Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

One-pot π-extension approach of iminoindoles-to-α-carbolines as blue-light emitters using the cooperative basic system

Rajni Lodhi,[a] S Banuprakash Goud[a] and Sampak Samanta*,[a]

[a]Department of Chemistry, Indian Institute of Technology Indore, Simrol, 453552, Indore, Madhya Pradesh, India.

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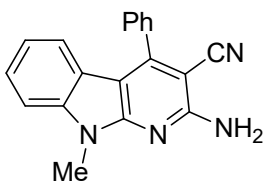
General Information: All the reactions were carried out either under an inert atmosphere or air and monitored by TLC using Merck 60 F_{254} pre-coated silica-gel plates and the products were visualized by UV detection. Flash chromatography was carried out using silica gel (200-300 mesh). ^{1}H and ^{13}C NMR spectra were recorded on 500 MHz and 125 MHz spectrometers, respectively. Data for ^{1}H NMR are reported as a chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant J (Hz), integration, and assignment, data for ^{13}C are reported as a chemical shift. High resolution mass spectrometry (HRMS) data analysis was carried out using ESI-TOF-MS. The UV-Vis experiments were monitored in a quartz cuvette (10 × 10 mm^2) using a Varian carry 100 Bio UV−vis spectrophotometer. Cyclic voltammetry was measured by using Metrohm Potentiostat/Galvanostat with the three-electrode system at room temperature. Melting points were recorded on an Electro thermal melting points apparatus and are uncorrected.

Starting materials: All the iminoindoles **(1a-i)**[1] and alkylidene malononitriles (**2a-x**)[2] were synthesized by literature known procedures. All the starting materials were known in the literatures. All the catalysts were purchased from commercial suppliers.

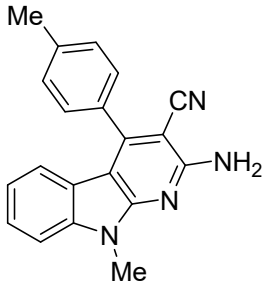
General experimental procedure for the synthesis of α-carboline derivative (3). To a stirred solution of compound iminoindole **1** (0.2 mmol), arylidene malononitrile **2** (0.24 mmol), DABCO (20 mol%) and $NaHCO_3$ (50 mol%) in DCE (2.0 mL) was heated at 60 °C under an argon-atmosphere. After completion of the reaction, the reaction mixture was extracted with EtOAc (3×10 mL), washed with brine and dried Na_2SO_4. The combined organic phases were evaporated by rotary evaporator under reduced pressure to give the crude mass, which was purified by column chromatography over silica-gel using a mixture of ethyl acetate and hexane to afford the pure α-carboline **3**. The products were characterized by their ^{1}H, ^{13}C NMR and HRMS data.

2-Amino-9-methyl-4-phenyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3aa): White solid;



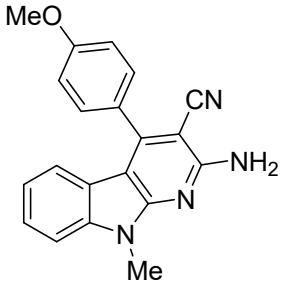
mp 202-204 °C; yield = 77%; R_f = 0.35 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.71-7.60 (m, 3H), 7.59-7.53 (m, 2H), 7.51 (d, J = 7.9 Hz, 1H), 7.32 (t, J = 7.3 Hz, 1H), 7.04-6.91 (m, 3H), 6.84 (d, J = 7.5 Hz, 1H), 3.78 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 160.0, 153.4, 150.0, 140.0, 136.1, 129.8, 129.3, 128.7, 125.5, 120.9, 120.7, 119.9, 118.1, 110.1, 105.2, 83.3, 28.0 ppm; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{19}H_{14}N_4Na^+$ 321.1111, found 321.1131.

2-Amino-9-methyl-4-(4-methylphenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ab):



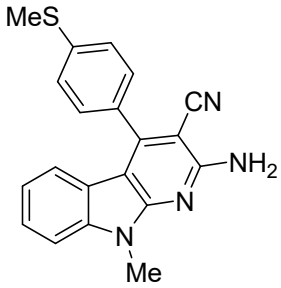
White solid; mp 181-183 °C; yield = 78%; R_f = 0.35 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, J = 7.8 Hz, 2H), 7.39 (d, J = 7.8 Hz, 2H), 7.36–7.31 (m, 2H), 7.23 (d, J = 7.8 Hz, 1H), 7.02 (t, J = 7.3 Hz, 1H), 5.26 (s, 2H), 3.83 (s, 3H), 2.50 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 153.2, 150.0, 140.0, 139.6, 132.5, 129.6, 128.5, 125.5, 121.0, 120.9, 120.7, 118.2, 108.9, 106.9, 84.1, 27.6, 21.5 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for $C_{20}H_{16}N_4Na^+$ 335.1267, found 335.1266.

2-Amino-4-(4-methoxyphenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile(3ac):



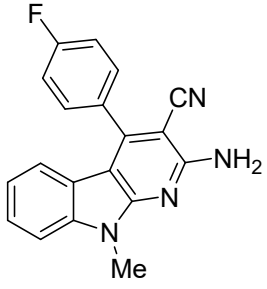
White solid; mp 196-198 °C; yield = 73%; R_f = 0.33 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, J = 7.1 Hz, 2H), 7.36-7.28 (m, 3H), 7.11 (d, J = 7.1 Hz, 2H), 7.04-6.98 (m, 1H), 5.26 (s, 2H), 3.93 (s, 3H), 3.83 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.6, 158.8, 153.2, 149.7, 140.0, 130.1, 127.6, 126.5, 125.5, 121.0, 120.7, 118.4, 114.3, 108.9, 107.0, 84.2, 55.4, 27.66 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for $C_{20}H_{16}N_4NaO^+$ 351.1216, found 351.1202.

2-Amino-9-methyl-4-(4-(methylthio)phenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile



(3ad): White solid; mp 187-189 °C; yield = 73%; R_f = 0.33 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (d, J = 7.9 Hz, 2H), 7.43 (d, J = 7.9 Hz, 2H), 7.37 (t, J = 7.4 Hz, 1H), 7.32 (d, J = 7.9 Hz, 1H), 7.25 (d, J = 5.1 Hz, 1H), 7.03 (t, J = 7.3 Hz, 1H), 5.28 (s, 2H), 3.82 (s, 3H), 2.59 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 153.2, 149.2, 140.8, 140.0, 131.7, 129.1, 126.1, 125.6, 121.0, 120.8, 120.7, 118.2, 109.0, 106.8, 83.9, 27.6, 15.2 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for $C_{20}H_{16}N_4NaS^+$ 367.0988, found 367.0962.

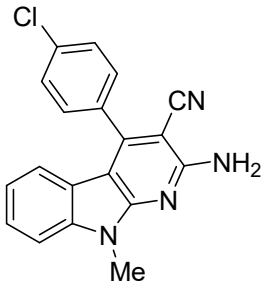
2-Amino-4-(4-fluorophenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ae):



White solid; mp 185-187 °C; yield = 81%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (dd, J = 8.4, 5.4 Hz, 2H), 7.38 (t, J = 7.5 Hz, 1H), 7.35–7.27 (m, 3H), 7.15 (d, J = 7.8 Hz, 1H),

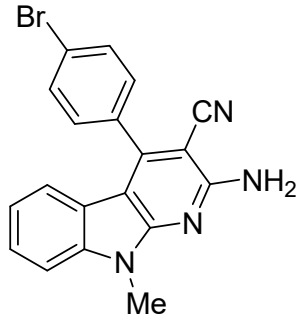
7.04 (t, J = 7.4 Hz, 1H), 5.31 (s, 2H), 3.82 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.4 (d, J = 249.7 Hz), 158.7, 153.2, 148.6, 140.1, 131.4 (d, J = 3.3 Hz), 130.6 (d, J = 8.4 Hz), 125.7, 120.9, 120.7, 120.6, 118.0, 116.1 (d, J = 21.9 Hz), 109.1, 106.9, 84.0, 27.6 ppm; ^{19}F NMR (470 MHz, $CDCl_3$) δ 114.1 ppm; HRMS (ESI-TOF) m/z z $[M + H]^+$ calcd for $C_{19}H_{14}FN_4^+$ 317.1197, found 317.1205.

2-Amino-4-(4-chlorophenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3af):



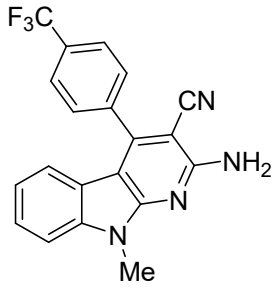
White solid; mp 189-191 °C; yield = 84%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, J = 8.3 Hz, 1H), 7.54 (d, J = 8.3 Hz, 1H), 7.39 (t, J = 7.5 Hz, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.16 (d, J = 7.8 Hz, 1H), 7.04 (t, J = 7.4 Hz, 1H), 5.31 (s, 1H), 3.82 (s, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 153.2, 148.3, 140.1, 135.7, 133.9, 130.0, 129.3, 125.8, 120.9, 120.8, 120.5, 117.9, 109.1, 106.8, 83.8, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{19}H_{14}ClN_4^+$ 333.0902, found 333.0888.

2-Amino-4-(4-bromophenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ag):



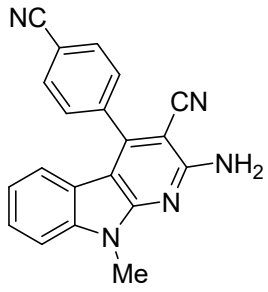
White solid; mp 192-194 °C; yield = 78%; R_f = 0.37 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, J = 8.3 Hz, 2H), 7.48 (d, J = 8.3 Hz, 2H), 7.39 (t, J = 7.5 Hz, 1H), 7.34 (d, J = 8.0 Hz, 1H), 7.16 (d, J = 7.8 Hz, 1H), 7.05 (t, J = 7.4 Hz, 1H), 5.29 (s, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 153.2, 148.2, 140.1, 134.4, 132.2, 130.3, 125.8, 124.0, 120.9, 120.8, 120.5, 117.9, 109.1, 106.7, 83.7, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{19}H_{14}BrN_4^+$ 377.0396, found 377.0414.

2-Amino-9-methyl-4-(4-(trifluoromethyl)phenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile



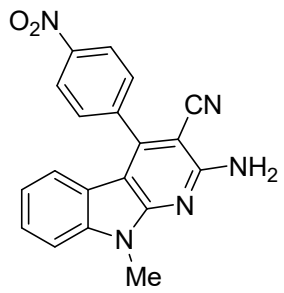
(3ah): White solid; mp 201-203 °C; yield = 77%; R_f = 0.31 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, J = 7.8 Hz, 2H), 7.73 (d, J = 7.8 Hz, 2H), 7.42–7.34 (m, 2H), 7.08 – 7.02 (m, 2H), 5.33 (s, 2H), 3.85 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 153.2, 147.8, 140.2, 139.2, 131.8, 131.5, 131.3, 129.2, 126.88–125.84 (1C, q), 121.0, 120.7, 120.3, 117.7, 109.2, 106.7, 83.6, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{20}H_{13}F_3N_4Na^+$ 389.0985, found 389.0963.

2-Amino-4-(4-cyanophenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ai):

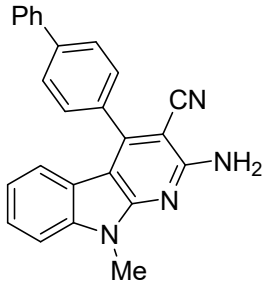


White solid; mp 205-207 °C; yield = 82%; R_f = 0.33 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, J = 8.1 Hz, 2H), 7.72 (d, J = 8.1 Hz, 2H), 7.44–7.32 (m, 2H), 7.09–6.96 (m, 2H), 5.33 (s, 2H), 3.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 153.2, 147.0, 140.3, 140.2, 132.8, 129.6, 126.1, 121.1, 120.5, 120.1, 118.3, 117.5, 113.6, 109.3, 106.5, 83.2, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{20}H_{14}N_5^+$ 324.1244, found 324.1263.

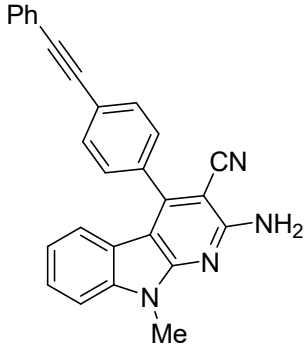
2-Amino-9-methyl-4-(4-nitrophenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3aj): White solid; mp 210-212 °C; yield = 81%; R_f = 0.34 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.47–7.32 (m, 2H), 7.11 – 6.91 (m, 2H), 5.34 (s, 2H), 3.85 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 153.2, 148.6, 146.7, 142.1, 140.3, 129.9, 126.2, 124.3, 121.1, 120.5, 120.1, 117.4, 109.4, 106.6, 83.2, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{19}H_{14}N_5O_2Na^+$ 366.0961, found 366.0946.



4-([1,1'-Biphenyl]-4-yl)-2-amino-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ak): White solid; mp 195-197 °C; yield = 79%; R_f = 0.34 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, J = 8.1 Hz, 2H), 7.74 (d, J = 7.4 Hz, 2H), 7.69 (d, J = 8.1 Hz, 2H), 7.51 (t, J = 7.6 Hz, 2H), 7.43–7.33 (m, 3H), 7.29 (d, J = 7.9 Hz, 1H), 7.04 (t, J = 7.3 Hz, 1H), 5.32 (s, 2H), 3.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 153.2, 149.4, 142.3, 140.3, 140.1, 134.3, 129.1, 128.9, 127.8, 127.5, 127.2, 125.6, 121.0, 120.9, 120.8, 118.2, 109.0, 106.9, 83.9, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{25}H_{18}N_4Na^+$ 397.1424, found 397.1401.

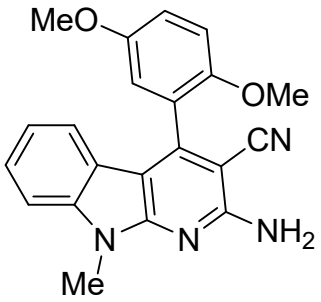


2-Amino-9-methyl-4-(4-(phenylethynyl)phenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3al): White solid; mp 208-210 °C; yield = 75%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, J = 7.9 Hz, 2H), 7.60 (d, J = 7.8 Hz, 4H), 7.40 -7.36 (m, 4H), 7.34 (d, J = 8.0 Hz, 1H), 7.21 (d, J = 7.9 Hz, 1H), 7.04 (t, J = 7.4 Hz, 1H), 5.32 (s, 2H), 3.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 153.2, 148.9, 140.1, 135.3, 132.1, 131.7, 128.7, 128.5,



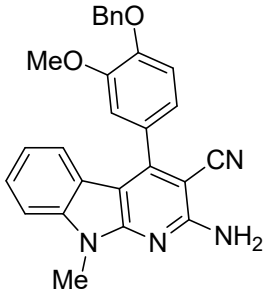
128.4, 125.7, 124.7, 123.0, 121.0, 120.9, 120.6, 117.9, 109.1, 106.7, 90.9, 88.8, 83.7, 27.7 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for for $C_{27}H_{18}N_4Na^+$ 421.1424, found 421.1450.

2-Amino-4-(2,5-dimethoxyphenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile

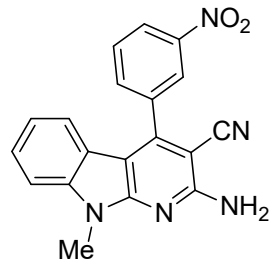


(3am): White solid; mp 199-201 °C; yield = 62%; R_f = 0.32 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 - 7.31 (m, 2H), 7.10–7.05 (m, 3H), 7.05–6.99 (m, 1H), 6.94 (s, 1H), 5.24 (s, 2H), 3.83 (s, 3H), 3.79 (s, 3H), 3.73 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.5, 153.7, 153.2, 150.6, 146.4, 140.0, 125.4, 124.9, 121.0, 120.9, 120.8, 118.0, 116.2, 115.4, 113.0, 108.8, 107.5, 84.9, 56.3, 55.9, 32.7, 27.6 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for $C_{21}H_{18}N_4NaO_2^+$ 381.1322, found 381.1346.

2-Amino-4-(4-(benzyloxy)-3-methoxyphenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3an): White solid; mp 180-182 °C; yield = 61%; R_f = 0.31 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52–7.47 (m, 2H), 7.45–7.39 (m, 2H), 7.39-7.31 (m, 3H), 7.30–7.26 (m, 1H), 7.17–7.09 (m, 3H), 7.06–6.99 (m, 1H), 5.27 (s, 4H), 3.90 (s, 3H), 3.83 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 153.2, 149.7, 149.6, 149.2, 140.0, 136.8, 128.6, 128.2, 128.0, 127.5, 125.5, 121.3, 121.1, 120.9, 120.7, 118.3, 113.8, 112.3, 109.0, 106.9, 84.1, 71.1, 56.1, 27.6 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for $C_{27}H_{22}N_4NaO_2^+$ 457.1635, found 457.1612.

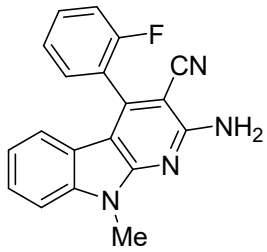


2-Amino-9-methyl-4-(3-nitrophenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ao):



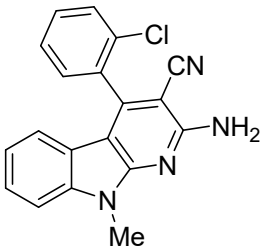
Light yellow solid; mp 210-212 °C; yield = 80%; R_f = 0.34 (EtOAc/hexane = 25:75); ^{1}H NMR(500 MHz, $CDCl_3$) δ 8.59–8.33 (m, 2H), 7.94 (d, J = 7.6 Hz, 1H), 7.82 (t, J = 7.9 Hz, 1H), 7.49–7.32 (m, 2H), 7.08–6.88 (m, 2H), 5.34 (s, 2H), 3.85 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.3, 152.4, 147.3, 145.3, 139.1, 136.4, 134.0, 129.4, 124.8, 123.3, 122.6, 119.9, 119.1, 118.9, 116.6, 108.4, 104.9, 82.1, 26.7 ppm; HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for $C_{19}H_{15}N_5O_2^+$ 344.1142, found 344.1116.

2-Amino-4-(2-fluorophenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ap):



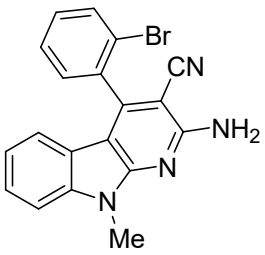
White solid; mp 183-185 °C; yield = 83%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67–7.57 (m, 1H), 7.52 (t, J = 6.9 Hz, 1H), 7.40–7.32 (m, 4H), 7.08–7.01 (m, 2H), 5.32 (s, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.05 (d, J = 248.2 Hz), 158.6, 153.1, 143.1, 140.1, 131.7 (d, J = 8.0 Hz), 130.7 (d, J = 2.6 Hz), 125.8, 124.7 (d, J = 3.6 Hz), 123.2 (d, J = 15.8 Hz), 121.0, 120.6, 120.5, 117.6, 116.51 (d, J = 21.3 Hz), 109.1, 107.6, 84.5, 27.6 ppm; ^{19}F NMR ($CDCl_3$, 470 MHz) δ 113.6 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{19}H_{14}FN_4^+$ 317.1197, found 317.1205.

2-Amino-4-(2-chlorophenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3aq):



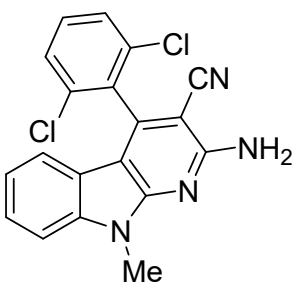
White solid; mp 198-200 °C; yield = 80%; R_f = 0.37 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, J = 8.0 Hz, 1H), 7.55–7.43 (m, 3H), 7.40–7.31 (m, 2H), 7.03 (t, J = 7.4 Hz, 1H), 6.83 (d, J = 7.8 Hz, 1H), 5.34 (s, 2H), 3.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.5, 153.1, 146.3, 140.1, 134.5, 132.6, 130.8, 130.2, 130.1, 127.4, 125.8, 121.1, 120.6, 117.4, 109.1, 107.4, 84.2, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{19}H_{13}ClN_4Na^+$ 355.0721, found 355.0706.

2-Amino-4-(2-bromophenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ar):



White solid; mp 205-207 °C; yield = 77%; R_f = 0.37 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, J = 8.0 Hz, 1H), 7.53 (t, J = 7.4 Hz, 1H), 7.50–7.40 (m, 2H), 7.40–7.32 (m, 2H), 7.02 (t, J = 7.4 Hz, 1H), 6.79 (d, J = 7.8 Hz, 1H), 5.34 (s, 2H), 3.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.5, 153.1, 147.8, 140.1, 136.6, 133.4, 130.9, 130.0, 128.0, 125.8, 122.0, 121.1, 120.7, 120.6, 117.4, 109.1, 107.3, 84.1, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{19}H_{14}BrN_4^+$ 377.0396, found 377.0414.

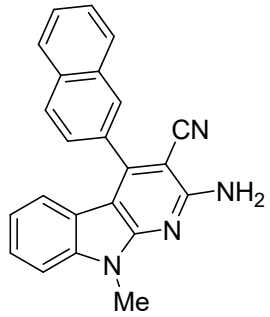
2-Amino-4-(2,6-dichlorophenyl)-9-methyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3as):



White solid; mp 209-211 °C; yield = 71%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, J = 8.1 Hz, 2H), 7.51–7.43 (m, 1H), 7.41–7.31 (m, 2H), 7.04 (t, J = 7.3 Hz, 1H), 6.75 (d, J = 7.8 Hz, 1H), 5.32 (s, 2H), 3.85 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 153.4, 143.5, 140.2,

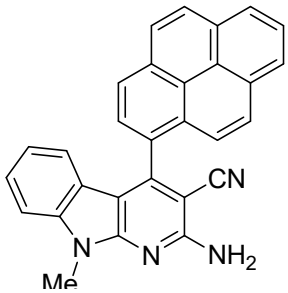
134.2, 133.3, 131.1, 128.6, 126.0, 121.3, 120.3, 120.1, 116.9, 109.2, 107.1, 83.8, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{19}H_{13}Cl_2N_4^+$ 367.0512, found 367.0520.

2-Amino-9-methyl-4-(naphthalen-2-yl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3at):

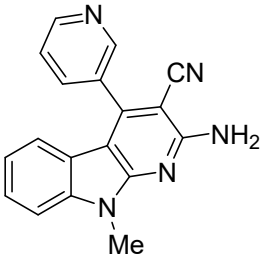


White solid; mp 190-192 °C; yield = 76%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (s, 1H), 8.10 (d, J = 8.1 Hz, 1H), 8.01 (d, J = 7.4 Hz, 1H), 7.97 (d, J = 7.2 Hz, 1H), 7.71 (d, J = 8.1 Hz, 1H), 7.68–7.57 (m, 2H), 7.45–7.31 (m, 2H), 7.15 (d, J = 7.4 Hz, 1H), 6.98 (d, J = 5.0 Hz, 1H), 5.37 (s, 2H), 3.88 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 153.2, 149.7, 140.1, 133.7, 133.2, 132.9, 128.7, 128.6, 128.2, 127.9, 127.1, 126.7, 126.0, 125.6, 121.0, 120.9, 120.8, 118.1, 109.0, 107.1, 84.2, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{23}H_{17}N_4^+$ 349.1448, found 349.1418.

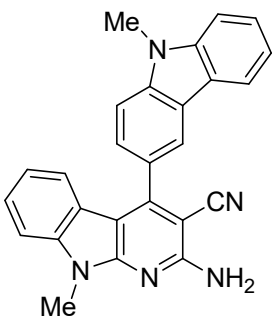
2-Amino-9-methyl-4-(pyren-1-yl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3au): White solid; mp 180-182 °C; yield = 73%; R_f = 0.35 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, J = 7.6 Hz, 1H), 8.20 (d, J = 7.3 Hz, 1H), 8.17–8.10 (m, 2H), 8.10 (d, J = 7.3 Hz, 1H), 8.01 (d, J = 7.7 Hz, 1H), 7.97 (t, J = 7.5 Hz, 1H), 7.88 (d, J = 9.1 Hz, 1H), 7.68 (d, J = 9.1 Hz, 1H), 7.24 (d, J = 7.8 Hz, 1H), 7.21–7.12 (m, 2H), 6.57 (t, J = 7.2 Hz, 1H), 6.15 (d, J = 7.6 Hz, 1H), 5.32 (s, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 153.1, 148.6, 140.1, 132.1, 131.3, 130.9, 130.1, 128.7, 128.4, 127.4, 126.4, 126.3, 125.8, 125.7, 125.6, 125.1, 124.8, 124.7, 124.2, 121.0, 120.9, 120.7, 117.9, 108.9, 108.6, 85.6, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + Na]^+$ calcd for $C_{29}H_{18}N_4Na^+$ 445.1424, found 445.1396.



2-Amino-9-methyl-4-(pyridin-3-yl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3av): White solid; mp 175-177 °C; yield = 78%; R_f = 0.31 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.87 (d, J = 7.0 Hz, 2H), 7.97 (d, J = 7.4 Hz, 1H), 7.62–7.55 (m, 1H), 7.42–7.33 (m, 2H), 7.09 (d, J = 7.6 Hz, 1H), 7.03 (t, J = 7.2 Hz, 1H), 5.33 (s, 2H), 3.85 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 153.2, 150.7, 149.2, 145.6, 140.2, 136.3, 126.0, 123.7, 121.1, 120.6, 120.4, 117.6, 109.2, 107.1, 83.8, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{18}H_{14}N_5^+$ 300.1244, found 300.1238.

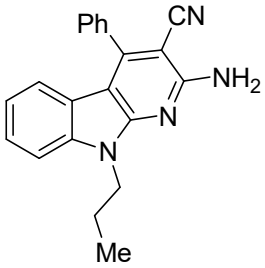


2-Amino-9-methyl-4-(9-methyl-9*H*-carbazol-3-yl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile

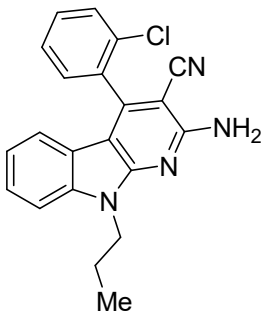


(3aw): White solid; mp 220-222 °C; yield = 66%; R_f = 0.33 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (s, 1H), 8.07 (d, J = 7.7 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.59 (d, J = 8.4 Hz, 1H), 7.52 (t, J = 7.6 Hz, 1H), 7.46 (d, J = 8.2 Hz, 1H), 7.32 (d, J = 3.9 Hz, 2H), 7.24 (t, J = 3.5 Hz, 1H), 7.18 (d, J = 7.9 Hz, 1H), 6.92 – 6.88 (m, 1H), 5.29 (s, 2H), 3.95 (s, 3H), 3.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 153.2, 151.1, 141.6, 141.5, 140.0, 126.3, 125.8, 125.4, 123.0, 122.7, 121.2, 121.0, 120.9, 120.7, 120.6, 119.4, 118.6, 108.93, 108.9, 108.7, 107.3, 84.7, 29.3, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{26}H_{20}N_5^+$ 402.1713, found 402.1685.

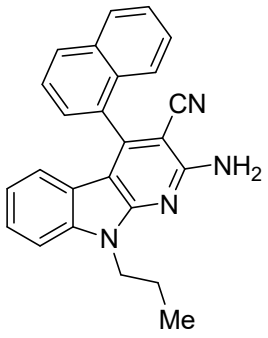
2-Amino-4-phenyl-9-propyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ba): White solid; mp 173-175 °C; yield = 79%; R_f = 0.35 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70-7.50 (m, 5H), 7.40-7.25 (m, 2H), 7.19–7.06 (m, 1H), 7.03–6.91 (m, 1H), 5.28 (s, 2H), 4.30 (s, 2H), 1.91 (s, 2H), 1.00 (s, 3H)ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.7, 153.0, 149.7, 139.5, 135.6, 129.5, 128.9, 128.5, 125.4, 121.0, 120.9, 120.5, 118.1, 109.3, 106.8, 84.1, 43.1, 21.9, 11.6 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{21}H_{19}N_4^+$ 327.1604, found 327.1619.



2-Amino-4-(2-chlorophenyl)-9-propyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3bq): White solid; mp 190-192 °C; yield = 80%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, J = 8.0 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.48 (t, J = 7.4 Hz, 1H), 7.44 (d, J = 7.3 Hz, 1H), 7.35 (d, J = 3.8 Hz, 2H), 7.01–6.98 (m, 1H), 6.82 (d, J = 7.8 Hz, 1H), 5.28 (s, 2H), 4.40–4.17 (m, 2H), 2.07–1.76 (m, 2H), 1.01 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 152.9, 146.2, 139.5, 134.6, 132.6, 130.7, 130.2, 130.1, 127.4, 125.6, 120.8, 120.7, 117.5, 109.3, 107.3, 84.2, 43.2, 22.0, 11.6 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{21}H_{18}ClN_4^+$ 361.1215, found 361.1206.

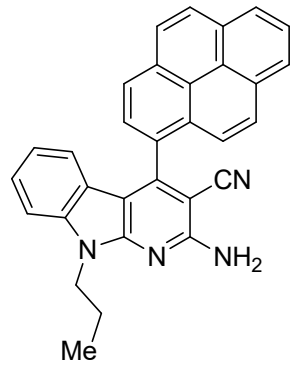


2-Amino-4-(naphthalen-1-yl)-9-propyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3bx):

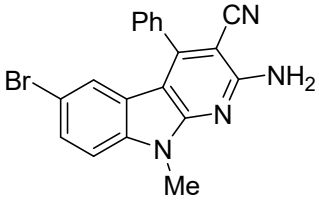


White solid; mp 182-184 °C; yield = 78%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, J = 8.2 Hz, 1H), 7.99 (d, J = 8.2 Hz, 1H), 7.66 (t, J = 7.6 Hz, 1H), 7.58 (d, J = 6.9 Hz, 1H), 7.55–7.45 (m, 2H), 7.35–7.31 (m, 2H), 7.27–7.21 (m, 1H), 6.76 (t, J = 7.5 Hz, 1H), 6.33 (d, J = 7.8 Hz, 1H), 5.31 (s, 2H), 4.54 – 4.21 (m, 2H), 2.08 – 1.81 (m, 2H), 1.04 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 152.8, 148.0, 139.5, 133.6, 133.2, 130.5, 129.7, 128.5, 126.9, 126.5, 126.4, 125.6, 125.4, 125.1, 121.1, 120.7, 120.6, 117.7, 109.2, 108.2, 85.2, 43.2, 22.0, 11.6ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{25}H_{21}N_4^+$ 377.1761, found 377.1748.

2-Amino-9-propyl-4-(pyren-1-yl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3bu): White solid; mp 203-205 °C; yield = 71%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, J = 7.8 Hz, 1H), 8.25 (d, J = 7.6 Hz, 1H), 8.22–8.16 (m, 2H), 8.15 (d, J = 7.5 Hz, 1H), 8.09 (d, J = 7.8 Hz, 1H), 8.02 (t, J = 7.6 Hz, 1H), 7.95 (d, J = 9.2 Hz, 1H), 7.78 (d, J = 9.1 Hz, 1H), 7.31 (d, J = 8.1 Hz, 1H), 7.23 – 7.19 (m, 1H), 6.62 (t, J = 7.6 Hz, 1H), 6.23 (d, J = 7.9 Hz, 1H), 5.39 (s, 2H), 4.49–4.17 (m, 2H), 2.14–1.80 (m, 2H), 1.04 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 152.9, 148.5, 139.6, 132.1, 131.3, 131.0, 130.2, 128.7, 128.5, 128.4, 127.4, 126.4, 126.3, 125.7, 125.6, 125.4, 125.1, 124.9, 124.8, 124.3, 121.1, 120.8, 120.7, 117.9, 109.2, 108.5, 85.6, 43.2, 22.0, 11.7 ppm; HRMS (ESI-TOF) m/z calcd for $C_{31}H_{22}N_4Na^+$ $[M + Na]^+$: 473.1737, found 473.1718.

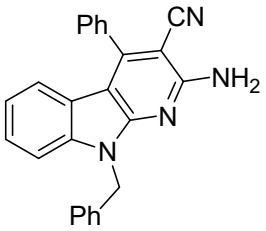


2-Amino-6-bromo-9-methyl-4-phenyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3da):

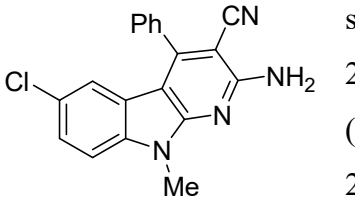


White solid; mp 193-195 °C; yield = 70%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64–7.59 (m, 3H), 7.57–7.55 (m, 2H), 7.45 – 7.43 (m, 1H), 7.23–7.19 (m, 1H), 7.18 (d, J = 8.5 Hz, 1H), 5.35 (s, 2H), 3.80 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 153.2, 150.4, 138.7, 134.9, 130.0, 129.0, 128.4, 128.2, 123.5, 122.5, 117.7, 113.7, 110.4, 105.8, 84.6, 27.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{19}H_{14}BrN_4^+$ 377.0396, found 377.0414.

