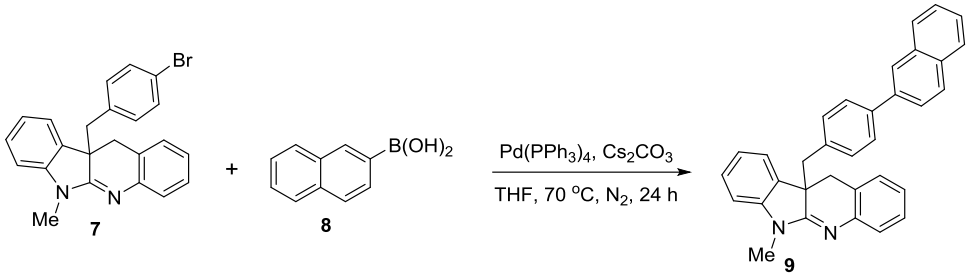


An oven-dried Schlenk tube equipped with a Teflon screw seal was charged with a magnetic stirbar, CuCl (30 μmol, 10 mol%), **1l** (0.33 mmol, 1.1 equiv), **2a** (0.3 mmol, 1.0 equiv) and K_2CO_3 (1.2 mmol, 4.0 equiv). The tube was evacuated and backfilled with argon; this procedure was carried out three times. The solids were dissolved in ^{t}BuOH (3.0 mL), the reaction tube was sealed, and the reaction mixture was stirred in a pre-heated oil-bath at 100 °C for 12 h. The solvent was then removed under vacuum, and the residue was purified by column chromatography on silica eluted with petroleum ether/EtOAc (10:1 in volume) to give the desired product **7** as a light yellow oil.

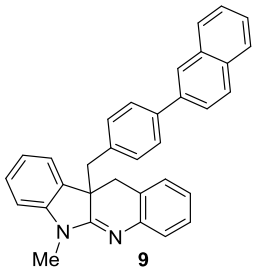


10b-(4-Bromobenzyl)-6-methyl-10b,11-dihydro-6*H*-indolo[2,3-*b*]quinoline (7): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 (d, *J* = 7.6 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.22 – 7.16 (m, 4H), 7.05 (t, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 7.0 Hz, 1H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.59 (d, *J* = 7.8 Hz, 1H), 6.49 (d, *J* = 8.2 Hz, 2H), 3.11 (s, 3H), 3.07 (d, *J* = 15.7 Hz, 1H), 2.99 (d, *J* = 15.7 Hz, 1H), 2.75 (d, *J* = 13.0 Hz, 1H), 2.60 (d, *J* = 13.0 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.0, 146.2, 145.7, 134.7, 131.9, 131.6, 130.4, 128.7, 128.5, 128.1, 124.5, 123.7, 123.3, 122.7, 120.7, 120.6, 107.3, 46.1, 39.4, 33.5, 27.2. HRMS (ESI$^+$): Calcd for $C_{23}H_{20}BrN_2$, $[M+H]^+$ m/z 403.0810. Found 403.0811.

2.6. Synthesis and Characterization of 9

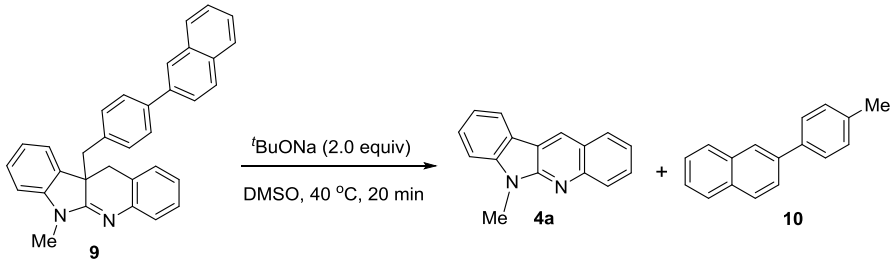


To a mixture of **7** (0.3 mmol, 1.0 equiv), **8** (0.6 mmol, 2.0 equiv), $Pd(PPh_3)_4$ (0.03 mmol, 0.1 eq) and Cs_2CO_3 (0.9 mmol, 3.0 equiv) was added 3 mL of THF under N_2, and the mixture was heated with stirring at 70 °C for 24 h. After removal of all volatiles *in vacuo*, the residue was purified by column chromatography on silica eluted with petroleum ether/EtOAc (15:1 in volume) to give the desired product **9** as a pale yellow solid, mp = 179-181 ℃.

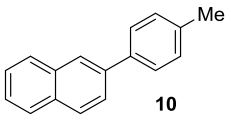


6-Methyl-10b-(4-(naphthalen-2-yl)benzyl)-10b,11-dihydro-6*H*-indolo[2,3-*b*]quinoline (9): ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (s, 1H), 7.85 (t, *J* = 7.2 Hz, 2H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.68 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.49 – 7.42 (m, 4H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.19 (m, 2H), 7.09 (t, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 6.6 Hz, 1H), 6.94 (t, *J* = 7.4 Hz, 1H), 6.77 (d, *J* = 8.0 Hz, 2H), 6.61 (d, *J* = 7.8 Hz, 1H), 3.19 – 3.14 (m, 4H), 3.01 (d, *J* = 15.6 Hz, 1H), 2.81 (d, *J* = 13.0 Hz, 1H), 2.77 (d, *J* = 13.0 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.6, 146.3, 145.7, 139.1, 138.1, 134.9, 133.6, 132.5, 132.3, 130.7, 128.8, 128.4, 128.4, 128.1, 127.6, 126.3, 126.3, 125.9, 125.4, 125.3, 124.5, 123.7, 123.7, 122.9, 120.7, 107.4, 46.3, 39.6, 33.3, 27.3. HRMS (ESI^+): Calcd for $C_{33}H_{27}N_2$, $[M+H]^+$ m/z 451.2174. Found 451.2173.

2.7. Synthesis and Characterization of 10



To a mixture of **9** (0.2 mmol, 1.0 equiv) and ^{t}BuONa (0.2 mmol, 2.0 equiv) was added 3 mL of THF under air or N_2, and the mixture was heated with stirring at 40 ℃ for 20 min. After removal of all volatiles *in vacuo*, the residue was purified by column chromatography on silica eluted with petroleum ether/EtOAc (100:1 in volume) to give the desired product **10** as a white solid, mp = 81-83 ℃.



10

2-(*p*-tolyl)naphthalene (10)[6]: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.88 (t, *J* = 8.2 Hz, 2H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.73 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.51 – 7.42 (m, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 138.5, 138.2, 137.2, 133.7, 132.5, 129.6, 128.4, 128.2, 127.7, 127.3, 126.3, 125.8, 125.6, 125.5, 21.2. EI-MS: Calcd for $C_{17}H_{14}$, M^+ m/z 218. Found 218.

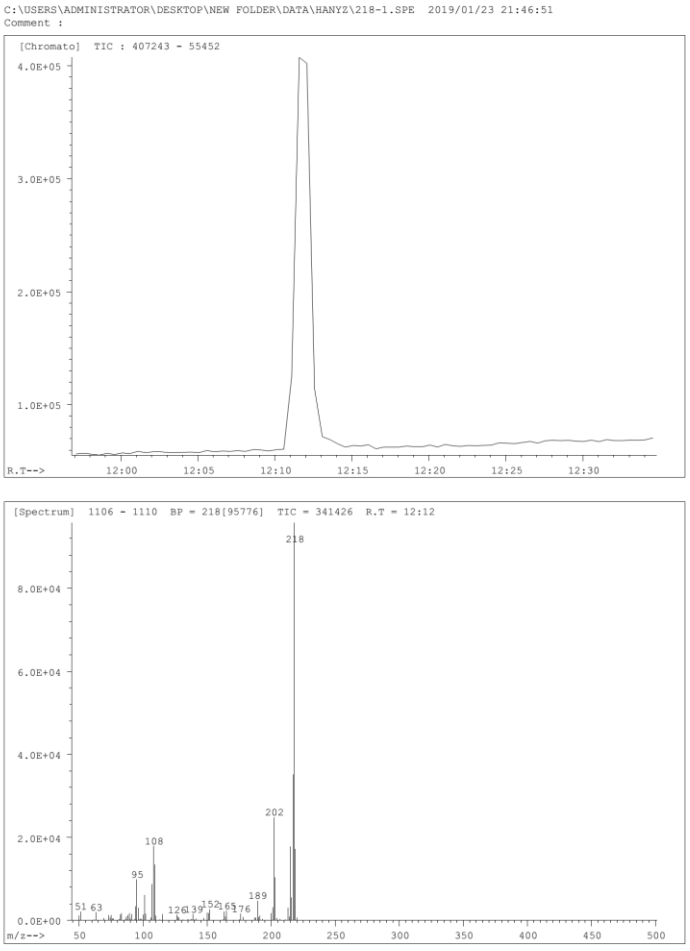


Figure S1. EI-MS data for compound **10** using GC-MS.

3. ICP-MS Data

The commercial available ^{t}BuONa from J & K Scientific Ltd. was examined by **ICP-MS** experiments. Possible critical transition metals, including Fe, Co, Ni, Cu, Pd, Ru, Ir were tested. The results were as **Table S1**.

Table S1. **ICP-MS** Analysis of Various Metals in ^{t}BuONa.

Element	Fe	Ni	Co	Pd	Ir	Cu	Ru
Amount	75.911	2.303	＜0.1	6.446	＜0.01	40.051	0.147

Unit: ng/g (ppb)

We found that the ^{t}BuONa from J & K Scientific Ltd., contained all these metals in the ppb level.

4. X-Ray Crystallographic Data for 4e

Single crystal X-ray data were collected on a Bruker APEXII X-ray diffractometer equipped with a CMOS PHOTON 100 detector with a Cu Kα X-ray source (Kα = 1.54178 Å). Data were indexed, integrated and scaled using DENZO and SCALEPACK from the HKL program suite. Structure of **4e**, was solved through direct method (SHELXS-97) and refined by full-matrix least-squares (SHELXL-2014) on F^2. Anisotropic thermal parameters were used for the non-hydrogen atoms and isotropic parameters for the hydrogen atoms. The data obtained were deposited at the Cambridge Crystallographic Data Centre.

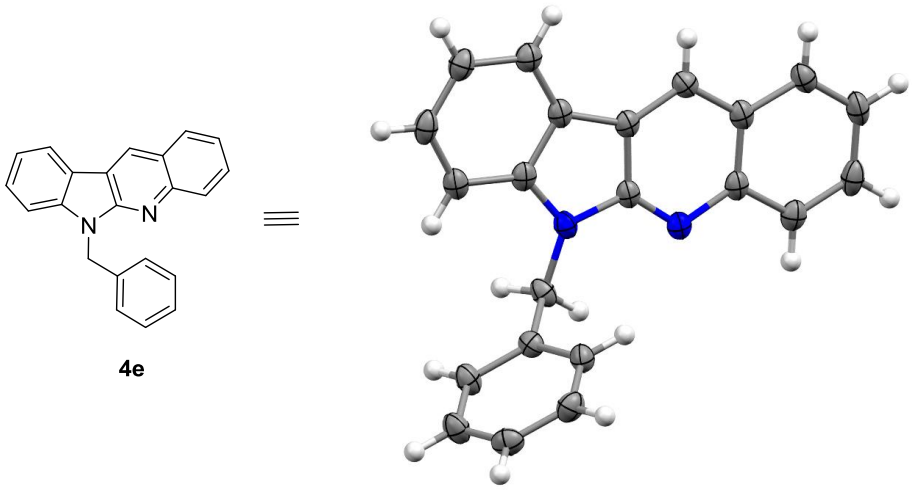


Figure S2. Crystal structure of 4e showing 50% probability displacement ellipsoids.

Table S2. Crystal Data and Structure Refinement for 4e.

Identification code	CCDC 1889682
Empirical formula	$C_{22}H_{16}N_2$
Formula weight	308.37
Temperature/K	108.9(7)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	4.84497(9)
b/Å	20.0214(4)
c/Å	15.7697(3)
α/°	90
β/°	96.9103(18)
γ/°	90
Volume/Å^3	1518.60(5)
Z	4
ρ_{calc}g/cm^3	1.349
μ/mm^{-1}	0.615
F(000)	648
Crystal size/mm^3	0.4 × 0.12 × 0.1
Radiation	CuK\α (λ = 1.54184)
2Θ range for data collection/°	7.134 to 142.328
Index ranges	-5 <= h <= 4, -23 <= k <= 23, -18 <= l <= 19
Reflections collected	9190
Independent reflections	2899 [R_{int} = 0.0328, R_{sigma} = 0.0309]
Data/restraints/parameters	2899/0/217
Goodness-of-fit on F^2	1.017
Final R indexes [I>=2σ (I)]	R_1 = 0.0406, wR_2 = 0.1010
Final R indexes [all data]	R_1 = 0.0501, wR_2 = 0.1083
Largest diff. peak/hole / e Å^{-3}	0.378/-0.226

5. References

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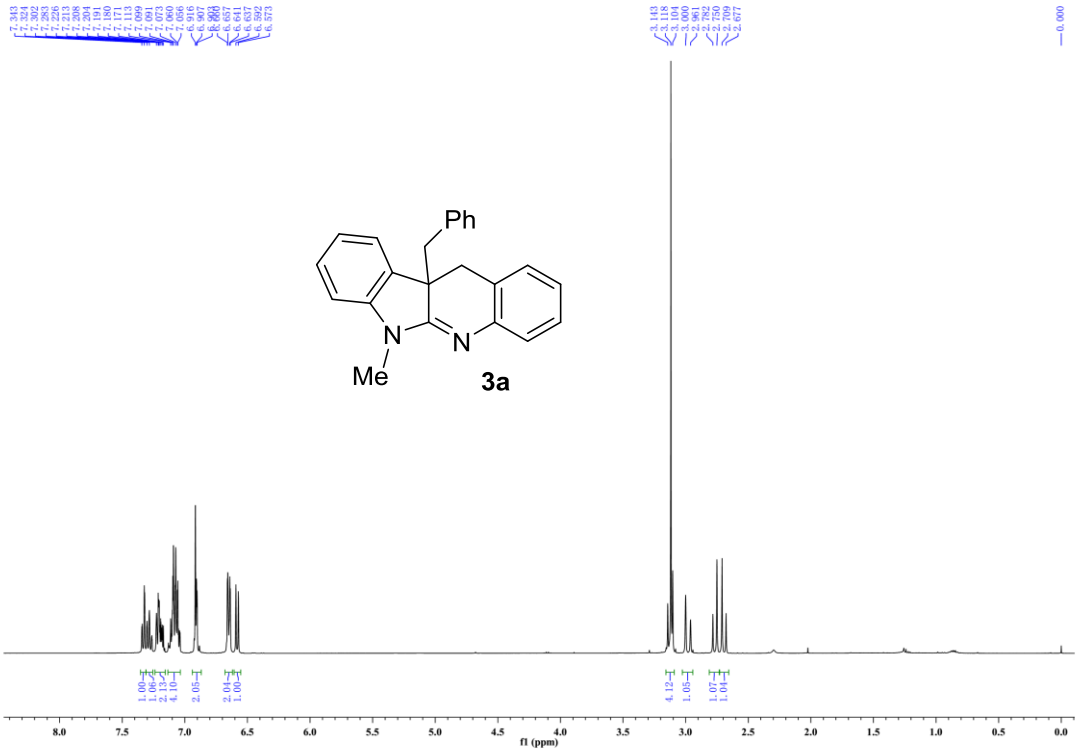
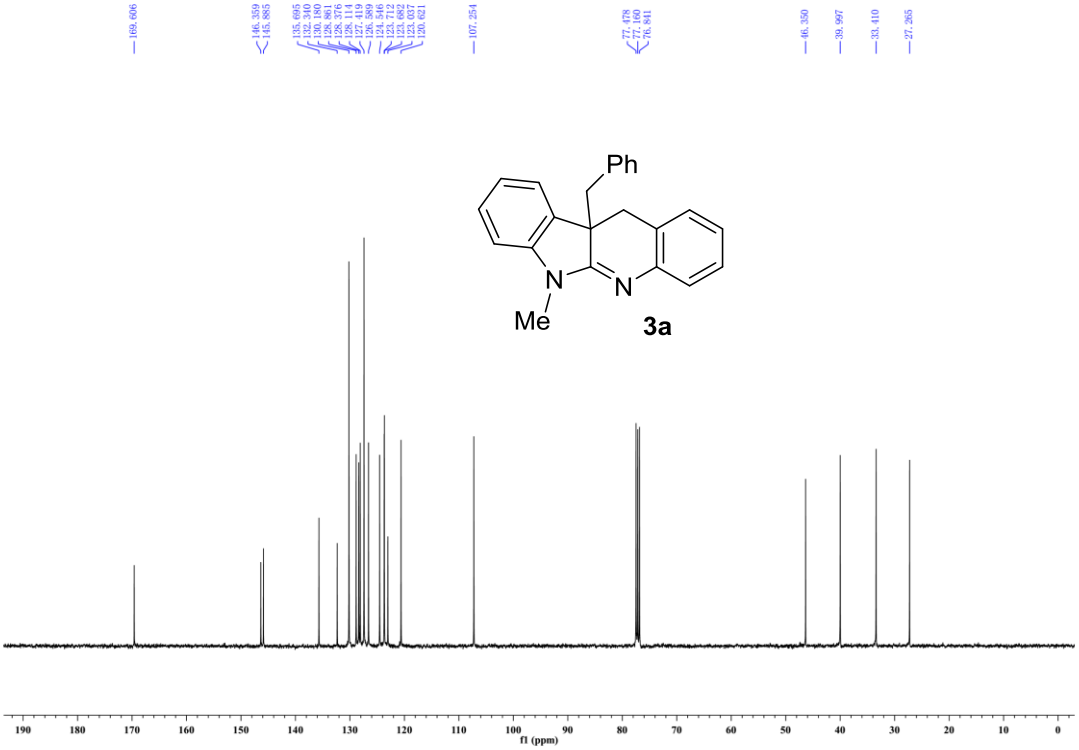
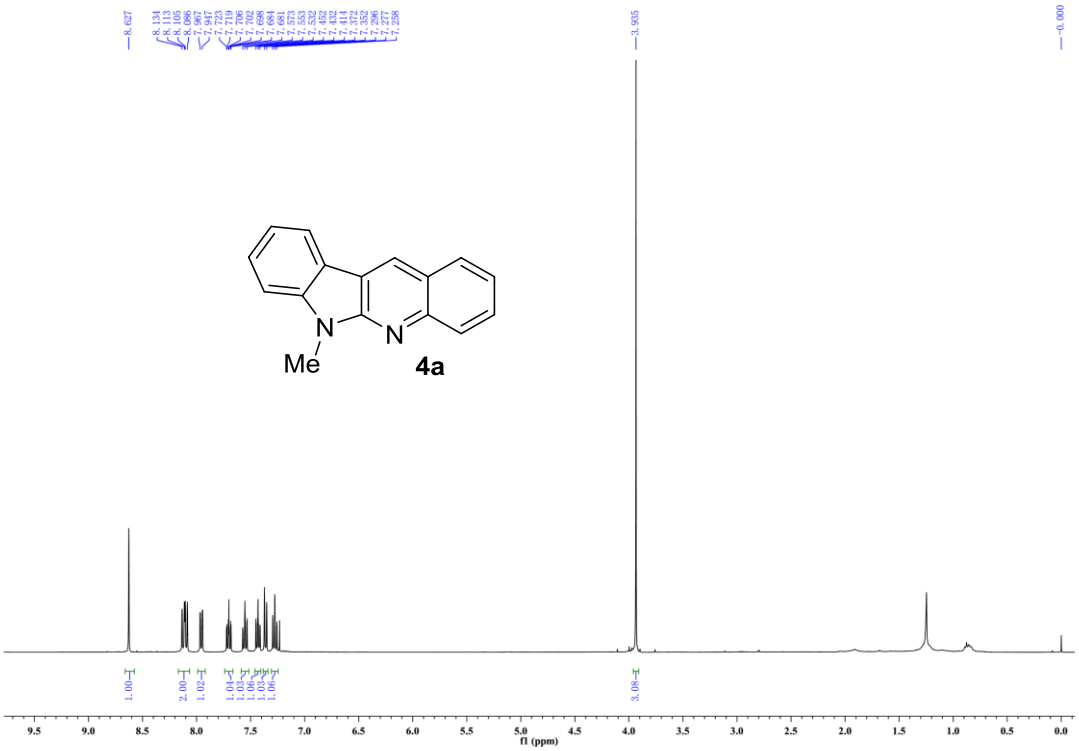
6. NMR Spectra of 3a, 4a–s, 5–7, 9 and 10