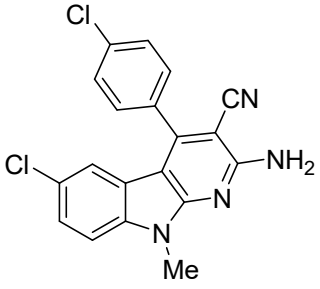
2-Amino-9-benzyl-4-phenyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile(3ca): White solid; mp 208-210 °C; yield = 73%; R_f = 0.35 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67–7.54 (m, 5H), 7.33 – 7.20 (m, 7H), 7.14 (d, J = 7.9 Hz, 1H), 6.97 (t, J = 7.2 Hz, 1H), 5.56 (s, 2H), 5.30 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 153.1, 150.0, 139.3, 136.6, 135.5, 129.6, 128.9, 128.7, 128.5, 127.6, 127.0, 125.6, 121.1, 121.0, 120.9, 118.0, 109.8, 106.8, 84.5, 45.0 ppm; HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for $C_{25}H_{19}N_4^+$ 375.1604, found 375.1599.



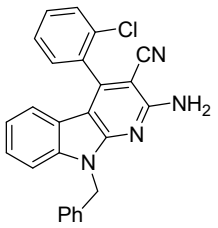
2-Amino-6-chloro-9-methyl-4-phenyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ea): White solid; mp 189-191 °C; yield = 71%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 – 7.53 (m, 5H), 7.32 (d, J = 8.4 Hz, 1H), 7.24 (d, J = 8.7 Hz, 1H), 7.08 (s, 1H), 5.34 (s, 2H), 3.82 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 153.4, 150.4, 138.4, 134.9, 129.9, 129.1, 128.4, 126.2, 125.5, 121.9, 120.6, 117.7, 109.9, 106.0, 84.6, 27.7 ppm; HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for $C_{19}H_{14}ClN_4^+$ 333.0902, found 333.0888.



2-Amino-6-chloro-9-methyl-4-(4-chlorophenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3ef): Light yellow solid; mp 215-217 °C; yield = 75%; R_f = 0.33 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64–7.57 (m, 2H), 7.56 – 7.49 (m, 2H), 7.33 (d, J = 5.7 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.12 (s, 1H), 5.34 (s, 2H), 3.82 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 153.4, 148.9, 138.4, 136.1, 133.3, 129.9, 129.5, 126.4, 125.8, 121.7, 120.4, 117.6, 110.0, 105.8, 84.4, 27.8 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for $C_{19}H_{12}Cl_2N_4Na^+$ 389.0512, found 389.0306.

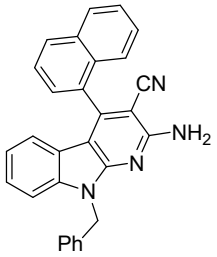


2-Amino-9-benzyl-4-(2-chlorophenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3cq): White solid; mp 185-187 °C; yield = 78%; R_f = 0.37 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, J = 7.2 Hz, 1H), 7.53 – 7.46 (m, 3H), 7.37–7.11 (m, 7H), 7.01–6.90 (m, 1H), 6.83 (d, J = 7.0 Hz, 1H), 5.63–5.49 (m, 2H), 5.30 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 153.1, 146.5, 139.4, 136.5, 134.5, 132.6, 130.8, 130.2, 130.1, 128.8, 127.6, 127.4, 127.1, 125.8, 121.2, 120.8, 120.7, 117.3,



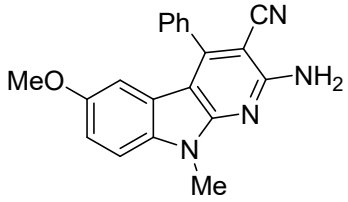
109.9, 107.4, 84.7, 45.0 ppm; HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for $C_{25}H_{18}ClN_4^+$ 409.1215, found 409.1210.

2-Amino-9-benzyl-4-(naphthalen-1-yl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3cx):



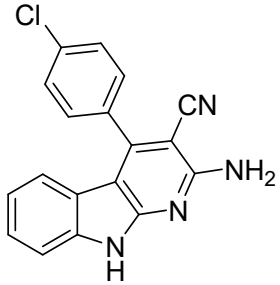
White solid; mp 199-201 °C; yield = 72%; R_f = 0.36 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, J = 8.0 Hz, 1H), 8.00 (d, J = 7.9 Hz, 1H), 7.67 (t, J = 7.5 Hz, 1H), 7.61 (d, J = 6.8 Hz, 1H), 7.52 (t, J = 7.5 Hz, 2H), 7.38–7.31 (m, 5H), 7.29 – 7.25 (m, 1H), 7.22 (d, J = 7.8 Hz, 1H), 7.17 (t, J = 7.5 Hz, 1H), 6.75 (t, J = 7.3 Hz, 1H), 6.34 (d, J = 7.7 Hz, 1H), 5.65–5.54 (m, 2H), 5.34 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.8, 152.9, 148.3, 139.3, 136.6, 133.6, 133.1, 130.4, 129.8, 128.8, 128.6, 127.6, 127.1, 127.0, 126.5, 126.4, 125.5, 125.0, 121.1, 121.0, 120.9, 117.6, 109.7, 108.2, 85.7, 45.1ppm; HRMS (ESI-TOF) m/z [M + H]$^+$ calcd for $C_{29}H_{21}N_4^+$ 425.1761, found 425.1786.

2-Amino-6-methoxy-9-methyl-4-phenyl-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3fa):

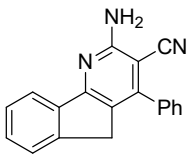


White solid; mp 194-196 °C; yield = 76%; R_f = 0.33 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71–7.49 (m, 5H), 7.20 (d, J = 8.7 Hz, 1H), 6.97 (d, J = 8.6 Hz, 1H), 6.63 (s, 1H), 5.33 (s, 2H), 3.77 (s, 3H), 3.61 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.6, 154.5, 153.2, 149.8, 135.3, 134.7, 129.6, 128.8, 128.6, 121.3, 118.1, 113.4, 109.5, 106.8, 105.0, 83.6, 55.6, 27.7 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for $C_{20}H_{16}N_4NaO^+$ 351.1216, found 351.1202.

2-Amino-4-(4-chlorophenyl)-9*H*-pyrido[2,3-*b*]indole-3-carbonitrile (3if): Yellow solid; mp 203-205 °C; yield = 83%; R_f = 0.31 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.98 (s, 1H), 8.10–9.99 (m, 1H), 7.81 – 7.64 (m, 4H), 7.54–7.38 (m, 2H), 7.27–7.08 (m, 1H), 6.43 (s, 2H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 156.5, 143.6, 143.5, 136.4, 134.8, 132.8, 131.6, 129.5, 129.2, 124.7, 121.4, 120.6, 119.8, 118.0, 112.7, 87.4 ppm; HRMS (ESI-TOF) m/z [M + Na]$^+$ calcd for $C_{18}H_{11}ClN_4Na^+$ 341.0564, found 341.0547.

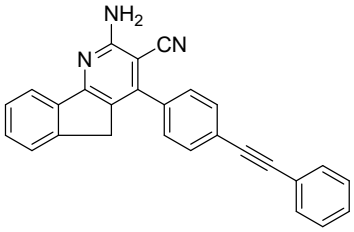


2-Amino-4-phenyl-5*H*-indeno[1,2-*b*]pyridine-3-carbonitrile(3ga): White solid; mp 191-193 °C; yield = 76%; R_f = 0.36 (EtOAc/hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, J = 6.8 Hz, 1H), 7.58–7.48 (m, 6H), 7.48–7.42



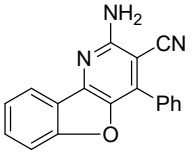
(m, 2H), 5.49 (s, 2H), 3.71 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9, 160.9, 150.4, 145.8, 139.6, 135.6, 130.0, 129.5, 128.8, 128.4, 127.5, 125.2, 125.1, 121.9, 117.5, 88.0, 33.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{19}H_{14}N_3^+$ 284.1182, found 284.1179.

2-Amino-4-(4-(phenylethynyl)phenyl)-5*H*-indeno[1,2-*b*]pyridine-3-carbonitrile(3gl):

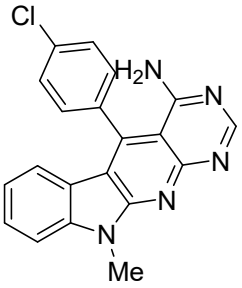


Light yellow solid; mp 195-197 °C; yield = 72%; R_f = 0.36 (EtOAc/hexane = 15:85); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10-8.01 (m, 1H), 7.71 (d, J = 7.9 Hz, 2H), 7.60–7.50 (m, 5H), 7.49 – 7.43 (m, 2H), 7.40 -7.30 (m, 3H), 5.50 (s, 2H), 3.74 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.7, 149.8, 145.8, 139.4, 135.1, 132.0, 131.7, 130.2, 128.6, 128.5, 128.4, 127.6, 125.2, 125.1, 124.8, 122.9, 122.1, 117.3, 91.1, 88.6, 87.7, 33.7 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{27}H_{18}N_3^+$ 384.1495, found 384.1523.

2-Amino-4-phenylbenzofuro[3,2-*b*]pyridine-3-carbonitrile(3ha):[3] White solid; mp 201-203 °C; yield = 75%; R_f = 0.34 (EtOAc/hexane = 25:75); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 6.3 Hz, 1H), 7.83 – 7.78 (m, 2H), 7.66 – 7.48 (m, 5H), 7.42 (d, J = 5.1 Hz, 1H), 5.37 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.1, 158.0, 146.1, 144.2, 141.0, 130.9, 130.7, 130.4, 129.6, 128.9, 123.7, 122.2, 122.0, 117.1, 112.5, 88.3 ppm; HRMS (ESI-TOF) m/z $[M + H]^+$ calcd for $C_{18}H_{12}N_3O^+$ 286.0975, found 286.0998.



5-(4-Chlorophenyl)-10-methyl-10*H*-pyrimido[5′,4′:5,6]pyrido[2,3-*b*]indol-4-amine (5af):



Yellow solid; mp 260-262 °C; yield = 91%; R_f = 0.35 (EtOAc/hexane = 80:20); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (s, 1H), 8.21 (d, J = 13.0 Hz, 2H), 7.71 (d, J = 8.1 Hz, 1H), 7.52 (dd, J = 18.4, 7.9 Hz, 2H), 7.41 (d, J = 8.1 Hz, 1H), 7.03 (t, J = 7.6 Hz, 1H), 6.61 (d, J = 7.8 Hz, 1H), 5.70 (s, 2H), 3.98 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9, 158.2, 157.3, 154.5, 142.6, 140.5, 136.2, 135.7, 130.6, 129.5, 128.3, 122.4, 121.0, 120.2, 116.7, 109.3, 102.1, 27.8 ppm; HRMS (ESI-TOF) m/z $[M+H]^+$ calcd for $C_{20}H_{15}ClN_5^+$ 360.1010, found 360.1040.

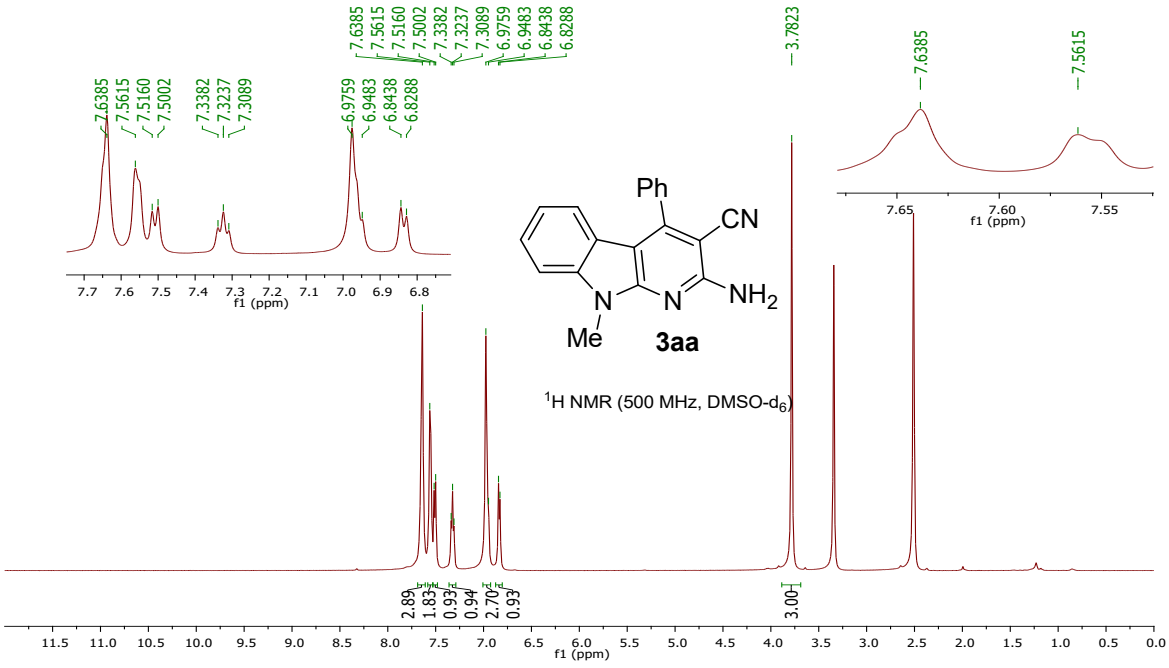
The relative quantum yield was evaluated by employing the following equation:

$\Phi = \Phi_S . I / I_S . OD_S / OD . \eta^2/\eta_S^2$

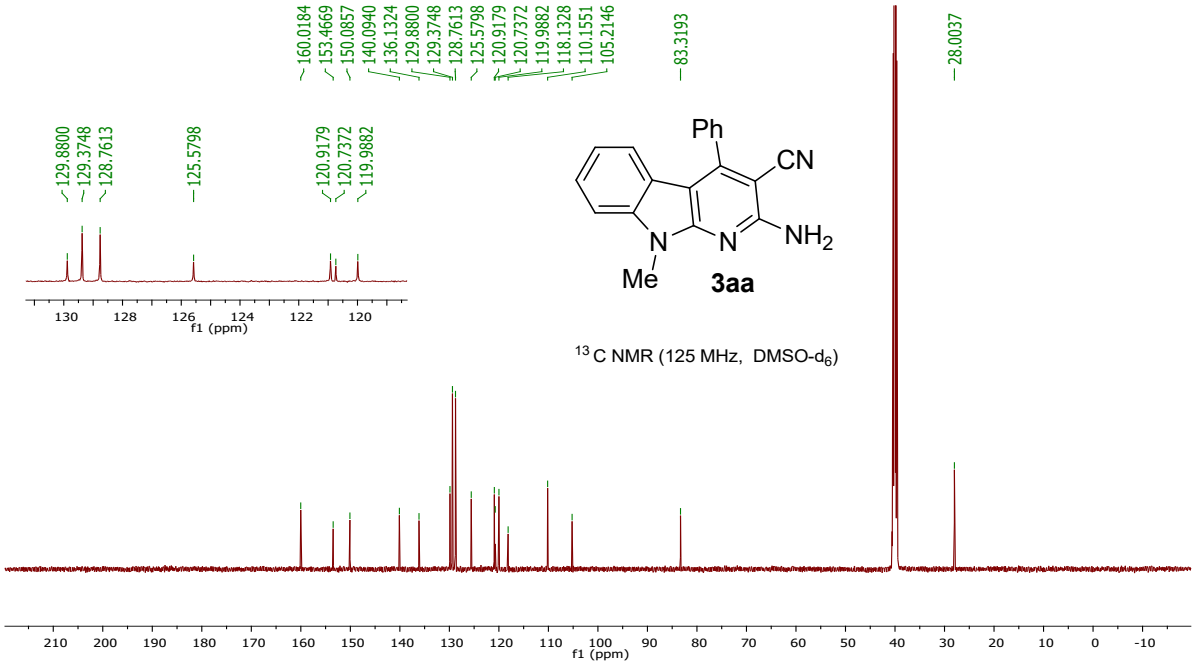
where, Φ is the quantum yield, I is the integrated intensity at a specified wavelength, OD is the optical density at the same excitation wavelength and η is the refractive index of the solvent used for dissolution. The subscript S refers to the standard quinine sulfate (Φ = 0.54 in 0.1M H_2SO_4).

References:

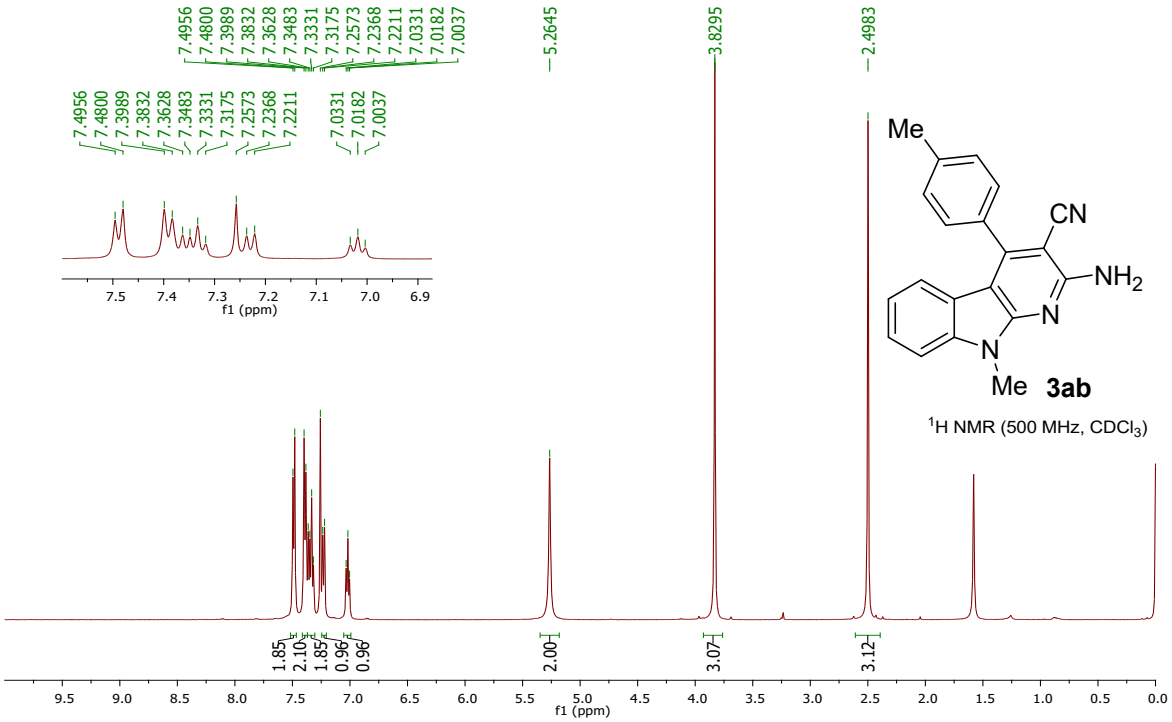
1. (a) K. Selvaraj and K. C. K. Swamy, *J. Org. Chem.*, 2018, **83**, 15043; (b) G. Sheng, K. Huang, Z. Chi, H. Ding, Y. Xing, P. Lu and Y. Wang, *Org. Lett.*, 2014, **16**, 5096. (c) S. Debnath, A. S. Kumar, S. Chauhan and K. C. Kumara Swamy, *J. Org. Chem.*, 2021, **86**, 11583; (d) G. Sheng, K. Huang, Z. Chi, H. Ding, Y. Xing, P. Lu and Y. Wang, *Org. Lett.*, 2014, **16**, 5096. (e) R. Ma, X. Wang, Q. Zhang, L. Chen, J. Gao, J. Feng, D. Wei and D. Du, *Org. Lett*., 2021, **23**, 4267.
2. (a) R.V. Hangarge, S.A. Sonwane, D.A. Jarikote and M. S. Shingare, *Green Chem.*, 2001, **3**, 310; (b) N. Salaverri, B. Carli, Gratal, B. Patrici, L. Marzo and J. Aleman, *Adv. Synth. Catal*., 2022, **364**, 1689; (c) M. Lian, J. Liu, S. Tang, G. Liu, C. Ma, Q. Meng, H. Peng and D. Zhu, *Org. Lett*., 2019, **21**, 2597.
3. Q. Wu, Y. Zhang and S. Cui, *Org. Lett*., 2014, **16**, 1350.



^{1}H NMR (500 MHz, DMSO-d_6)



^{13}C NMR (125 MHz, DMSO-d_6)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7.3989
7.3832
7.3628
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7.3331
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7.2573
7.2368
7.2211
7.0331
7.0182
7.0037
5.2645
3.8295
2.4983
Me
CN
NH2
N
N
Me
3ab
1H NMR (500 MHz, CDCl3)
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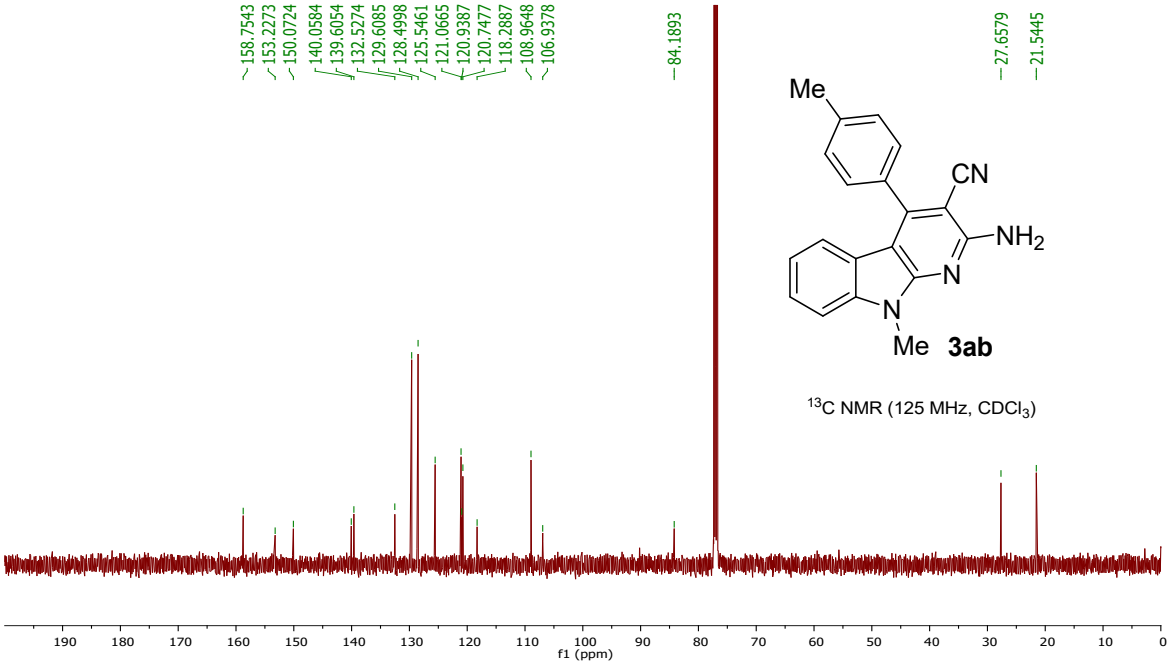
2.10
1.85
0.96
0.96
2.00
3.07
3.12
f1 (ppm)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150.0724
140.0584
139.6054
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125.5461
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120.9387
120.7477
118.2887
108.9648
106.9378
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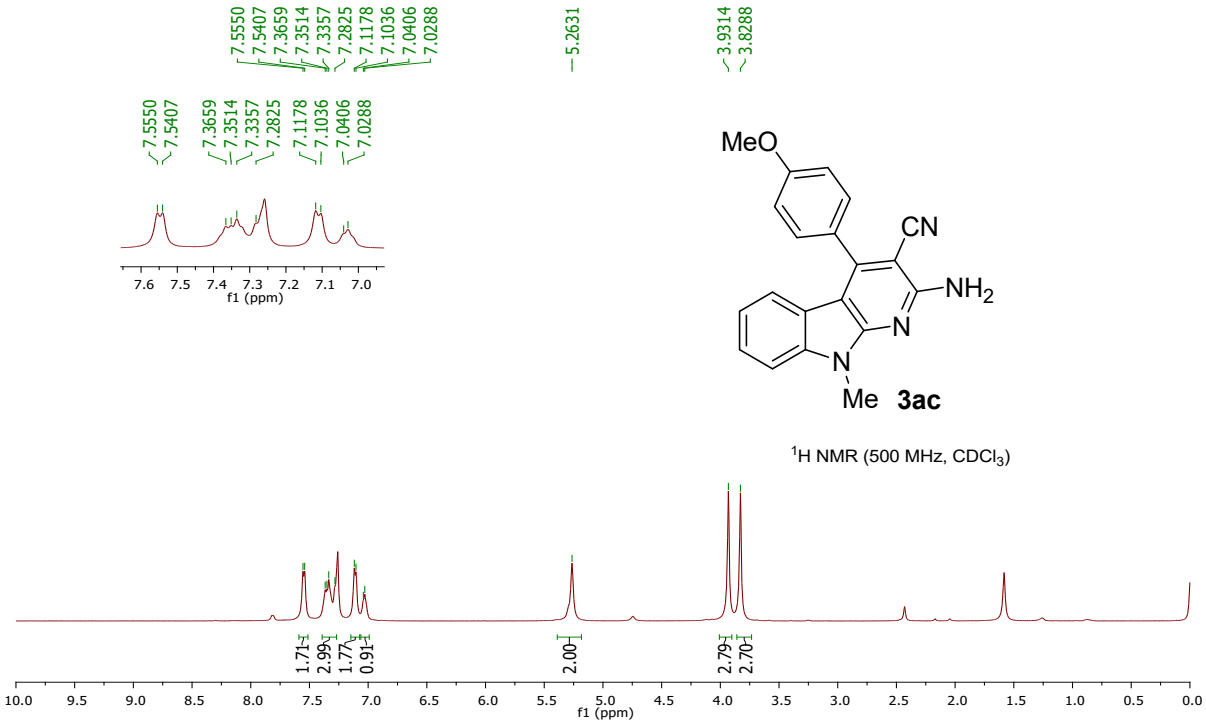
27.6579
21.5445
Me
CN
NH2
N
N
Me
3ab
13C NMR (125 MHz, CDCl3)
f1 (ppm)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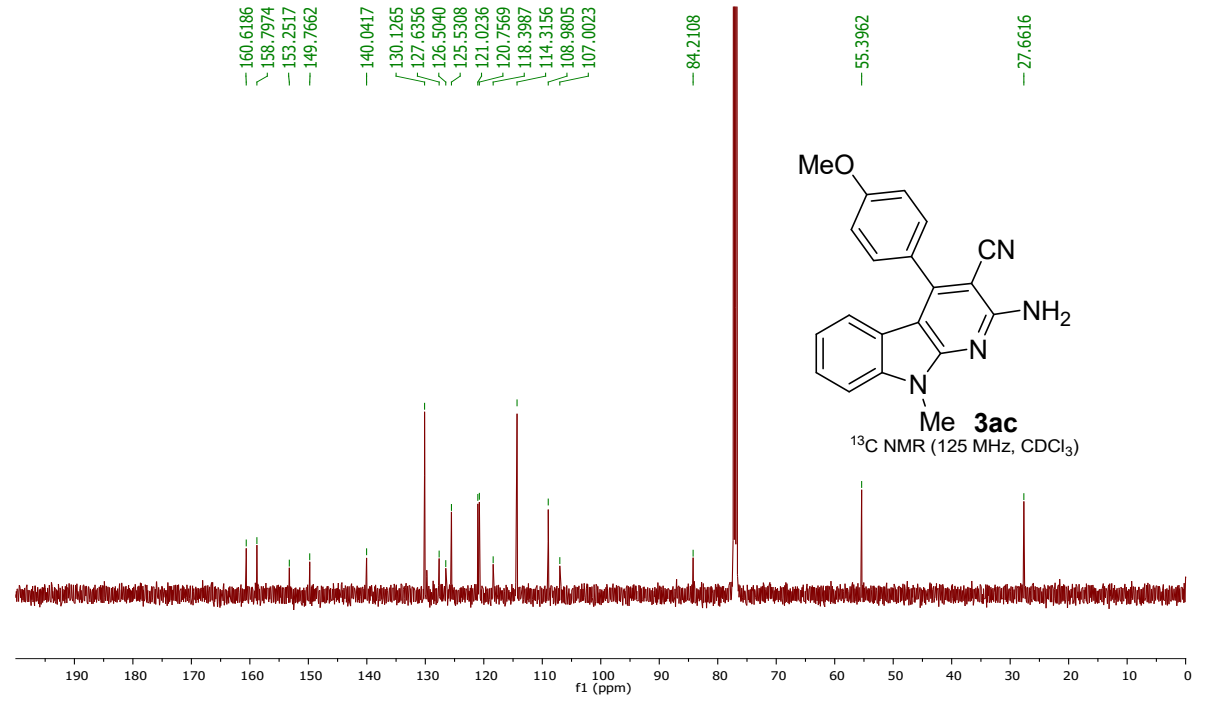
7.3357
7.2825
7.1178
7.1036
7.0406
7.0288
5.2631
3.9314
3.8288
MeO
CN
NH2
N
N
Me
3ac
1H NMR (500 MHz, CDCl3)
1.71
2.99
1.77
0.91
2.00
2.79
2.70
f1 (ppm)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120.7569
118.3987
114.3156
108.9805
107.0023
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MeO
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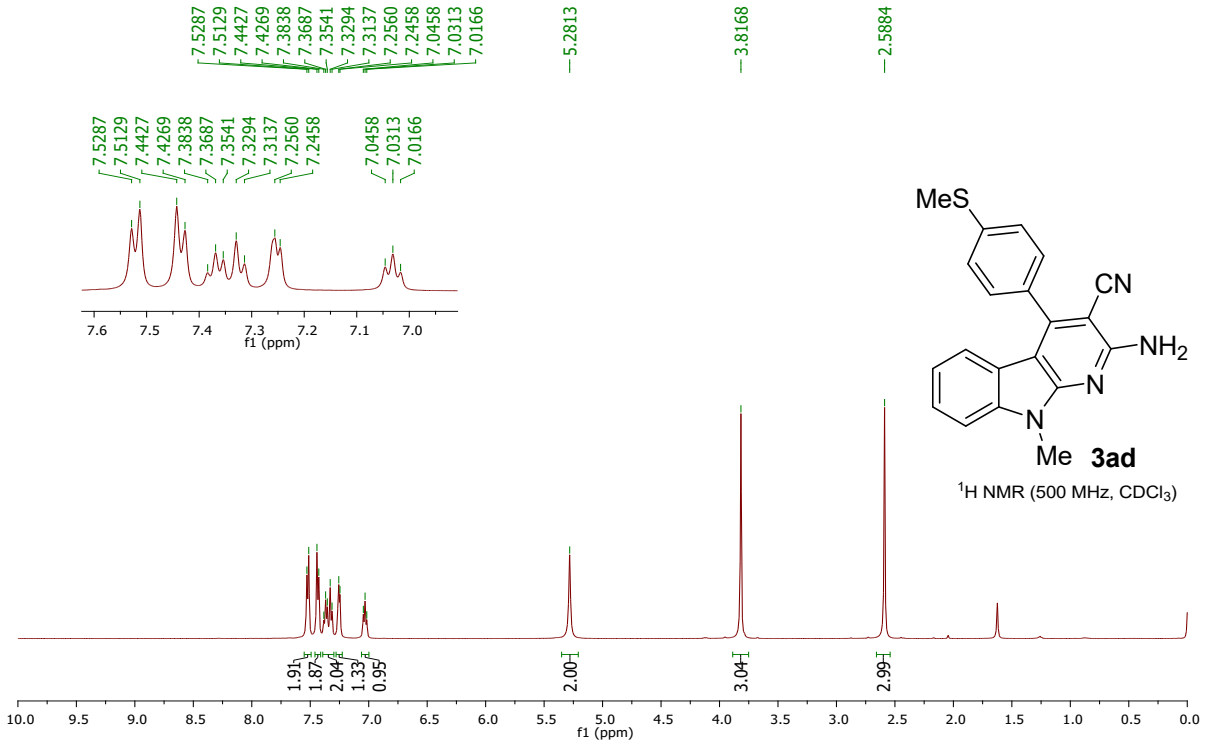
NH2
N
N
Me
3ac
13C NMR (125 MHz, CDCl3)
f1 (ppm)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7.2458
7.0458
7.0313
7.0166
5.2813
3.8168
2.5884
f1 (ppm)
MeS
CN
NH2
N
N
Me
3ad
1H NMR (500 MHz, CDCl3)
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1.33
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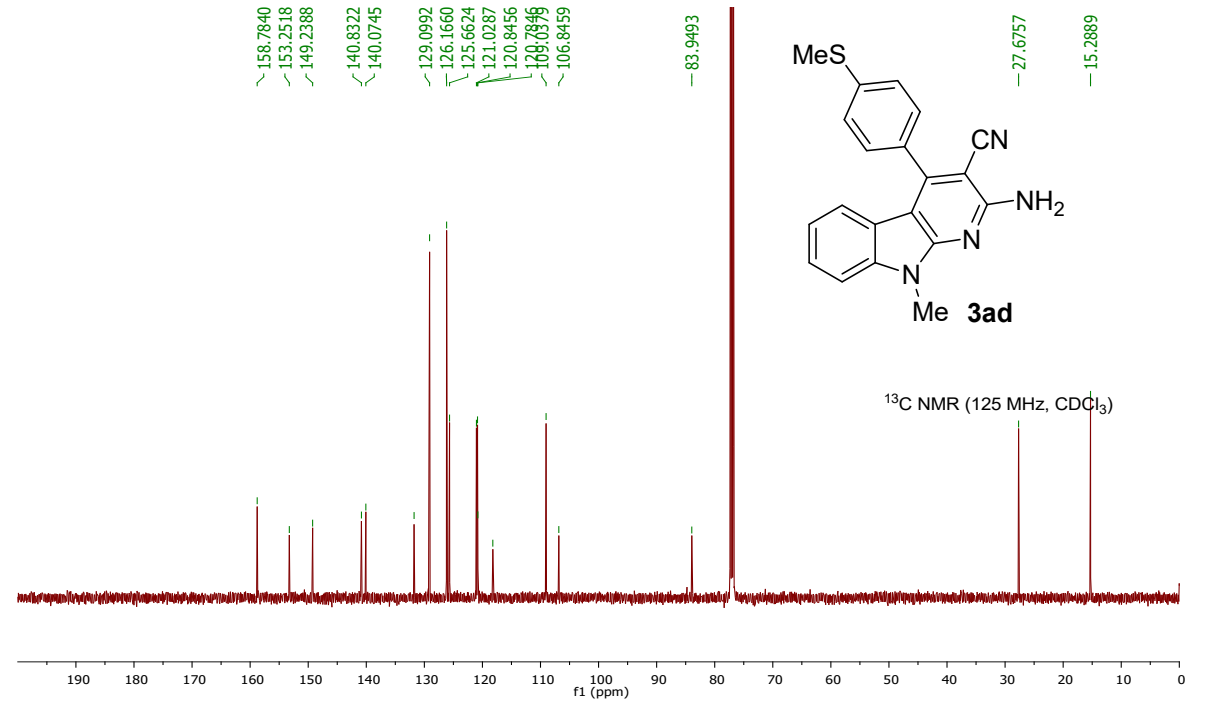
2.99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106.8459
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f1 (ppm)
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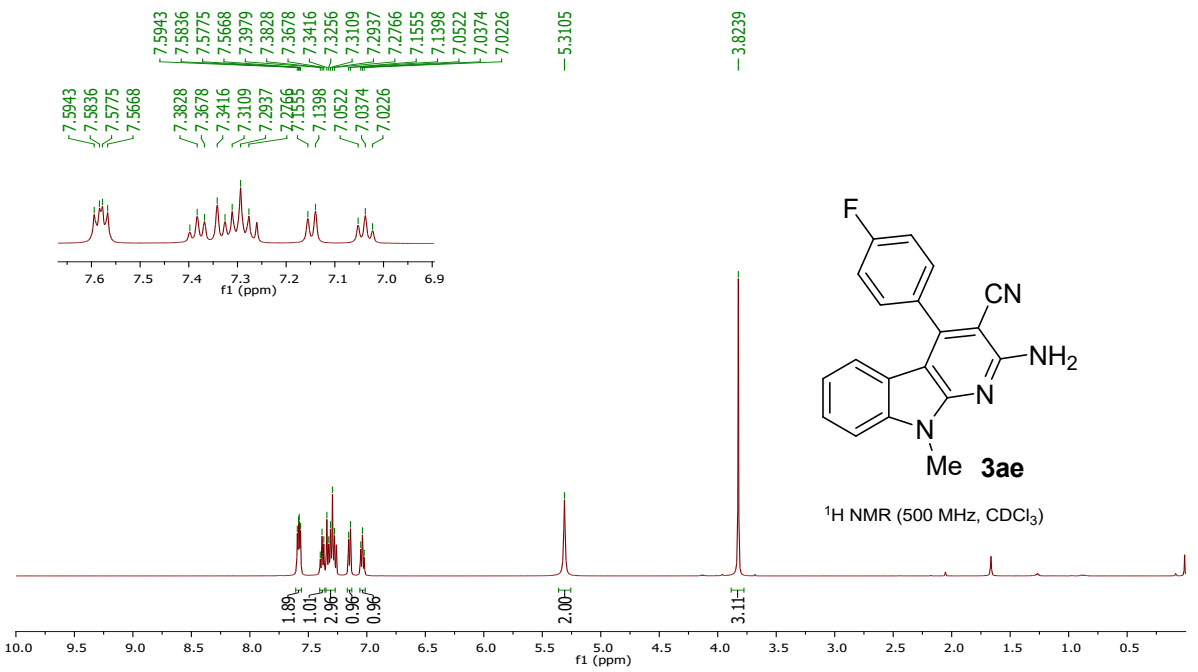
CN
NH2
N
N
Me
3ad
13C NMR (125 MHz, CDCl3)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7.3416
7.3256
7.3109
7.2937
7.2766
7.1555
7.1398
7.0522
7.0374
7.0226
5.3105
3.8239
F
CN
NH2
N
N
Me
3ae
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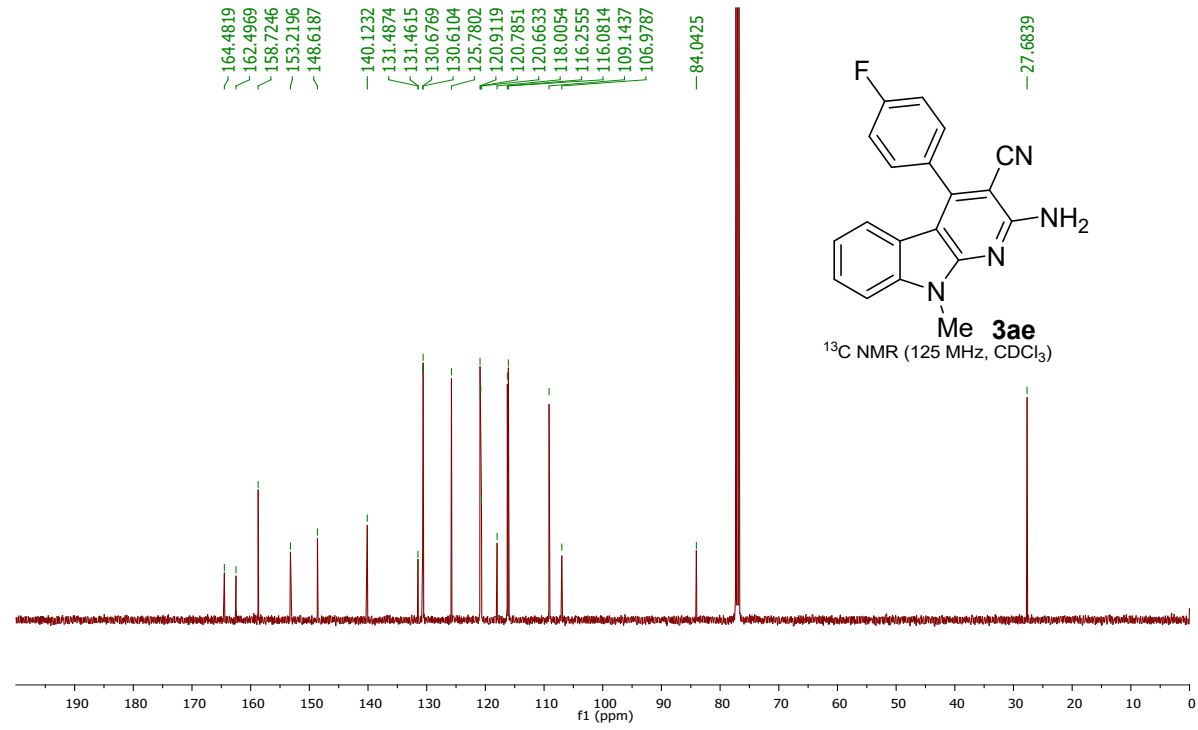
1.01
2.96
0.96
0.96
2.00
3.11
f1 (ppm)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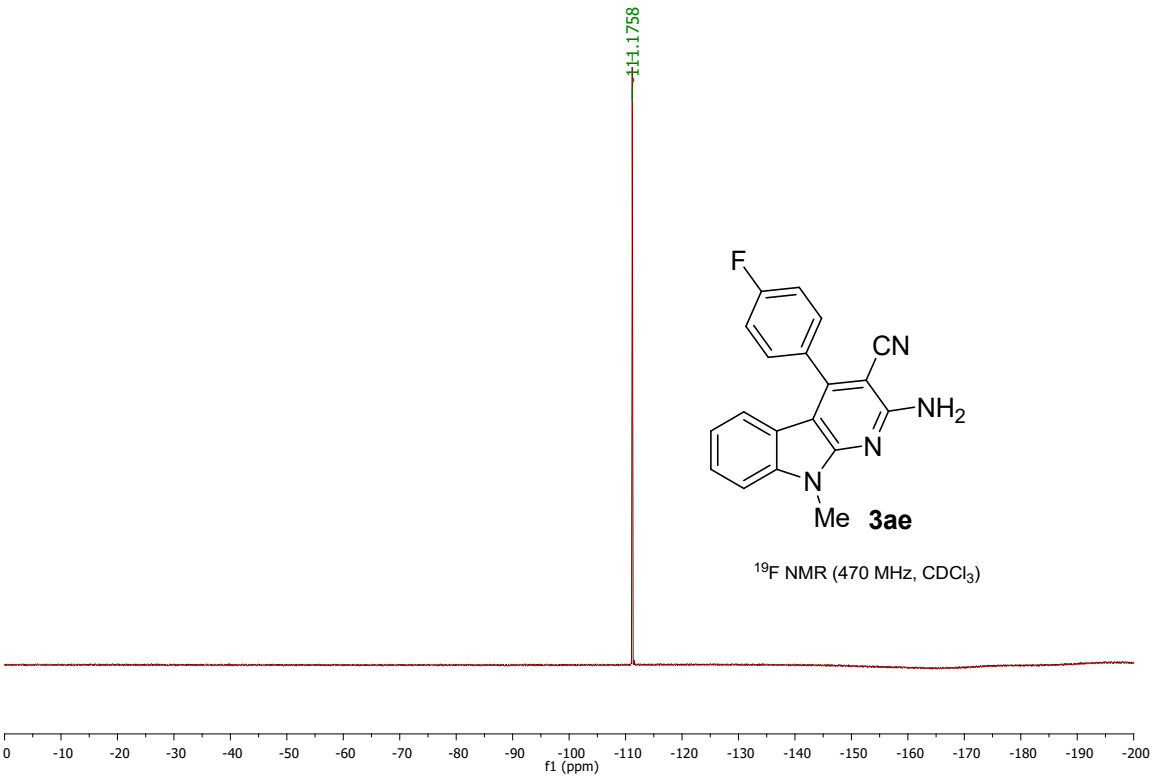
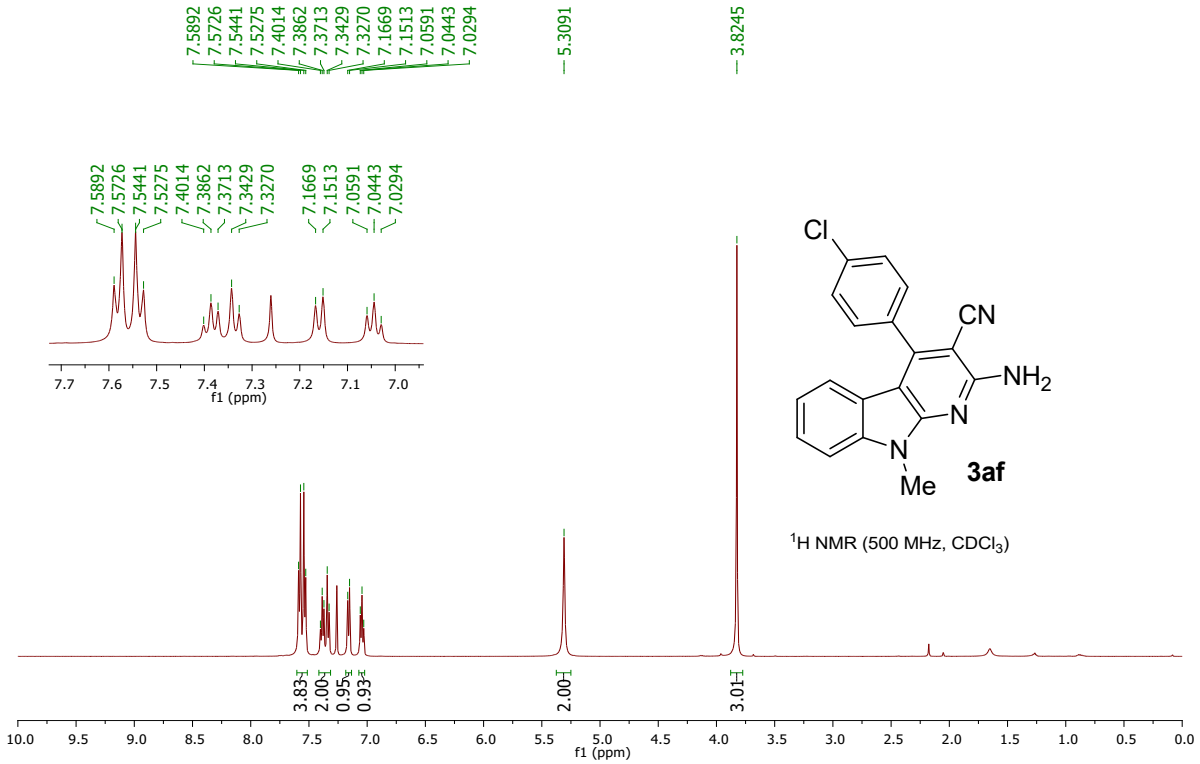
125.7802
120.9119
120.7851
120.6633
118.0054
116.2555
116.0814
109.1437
106.9787
84.0425
27.6839
F
CN
NH2
N
N
Me
3ae
13C NMR (125 MHz, CDCl3)
f1 (ppm)


-111.1758
F
CN
NH2
N
N
Me
3ae
19F NMR (470 MHz, CDCl3)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)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5.3091
3.8245
Cl
CN
NH2
N
N
Me
3af
1H NMR (500 MHz, CDCl3)
3.83
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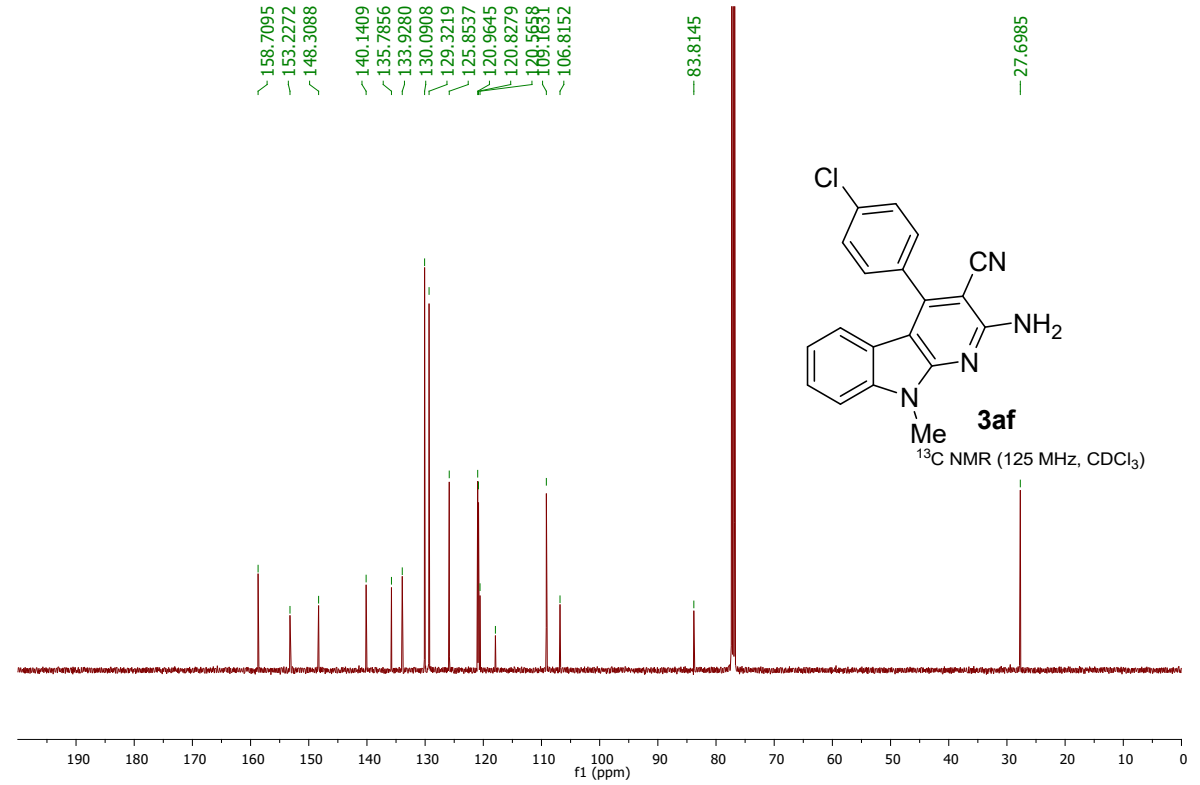
0.95
0.93
2.00
3.01
f1 (ppm)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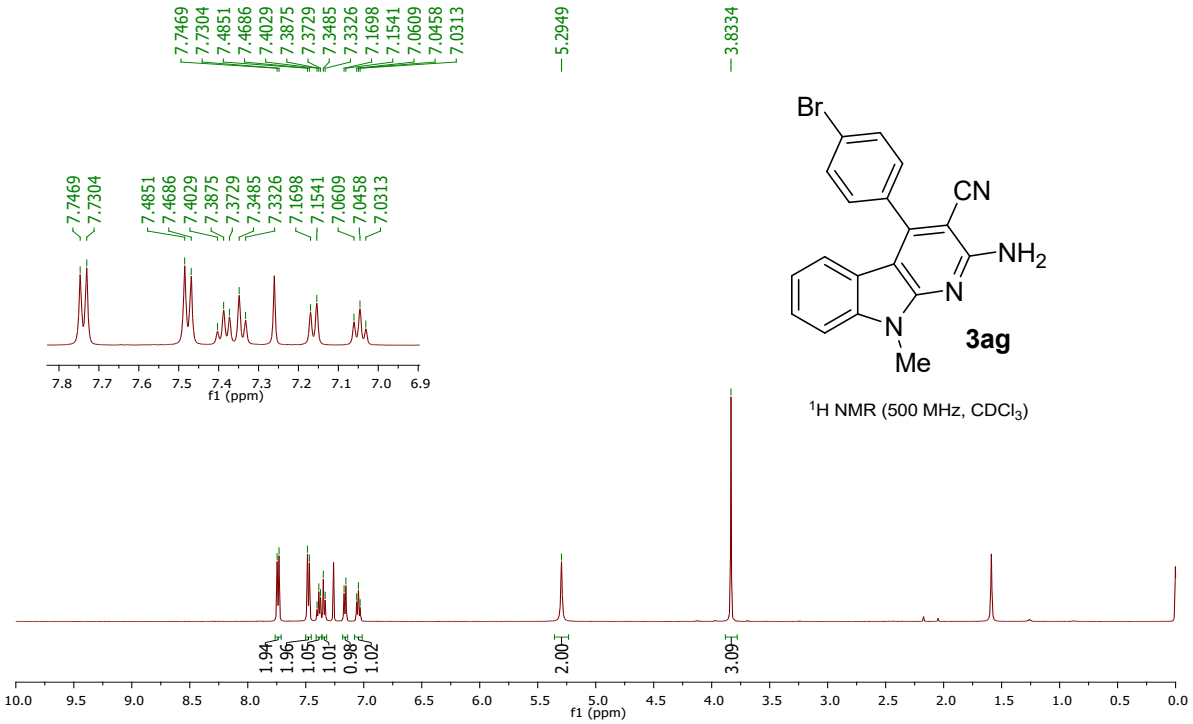
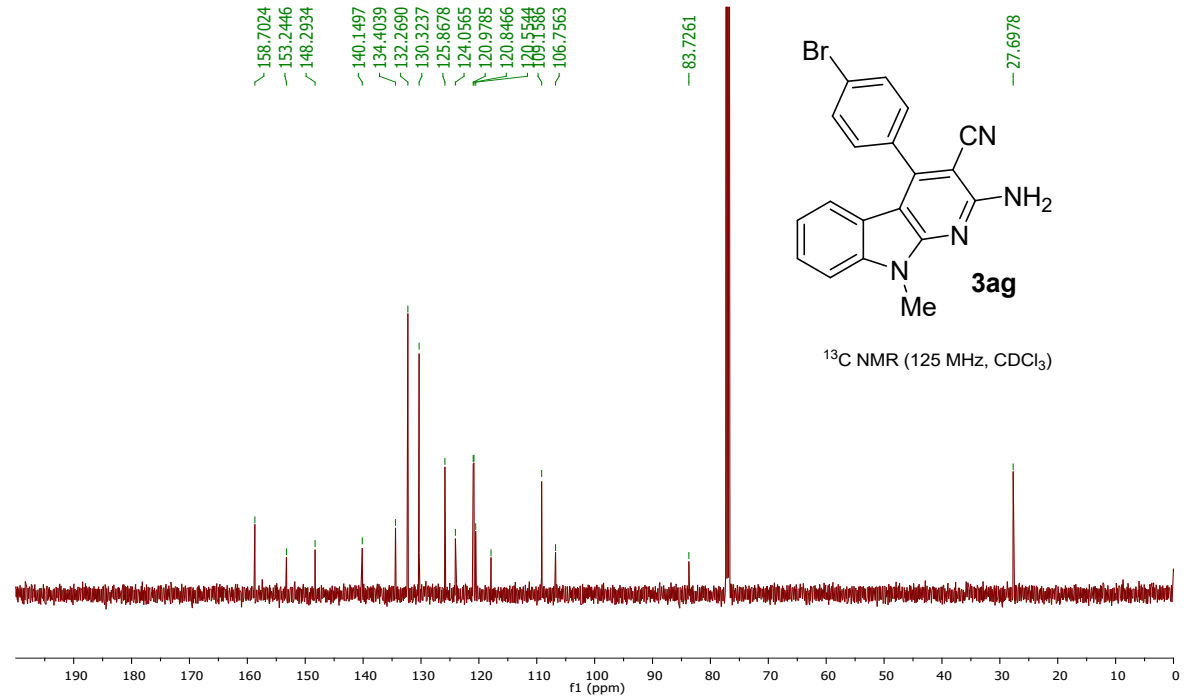
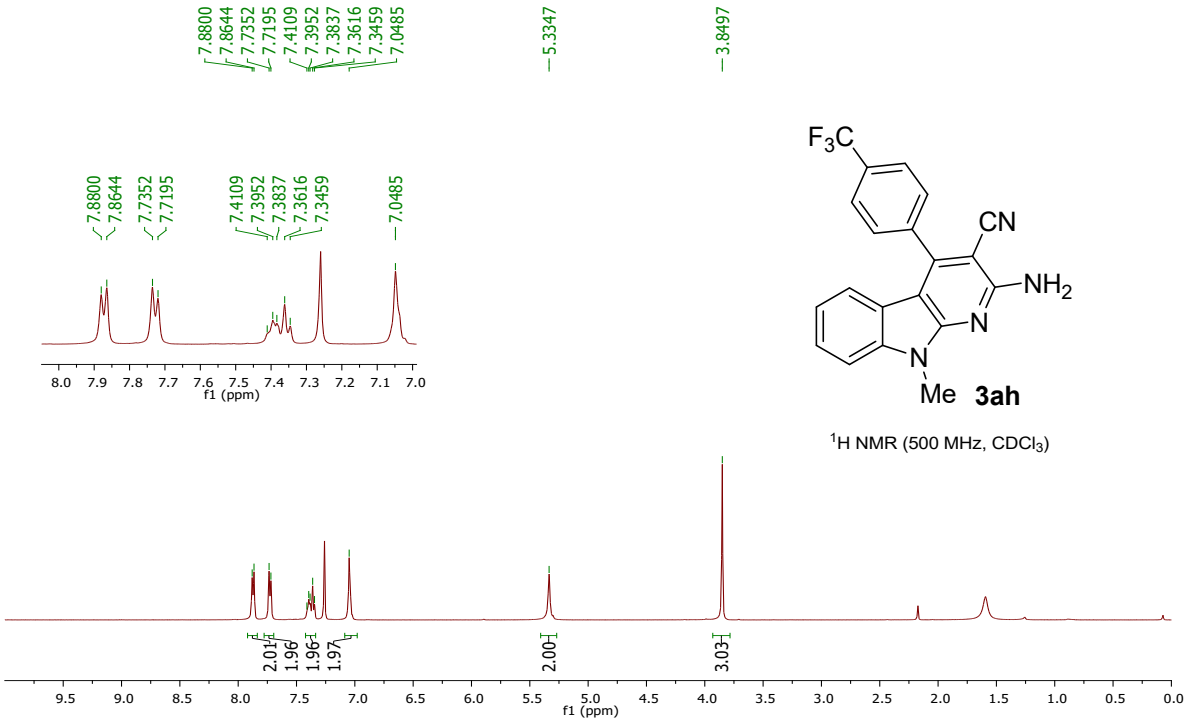
109.1631
106.8152
83.8145
27.6985
Cl
CN
NH2
N
N
Me
3af
13C NMR (125 MHz, CDCl3)
f1 (ppm)

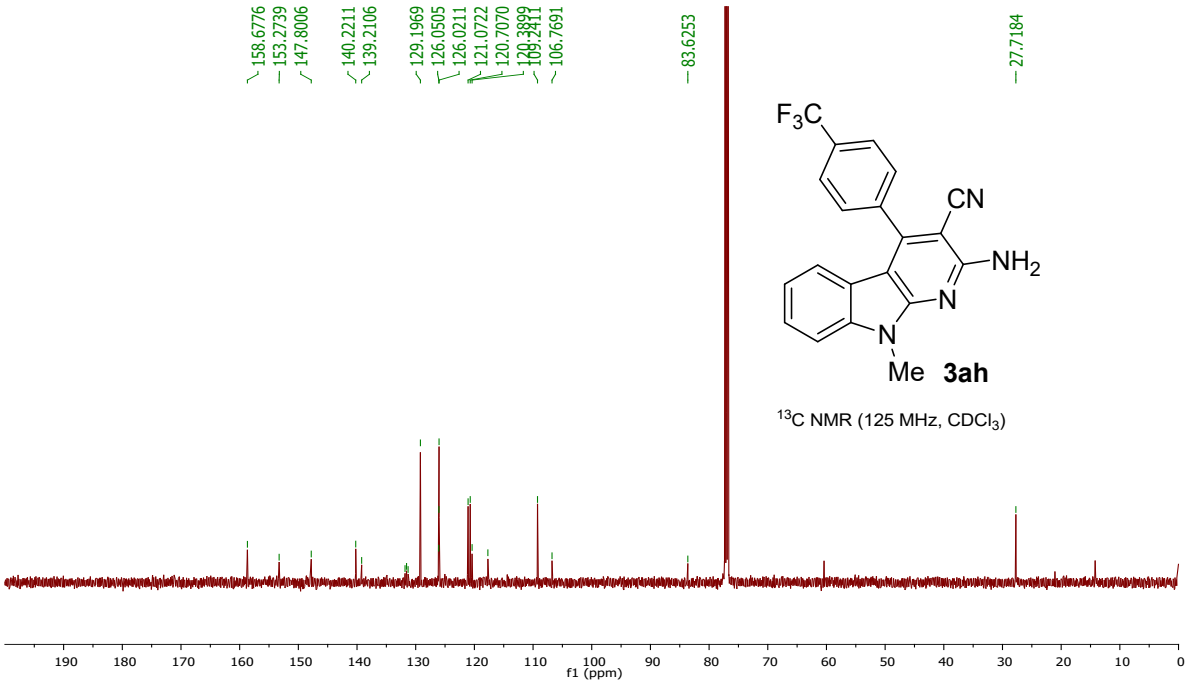


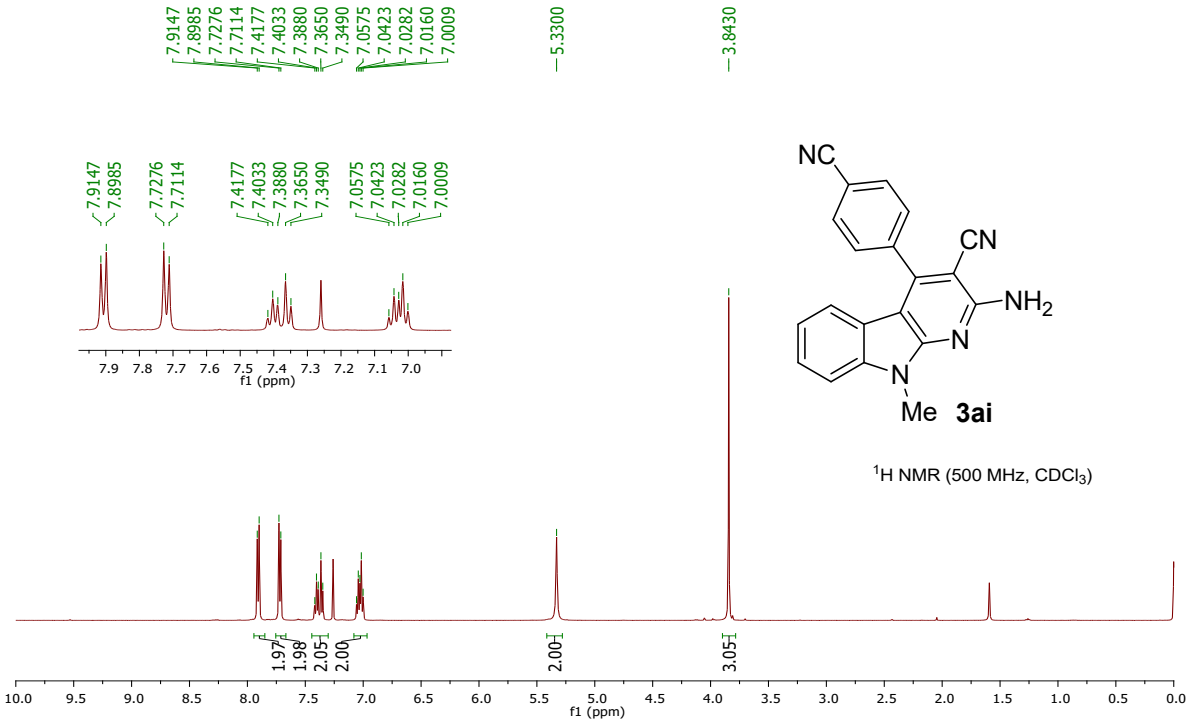
^{1}H NMR (500 MHz, $CDCl_3$)