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8.134
8.113
8.105
8.086
7.967
7.947
7.723
7.719
7.706
7.702
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7.684
7.681
7.673
7.533
7.530
7.532
7.432
7.422
7.414
7.372
7.352
7.306
7.277
7.258
3.935
0.000
N
N
Me
4a
1.00
2.00
1.02
1.04
1.03
1.06
1.05
1.06
3.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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1.0
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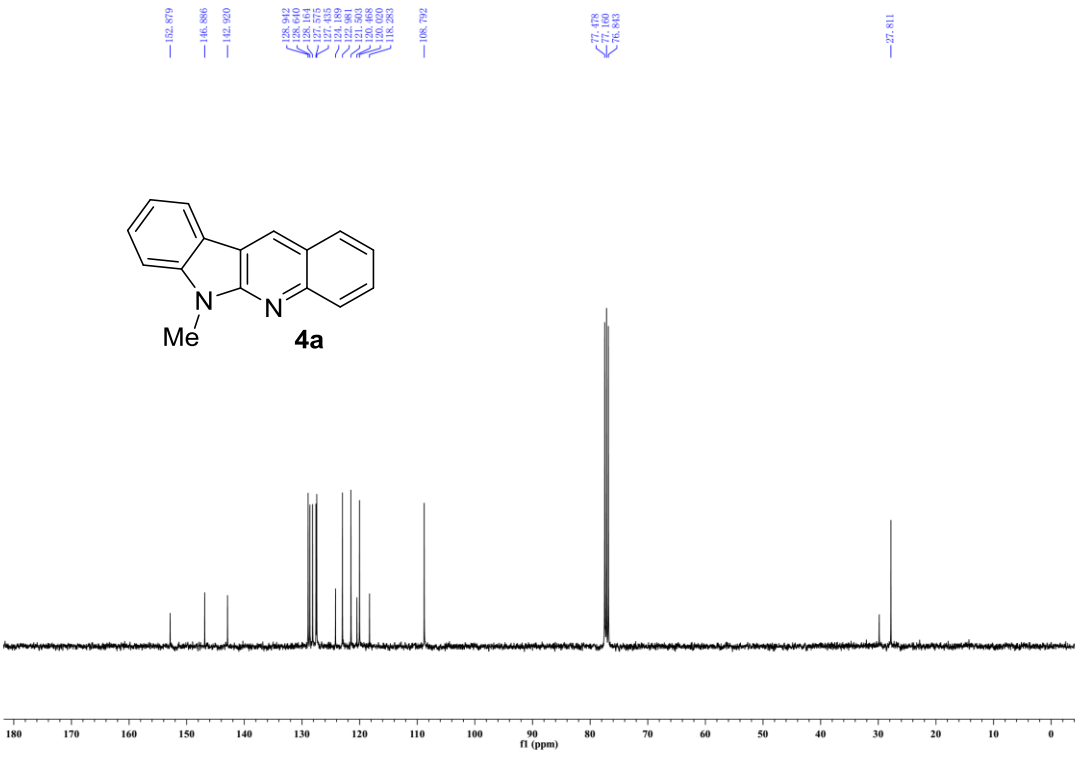
f1 (ppm)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122.901
121.553
120.468
120.020
118.283
108.792
77.478
77.160
76.843
27.811
N
N
Me
4a
180
170
160
150
140
130
120
110
100
90
80
70
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50
40
30
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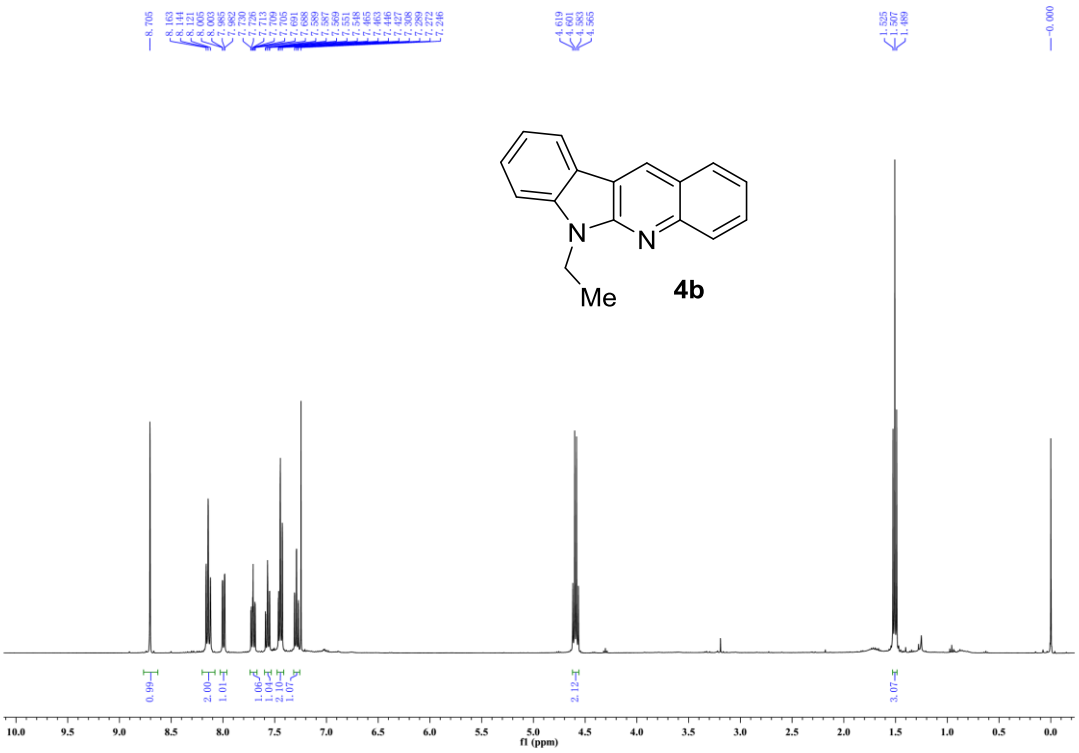
f1 (ppm)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7.982
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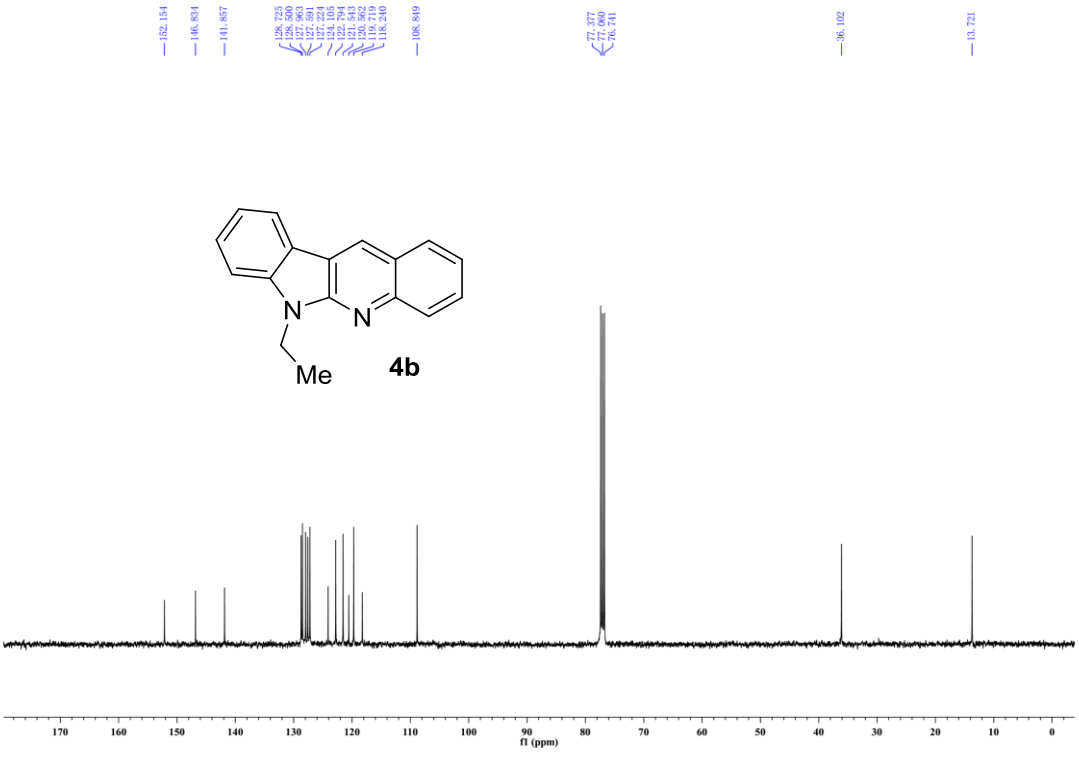
7.728
7.713
7.709
7.705
7.691
7.688
7.599
7.597
7.569
7.551
7.518
7.465
7.463
7.446
7.427
7.308
7.299
7.272
7.246
4.619
4.601
4.583
4.565
1.525
1.497
1.469
0.000
N
N
Me
4b
0.99
2.06
1.01
1.06
1.04
2.10
1.07
2.12
3.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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119.379
118.240
108.819
77.377
77.060
76.741
36.102
13.721
N
N
Me
4b
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50
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30
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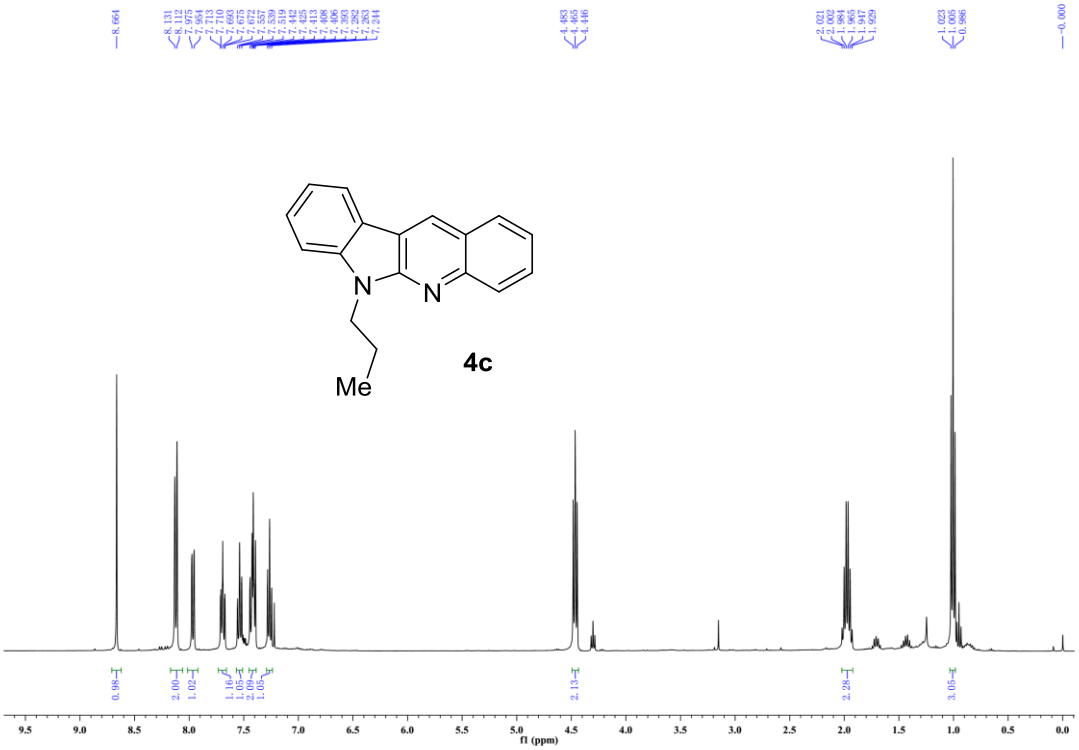
10
0
f1 (ppm)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8.112
7.975
7.954
7.713
7.710
7.693
7.675
7.672
7.558
7.539
7.519
7.442
7.435
7.413
7.408
7.406
7.360
7.282
7.283
7.244
4.483
4.465
4.446
2.021
2.002
1.984
1.965
1.947
1.929
1.023
1.000
0.986
0.000
N
N
Me
4c
0.98
2.00
1.02
1.16
1.05
2.08
1.05
2.13
2.28
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
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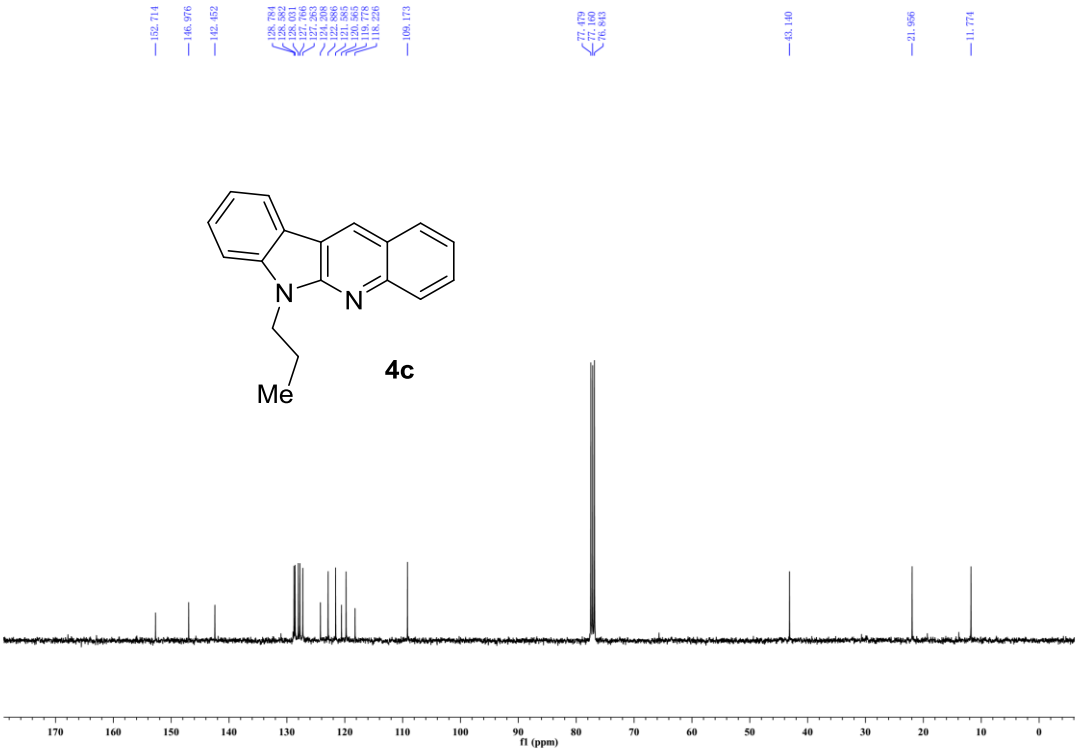
1.0
0.5
0.0
f1 (ppm)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121.360
120.565
119.778
118.226
109.173
77.479
77.160
76.843
63.140
21.956
11.774
N
N
Me
4c
170
160
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130
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50