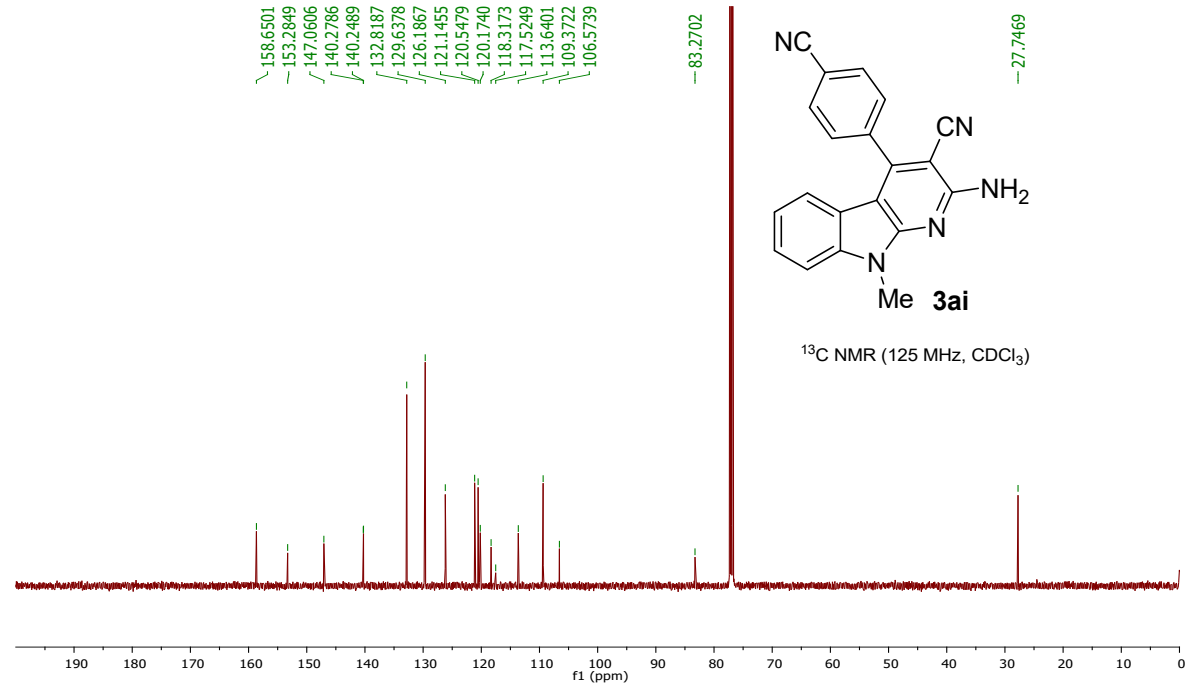
^{13}C NMR (125 MHz, $CDCl_3$)


7.8800
7.8644
7.7352
7.7195
7.4109
7.3952
7.3837
7.3616
7.3459
7.0485
5.3347
3.8497
F3C
CN
NH2
N
N
Me
3ah
1H NMR (500 MHz, CDCl3)
2.01
1.96
1.96
1.97
2.00
3.03
f1 (ppm)

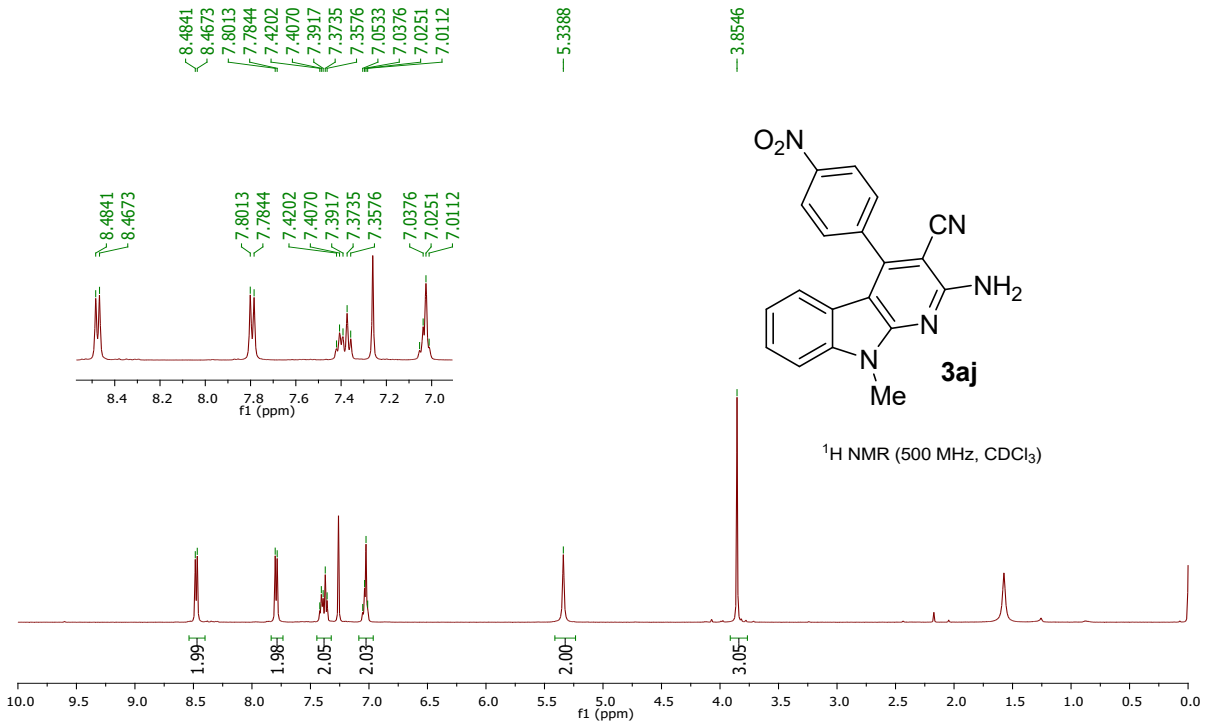

158.6776
153.2739
147.8006
140.2211
139.2106
129.1969
126.0505
126.0211
121.0722
120.7070
109.2411
106.7691
83.6253
27.7184
F3C
CN
NH2
N
N
Me
3ah
13C NMR (125 MHz, CDCl3)
f1 (ppm)



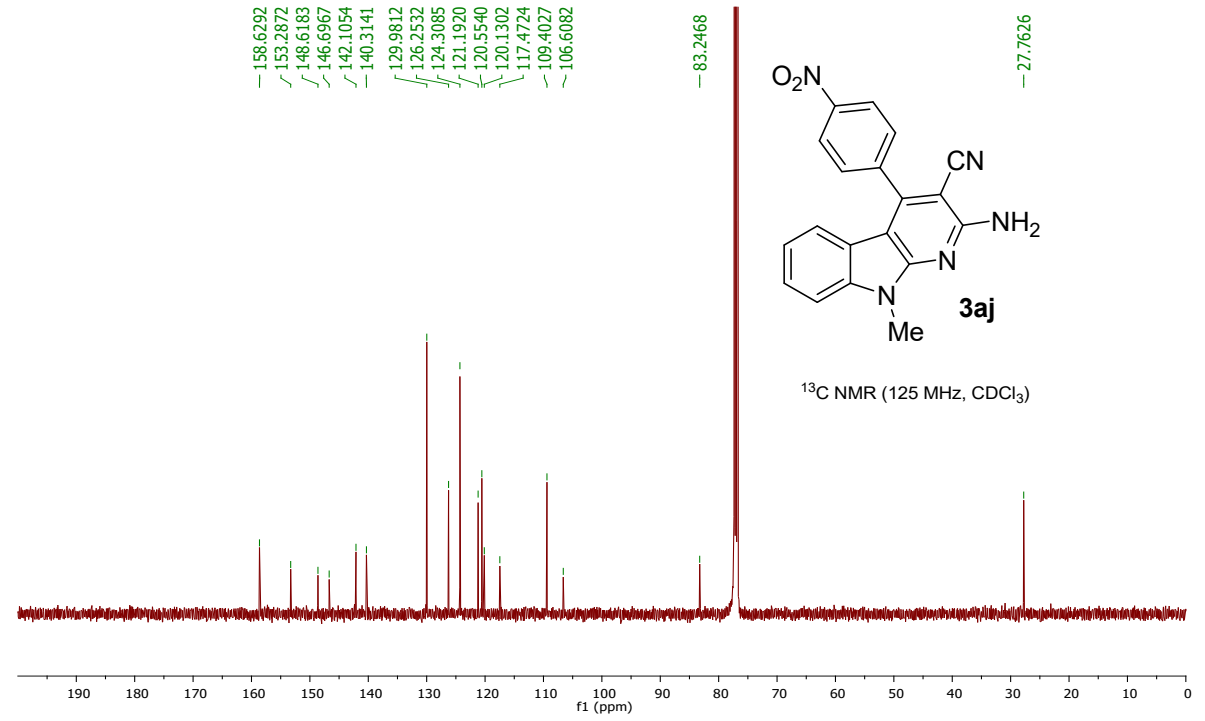
^{1}H NMR (500 MHz, $CDCl_3$)



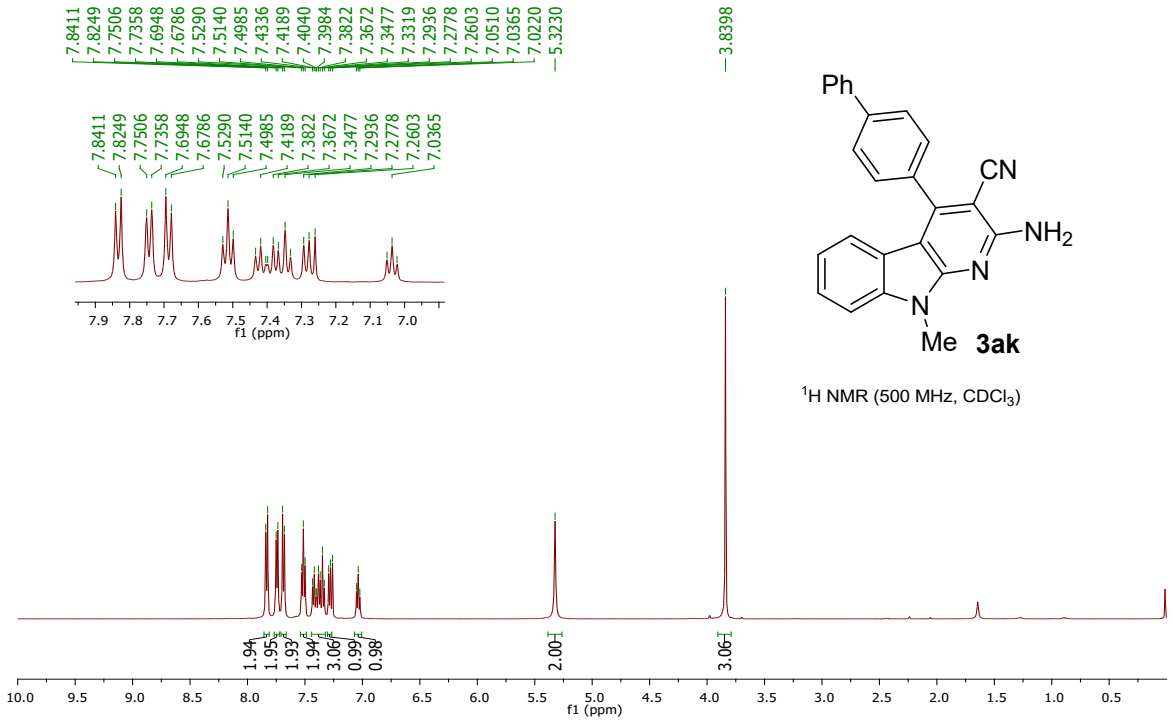
^{13}C NMR (125 MHz, $CDCl_3$)

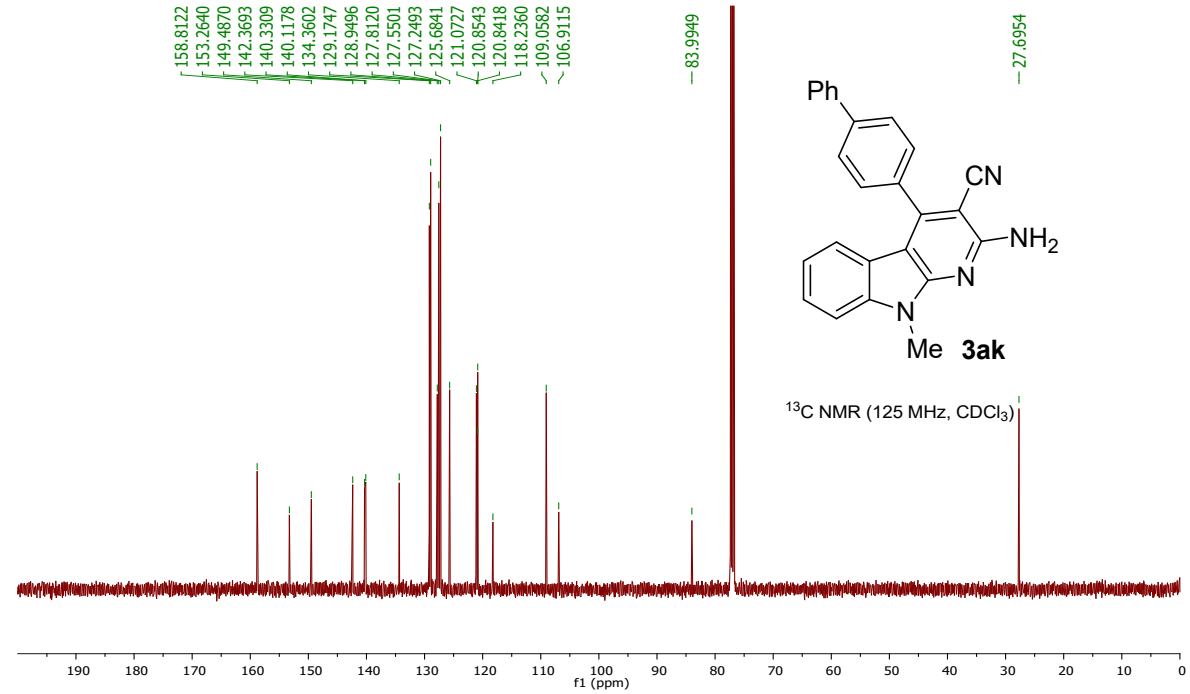


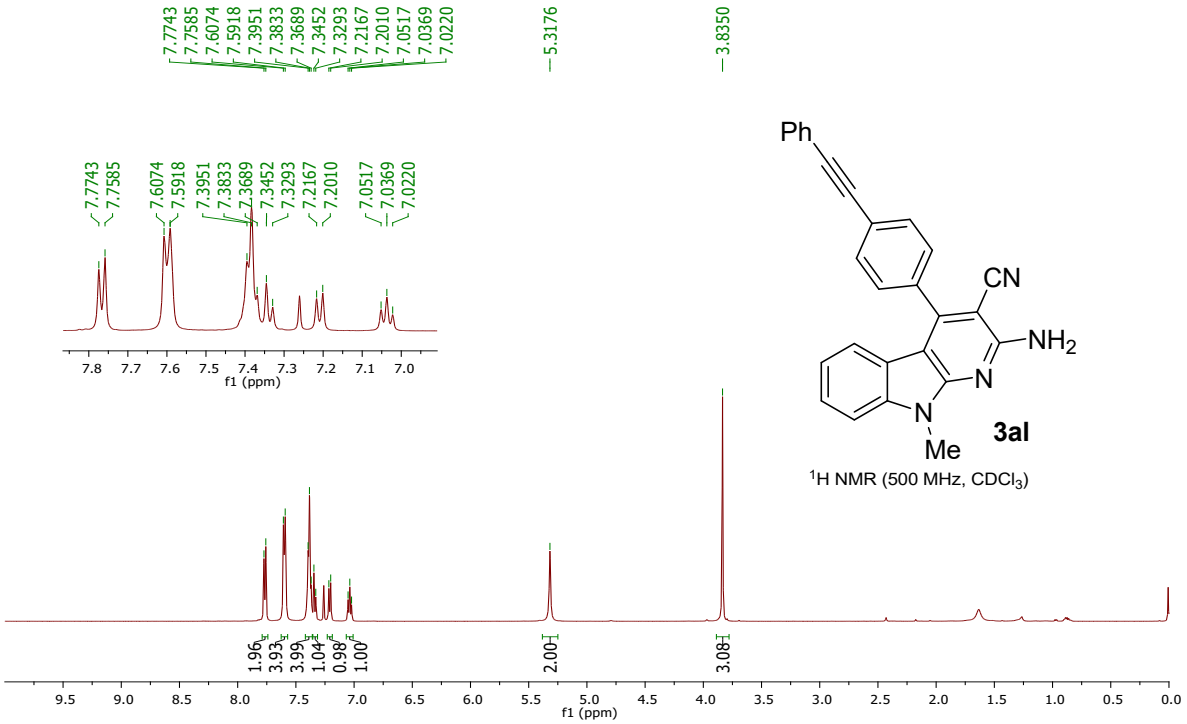
^{1}H NMR (500 MHz, $CDCl_3$)

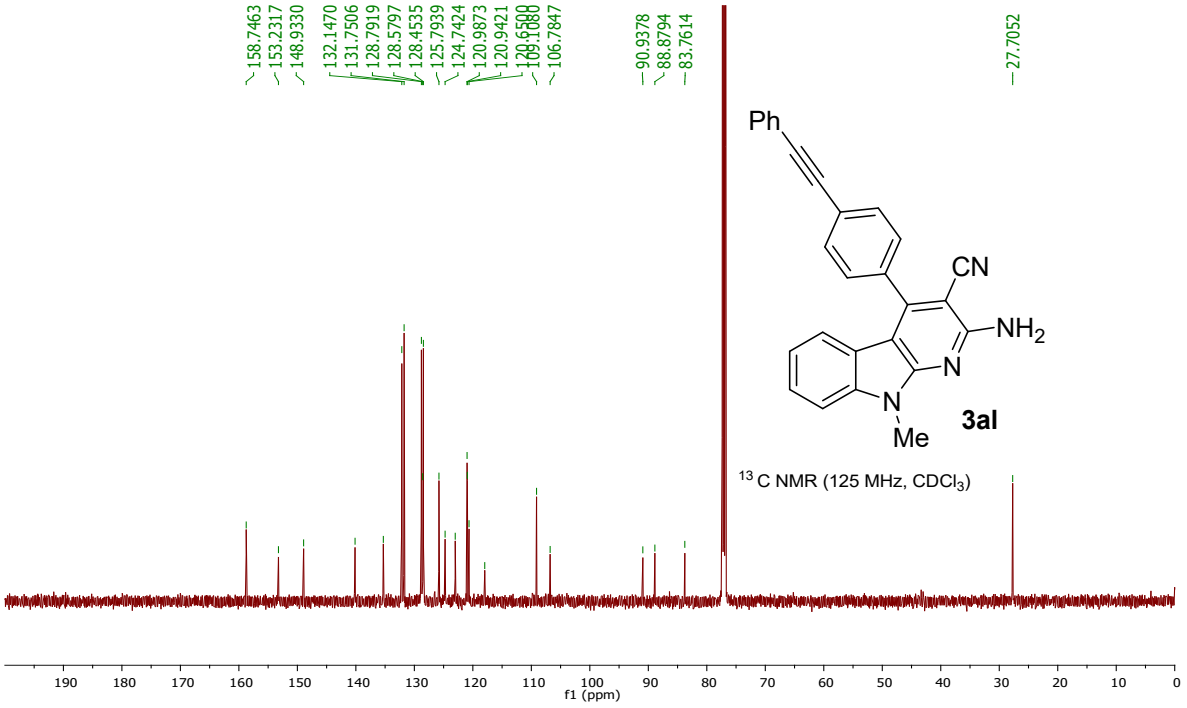


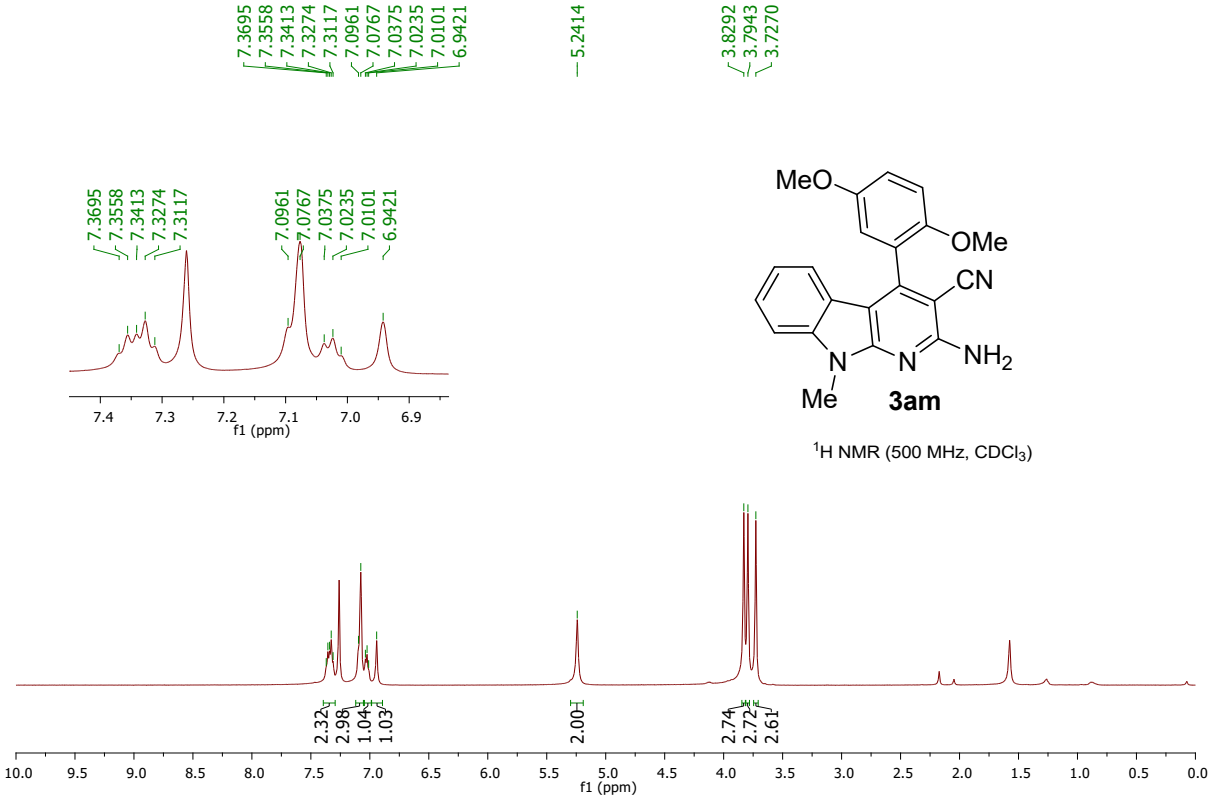
^{13}C NMR (125 MHz, $CDCl_3$)


7.8411
7.8249
7.7506
7.7358
7.6948
7.6786
7.5290
7.5140
7.4985
7.4336
7.4189
7.4040
7.3984
7.3822
7.3672
7.3477
7.3319
7.2936
7.2778
7.2603
7.0510
7.0365
7.0220
5.3230
3.8398
f1 (ppm)
Ph
CN
NH2
N
N
Me
3ak
1H NMR (500 MHz, CDCl3)
1.94
1.95
1.93
1.94
3.06
0.99
0.98
2.00
3.06

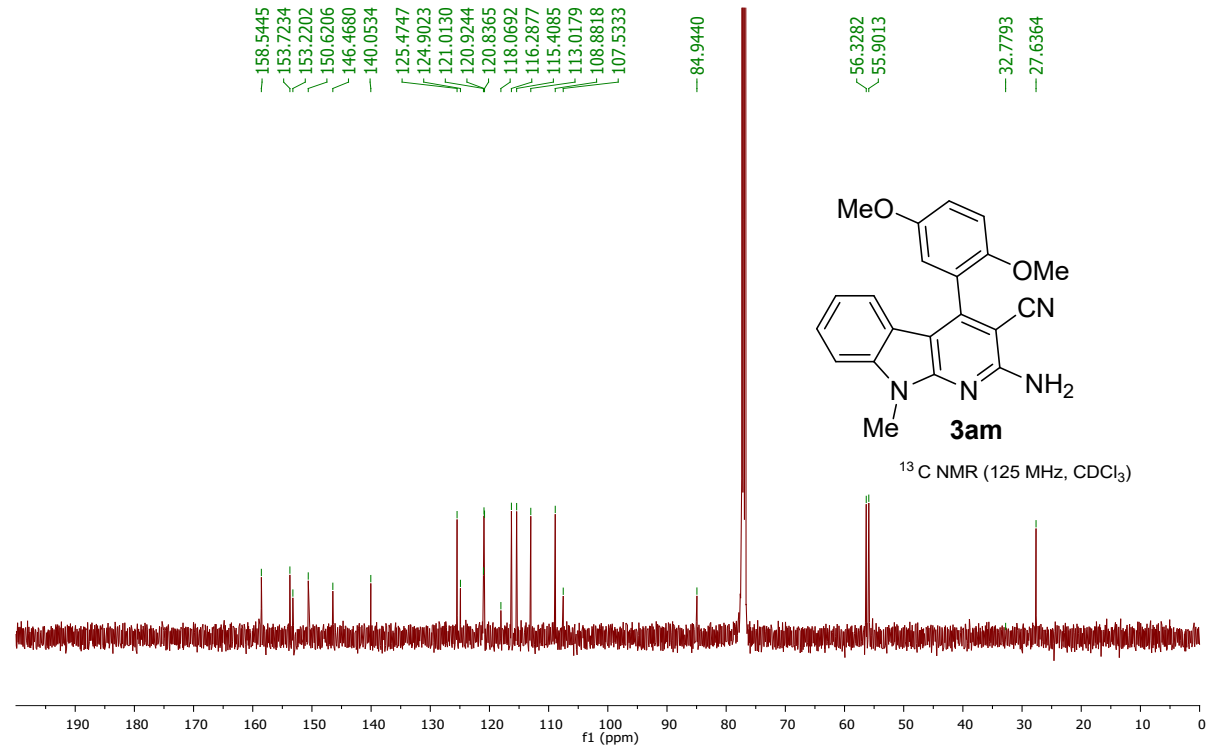

158.8122
153.2640
149.4870
142.3693
140.3309
140.1178
134.3602
129.1747
128.9496
127.8120
127.5501
127.2493
125.6841
121.0727
120.8543
120.8418
118.2360
109.0582
106.9115
83.9949
27.6954
f1 (ppm)
Ph
CN
NH2
N
N
Me
3ak
13C NMR (125 MHz, CDCl3)


7.7743
7.7585
7.6074
7.5918
7.3951
7.3833
7.3689
7.3452
7.3293
7.2167
7.2010
7.0517
7.0369
7.0220
5.3176
3.8350
Ph
CN
NH2
N
N
Me
3al
1H NMR (500 MHz, CDCl3)
1.96
3.93
3.99
1.04
0.98
1.00
2.00
3.08
f1 (ppm)

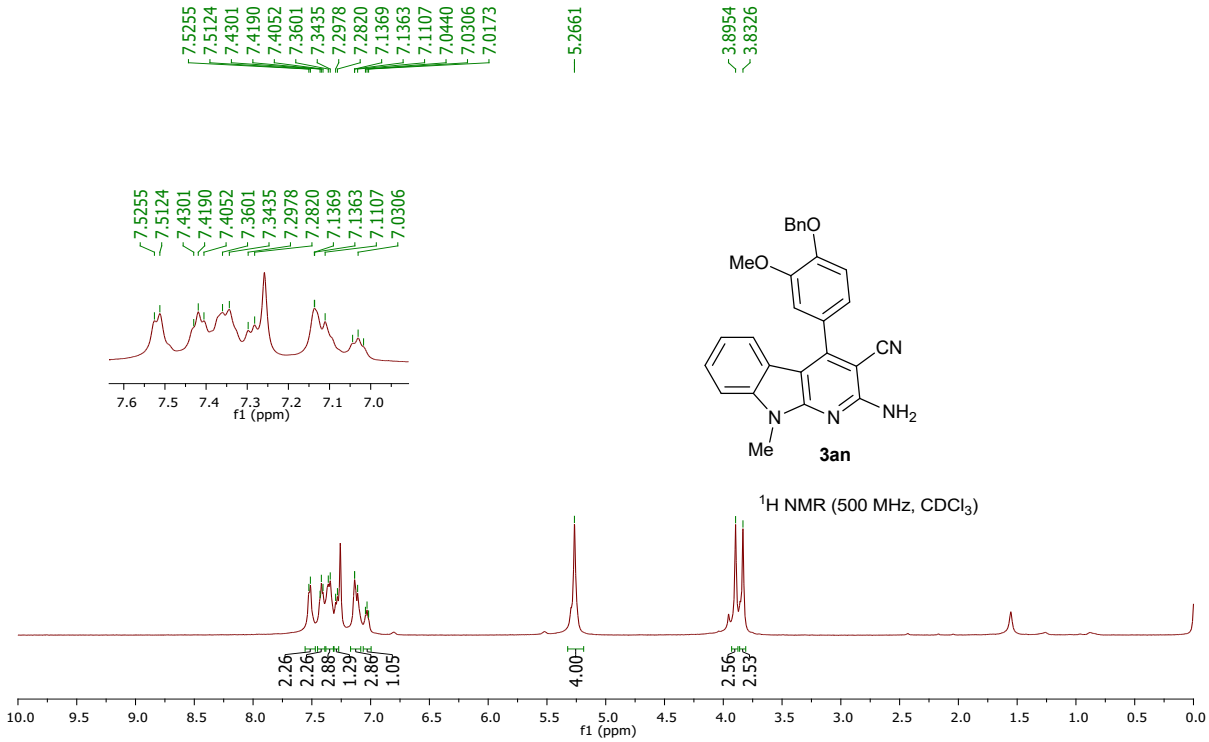

158.7463
153.2317
148.9330
132.1470
131.7506
128.7919
128.5797
128.4535
125.7939
124.7424
120.9873
120.9421
109.1080
106.7847
90.9378
88.8794
83.7614
27.7052
Ph
CN
NH2
N
N
Me
3al
13C NMR (125 MHz, CDCl3)
f1 (ppm)

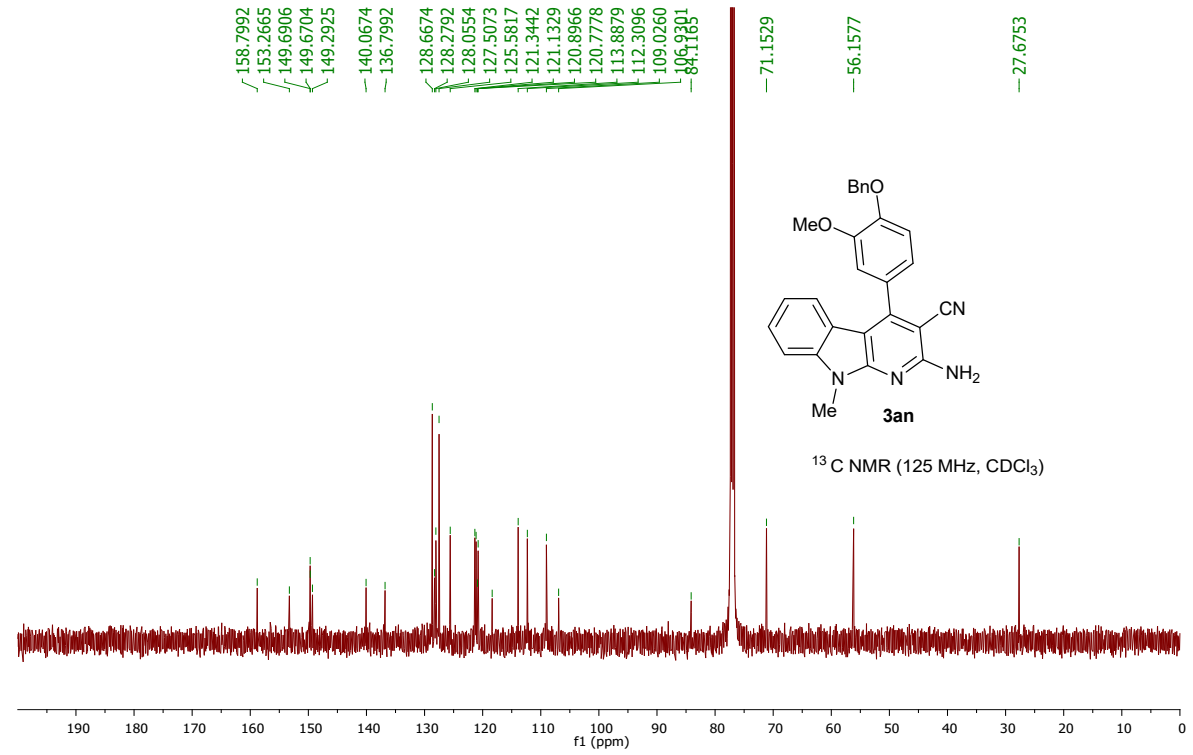


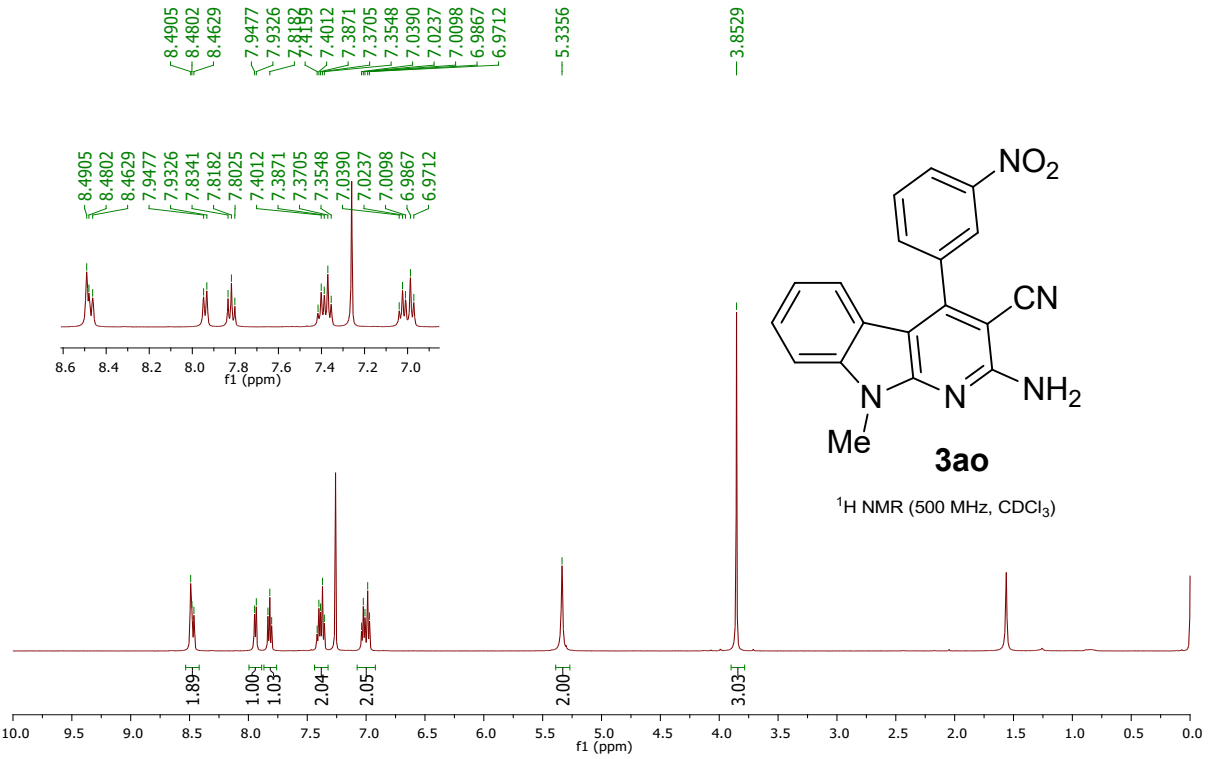
^{1}H NMR (500 MHz, $CDCl_3$)

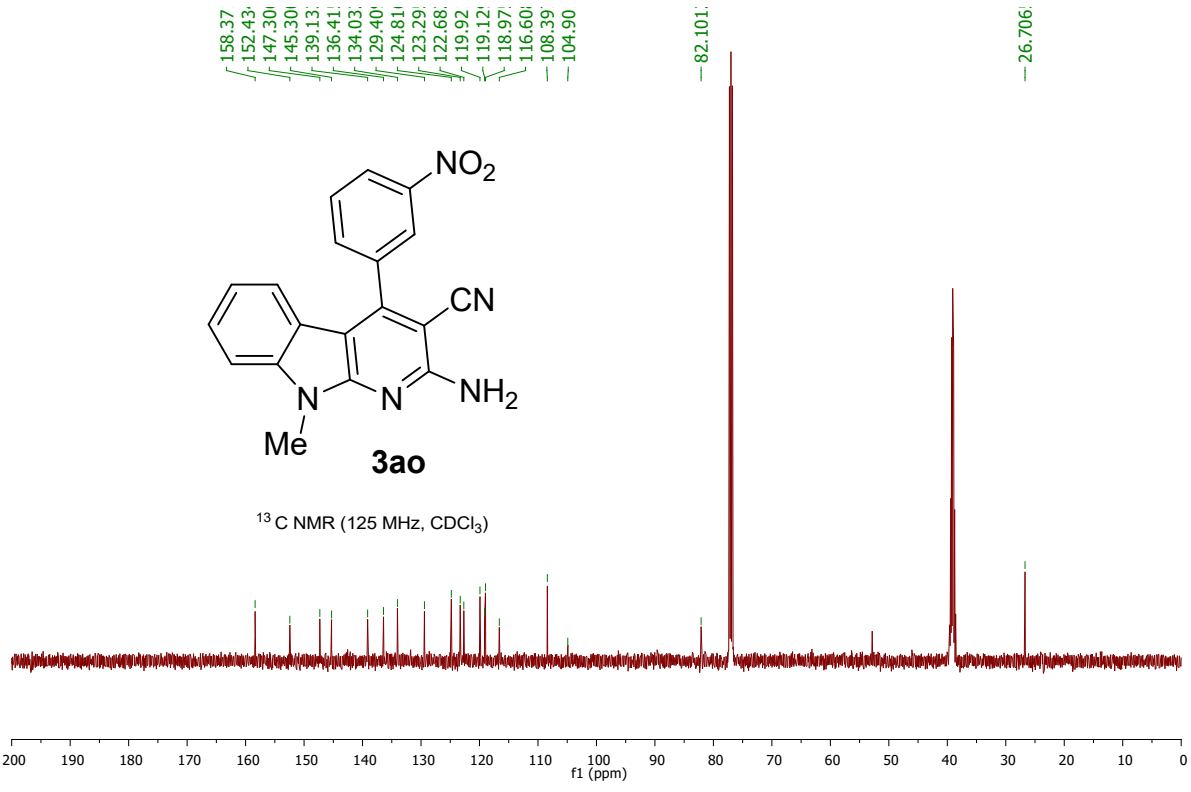


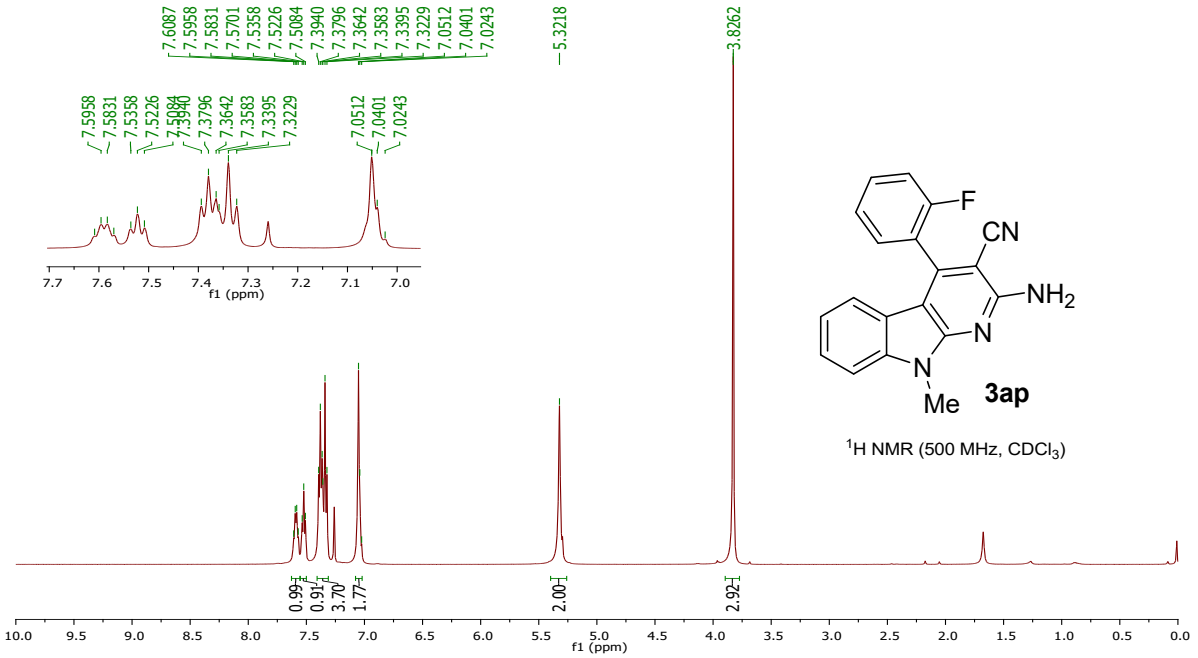
^{13}C NMR (125 MHz, $CDCl_3$)


7.5255
7.5124
7.4301
7.4190
7.4052
7.3601
7.3435
7.2978
7.2820
7.1369
7.1363
7.1107
7.0440
7.0306
7.0173
5.2661
3.8954
3.8326
BnO
MeO
CN
NH2
N
N
Me
3an
1H NMR (500 MHz, CDCl3)
2.26
2.26
2.88
1.29
2.86
1.05
4.00
2.56
2.53
f1 (ppm)


158.7992
153.2665
149.6906
149.6704
149.2925
140.0674
136.7992
128.6674
128.2792
128.0554
127.5073
125.5817
121.3442
121.1329
120.8966
120.7778
113.8879
112.3096
109.0260
106.9301
84.1165
71.1529
56.1577
27.6753
BnO
MeO
CN
NH2
N
N
Me
3an
13C NMR (125 MHz, CDCl3)
f1 (ppm)

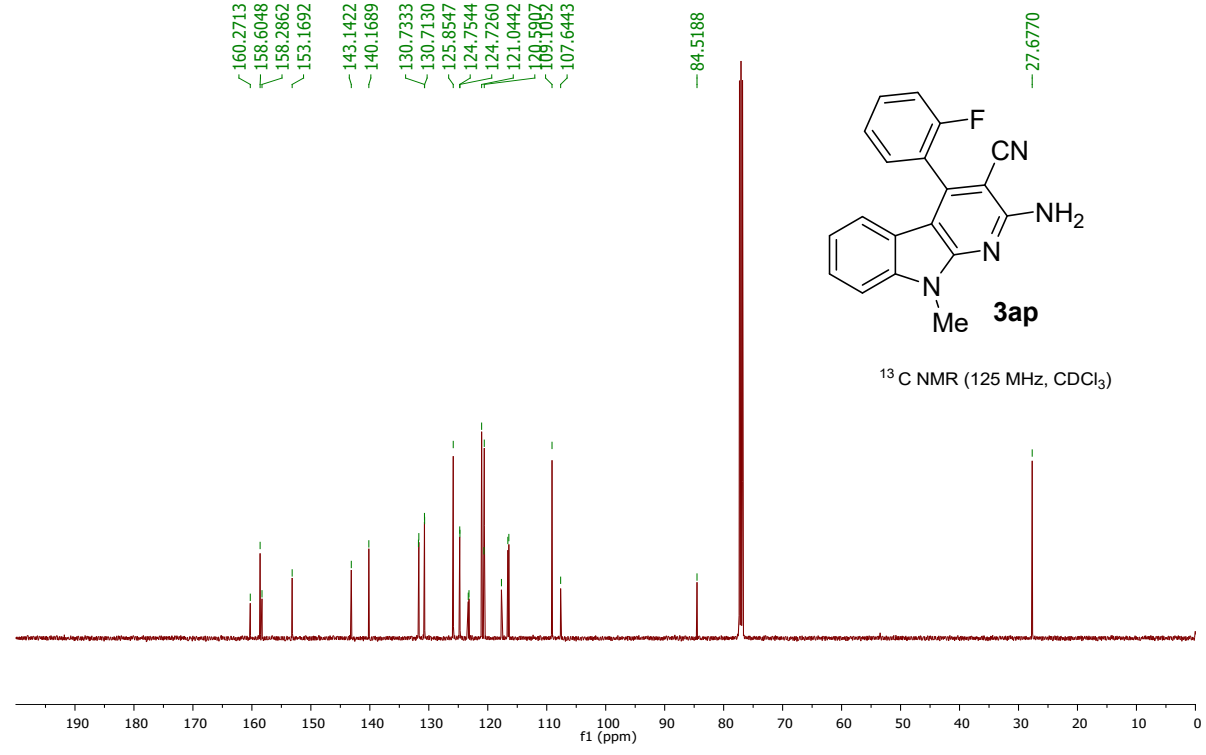

8.4905
8.4802
8.4629
7.9477
7.9326
7.8341
7.8182
7.8025
7.4012
7.3871
7.3705
7.3548
7.0390
7.0237
7.0098
6.9867
6.9712
5.3356
3.8529
f1 (ppm)
NO2
CN
NH2
N
N
Me
3ao
1H NMR (500 MHz, CDCl3)
1.89
1.00
1.03
2.04
2.05
2.00
3.03
f1 (ppm)


158.37
152.43
147.30
145.30
139.13
136.41
134.03
129.40
124.81
123.29
122.68
119.92
119.12
118.97
116.60
108.39
104.90
82.101
26.706
NO2
CN
NH2
N
N
Me
3ao
13C NMR (125 MHz, CDCl3)
f1 (ppm)



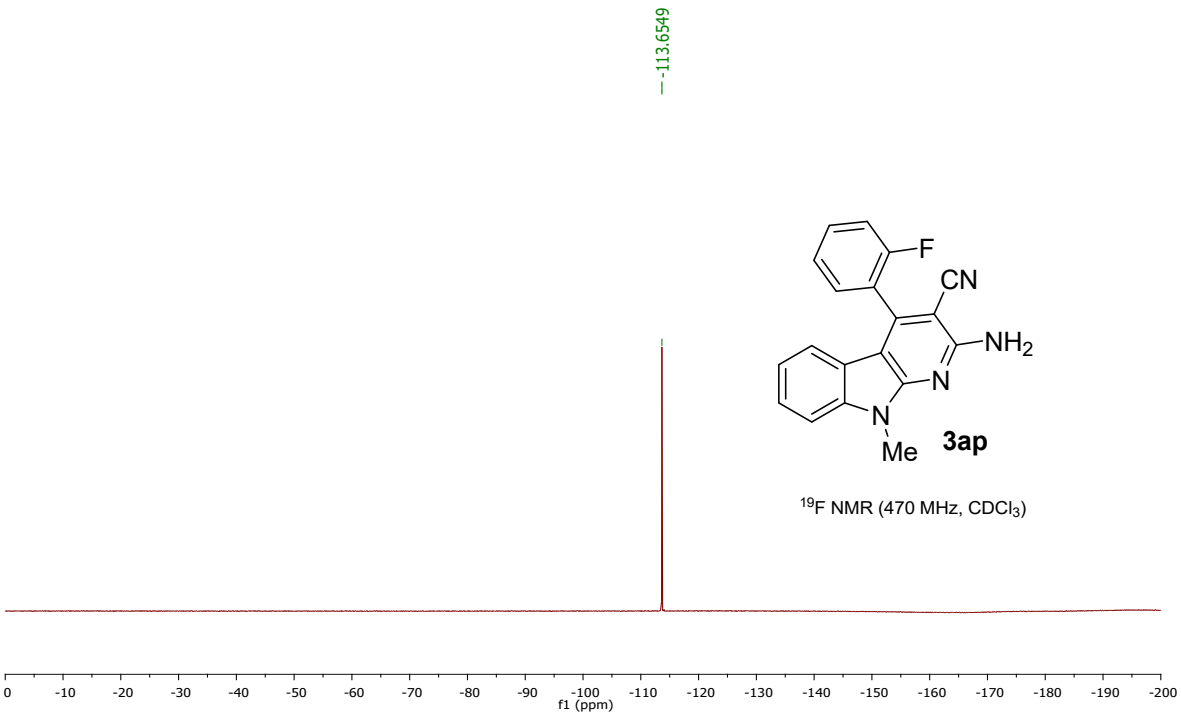
3ap

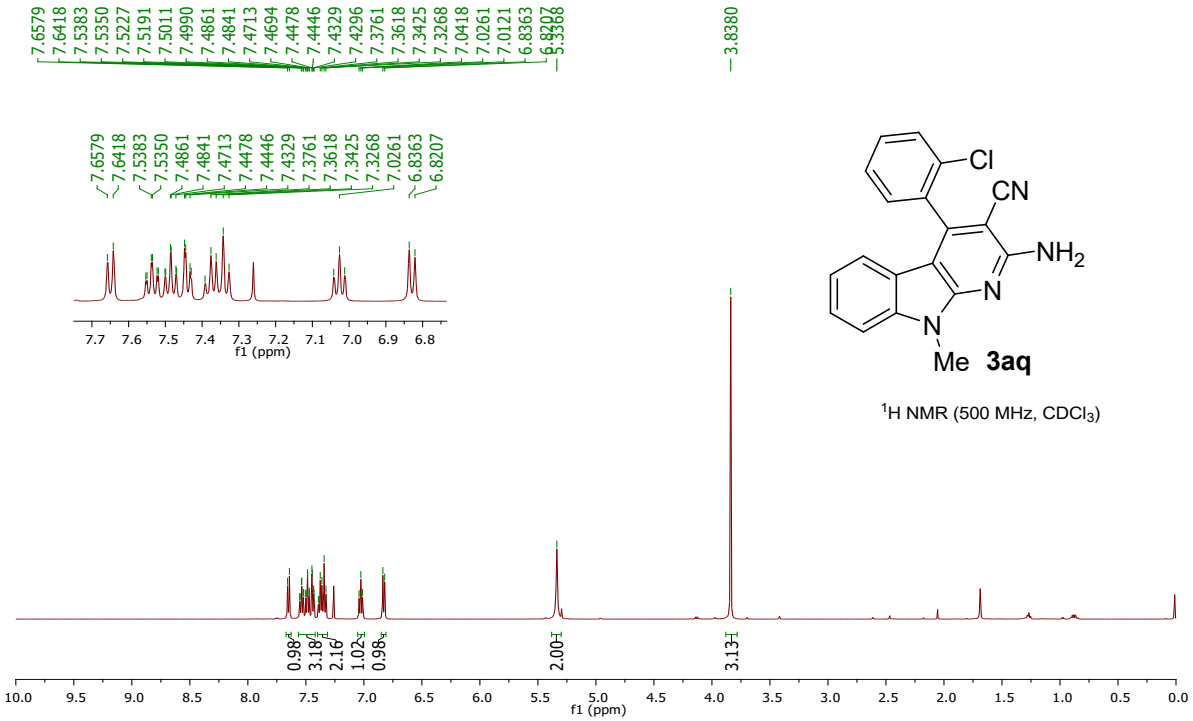
^{1}H NMR (500 MHz, $CDCl_3$)



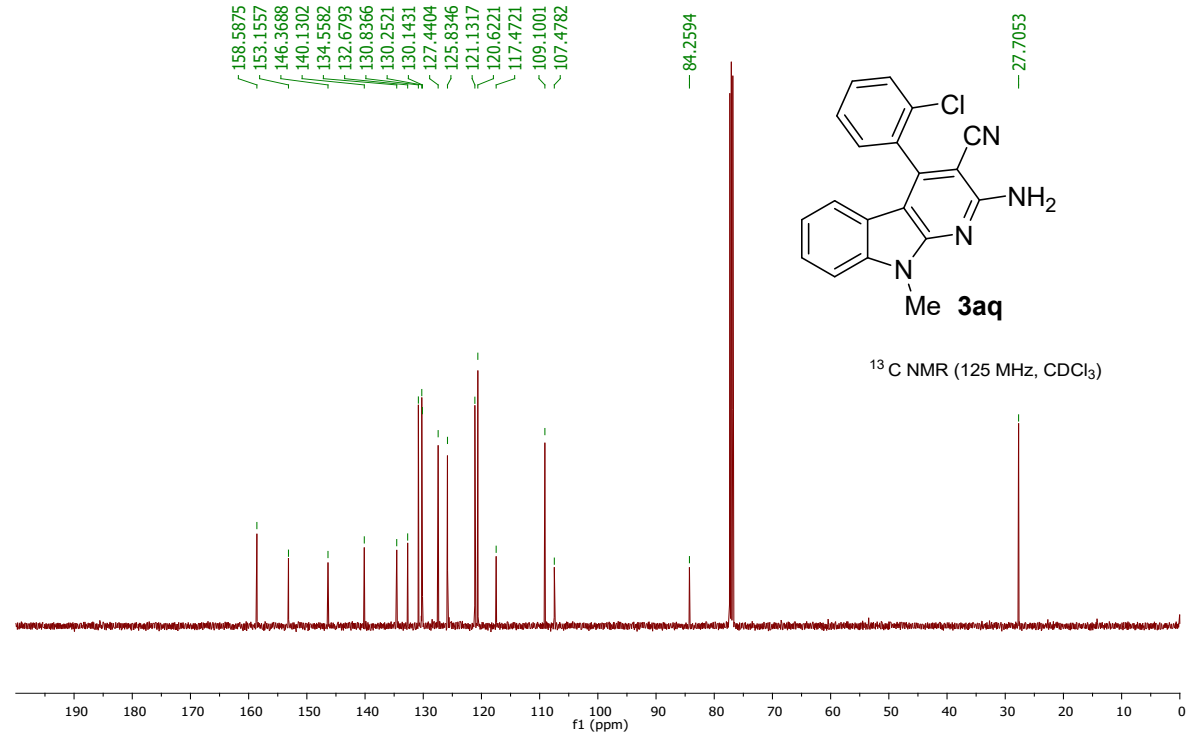
3ap

^{13}C NMR (125 MHz, $CDCl_3$)

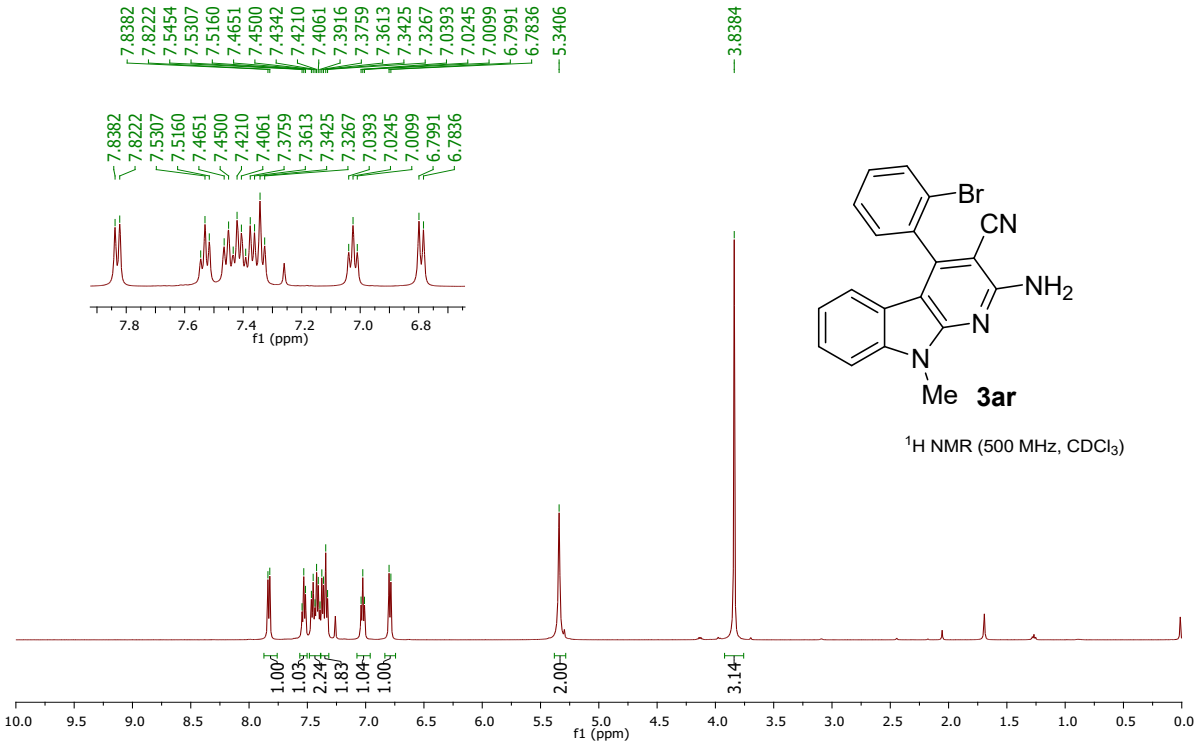

-113.6549
F
CN
NH2
N
N
Me
3ap
19F NMR (470 MHz, CDCl3)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

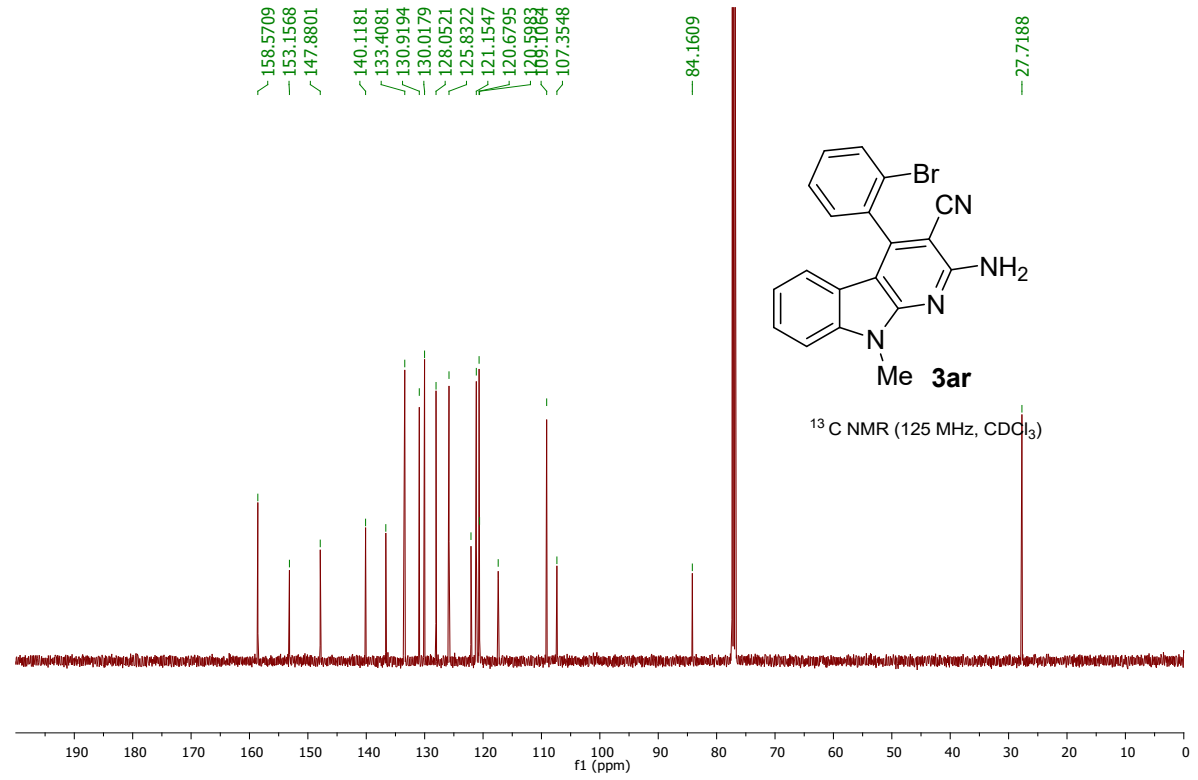


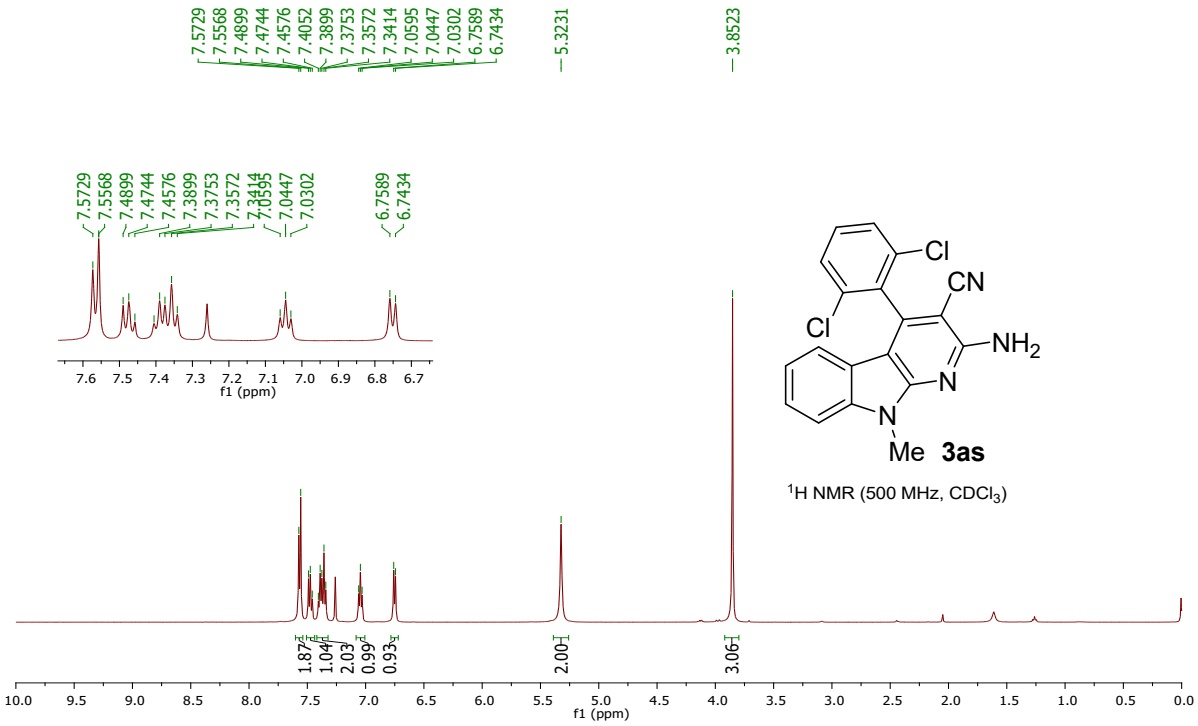
^{1}H NMR (500 MHz, $CDCl_3$)

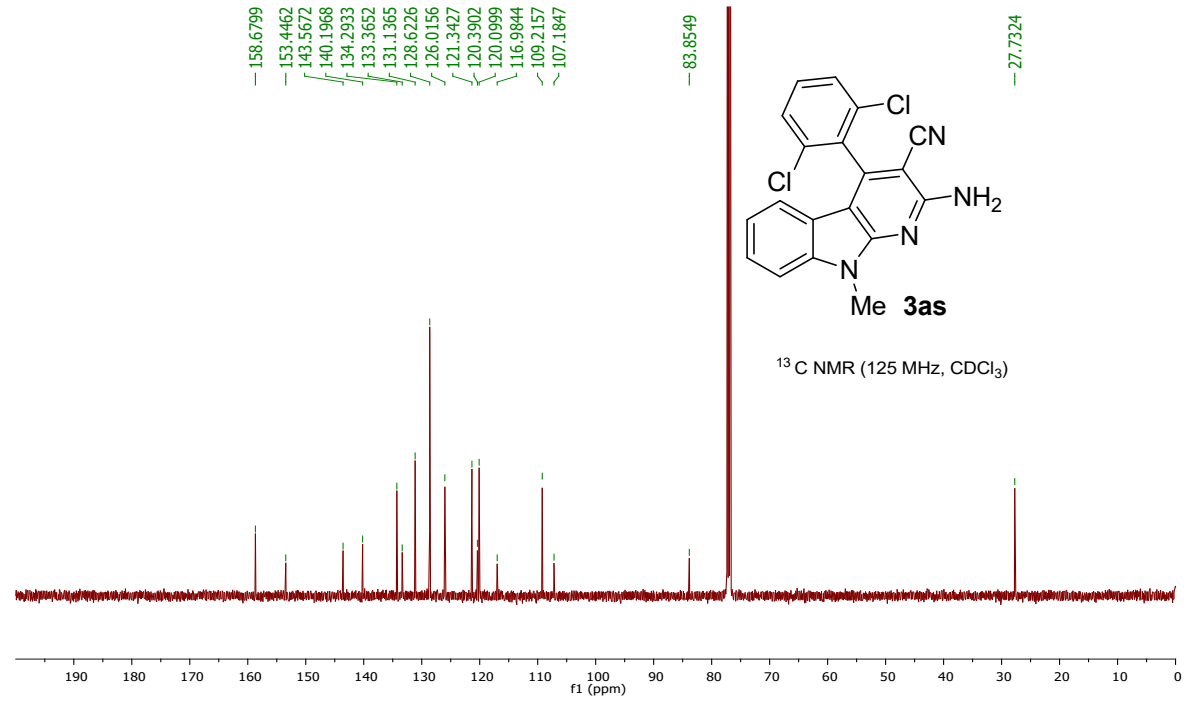


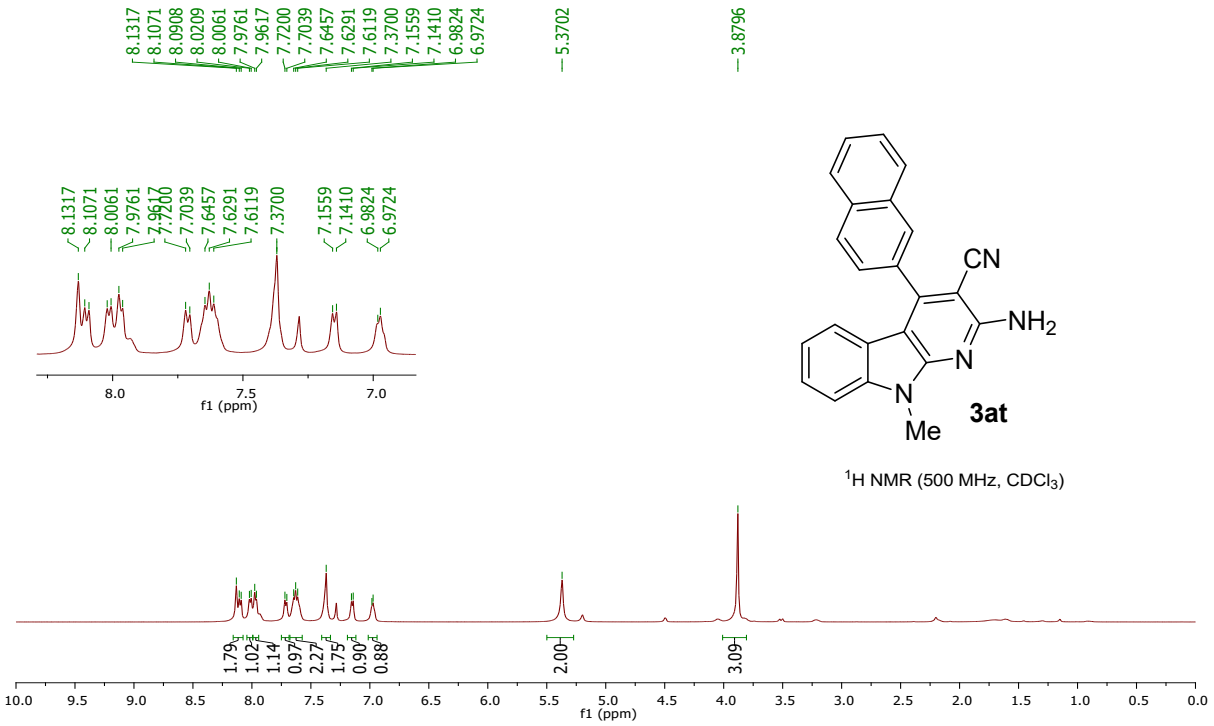
^{13}C NMR (125 MHz, $CDCl_3$)