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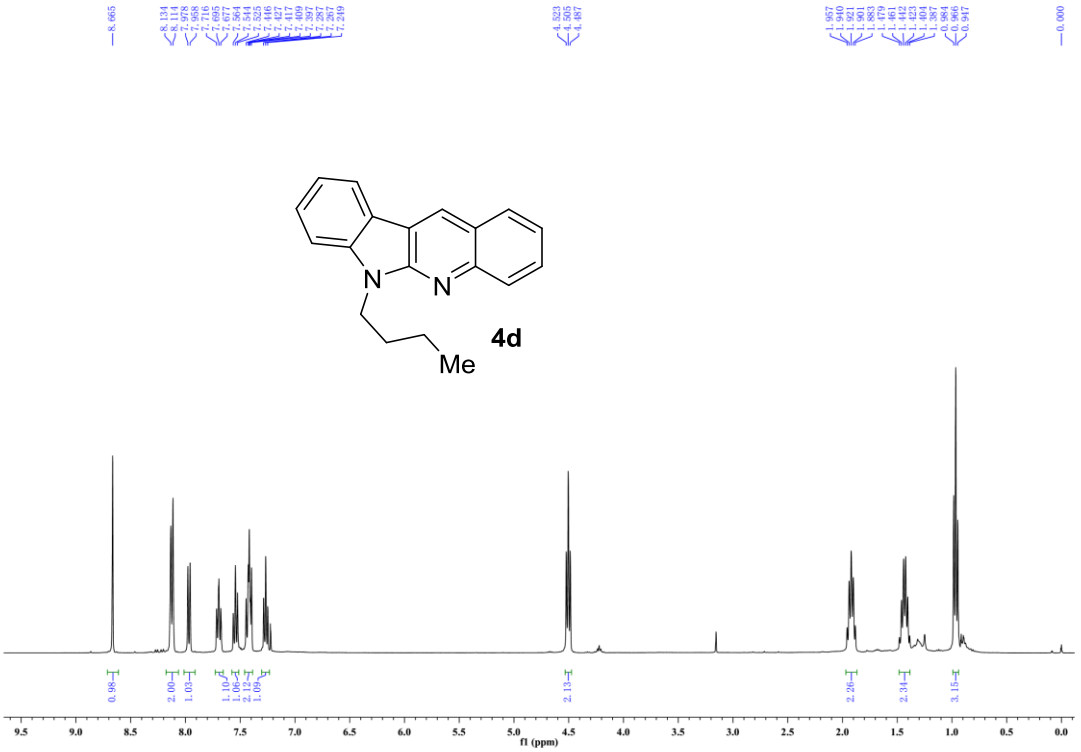
30
20
10
0
f1 (ppm)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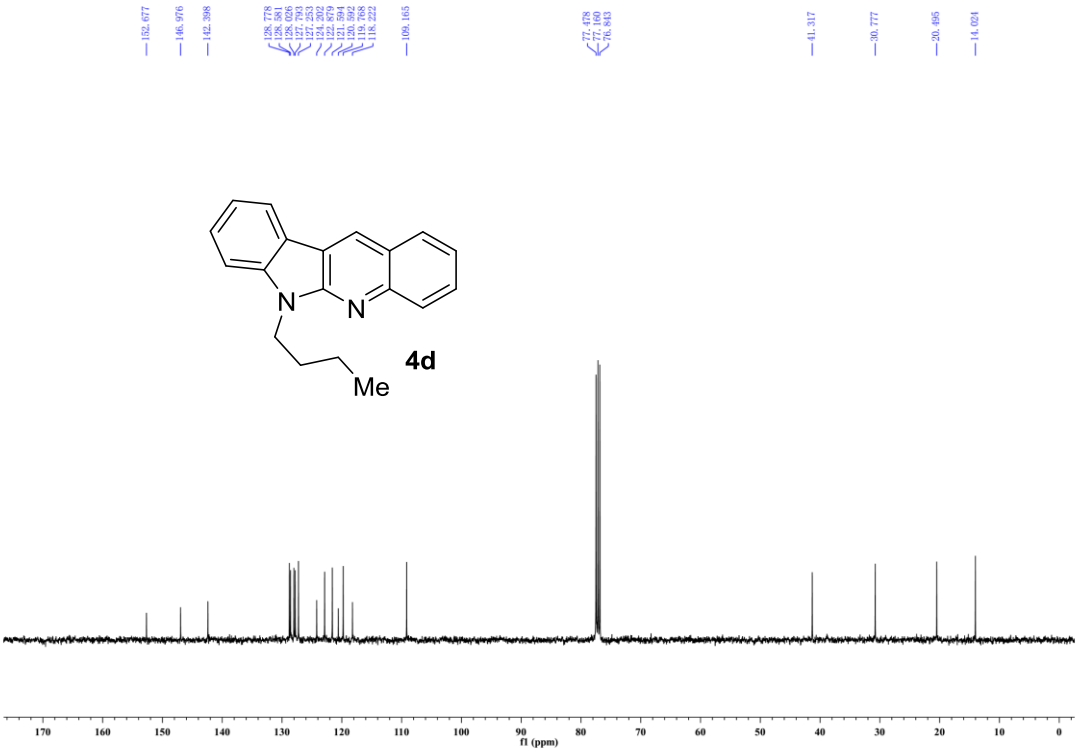
7.958
7.716
7.695
7.677
7.564
7.544
7.525
7.446
7.427
7.417
7.409
7.397
7.267
7.249
4.523
4.505
4.487
1.957
1.940
1.921
1.901
1.883
1.479
1.461
1.442
1.423
1.404
1.387
0.984
0.966
0.947
0.000
N
N
Me
4d
0.98
2.00
1.03
1.10
1.06
1.13
1.09
2.13
2.26
2.34
3.15
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.495
127.793
127.553
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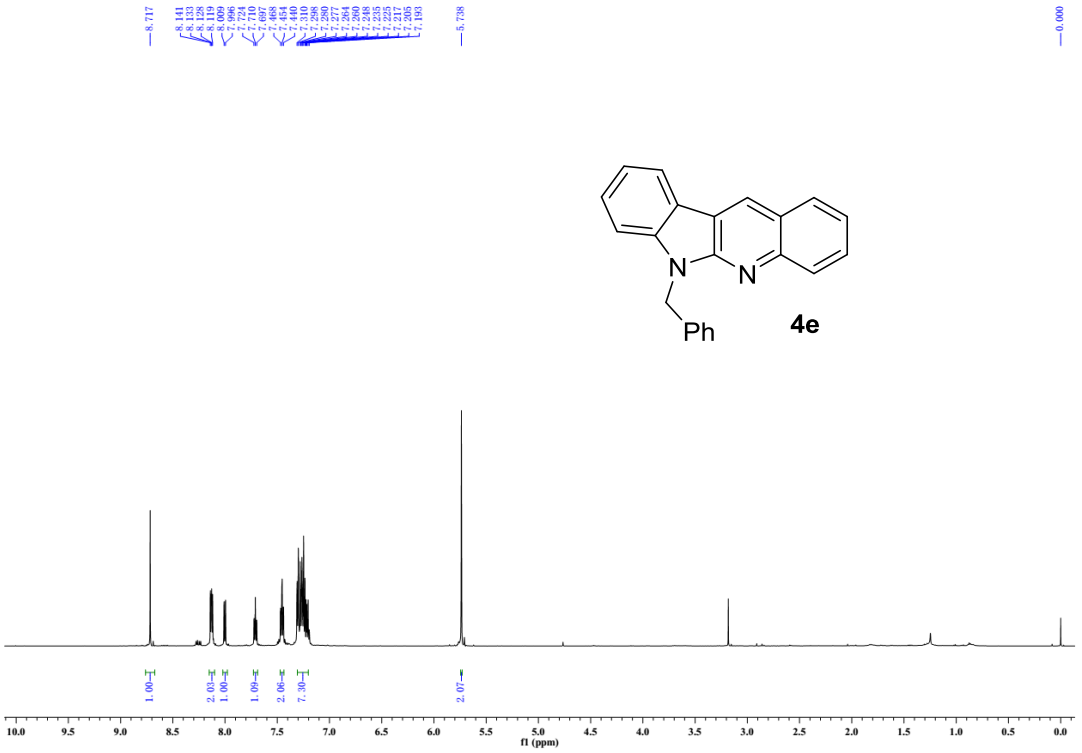
124.679
121.594
120.992
118.398
116.222
109.165
77.478
77.160
76.843
41.317
30.777
20.495
14.024
N
N
Me
4d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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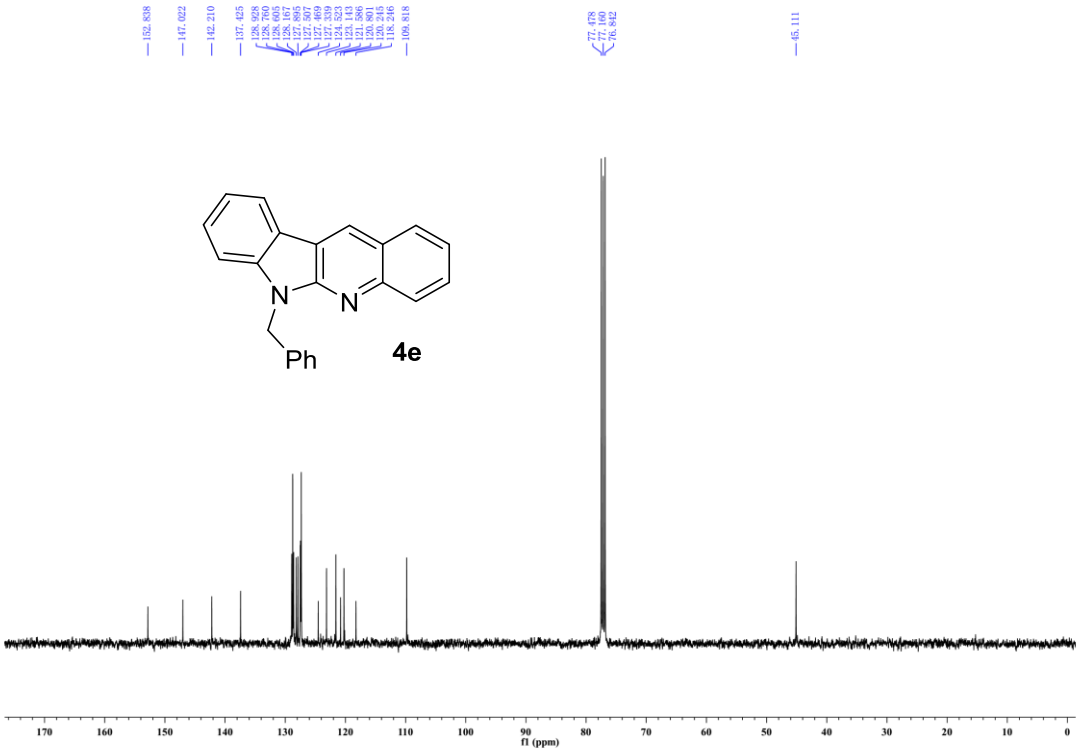
8.128
8.119
8.069
7.996
7.724
7.710
7.697
7.468
7.454
7.440
7.310
7.298
7.290
7.277
7.264
7.260
7.248
7.235
7.225
7.217
7.205
7.193
5.738
0.000
N
N
Ph
4e
1.00
2.03
1.00
1.09
2.06
7.30
2.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.700
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128.167
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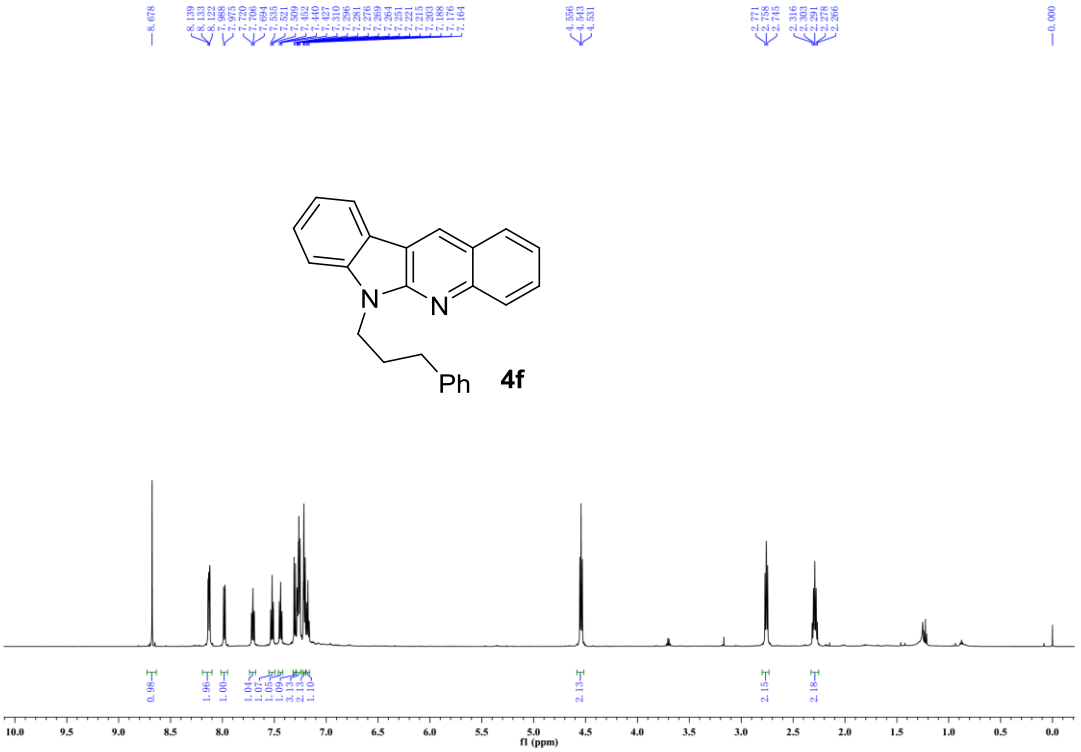
127.697
127.577
127.359
124.523
123.143
121.586
120.801
120.245
118.246
109.818
77.478
77.160
76.842
45.111
N
N
Ph
4e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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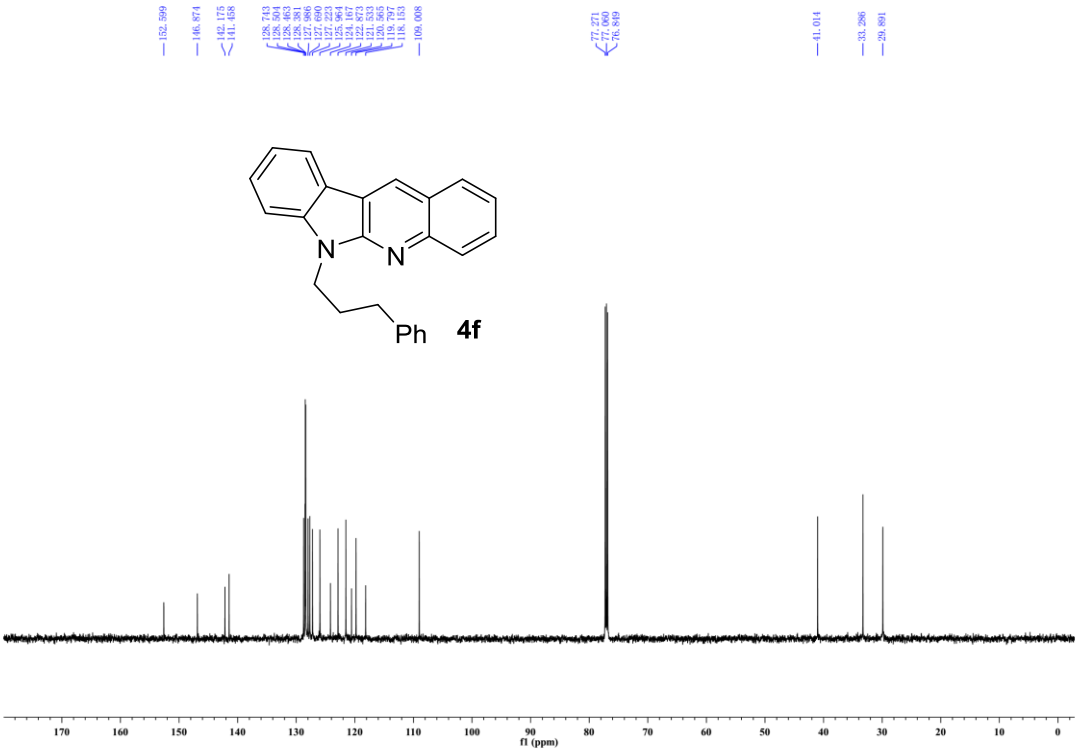
7.975
7.720
7.706
7.684
7.534
7.521
7.509
7.452
7.449
7.427
7.310
7.306
7.281
7.276
7.269
7.264
7.255
7.221
7.215
7.203
7.188
7.176
7.164
4.556
4.543
4.531
2.771
2.758
2.745
2.316
2.303
2.291
2.278
2.266
0.000
N
N
Ph
4f
0.98
1.96
1.00
1.04
1.07
1.05
1.09
1.13
2.13
1.10
2.13
2.15
2.18
10.0
9.5
9.0
8.5
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)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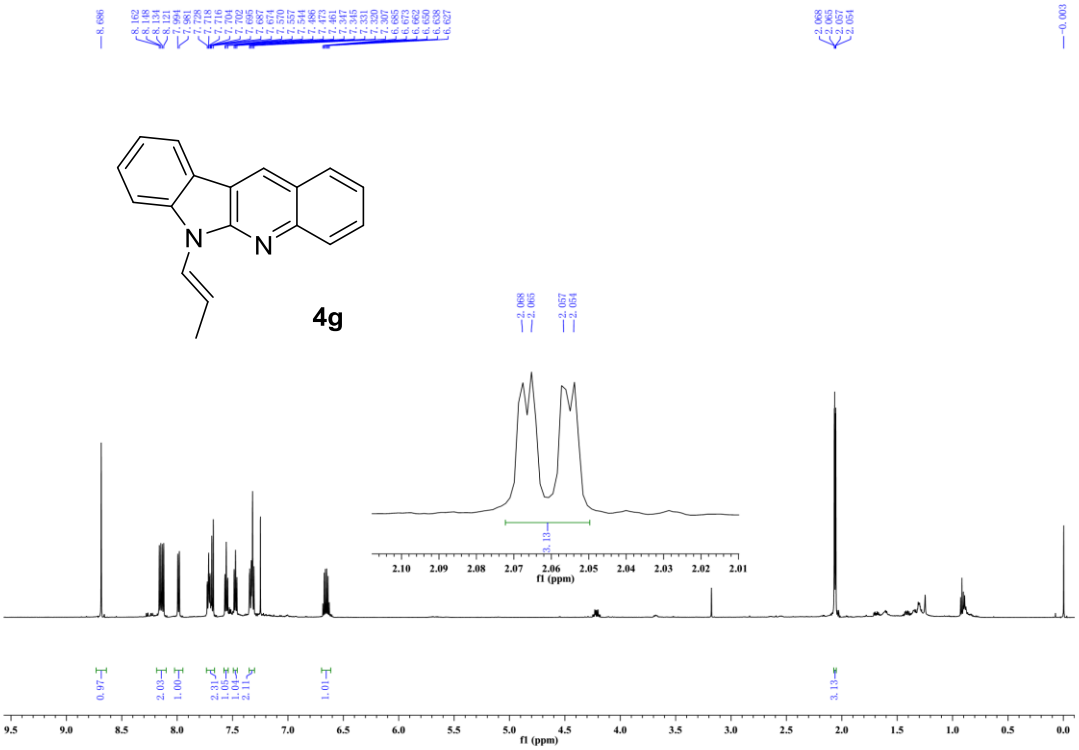
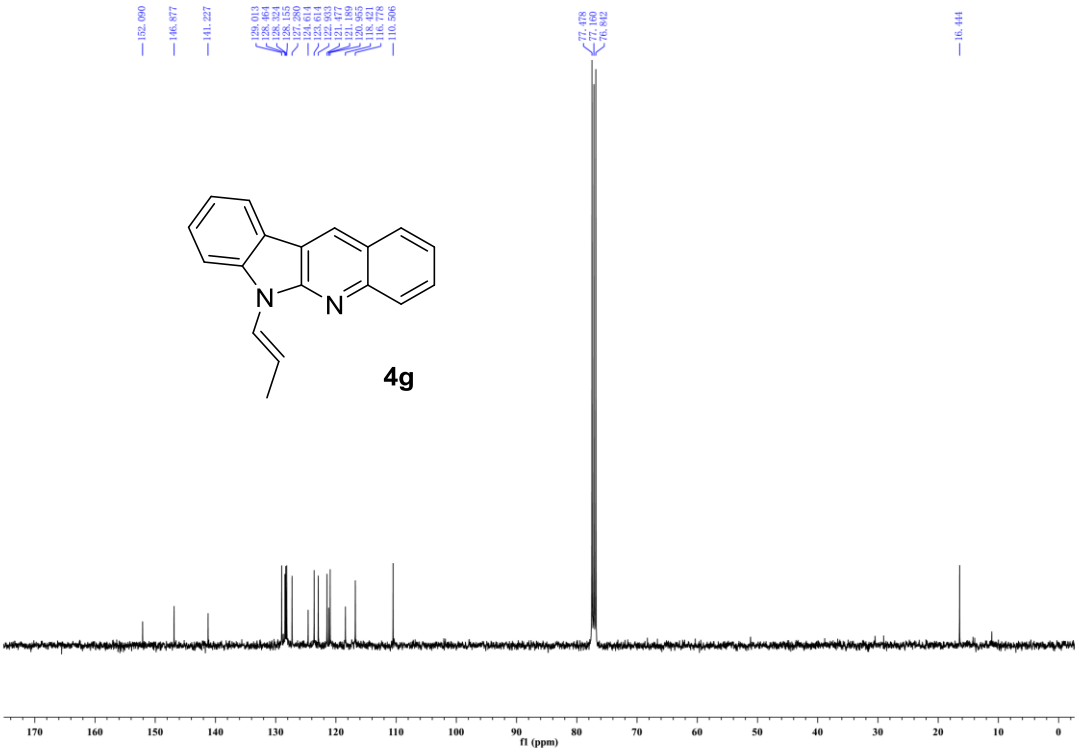
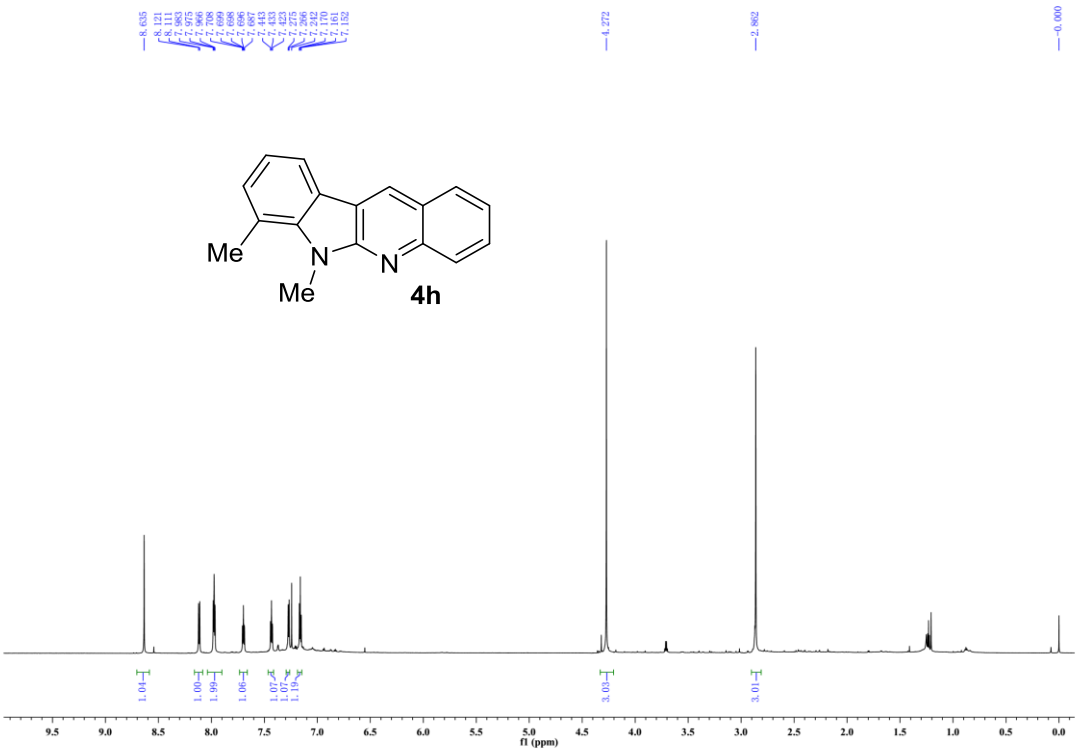
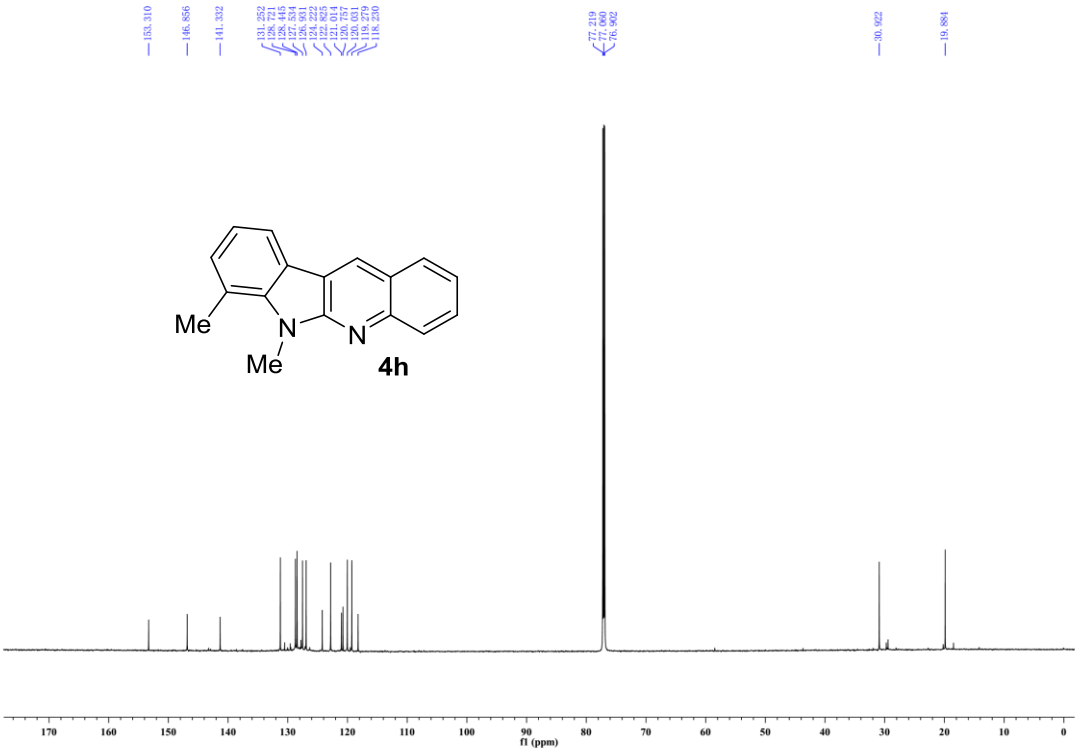
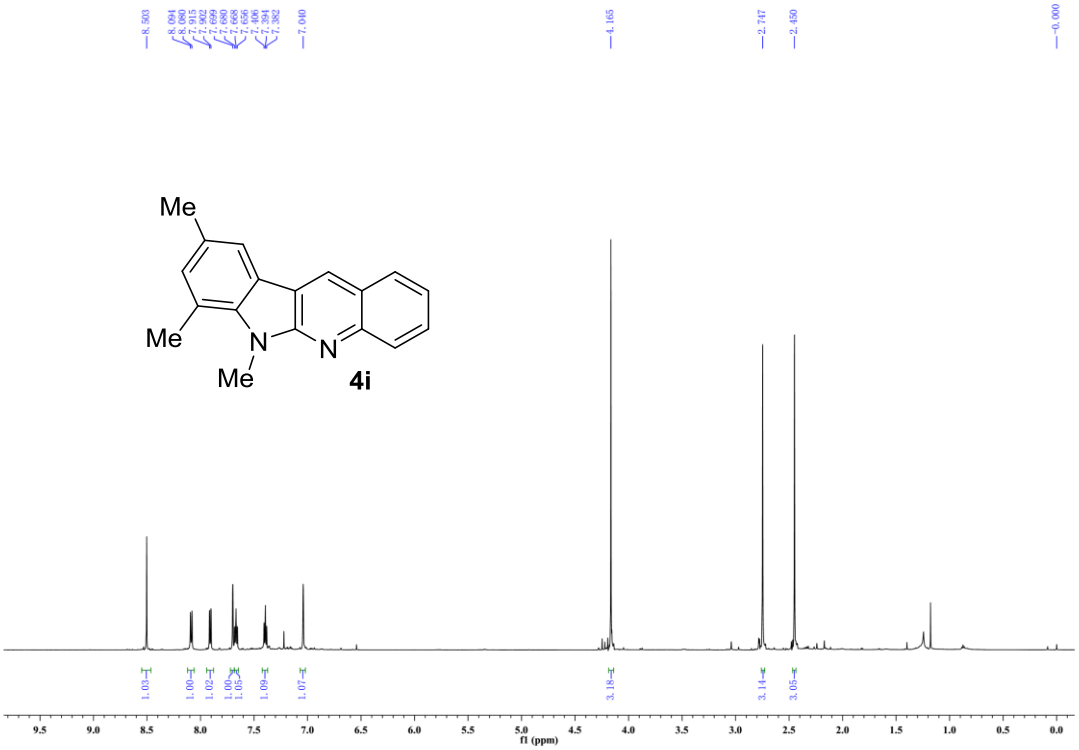
127.690
127.223
125.964
124.697
124.452
121.533
120.365
119.797
118.153
109.008
77.271
77.060
76.849
41.014
33.286
29.891
N
N
Ph
4f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4g
fl (ppm)