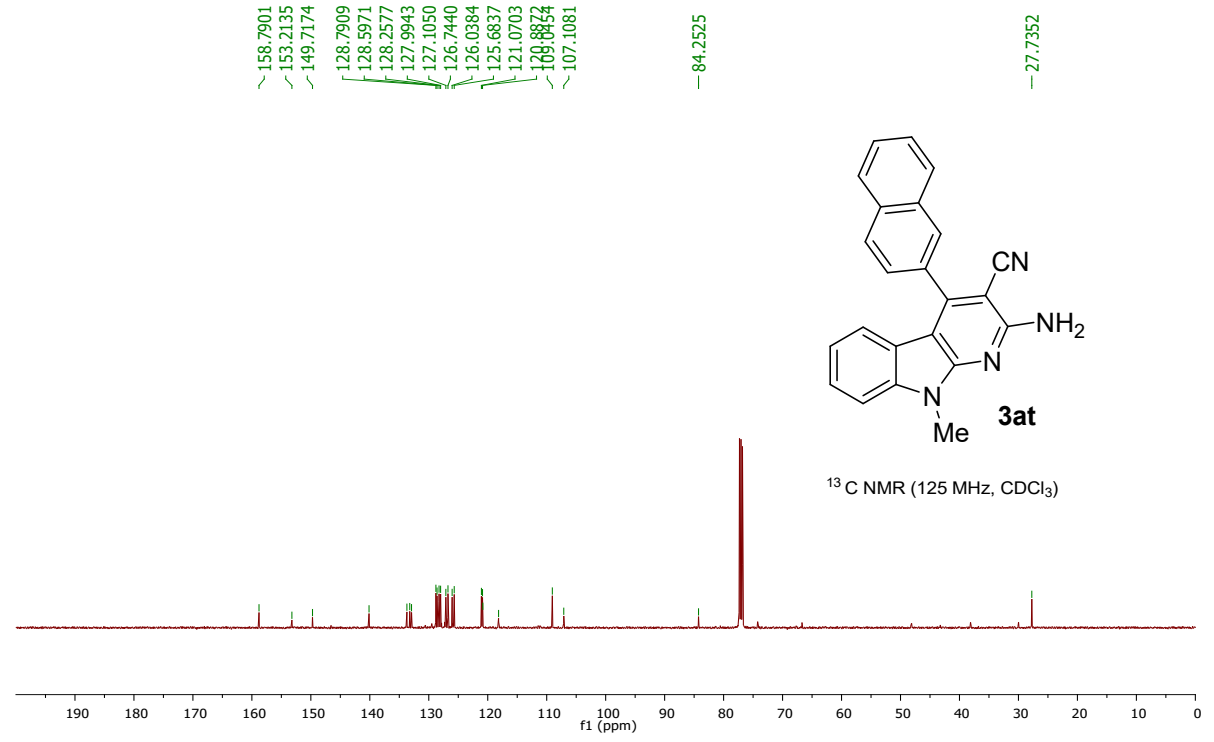

7.8382
7.8222
7.5454
7.5307
7.5160
7.4651
7.4500
7.4342
7.4210
7.4061
7.3916
7.3759
7.3613
7.3425
7.3267
7.0393
7.0245
7.0099
6.7991
6.7836
5.3406
3.8384
f1 (ppm)
Br
CN
NH2
N
N
Me
3ar
1H NMR (500 MHz, CDCl3)
1.00
1.03
2.24
1.83
1.04
1.00
2.00
3.14
f1 (ppm)

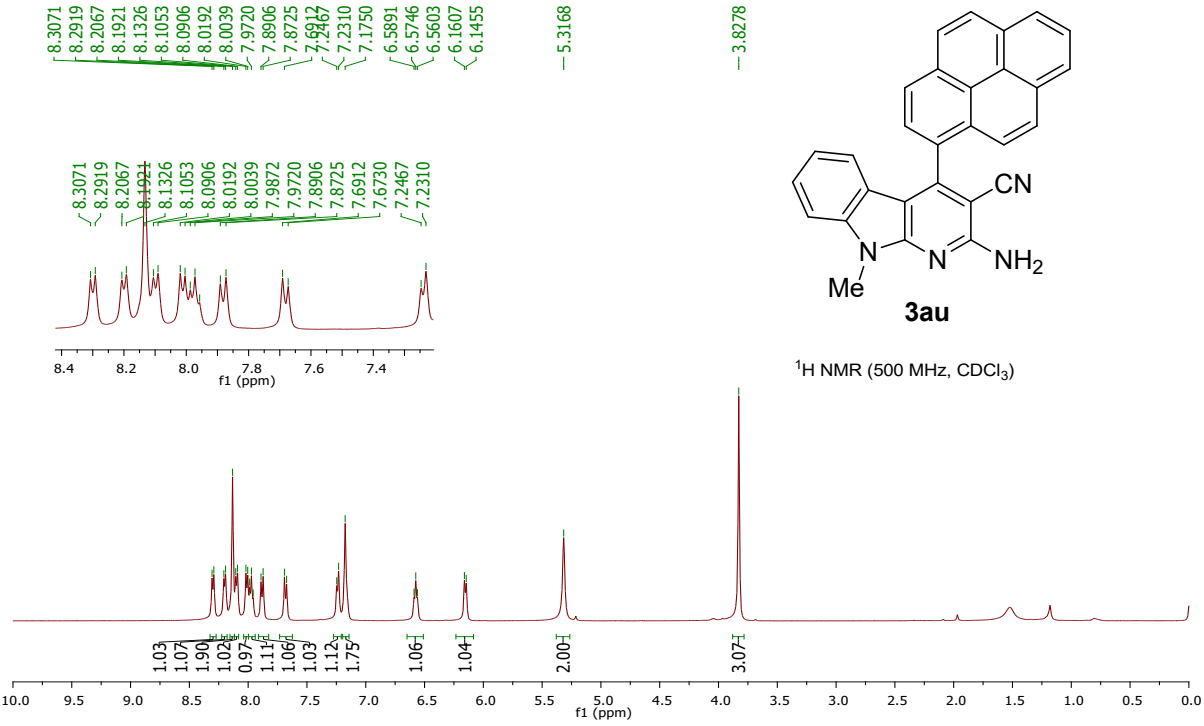

158.5709
153.1568
147.8801
140.1181
133.4081
130.9194
130.0179
128.0521
125.8322
121.1547
120.6795
107.3548
84.1609
27.7188
Br
CN
NH2
N
N
Me
3ar
13 C NMR (125 MHz, CDCl3)
f1 (ppm)

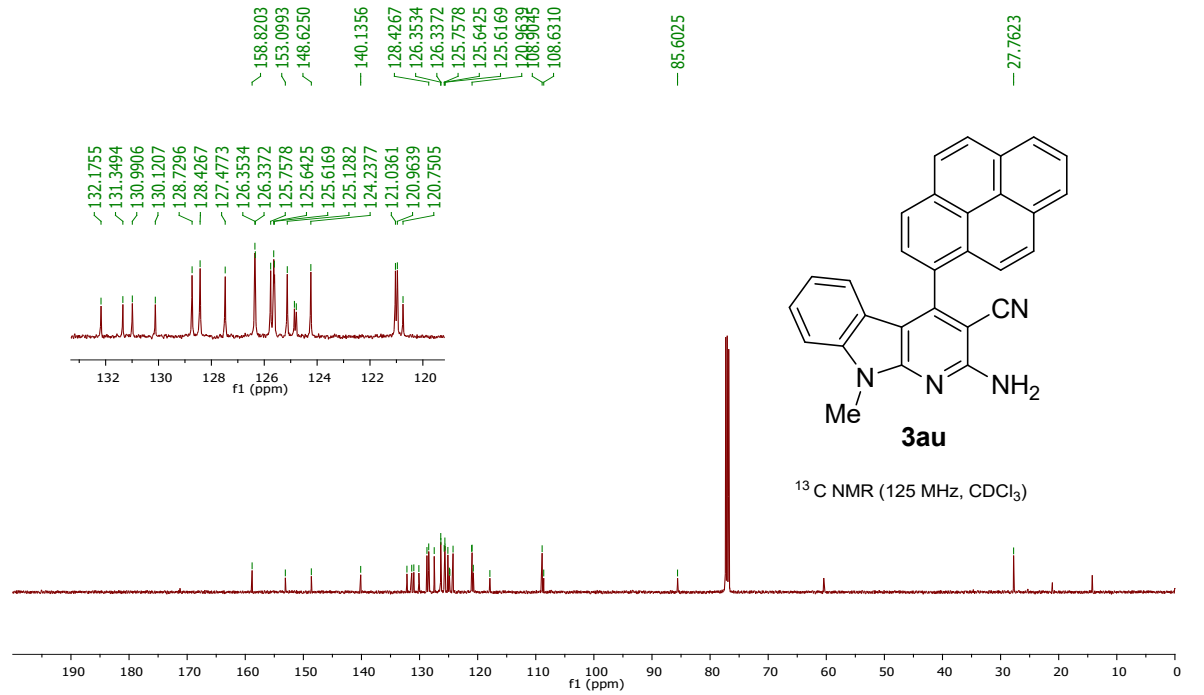

7.5729
7.5568
7.4899
7.4744
7.4576
7.4052
7.3899
7.3753
7.3572
7.3414
7.0595
7.0447
7.0302
6.7589
6.7434
5.3231
3.8523
Cl
CN
Cl
NH2
N
N
Me
3as
1H NMR (500 MHz, CDCl3)
1.87
1.04
2.03
0.99
0.93
2.00
3.06
f1 (ppm)

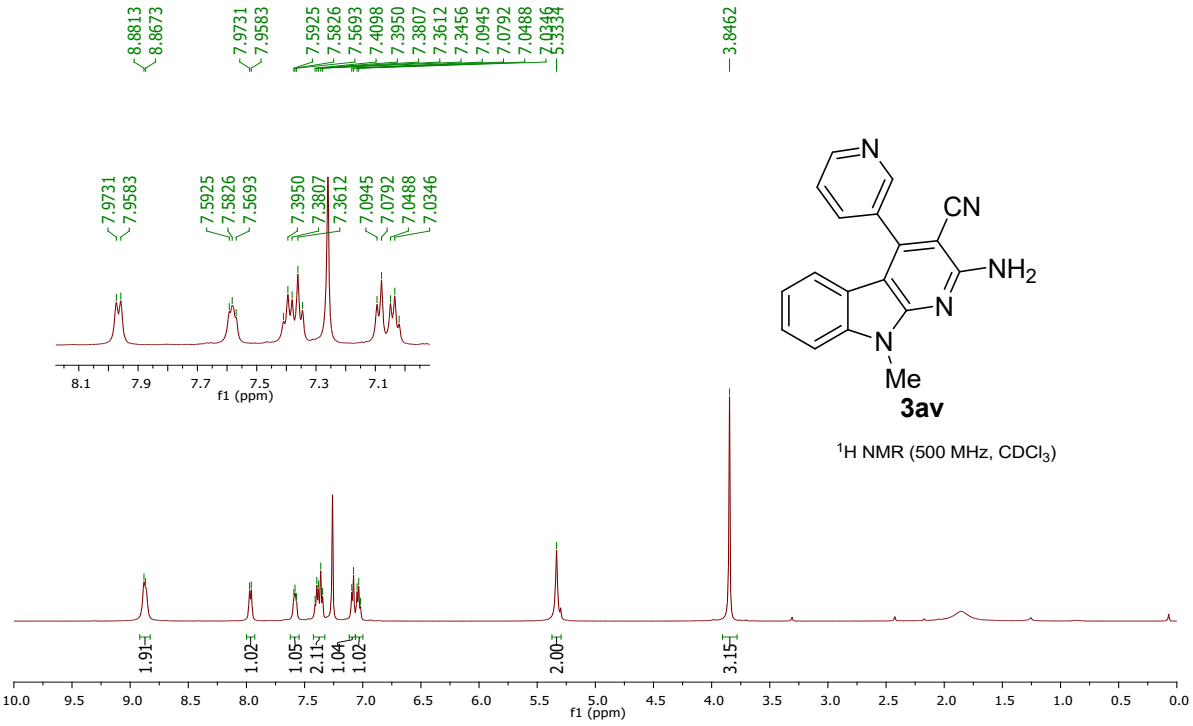

158.6799
153.4462
143.5672
140.1968
134.2933
133.3652
131.1365
128.6226
126.0156
121.3427
120.3902
120.0999
116.9844
109.2157
107.1847
83.8549
27.7324
Cl
CN
Cl
NH2
N
N
Me
3as
13 C NMR (125 MHz, CDCl3)
f1 (ppm)

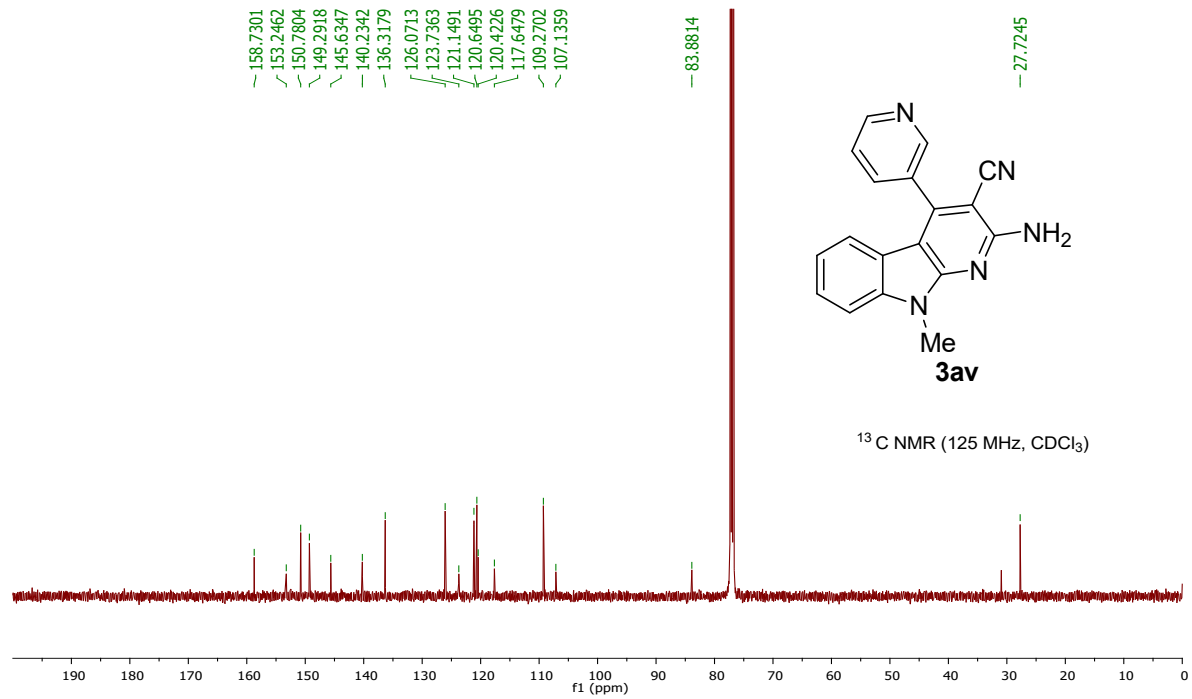

8.1317
8.1071
8.0908
8.0209
8.0061
7.9761
7.9617
7.7200
7.7039
7.6457
7.6291
7.6119
7.3700
7.1559
7.1410
6.9824
6.9724
5.3702
3.8796
f1 (ppm)
CN
NH2
N
N
Me
3at
1H NMR (500 MHz, CDCl3)
1.79
1.02
1.14
0.97
2.27
1.75
0.90
0.88
2.00
3.09
f1 (ppm)

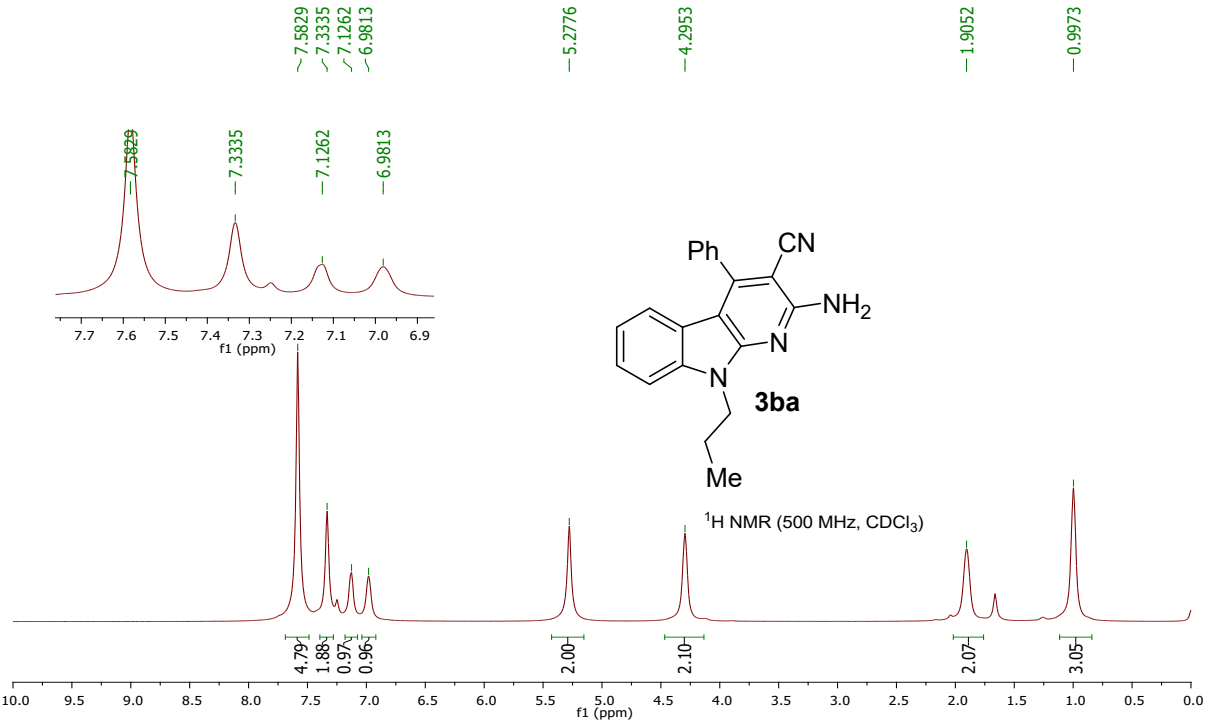

158.7901
153.2135
149.7174
128.7909
128.5971
128.2577
127.9943
127.1050
126.7440
126.0384
125.6837
121.0703
107.1081
84.2525
27.7352
CN
NH2
N
N
Me
3at
13C NMR (125 MHz, CDCl3)
f1 (ppm)

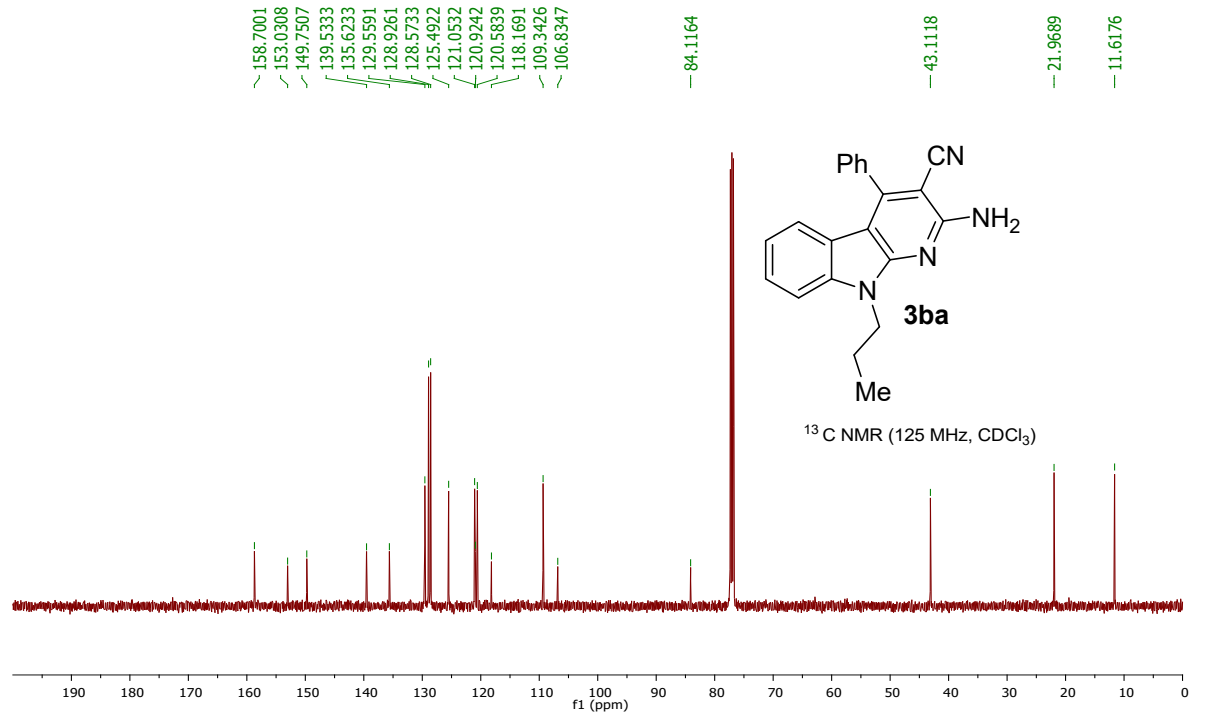

8.3071
8.2919
8.2067
8.1921
8.1326
8.1053
8.0906
8.0192
8.0039
7.9720
7.8906
7.8725
7.6912
7.6730
7.2467
7.2310
7.1750
6.5891
6.5746
6.5603
6.1607
6.1455
5.3168
3.8278
CN
N
N
NH2
Me
3au
1H NMR (500 MHz, CDCl3)
f1 (ppm)

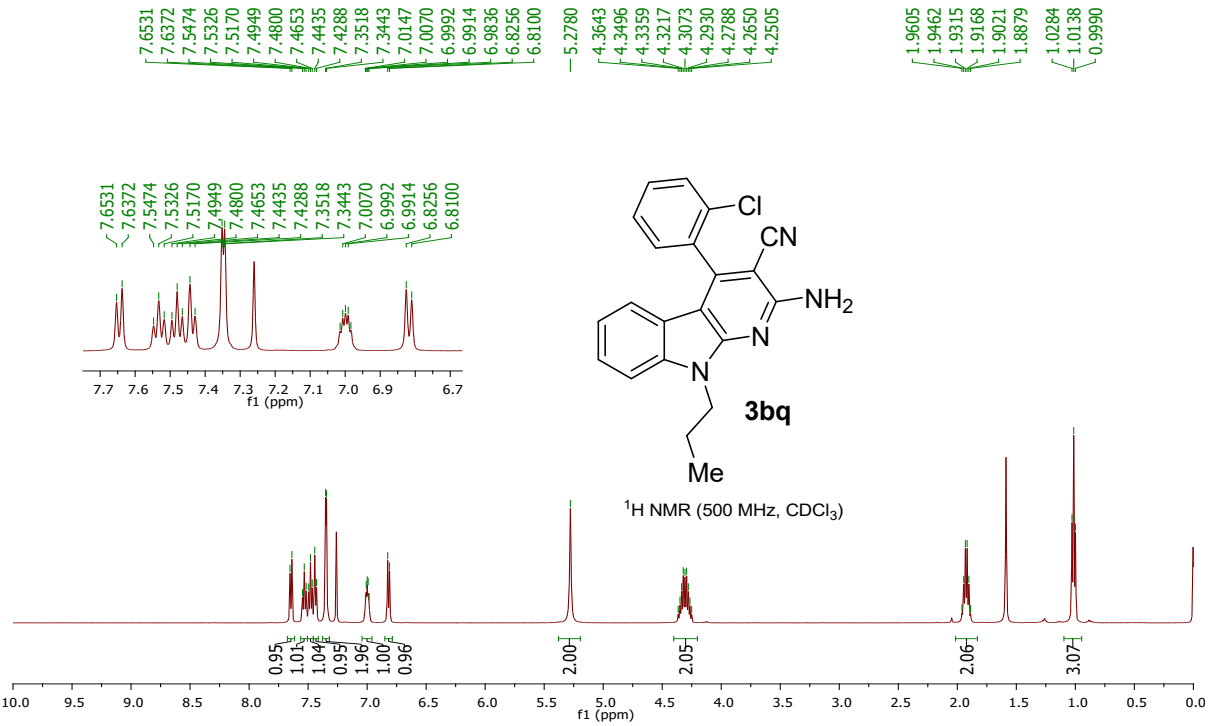

158.8203
153.0993
148.6250
140.1356
128.4267
126.3534
126.3372
125.7578
125.6425
125.6169
120.9639
108.6310
85.6025
27.7623
132.1755
131.3494
130.9906
130.1207
128.7296
128.4267
127.4773
126.3534
126.3372
125.7578
125.6425
125.6169
125.1282
124.2377
121.0361
120.9639
120.7505
CN
N
N
NH2
Me
3au
13C NMR (125 MHz, CDCl3)
f1 (ppm)

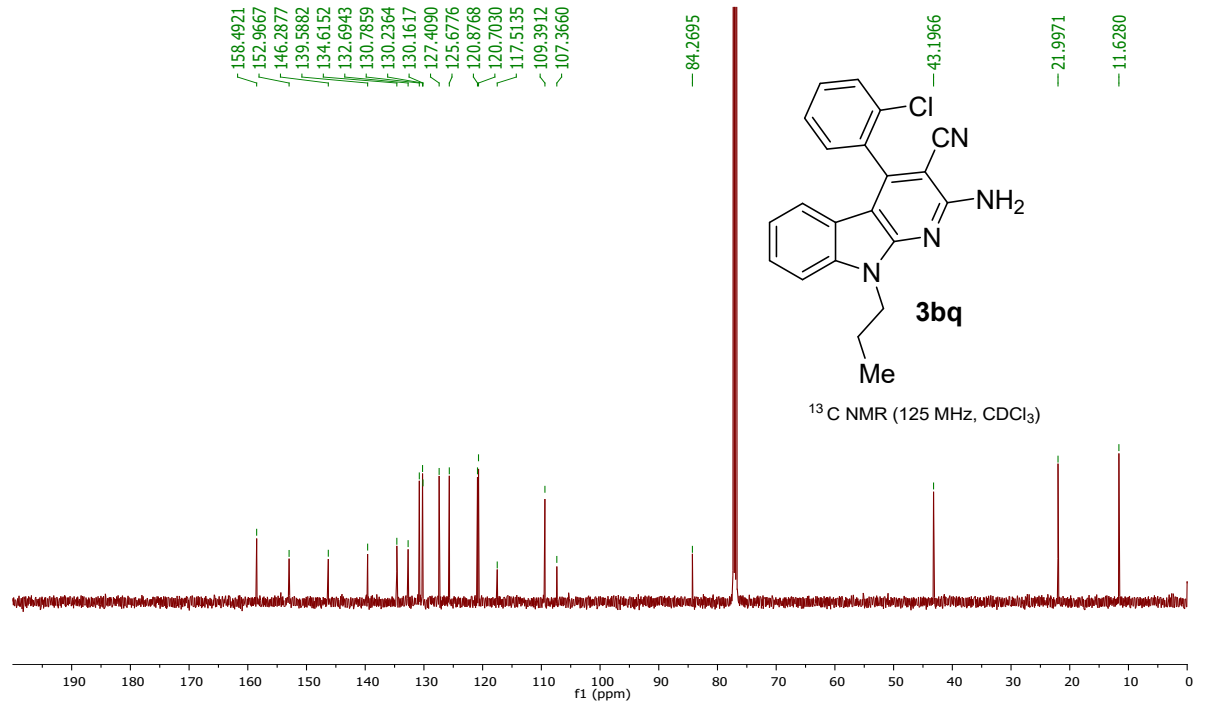

8.8813
8.8673
7.9731
7.9583
7.5925
7.5826
7.5693
7.4098
7.3950
7.3807
7.3612
7.3456
7.0945
7.0792
7.0488
7.0346
5.3334
3.8462
CN
NH2
N
N
Me
3av
1H NMR (500 MHz, CDCl3)
1.91
1.02
1.05
2.11
1.04
1.02
2.00
3.15
f1 (ppm)

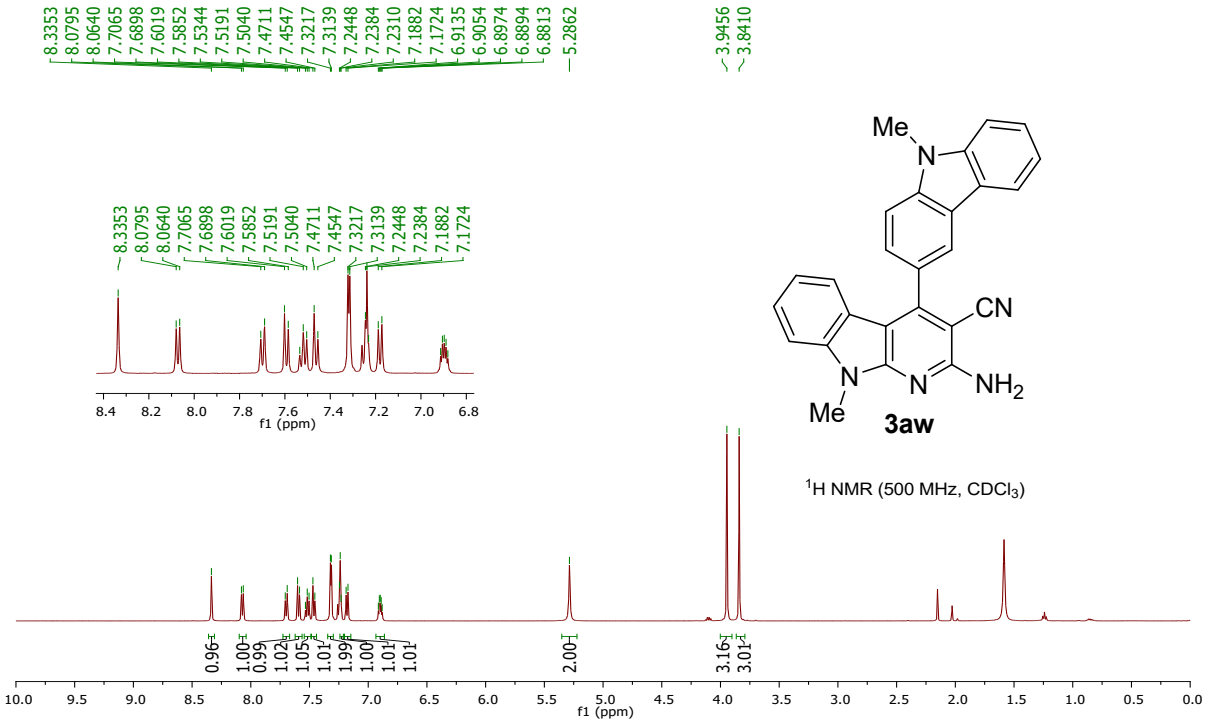

158.7301
153.2462
150.7804
149.2918
145.6347
140.2342
136.3179
126.0713
123.7363
121.1491
120.6495
120.4226
117.6479
109.2702
107.1359
83.8814
27.7245
CN
NH2
N
N
Me
3av
13 C NMR (125 MHz, CDCl3)
f1 (ppm)