4g
fl (ppm)


Me
N
N
Me
4h
f1 (ppm)


Me
N
N
Me
4h
f1 (ppm)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7.688
7.656
7.406
7.394
7.382
7.040
4.165
2.747
2.450
0.000
Me
Me
N
N
Me
4i
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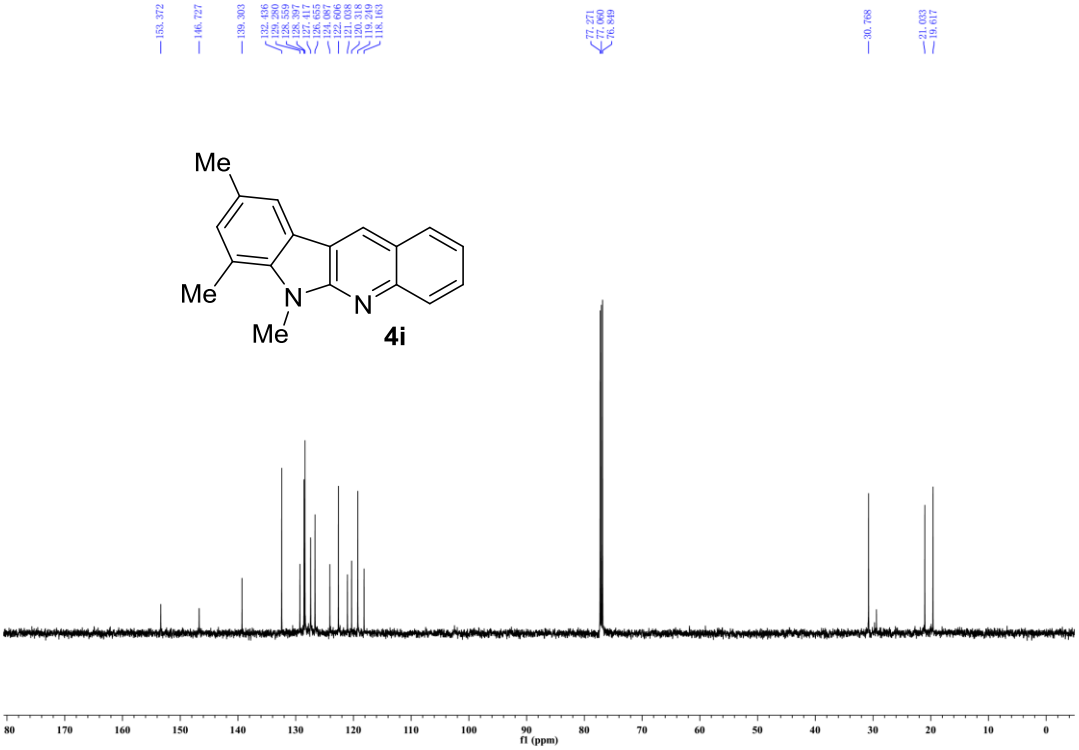
1.02
1.06
1.05
1.09
1.07
3.18
3.14
3.05
f1 (ppm)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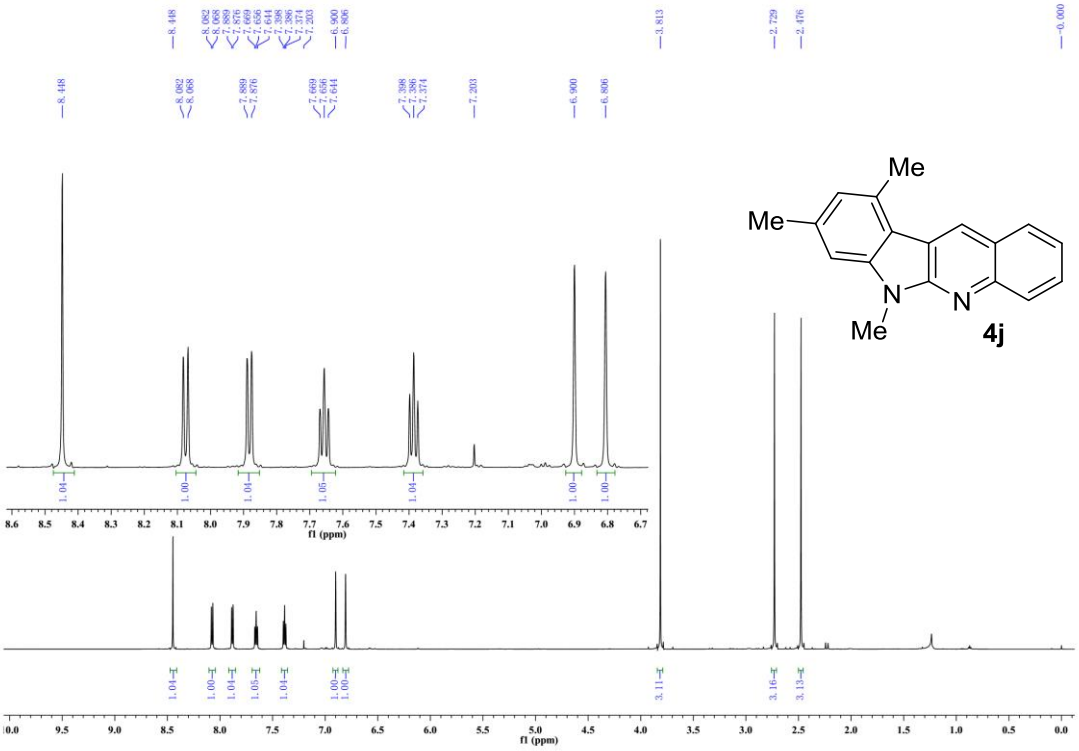
139.303
132.436
129.800
128.559
128.397
127.417
126.455
124.087
122.606
121.338
121.135
119.219
118.163
77.271
77.060
76.849
30.768
21.033
19.617
Me
Me
N
N
Me
4i
f1 (ppm)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7.644
7.398
7.386
7.374
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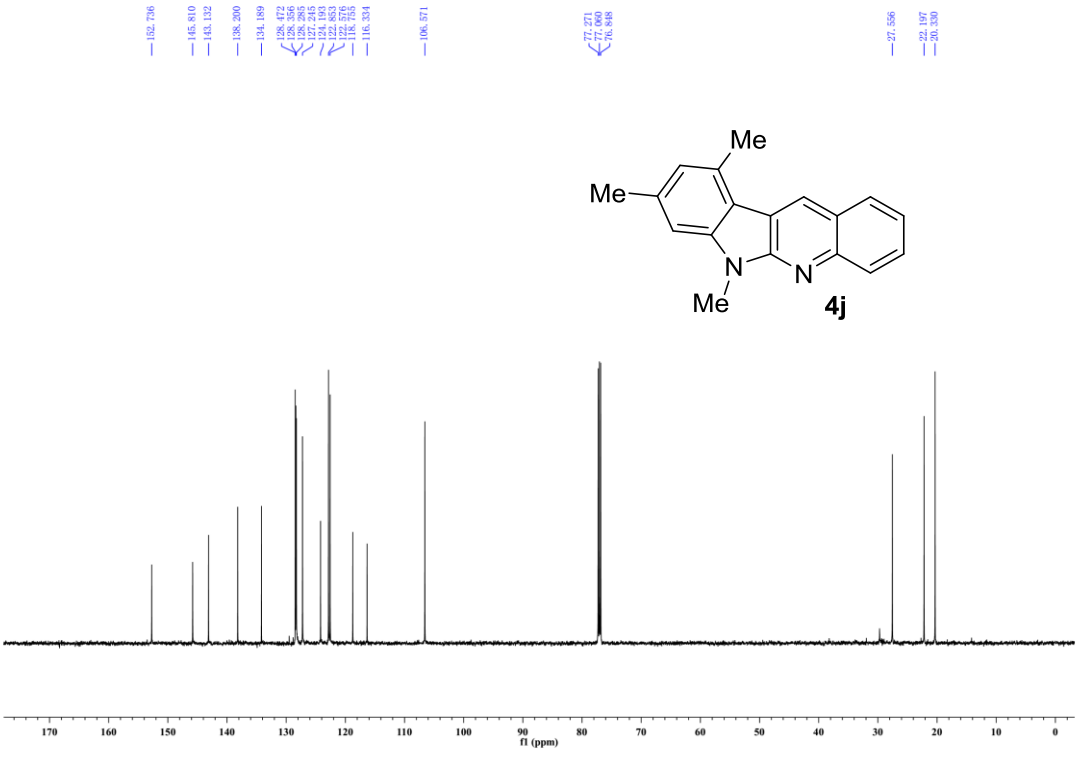
6.900
6.806
3.813
2.729
2.476
0.000
Me
Me
N
N
Me
4j
f1 (ppm)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128.472
128.366
128.285
127.245
124.193
122.653
122.576
118.755
116.334
106.571
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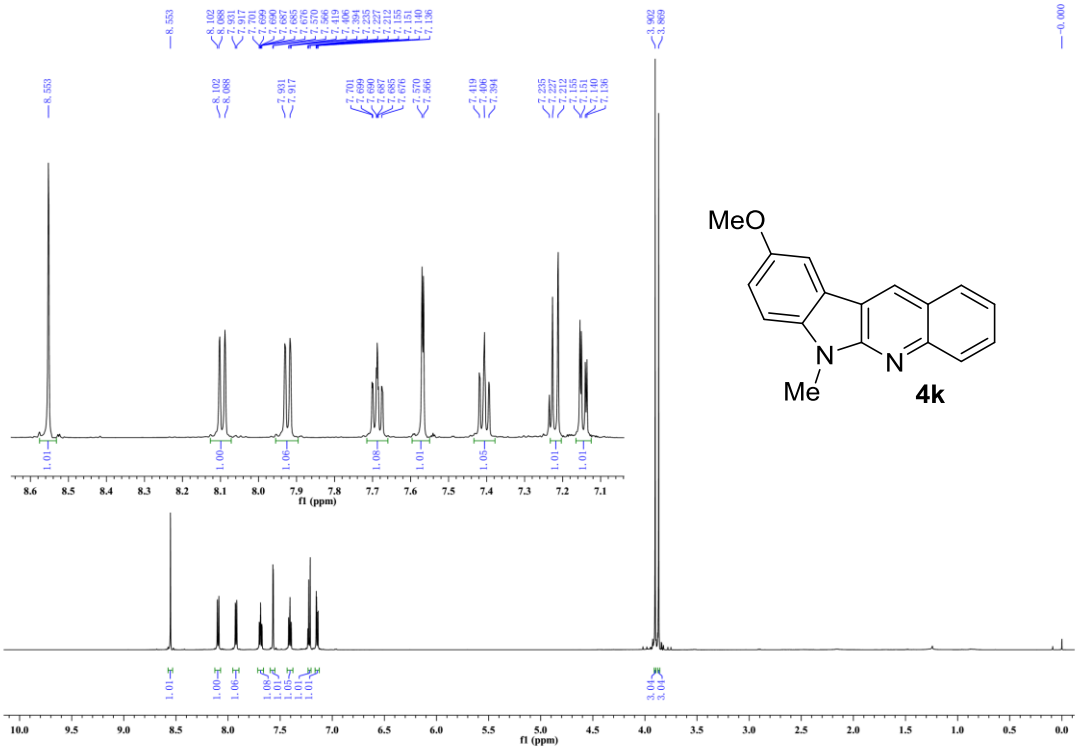
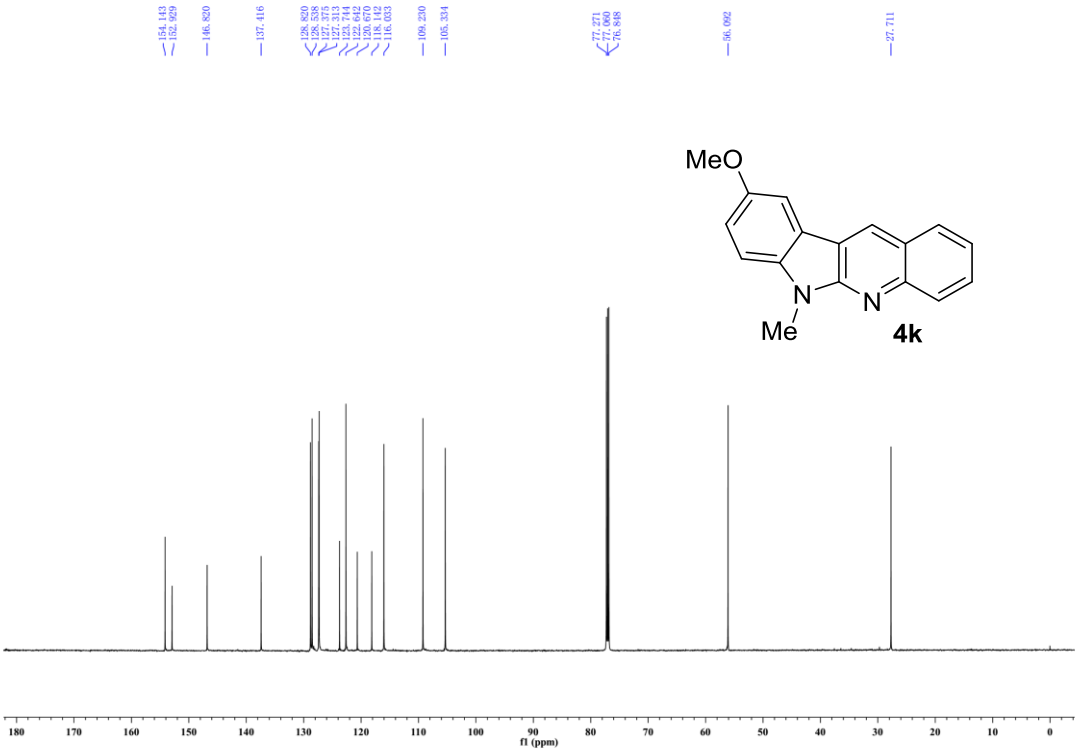
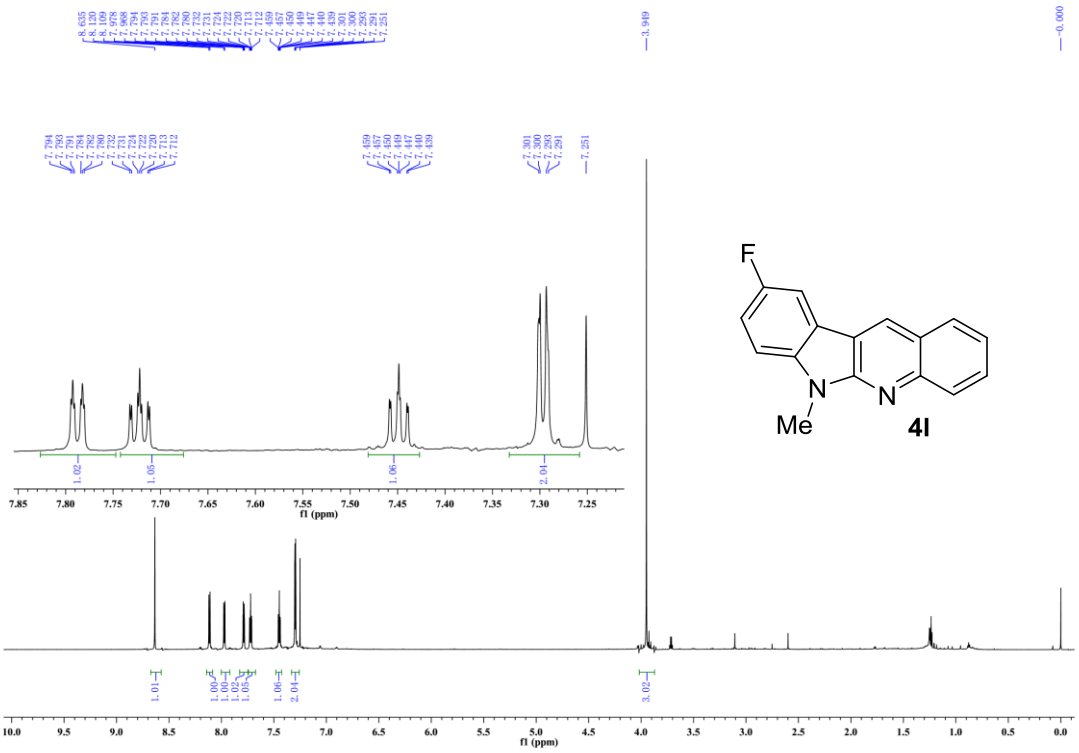
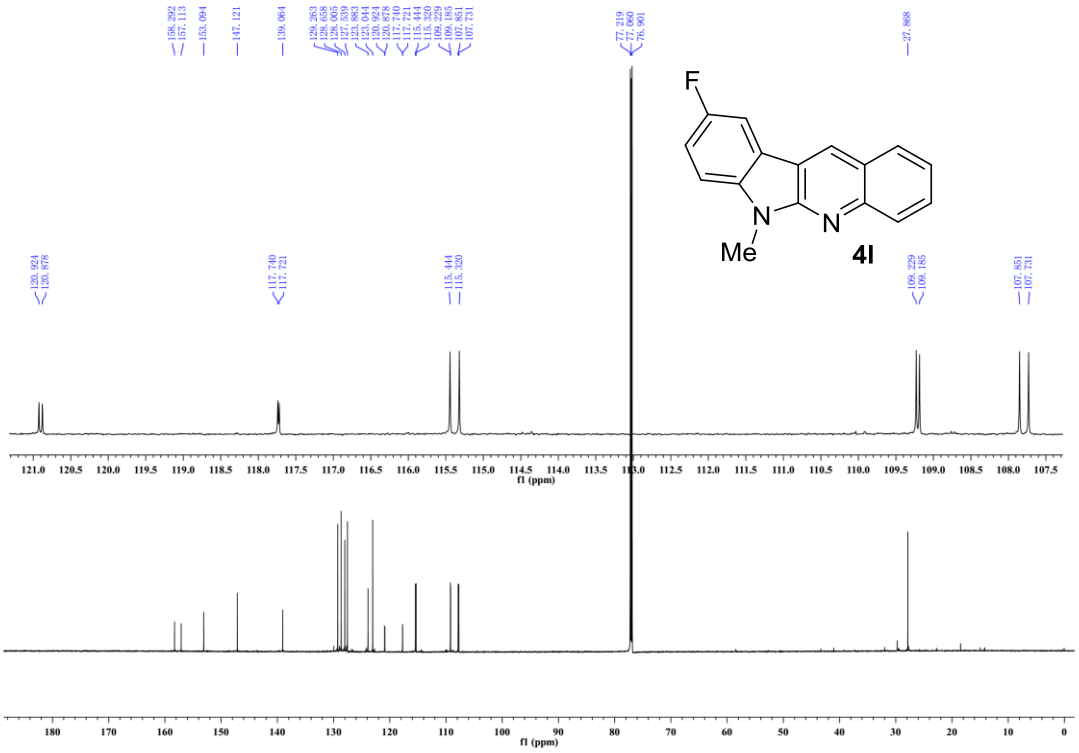
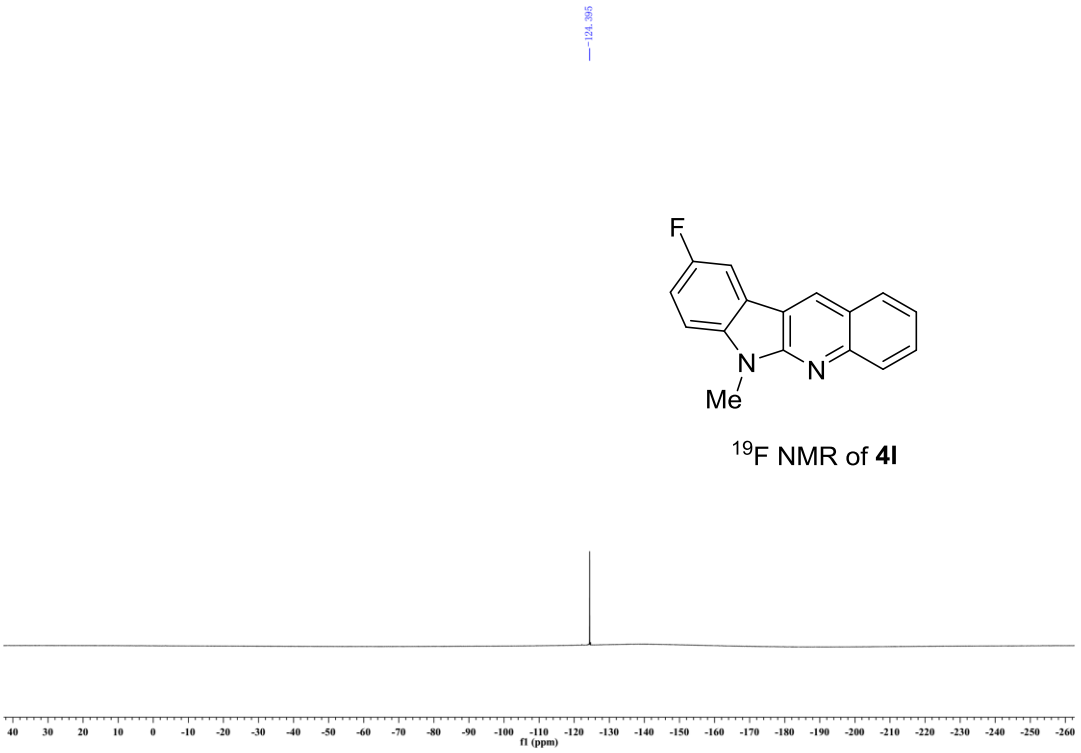
77.060
76.848
27.556
22.197
20.330
Me
Me
N
N
Me
4j
f1 (ppm)


MeO
N
N
Me
4k
fl (ppm)


MeO
N
N
Me
4k
fl (ppm)


F
N
N
Me
4l
fl (ppm)


F
N
N
Me
4l
fl (ppm)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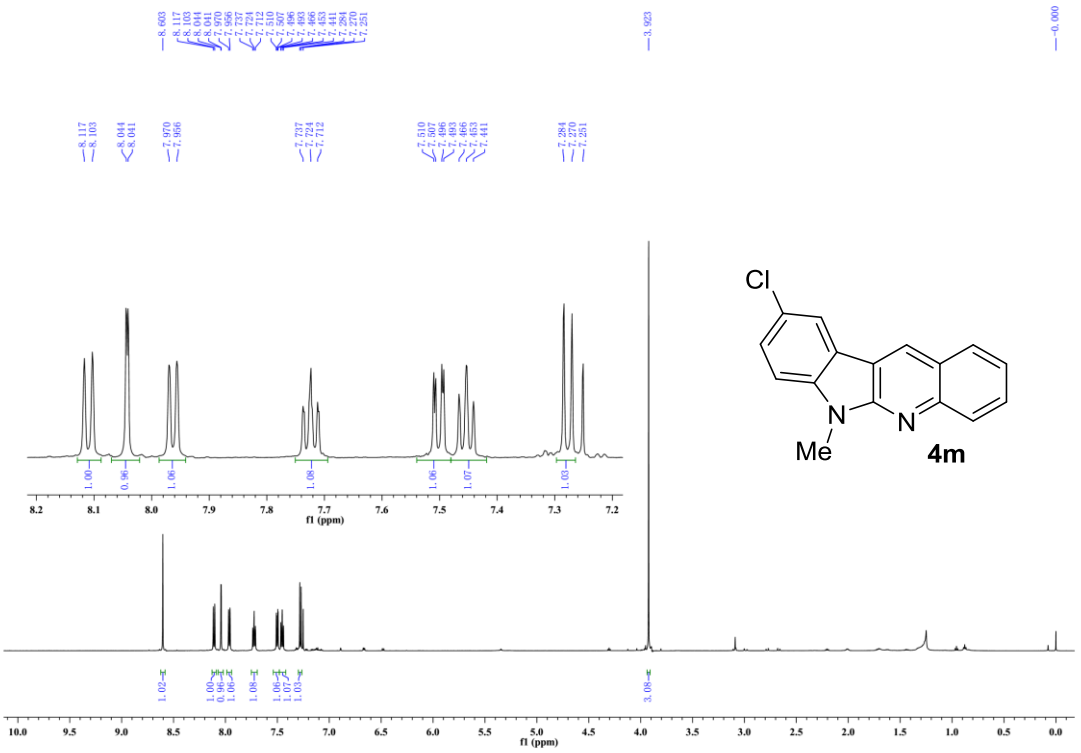
F
N
N
Me
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260
f1 (ppm)

^{19}F NMR of **4l**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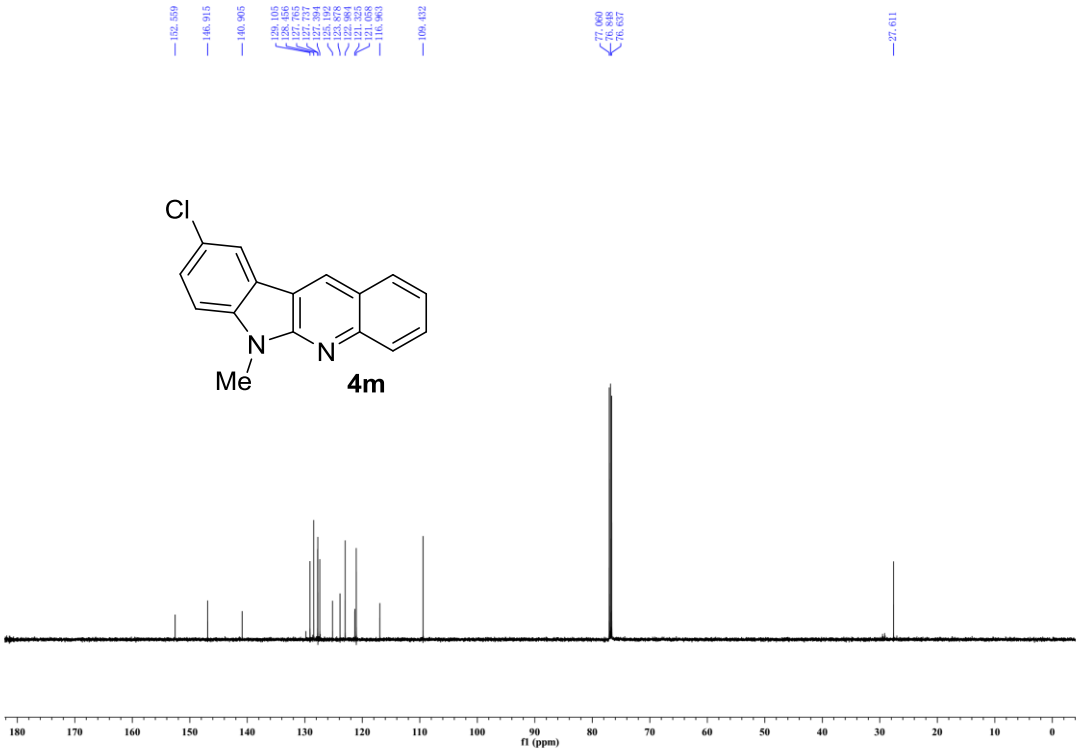
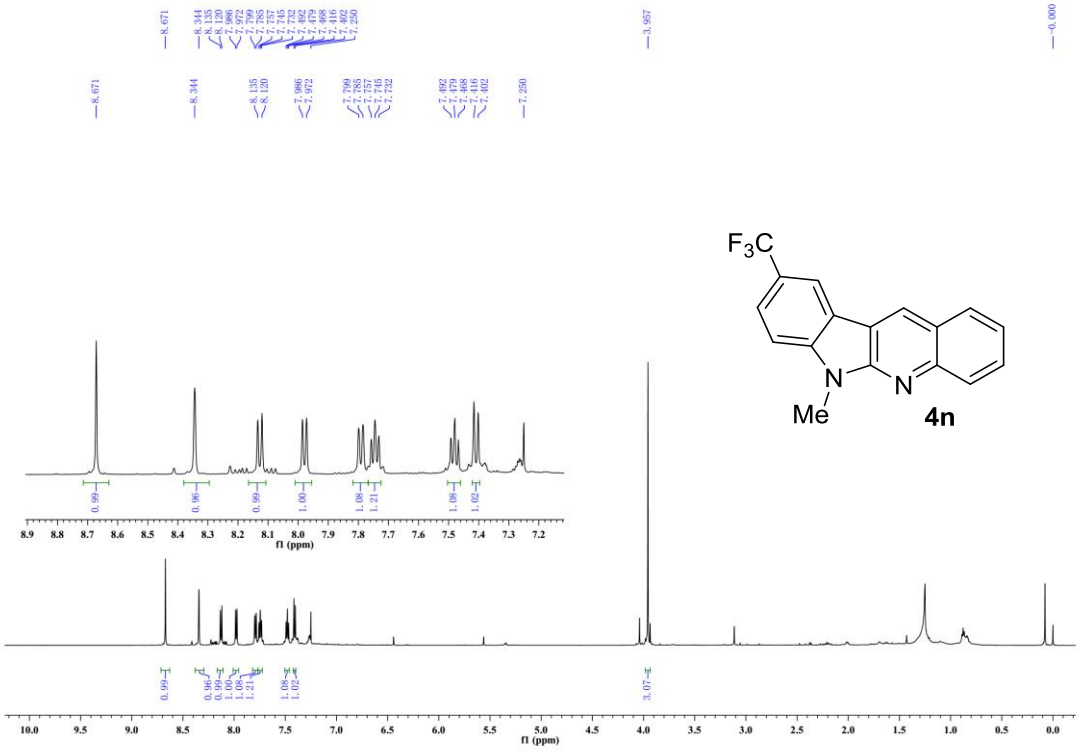
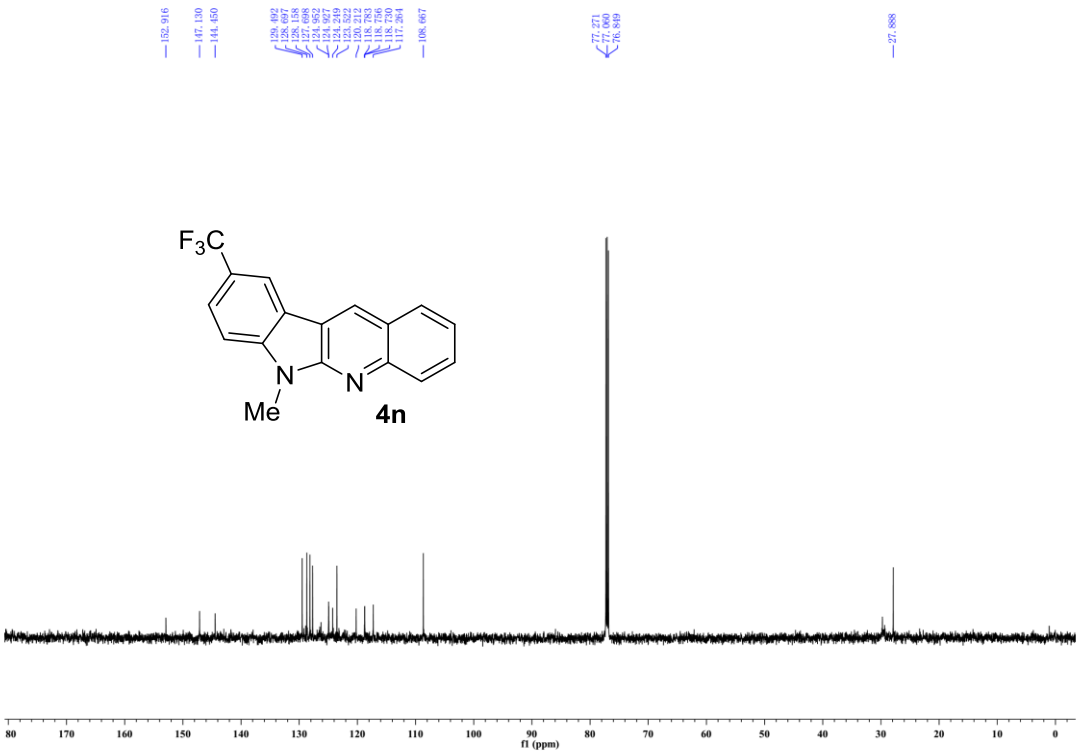
8.044
8.041
7.970
7.956
7.737
7.724
7.712
7.510
7.507
7.496
7.493
7.466
7.463
7.441
7.284
7.270
7.251
3.923
-0.000
Cl
N
N
Me
4m
1.00
0.96
1.06
1.08
1.06
1.07
1.03
1.02
3.08
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Cl
N
N
Me
4m
f1 (ppm)