7.5829
7.3335
7.1262
6.9813
5.2776
4.2953
1.9052
0.9973
Ph
CN
NH2
N
N
Me
3ba
1H NMR (500 MHz, CDCl3)
4.79
1.88
0.97
0.96
2.00
2.10
2.07
3.05
f1 (ppm)

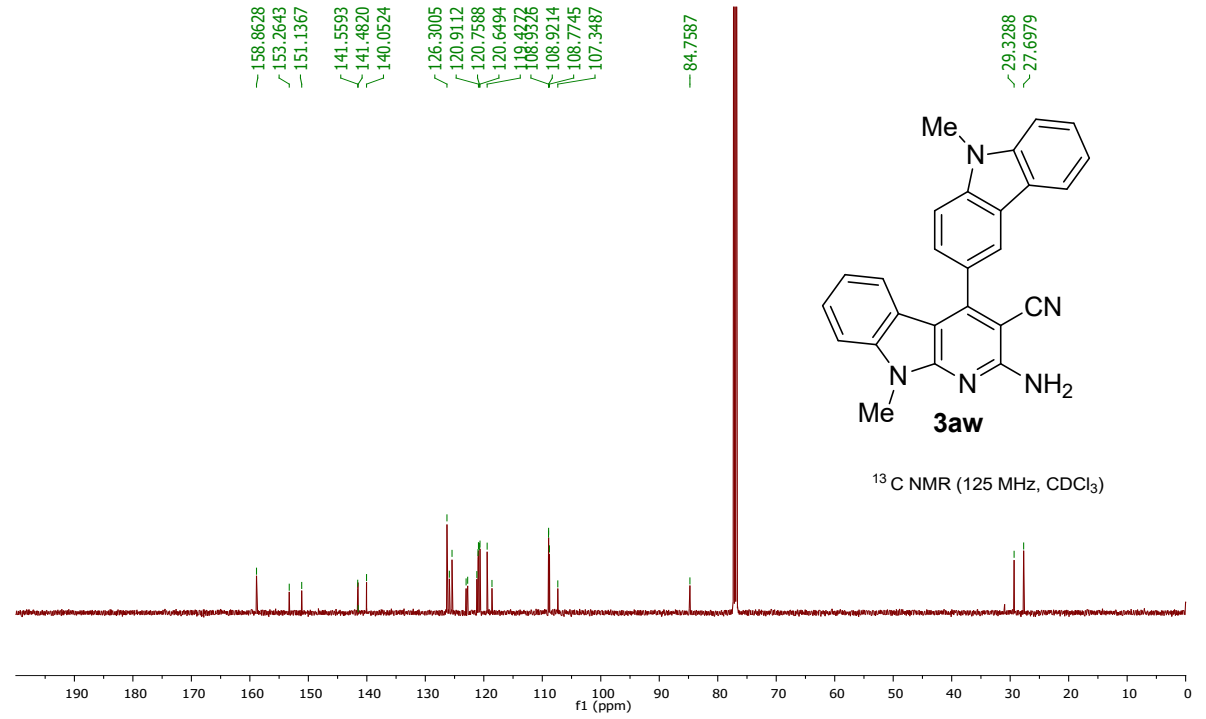

158.7001
153.0308
149.7507
139.5333
135.6233
129.5591
128.9261
128.5733
125.4922
121.0532
120.9242
120.5839
118.1691
109.3426
106.8347
84.1164
43.1118
21.9689
11.6176
Ph
CN
NH2
N
N
Me
3ba
13 C NMR (125 MHz, CDCl3)
f1 (ppm)


7.6531
7.6372
7.5474
7.5326
7.5170
7.4949
7.4800
7.4653
7.4435
7.4288
7.3518
7.3443
7.0147
7.0070
6.9992
6.9914
6.9836
6.8256
6.8100
5.2780
4.3643
4.3496
4.3359
4.3217
4.3073
4.2930
4.2788
4.2650
4.2505
1.9605
1.9462
1.9315
1.9168
1.9021
1.8879
1.0284
1.0138
0.9990
Cl
CN
NH2
N
N
Me
3bq
1H NMR (500 MHz, CDCl3)
0.95
1.01
1.04
0.95
1.96
1.00
0.96
2.00
2.05
2.06
3.07
f1 (ppm)

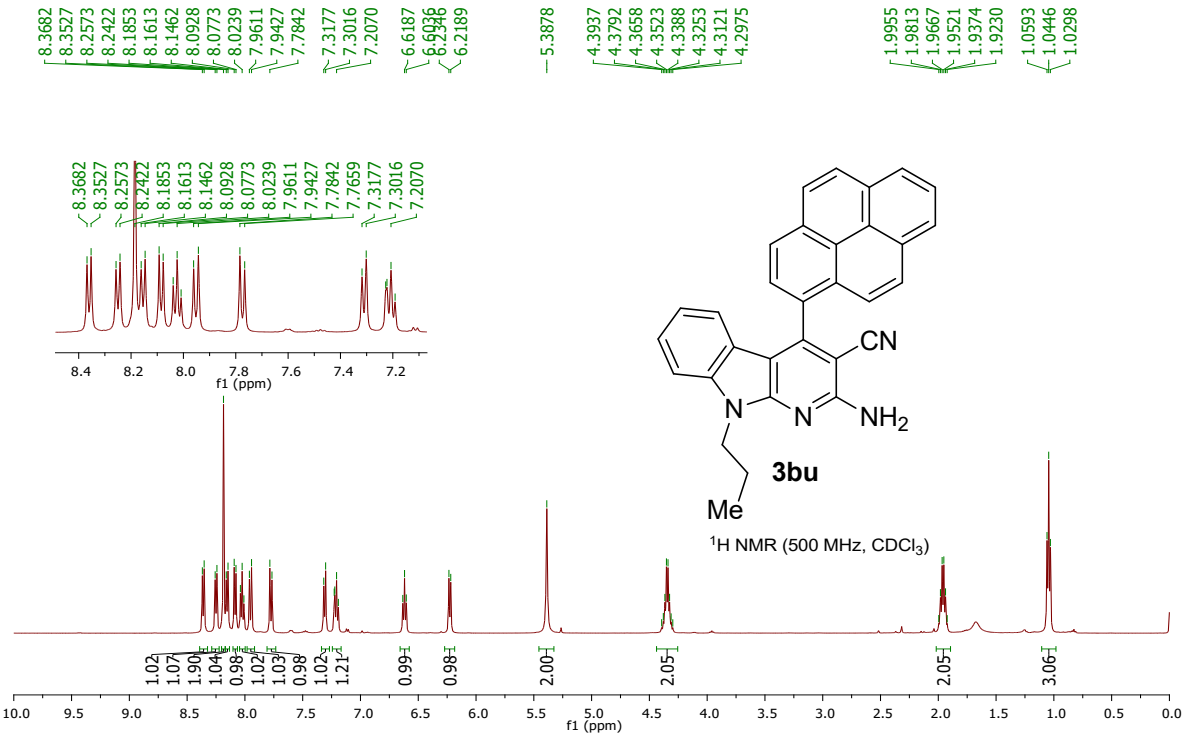

158.4921
152.9667
146.2877
139.5882
134.6152
132.6943
130.7859
130.2364
130.1617
127.4090
125.6776
120.8768
120.7030
117.5135
109.3912
107.3660
84.2695
43.1966
21.9971
11.6280
Cl
CN
NH2
N
N
Me
3bq
13C NMR (125 MHz, CDCl3)
f1 (ppm)

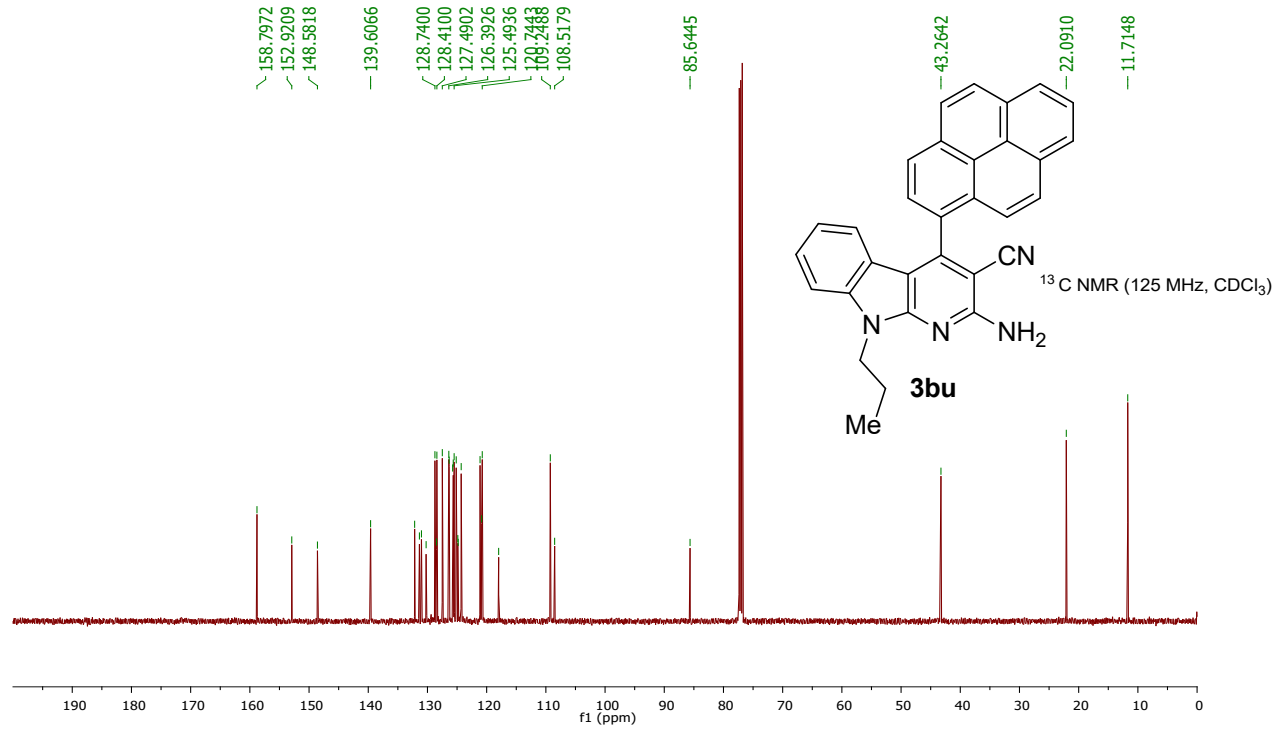


^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)


8.3682
8.3527
8.2573
8.2422
8.1853
8.1613
8.1462
8.0928
8.0773
8.0239
7.9611
7.9427
7.7842
7.3177
7.3016
7.2070
6.6187
6.2189
5.3878
4.3937
4.3792
4.3658
4.3523
4.3388
4.3253
4.3121
4.2975
1.9955
1.9813
1.9667
1.9521
1.9374
1.9230
1.0593
1.0446
1.0298
CN
N
N
NH2
Me
3bu
1H NMR (500 MHz, CDCl3)
f1 (ppm)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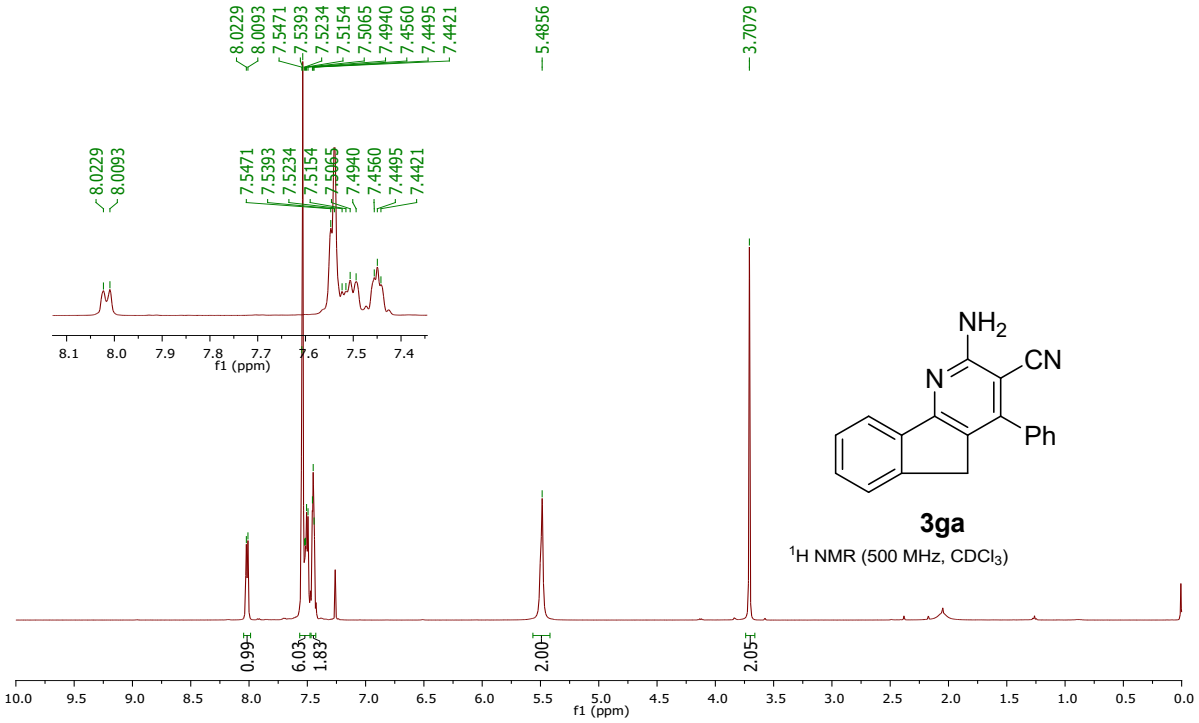
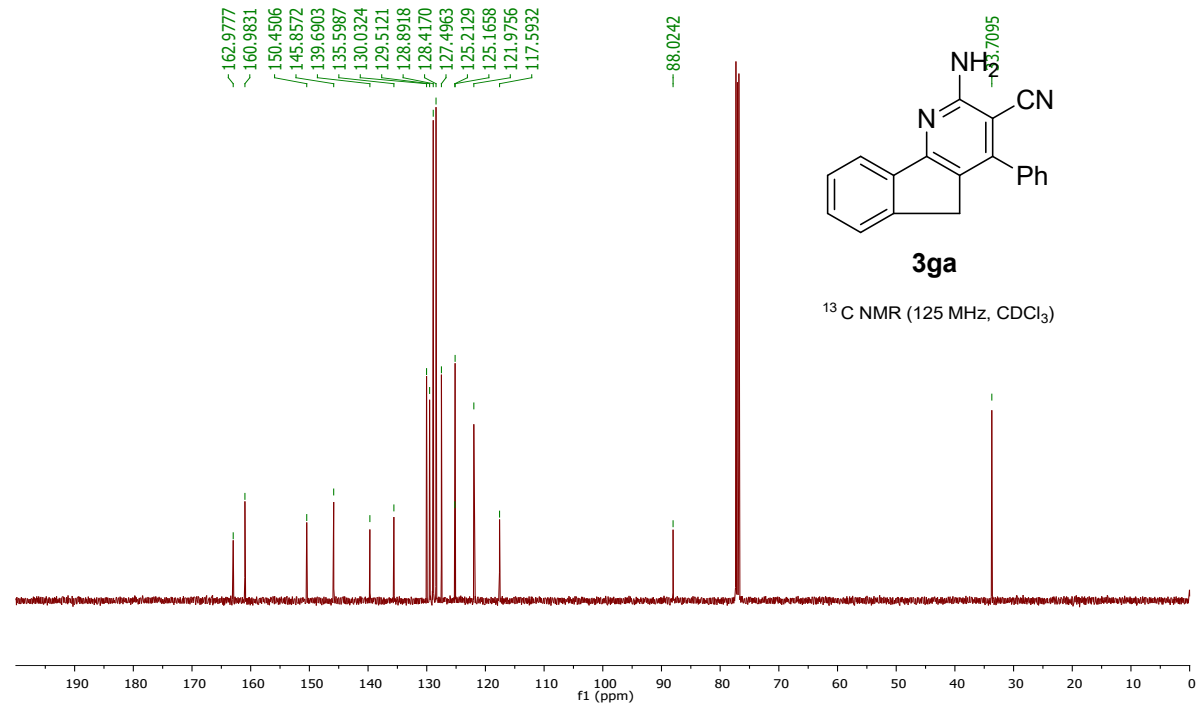
148.5818
139.6066
128.7400
128.4100
127.4902
126.3926
125.4936
120.7443
109.2488
108.5179
85.6445
43.2642
22.0910
11.7148
CN
N
N
NH2
Me
3bu
13C NMR (125 MHz, CDCl3)
f1 (ppm)



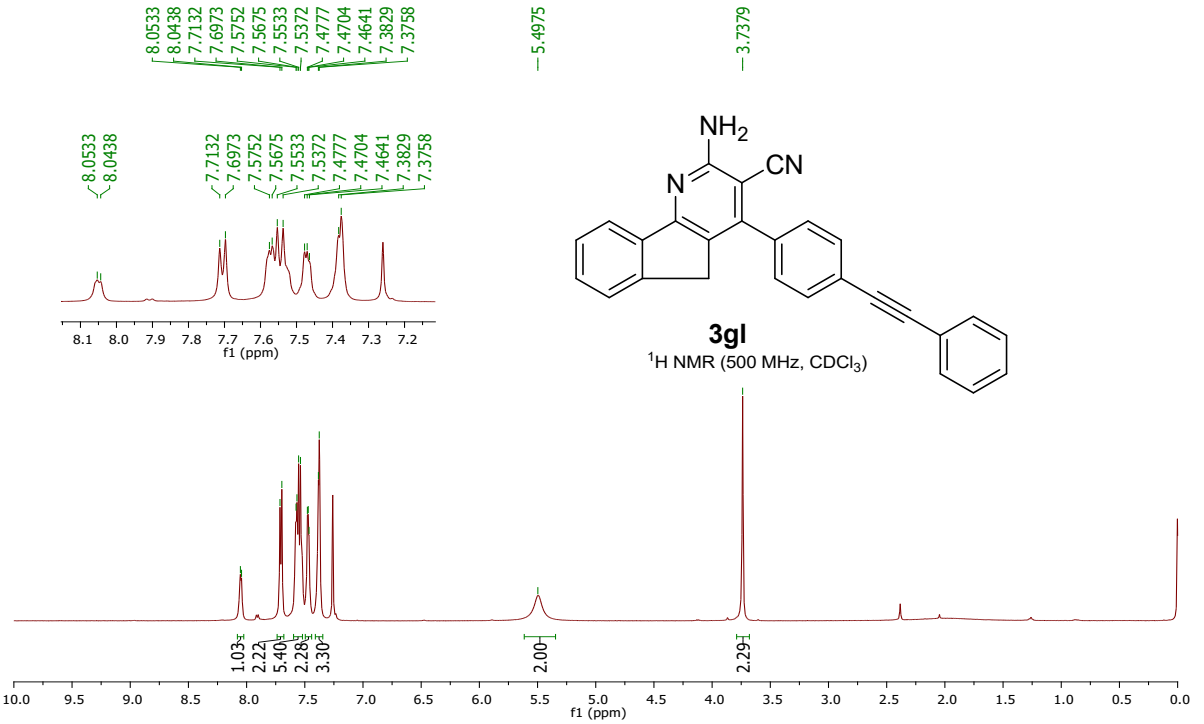
3ga

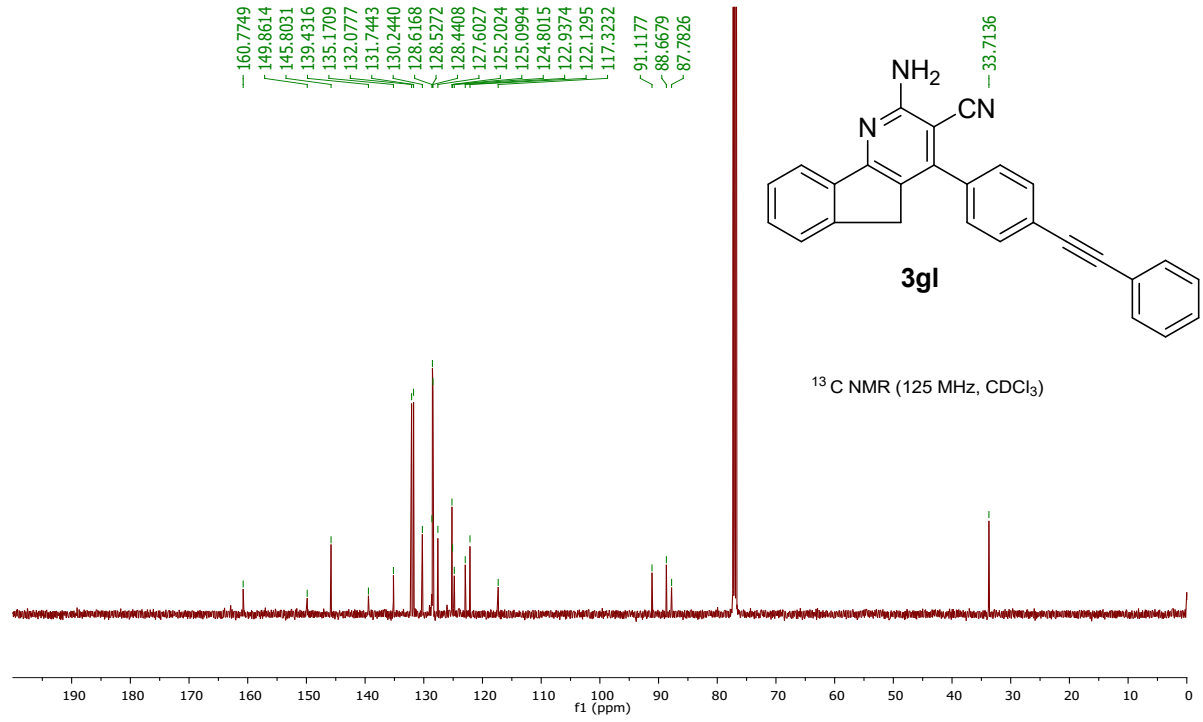
^{1}H NMR (500 MHz, $CDCl_3$)

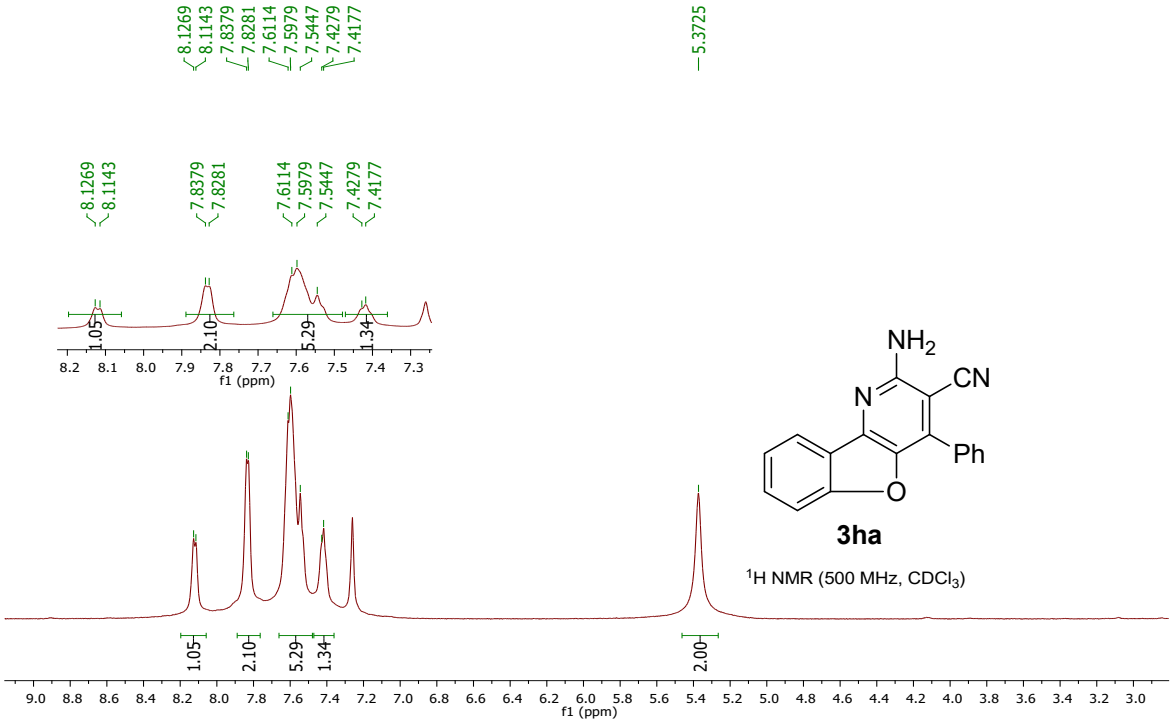


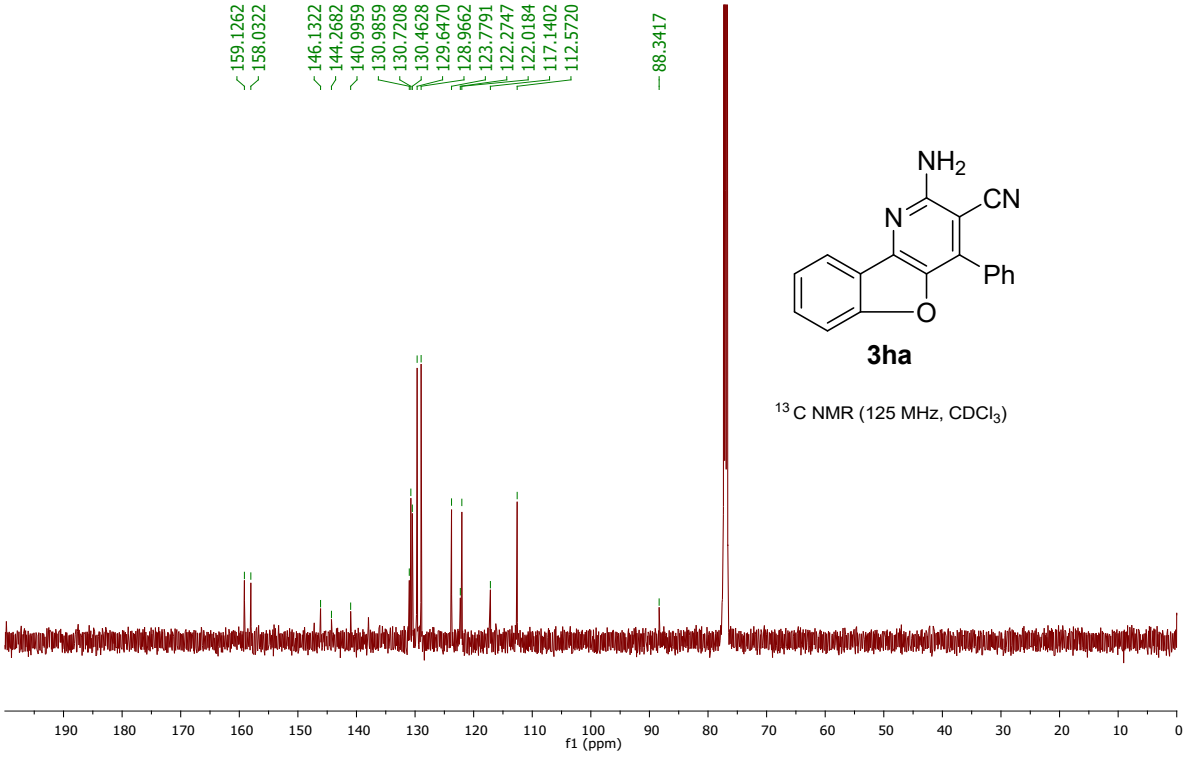
3ga

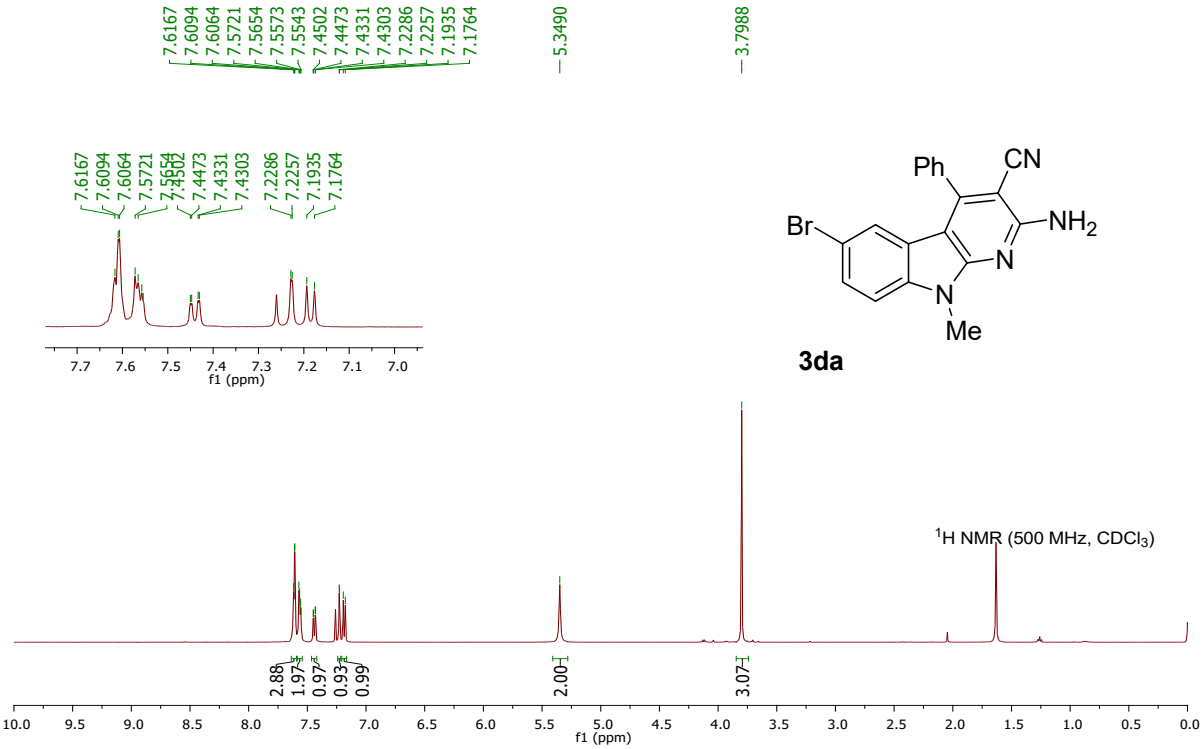
^{13}C NMR (125 MHz, $CDCl_3$)