F3C
N
N
Me
4n
f1 (ppm)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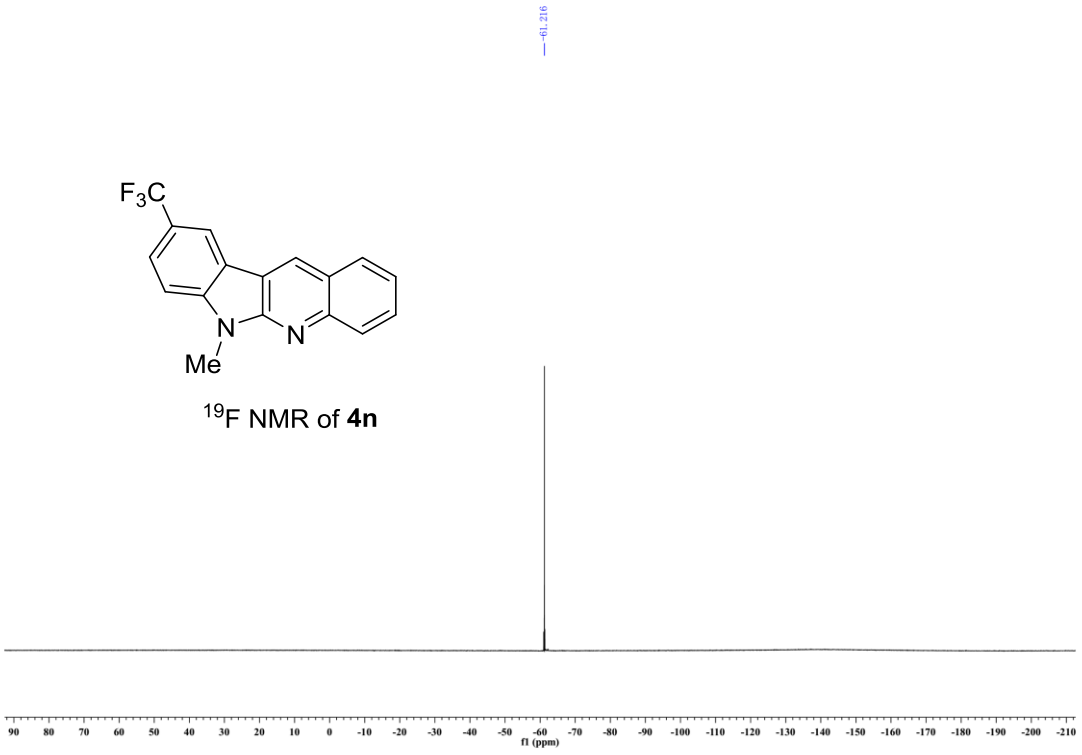
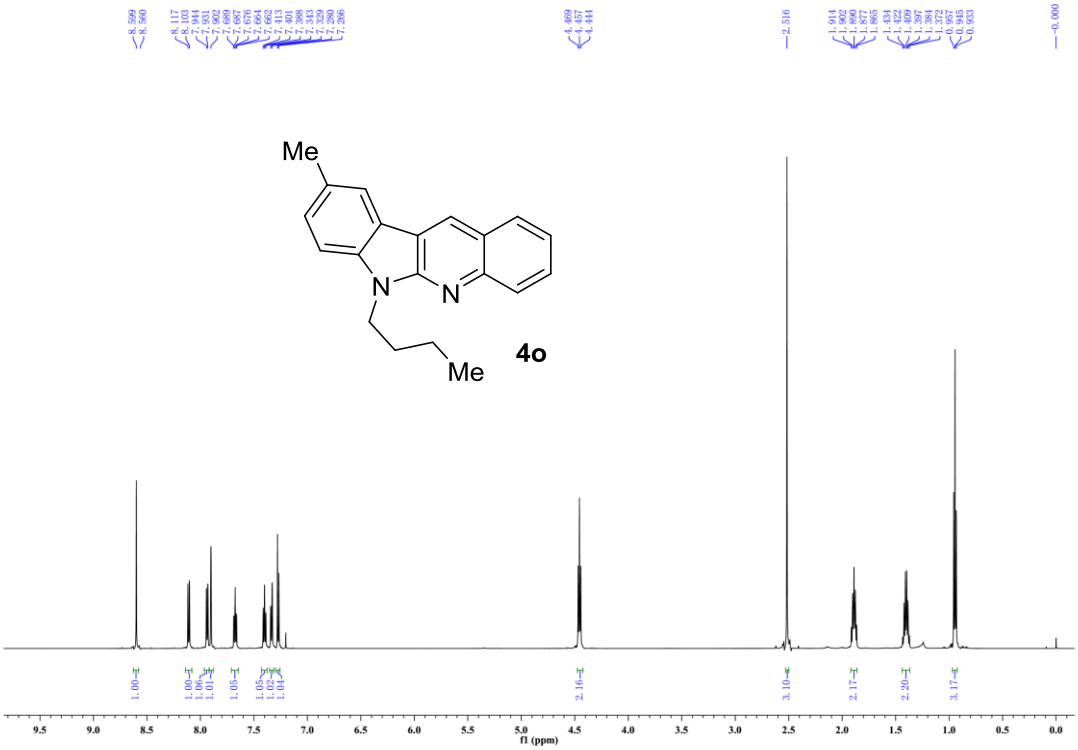
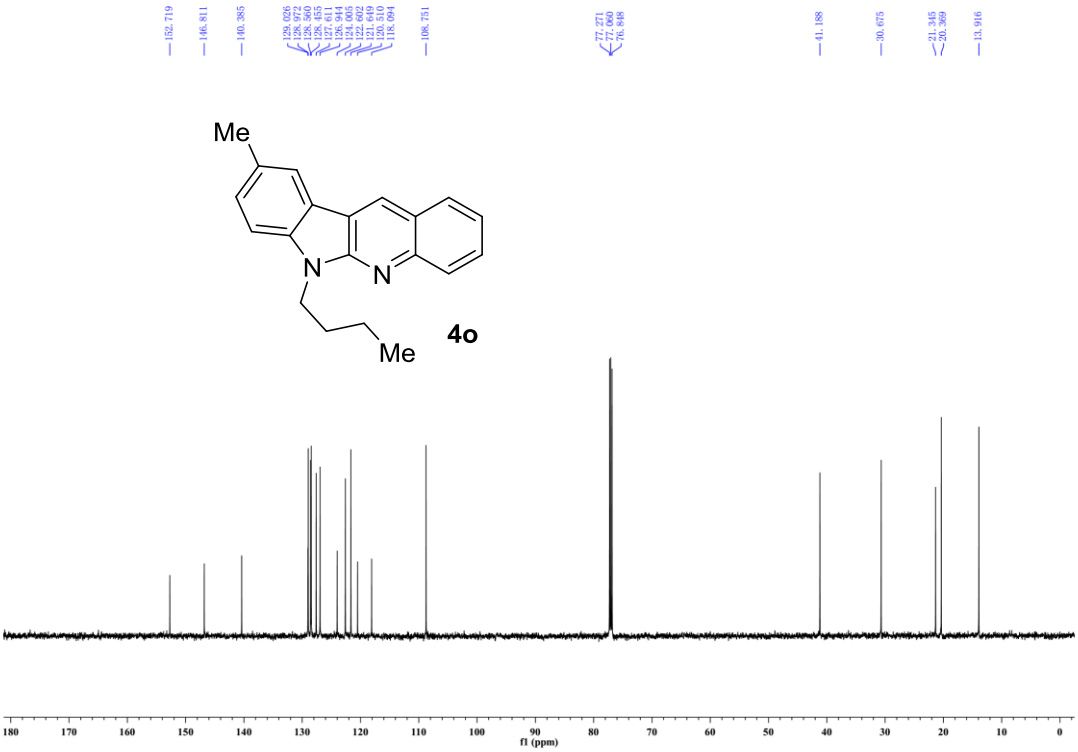
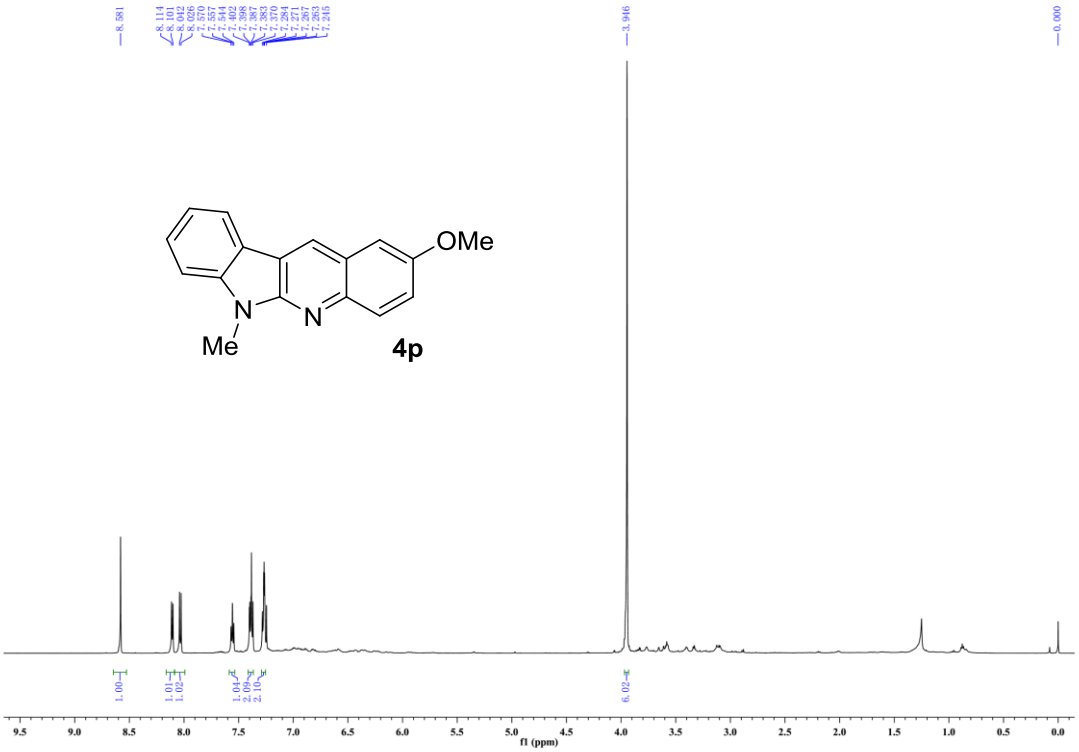
128.697
128.158
127.668
124.952
124.927
124.249
123.522
120.212
118.783
118.756
118.730
117.284
108.667
77.271
77.060
76.849
27.888
F3C
N
N
Me
4n
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

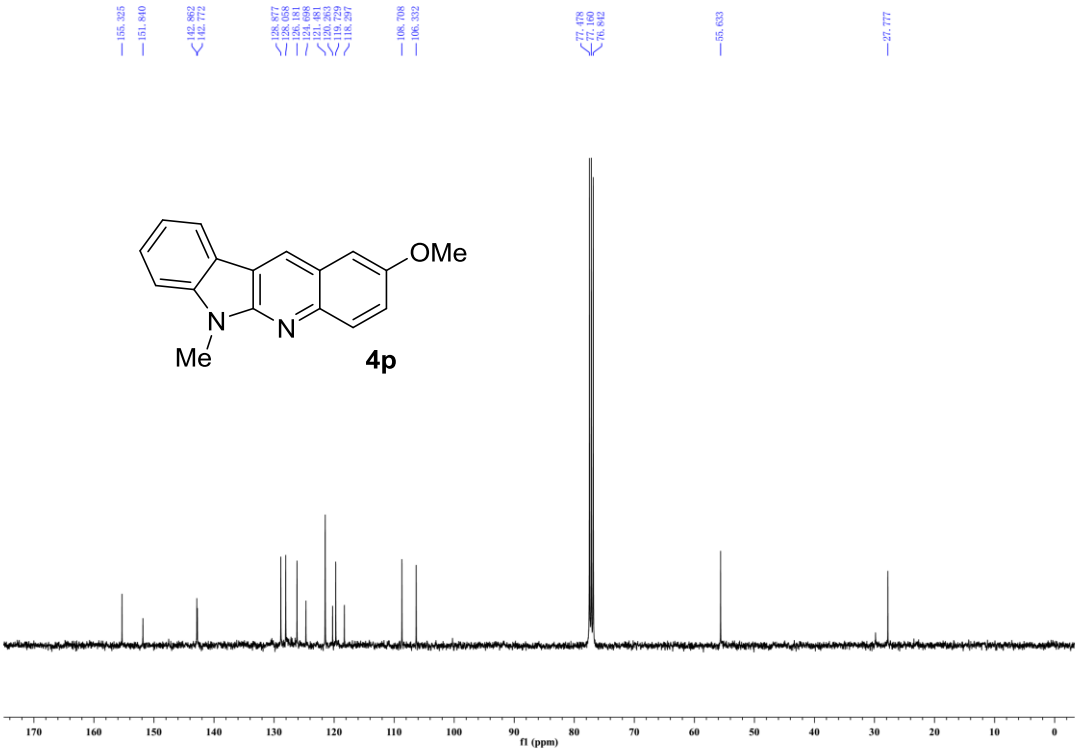

61.216
F3C
N
N
Me
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

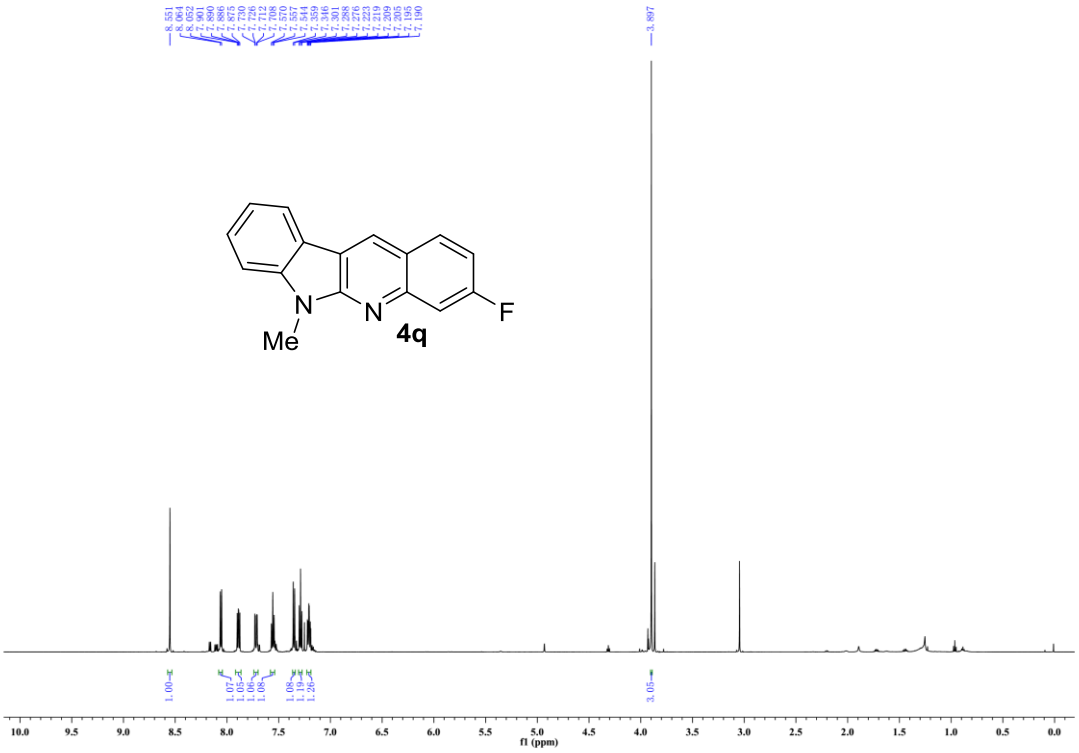
^{19}F NMR of **4n**

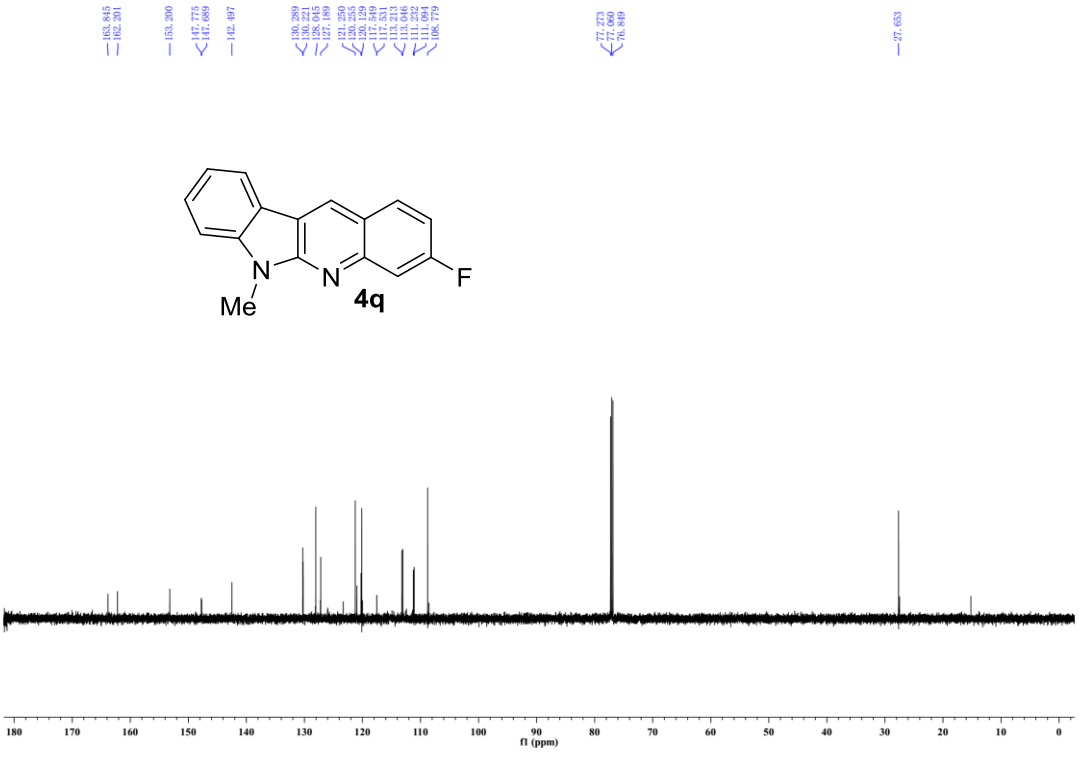

Me
N
N
Me
4o
fl (ppm)

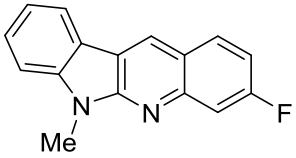

Me
N
N
Me
4o
fl (ppm)


8.581
8.114
8.101
8.042
8.026
7.570
7.557
7.414
7.402
7.398
7.387
7.373
7.370
7.284
7.271
7.265
7.263
7.245
3.946
0.000
OMe
N
N
Me
4p
1.00
1.01
1.02
1.04
1.04
2.10
6.02
fl (ppm)


155.325
151.840
142.862
142.772
128.877
128.658
126.181
124.698
121.861
120.283
119.729
118.297
108.708
106.332
77.478
77.160
76.842
55.633
27.777
OMe
N
N
Me
4p
fl (ppm)

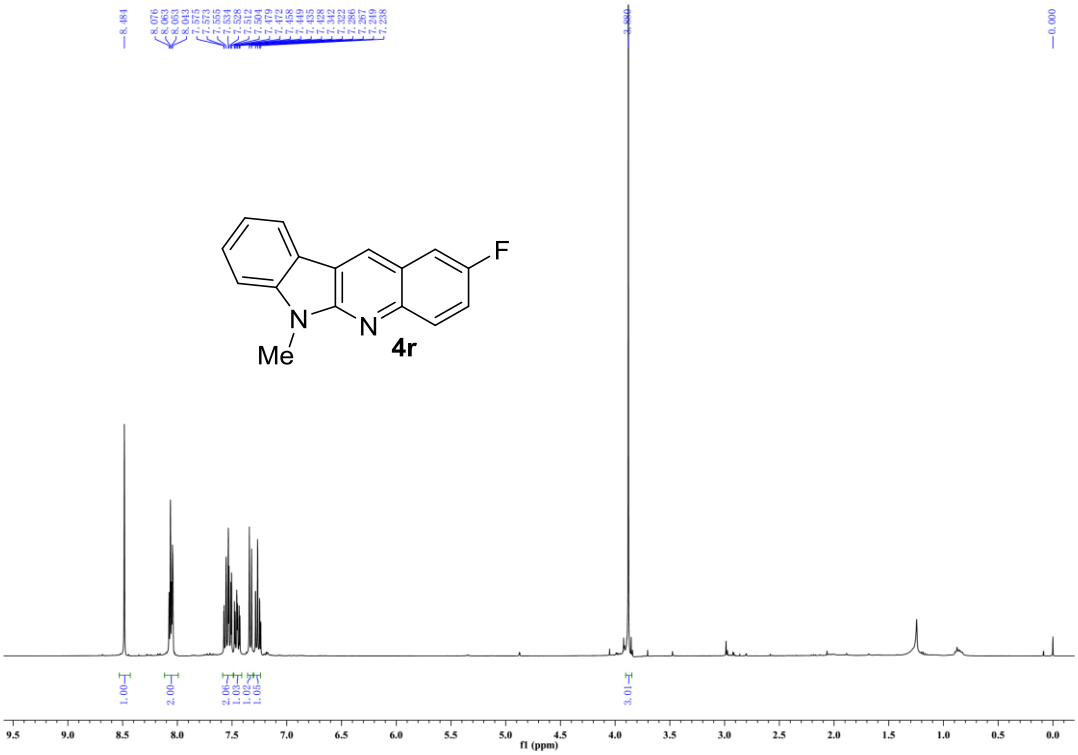

8.551
8.064
8.052
7.901
7.890
7.886
7.875
7.730
7.726
7.712
7.708
7.570
7.557
7.544
7.359
7.346
7.301
7.298
7.276
7.223
7.219
7.209
7.205
7.195
7.190
3.897
1.00
1.07
1.05
1.06
1.06
1.08
1.19
1.26
3.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
N
Me
N
F
4q

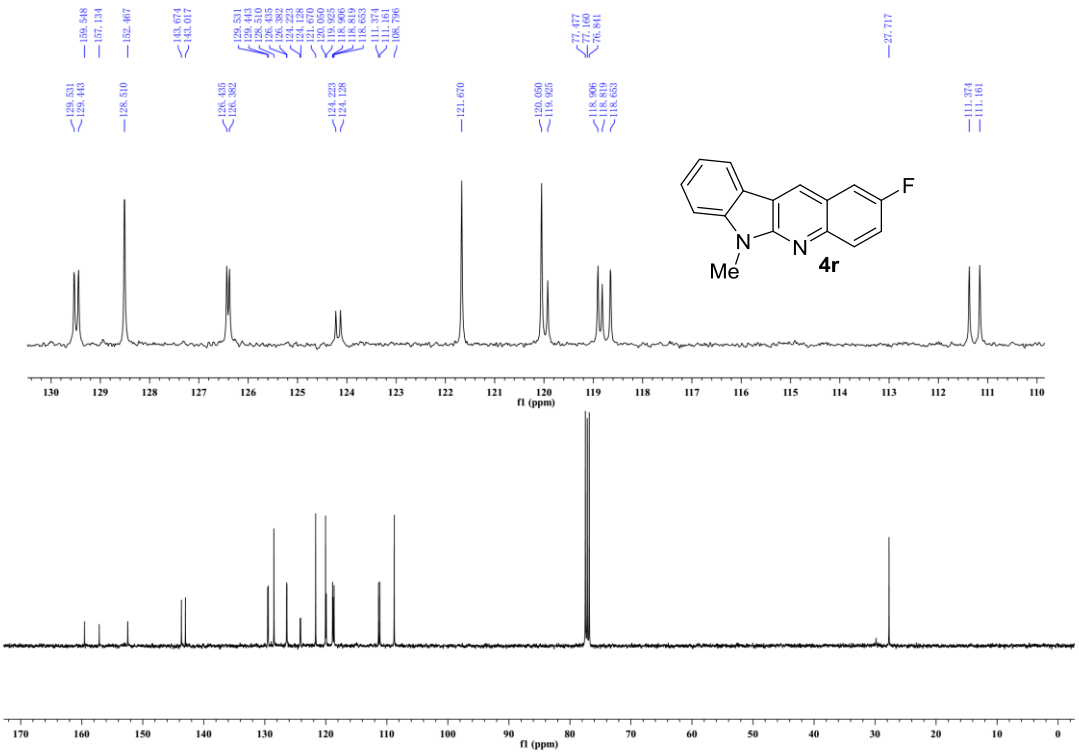

163.845
162.201
153.200
147.775
147.689
142.497
130.289
130.211
128.645
127.189
121.250
120.255
120.159
117.549
117.531
113.213
113.166
111.252
111.094
108.779
77.273
77.060
76.849
27.653
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
N
Me
N
F
4q

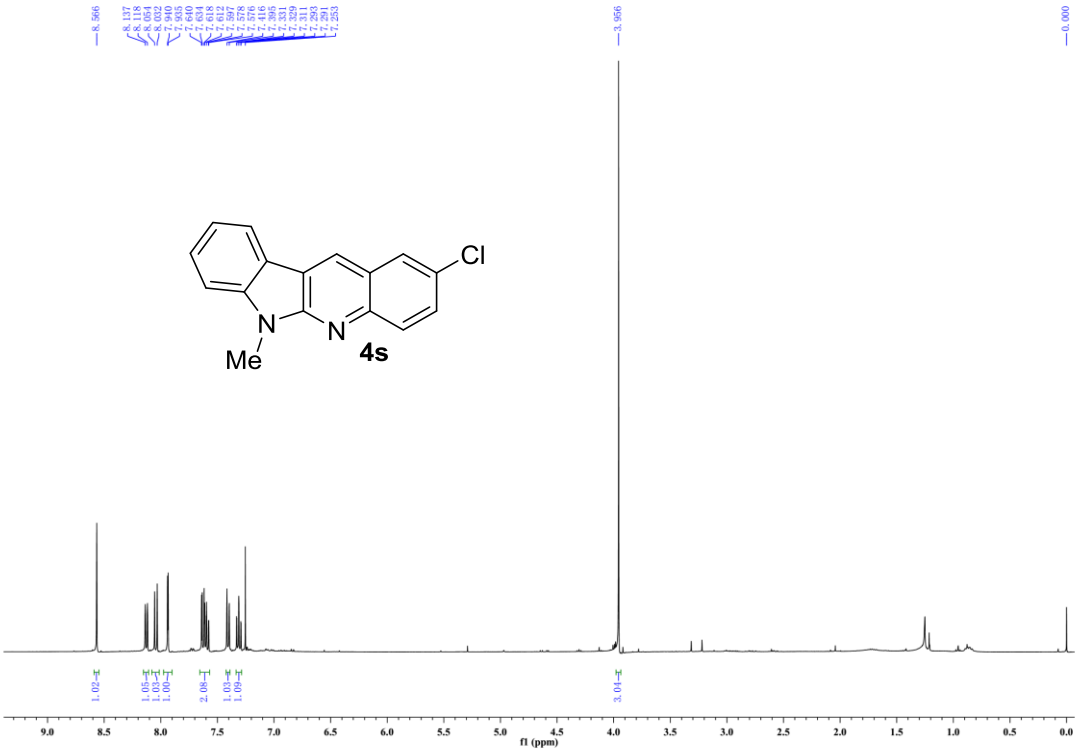

N
N
F
Me

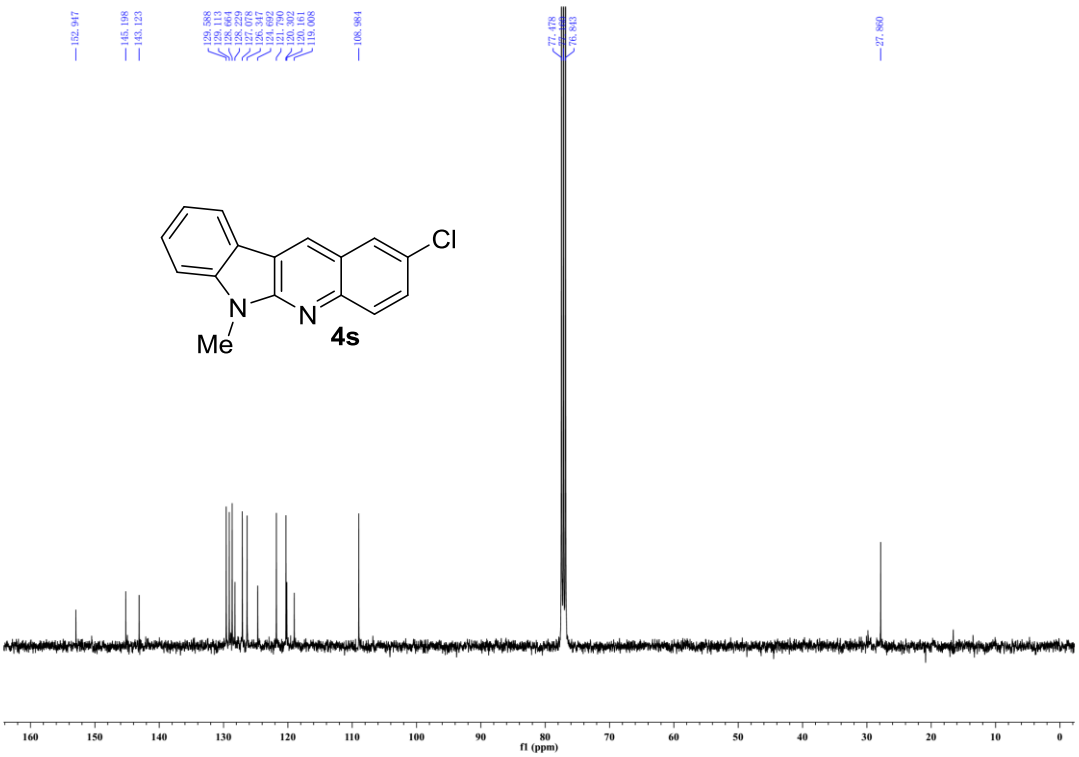
^{19}F NMR of **4q**

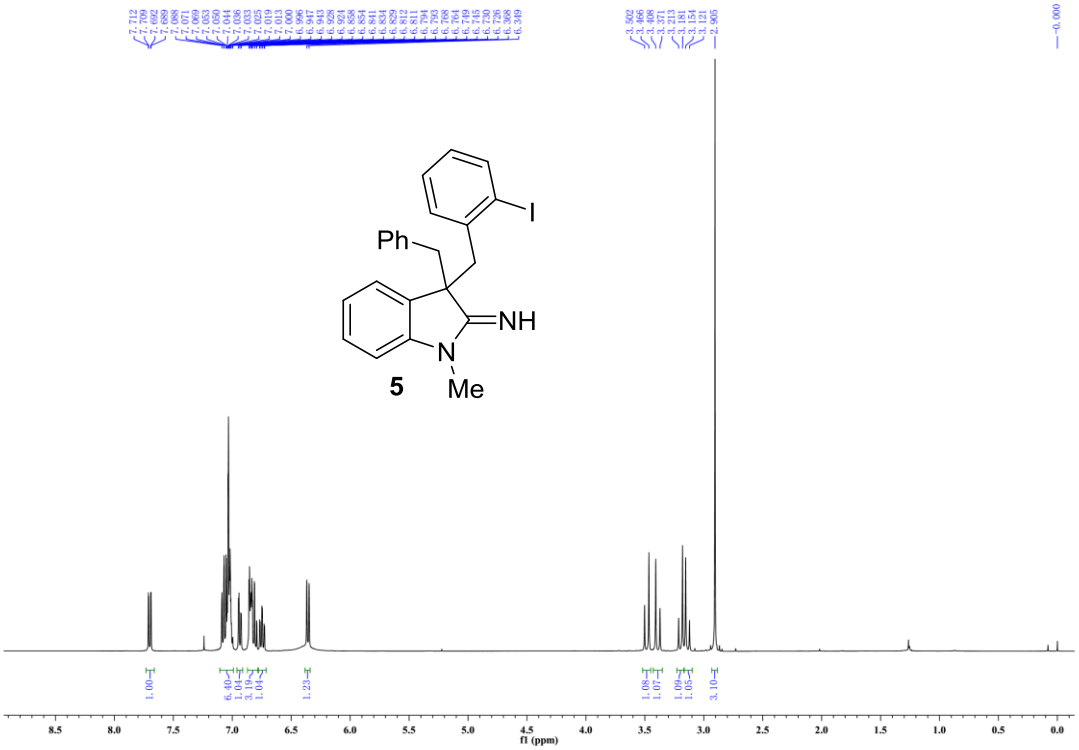
-111.731
10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -21
f1 (ppm)

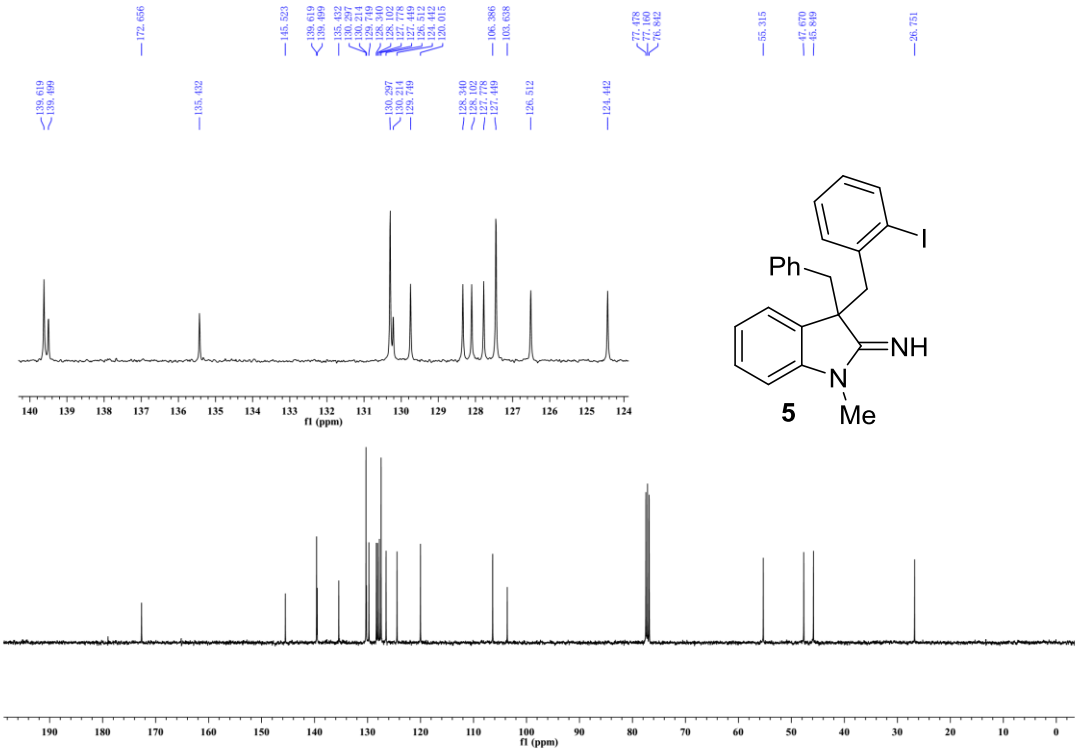

8.484
8.076
8.063
8.053
8.043
7.575
7.573
7.555
7.534
7.528
7.512
7.504
7.479
7.472
7.466
7.449
7.435
7.428
7.342
7.322
7.286
7.257
7.249
7.238
3.880
0.000
F
N
N
Me
4r
1.00
2.00
2.06
1.03
1.02
1.05
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

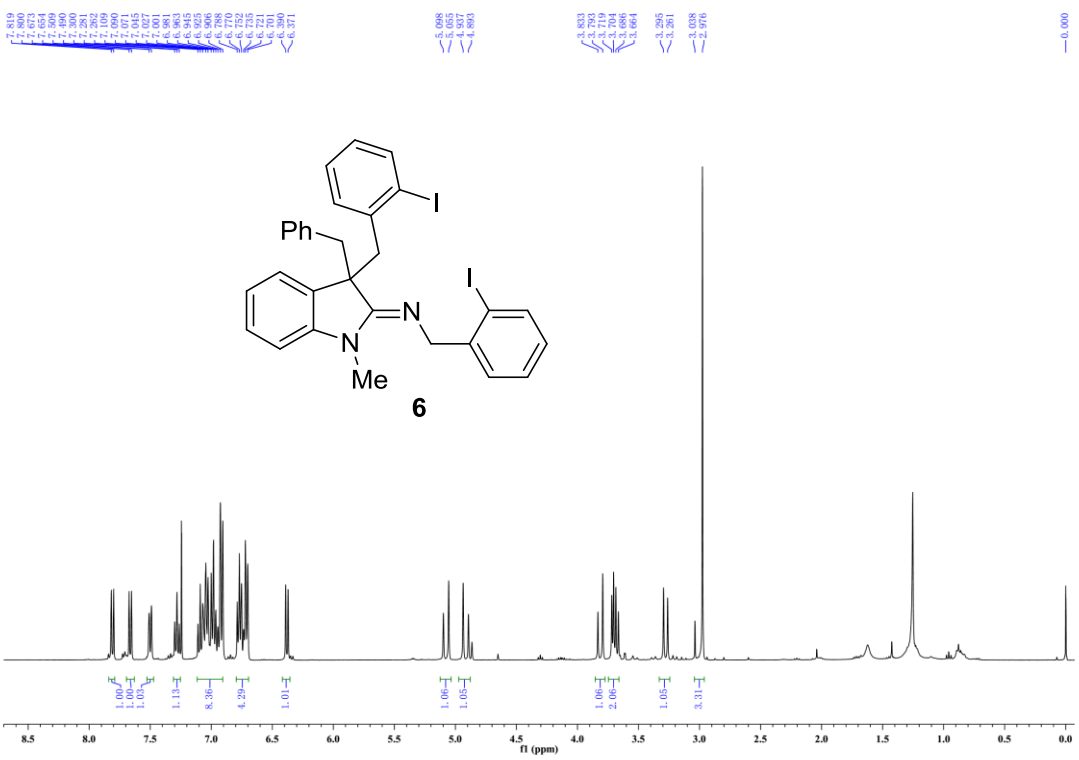

F
N
N
Me
4r
f1 (ppm)

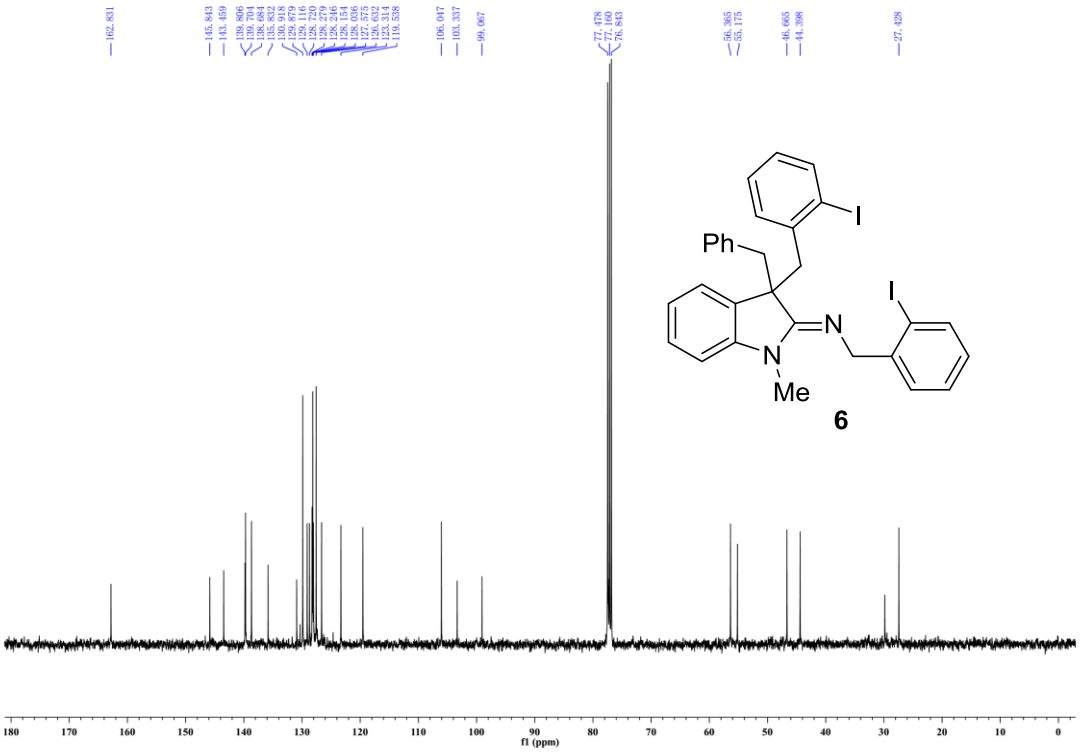

Cl
N
N
Me
4s
f1 (ppm)

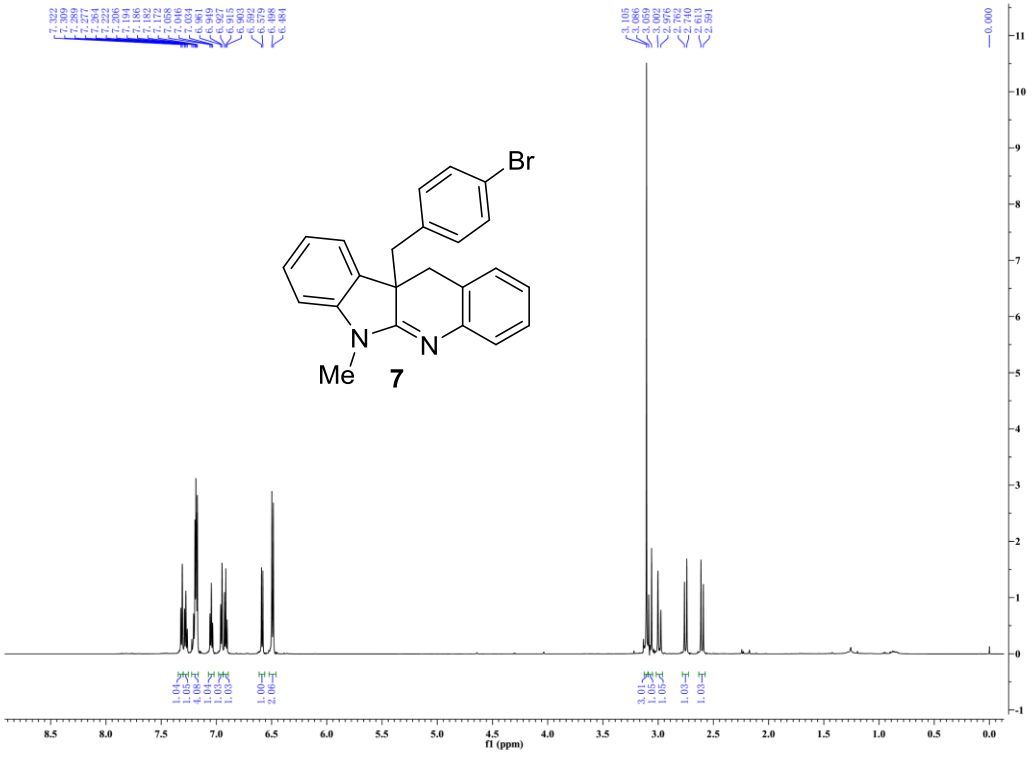

Cl
N
N
Me
4s
fl (ppm)

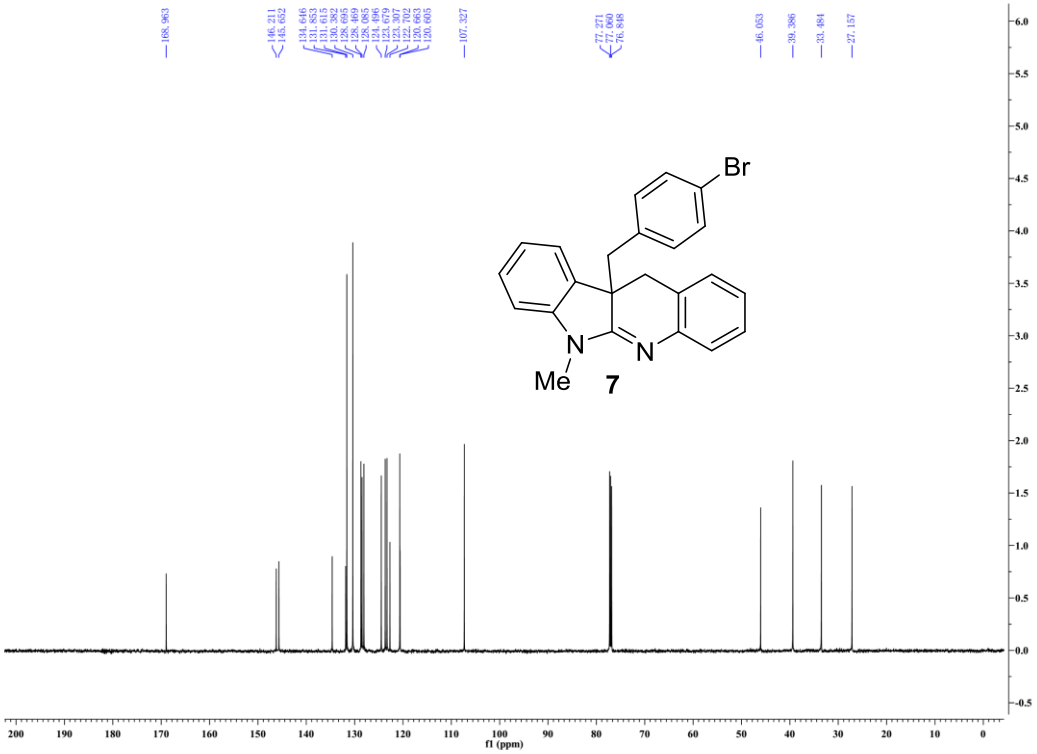

I
Ph
NH
N
Me
5
fl (ppm)

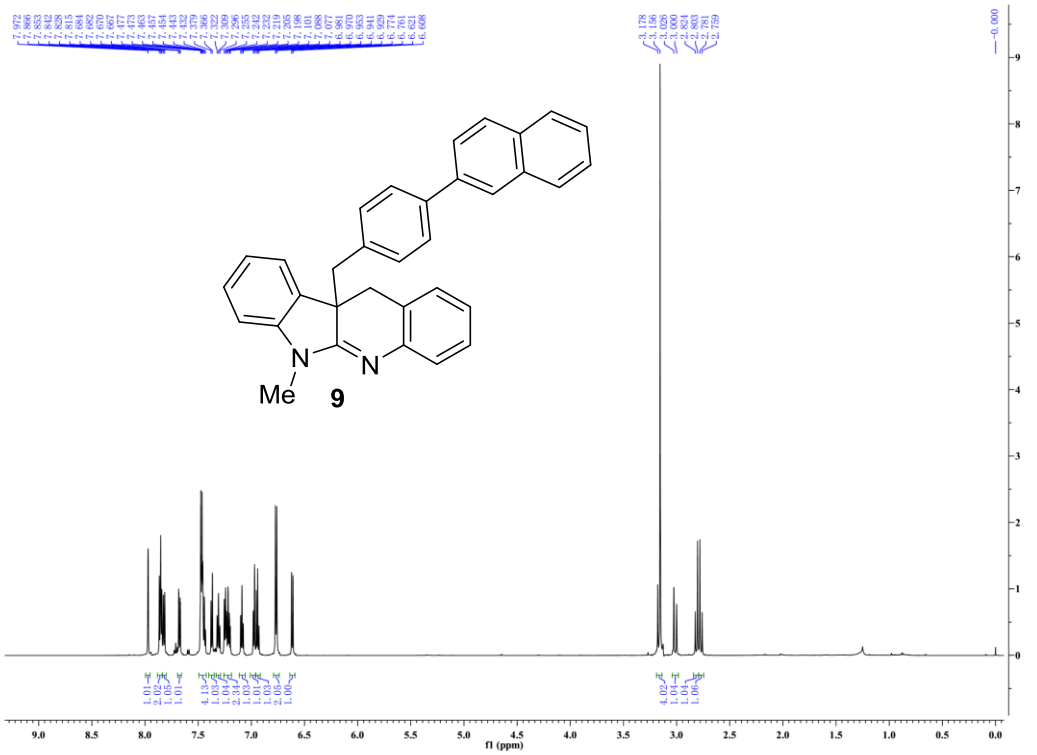

172.656
145.523
139.619
139.499
135.432
130.297
130.214
129.749
128.340
128.192
127.776
127.449
126.512
124.442
120.015
106.386
103.638
77.478
77.160
76.842
55.315
47.670
45.849
26.751
I
Ph
NH
N
Me
5
fl (ppm)

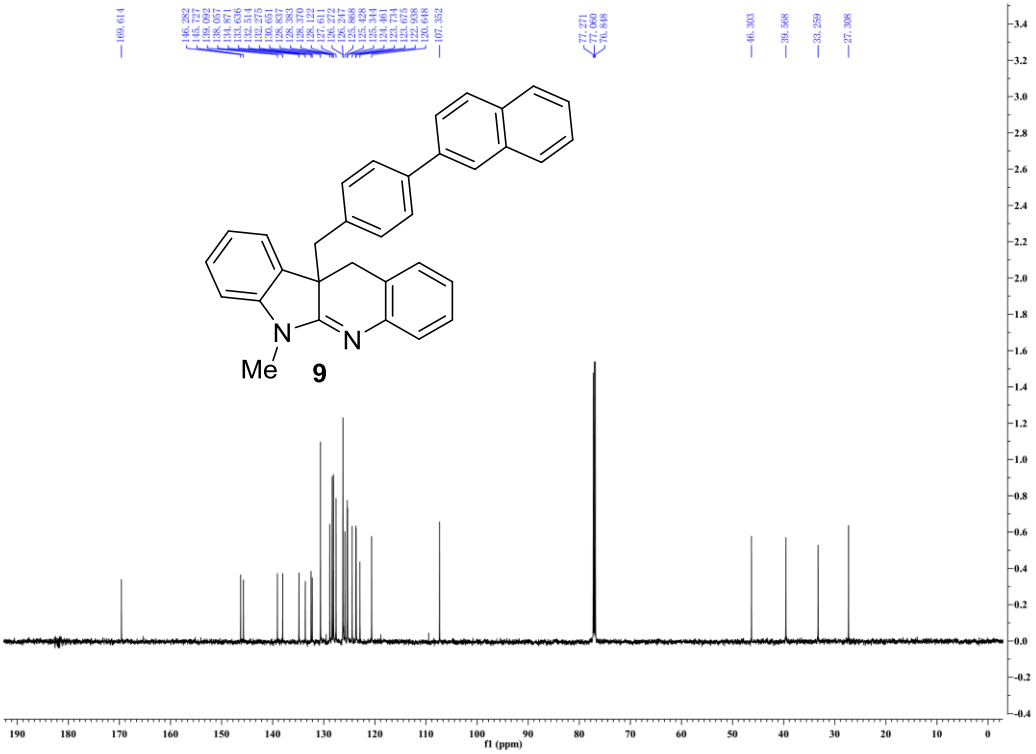

7.819
7.800
7.673
7.654
7.599
7.490
7.300
7.281
7.252
7.109
7.090
7.071
7.045
7.027
7.001
6.981
6.965
6.945
6.925
6.906
6.886
6.770
6.752
6.735
6.721
6.701
6.380
6.371
5.098
5.055
4.857
4.838
3.833
3.793
3.719
3.704
3.686
3.664
3.295
3.281
3.038
2.976
0.000
I
Ph
I
N
N
Me
6
fl (ppm)

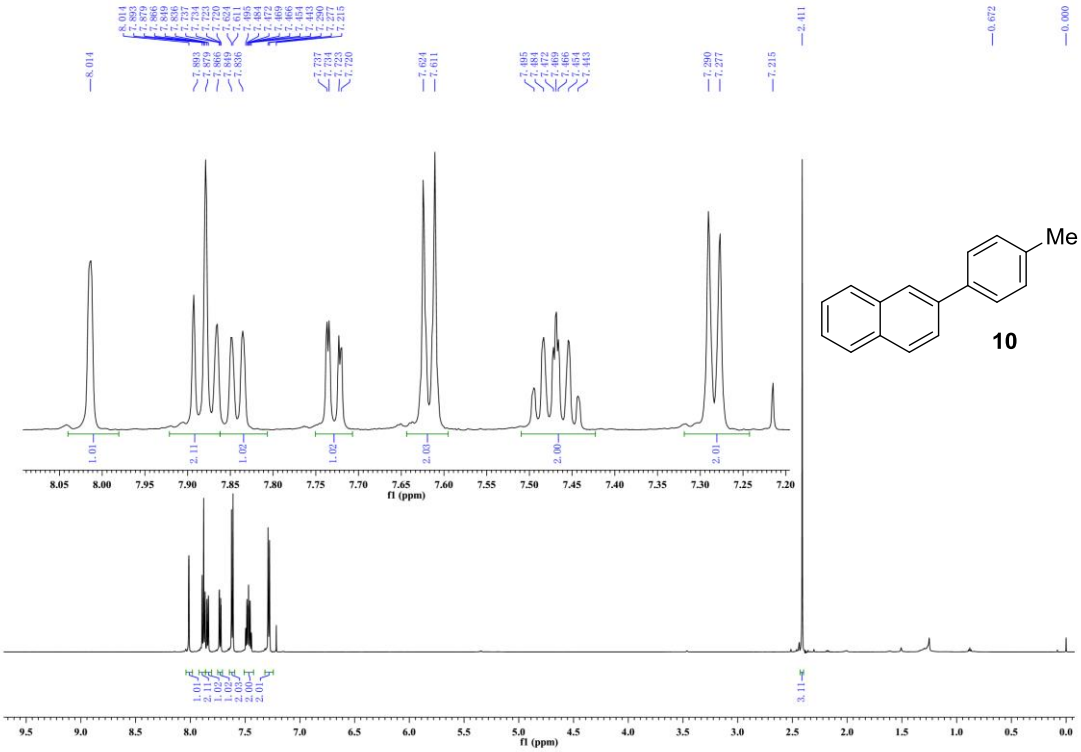

162.831
145.843
143.459
139.806
139.704
138.684
135.832
130.918
130.579
129.116
128.720
128.279
128.246
128.154
128.036
127.575
126.652
123.314
119.538
106.047
103.337
99.067
77.478
77.160
76.843
56.395
55.176
46.665
44.398
27.428
I
Ph
I
N
N
Me
6
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

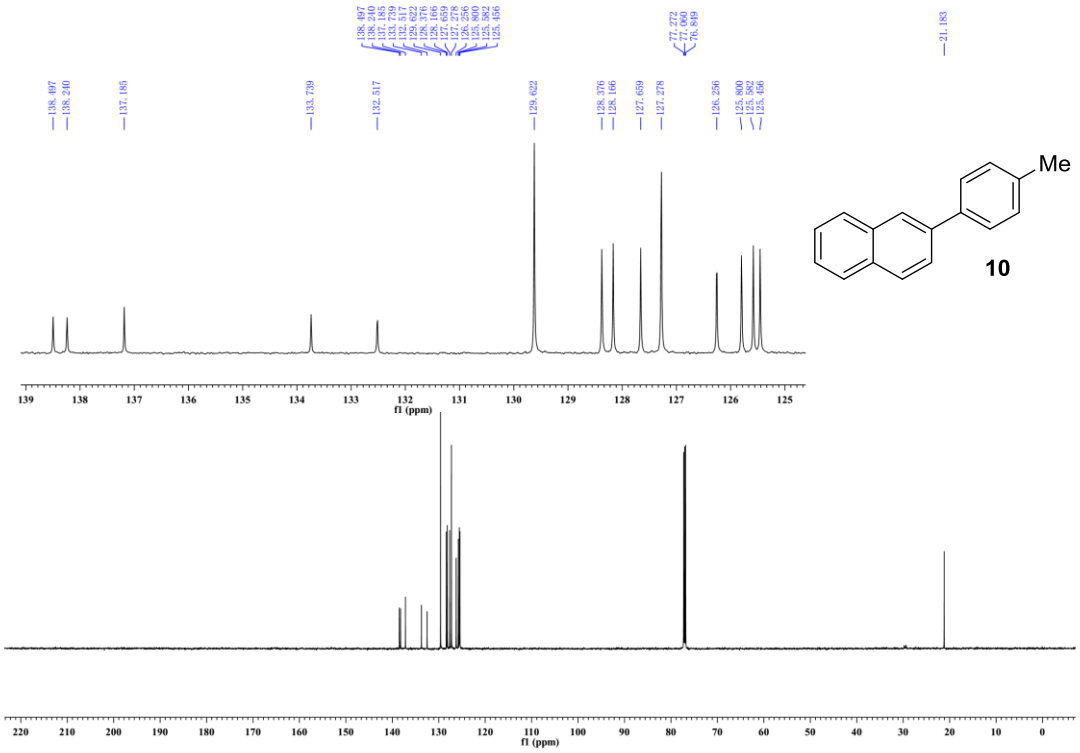

7.322
7.309
7.289
7.277
7.264
7.222
7.206
7.194
7.186
7.182
7.172
7.038
7.006
7.034
6.961
6.949
6.937
6.915
6.903
6.592
6.579
6.498
6.484
3.105
3.086
3.059
3.032
3.005
2.976
2.762
2.740
2.543
2.521
2.501
0.000
Br
N
N
Me
7
1.04
1.05
4.08
1.04
1.03
1.03
1.00
2.06
3.01
1.05
1.05
1.03
1.03
8.5
8.0
7.5
7.0
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)


Br
N
N
Me
7
f1 (ppm)


N
N
Me
9
f1 (ppm)


Me
N
N
9
f1 (ppm)


Me
10
f1 (ppm)


138.497
138.240
137.185
133.739
132.517
129.622
128.376
126.166
127.659
127.278
126.256
125.800
125.382
125.456
77.272
77.000
76.889
21.183
Me
10
fl (ppm)
fl (ppm)