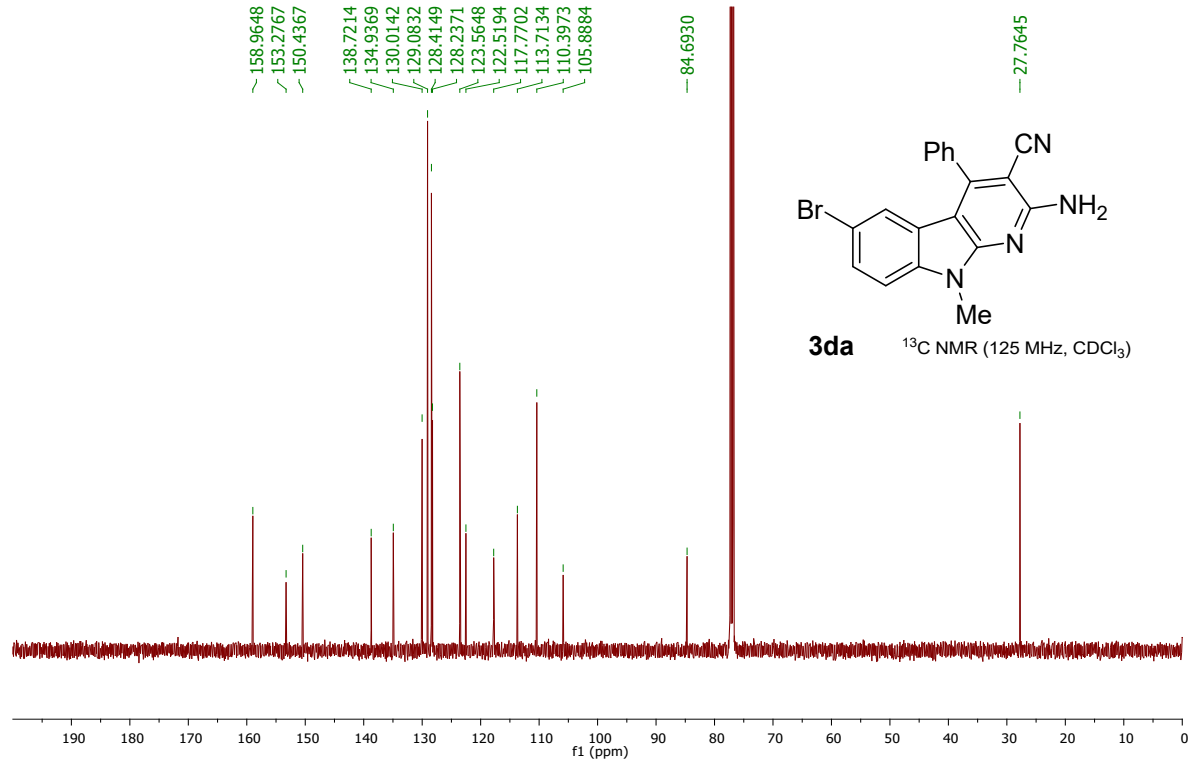

8.0533
8.0438
7.7132
7.6973
7.5752
7.5675
7.5533
7.5372
7.4777
7.4704
7.4641
7.3829
7.3758
5.4975
3.7379
NH2
CN
N
3gl
1H NMR (500 MHz, CDCl3)
1.03
2.22
5.40
2.28
3.30
2.00
2.29
f1 (ppm)


160.7749
149.8614
145.8031
139.4316
135.1709
132.0777
131.7443
130.2440
128.6168
128.5272
128.4408
127.6027
125.2024
125.0994
124.8015
122.9374
122.1295
117.3232
91.1177
88.6679
87.7826
33.7136
NH2
CN
N
3gl
13C NMR (125 MHz, CDCl3)
f1 (ppm)


8.1269
8.1143
7.8379
7.8281
7.6114
7.5979
7.5447
7.4279
7.4177
5.3725
1.05
2.10
5.29
1.34
2.00
f1 (ppm)
NH2
CN
N
Ph
O
3ha
1H NMR (500 MHz, CDCl3)


159.1262
158.0322
146.1322
144.2682
140.9959
130.9859
130.7208
130.4628
129.6470
128.9662
123.7791
122.2747
122.0184
117.1402
112.5720
88.3417
f1 (ppm)
NH2
CN
N
Ph
O
3ha
13C NMR (125 MHz, CDCl3)


7.6167
7.6094
7.6064
7.5721
7.5654
7.5573
7.5543
7.4502
7.4473
7.4331
7.4303
7.2286
7.2257
7.1935
7.1764
5.3490
3.7988
Ph
CN
Br
NH2
N
N
Me
3da
f1 (ppm)
1H NMR (500 MHz, CDCl3)
2.88
1.97
0.97
0.93
0.99
2.00
3.07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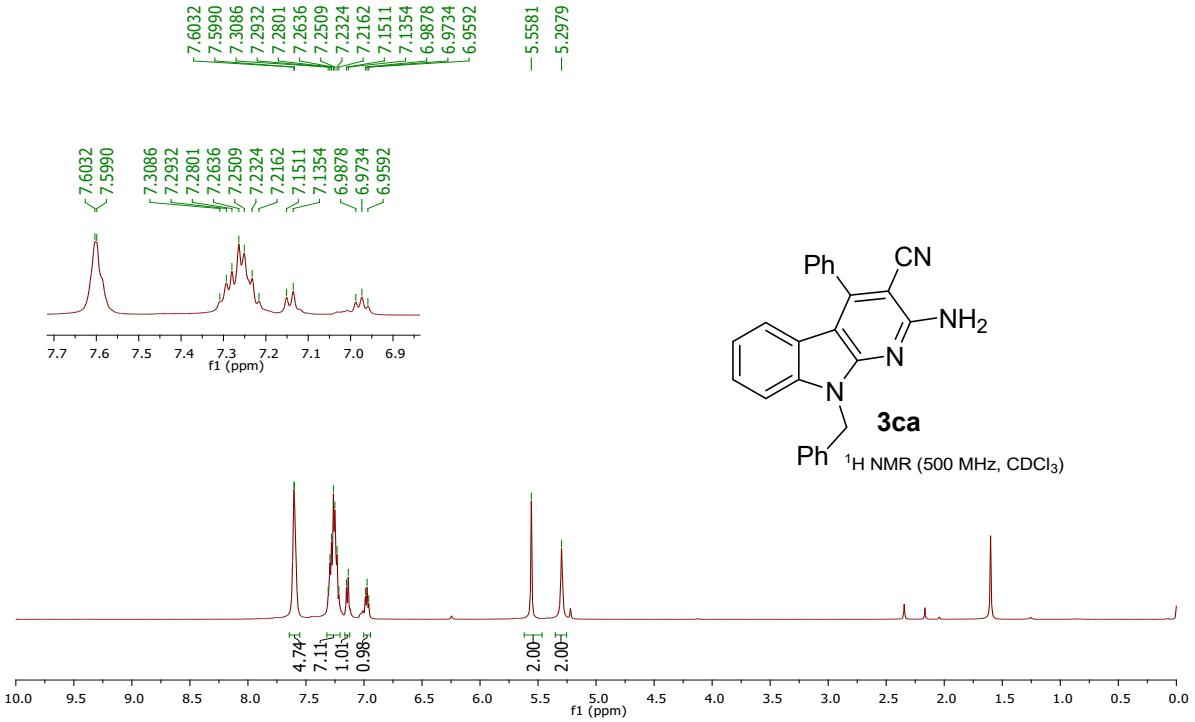
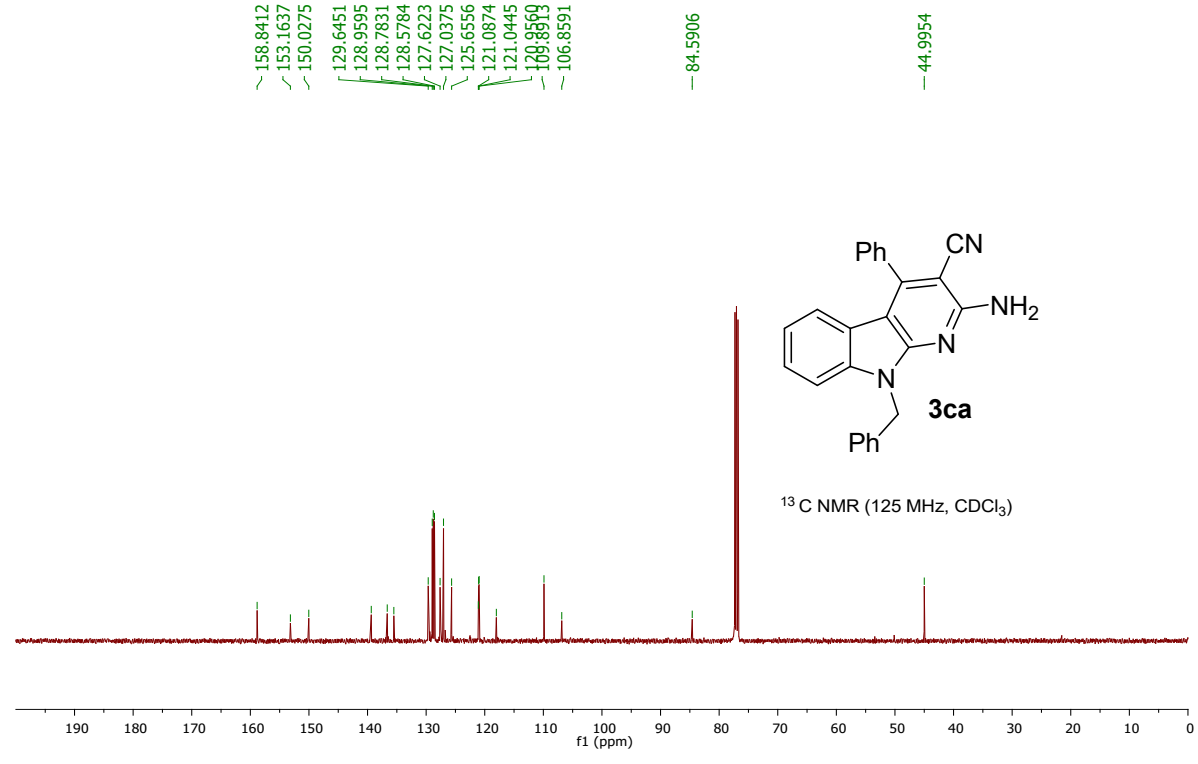
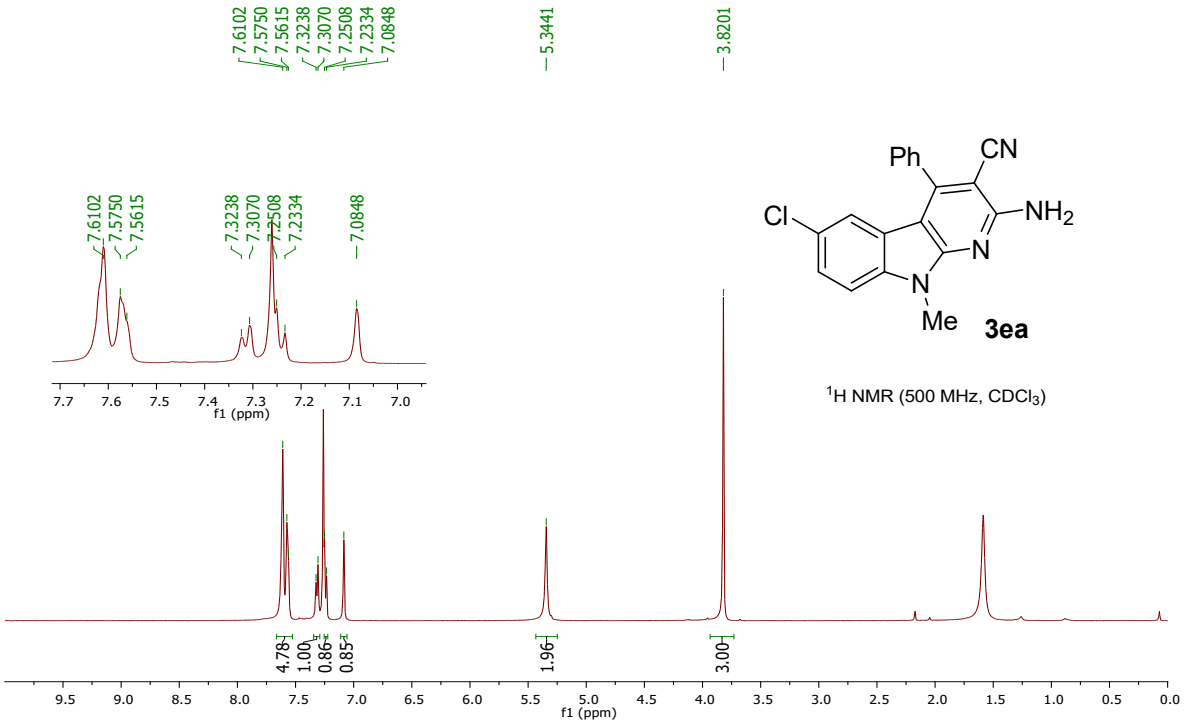
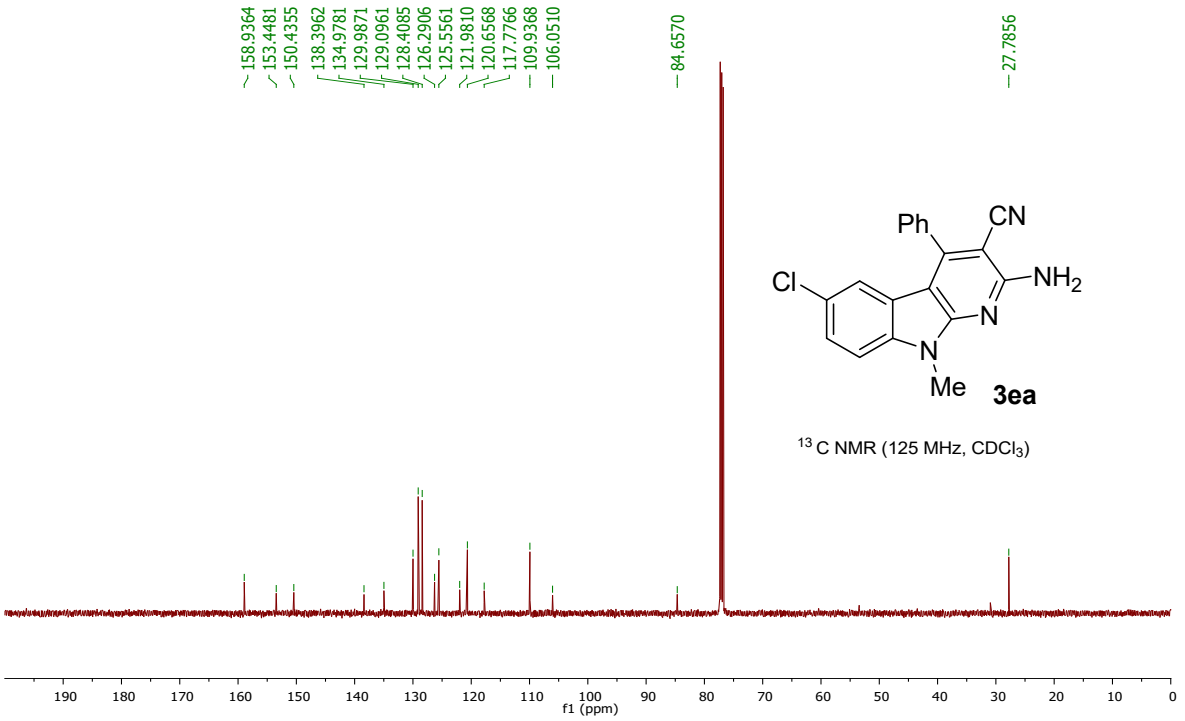
150.4367
138.7214
134.9369
130.0142
129.0832
128.4149
128.2371
123.5648
122.5194
117.7702
113.7134
110.3973
105.8884
84.6930
27.7645
Ph
CN
Br
NH2
N
N
Me
3da
13C NMR (125 MHz, CDCl3)
f1 (ppm)


7.6032
7.5990
7.3086
7.2932
7.2801
7.2636
7.2509
7.2324
7.2162
7.1511
7.1354
6.9878
6.9734
6.9592
5.5581
5.2979
f1 (ppm)
Ph
CN
NH2
N
N
Ph
3ca
1H NMR (500 MHz, CDCl3)
4.74
7.11
1.01
0.98
2.00
2.00
f1 (ppm)

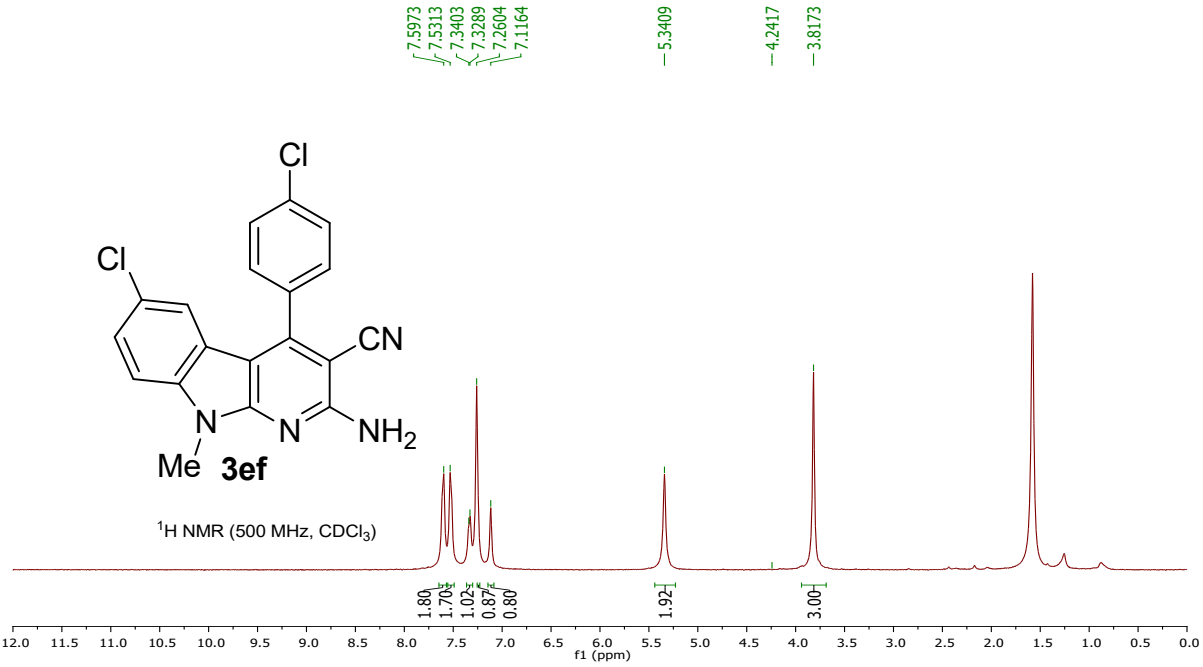

158.8412
153.1637
150.0275
129.6451
128.9595
128.7831
128.5784
127.6223
127.0375
125.6556
121.0874
121.0445
106.8591
84.5906
44.9954
Ph
CN
NH2
N
N
Ph
3ca
13C NMR (125 MHz, CDCl3)
f1 (ppm)

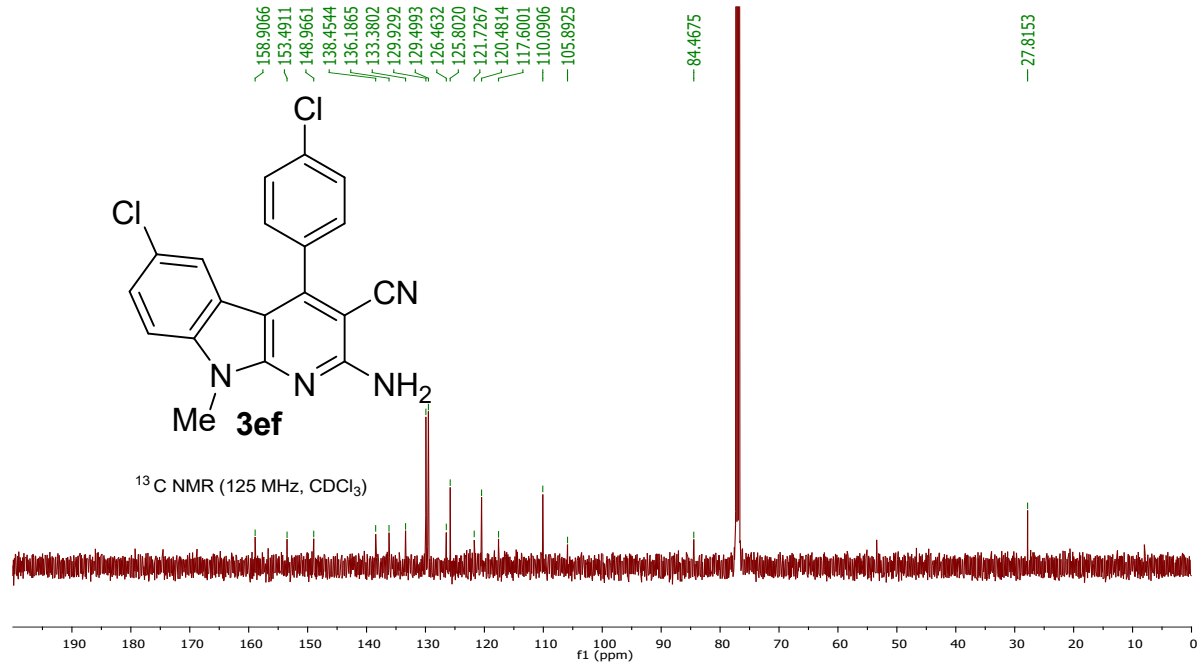


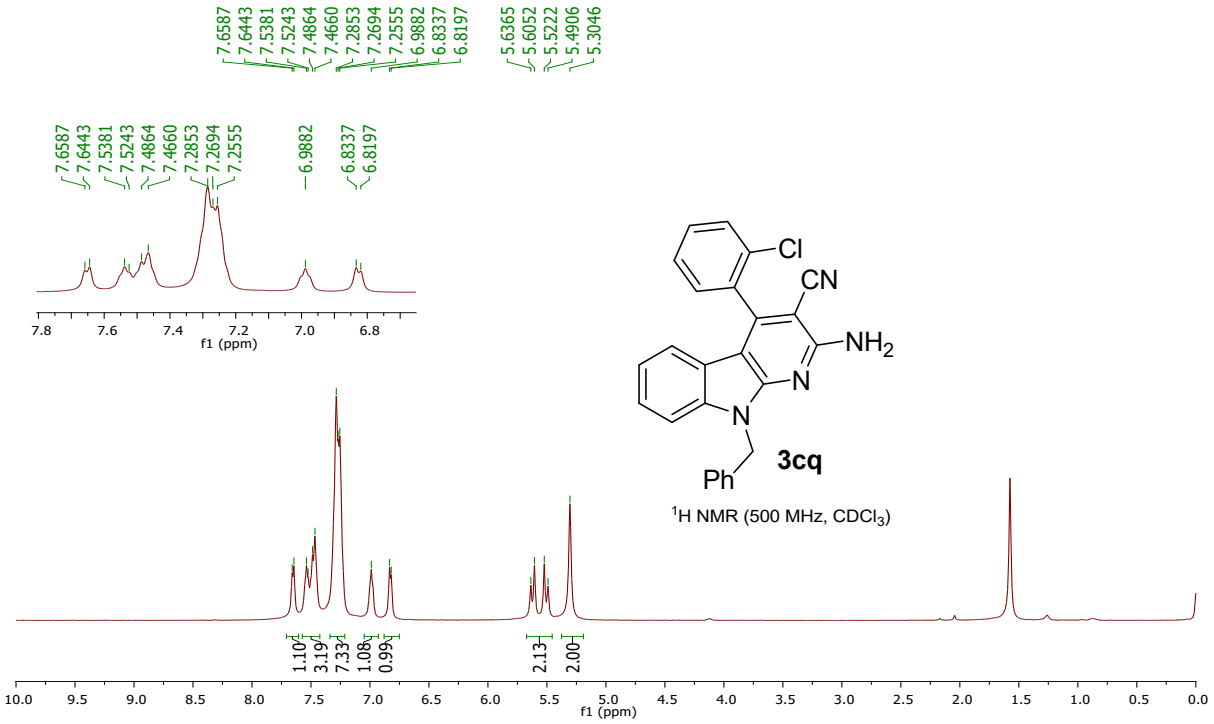
^{1}H NMR (500 MHz, $CDCl_3$)

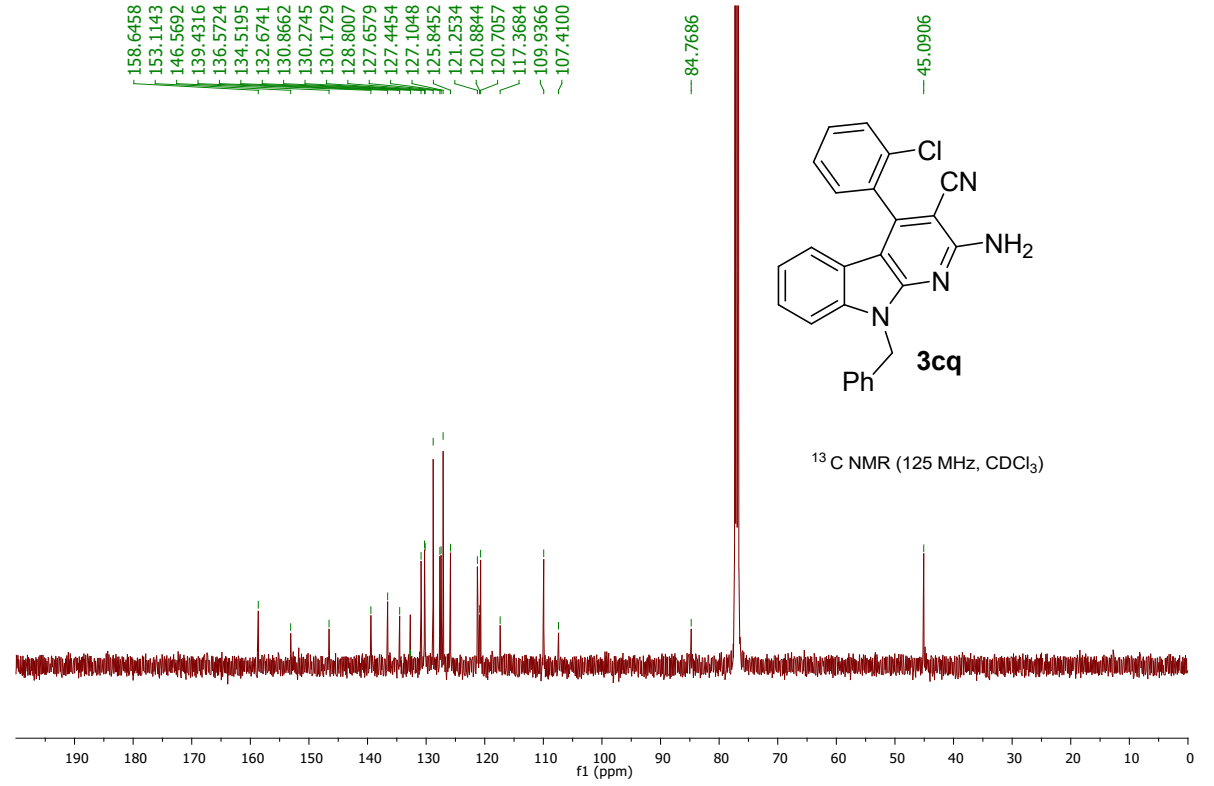


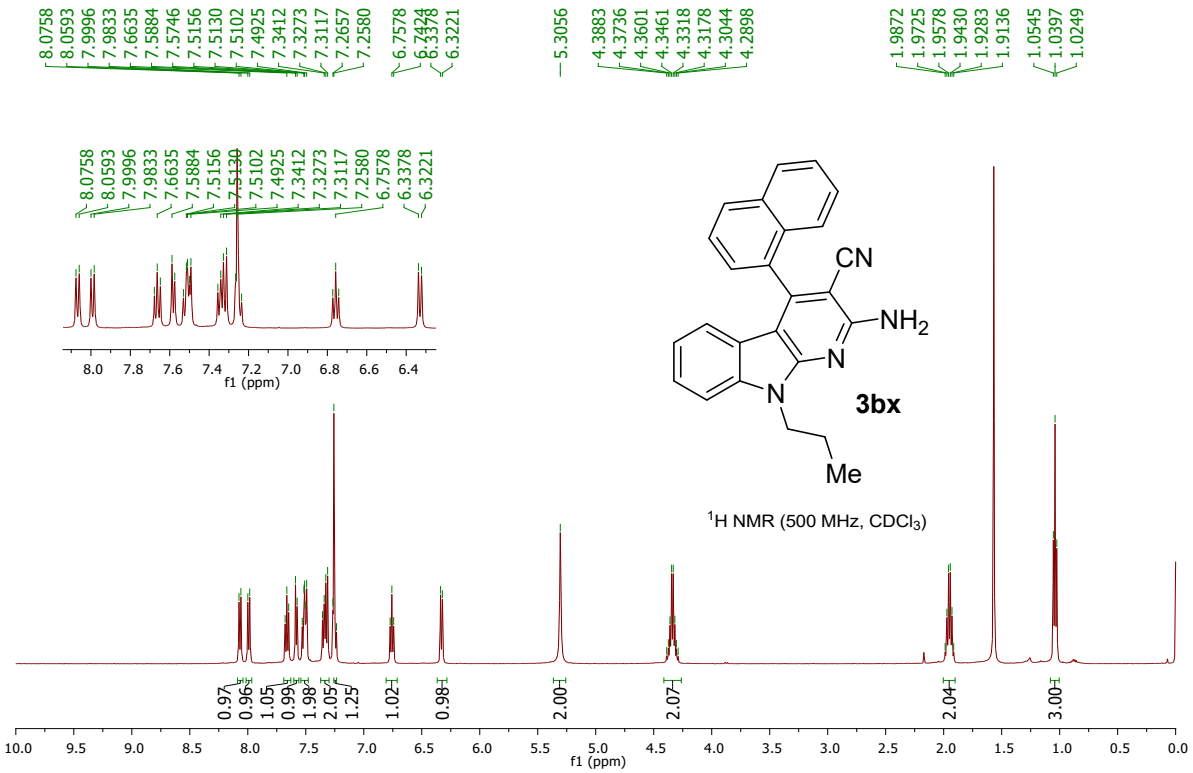
^{13}C NMR (125 MHz, $CDCl_3$)


7.5973
7.5313
7.3403
7.3289
7.2604
7.1164
5.3409
4.2417
3.8173
Cl
Cl
CN
N
N
NH2
Me
3ef
1H NMR (500 MHz, CDCl3)
1.80
1.70
1.02
0.87
0.80
1.92
3.00
f1 (ppm)

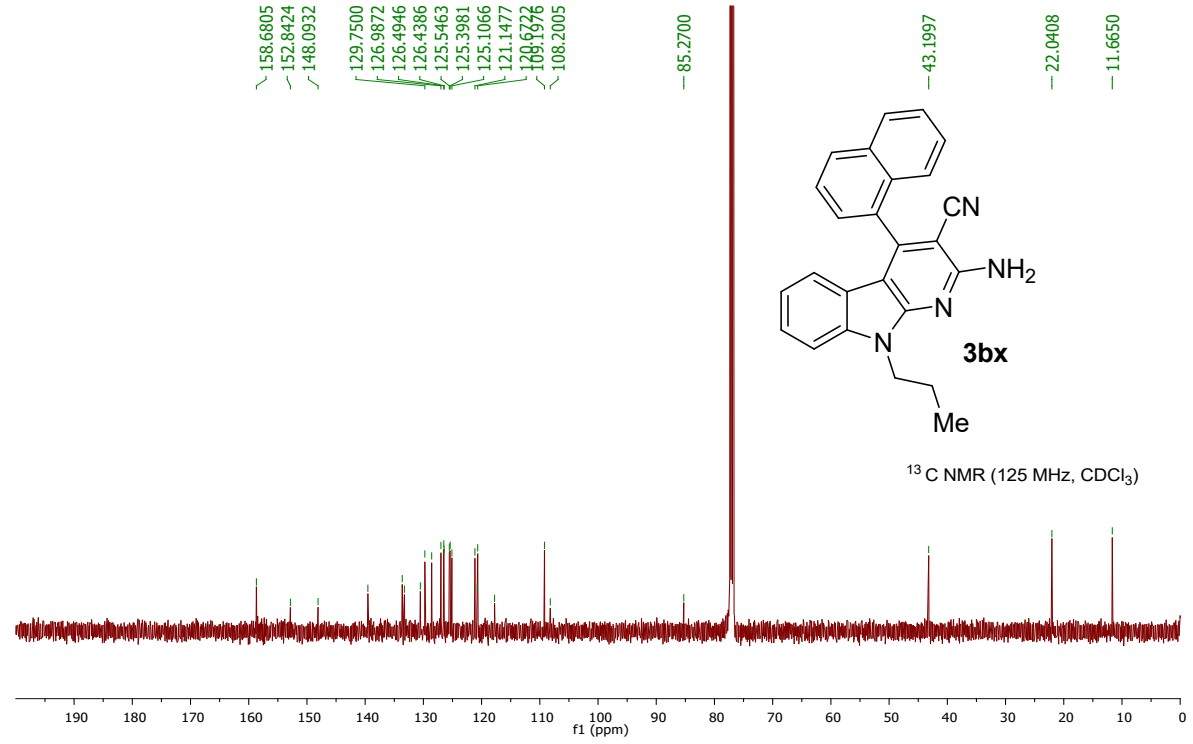

158.9066
153.4911
148.9661
138.4544
136.1865
133.3802
129.9292
129.4993
126.4632
125.8020
121.7267
120.4814
117.6001
110.0906
105.8925
84.4675
27.8153
Cl
Cl
CN
N
N
NH2
Me
3ef
13C NMR (125 MHz, CDCl3)
f1 (ppm)


7.6587
7.6443
7.5381
7.5243
7.4864
7.4660
7.2853
7.2694
7.2555
6.9882
6.8337
6.8197
5.6365
5.6052
5.5222
5.4906
5.3046
Cl
CN
NH2
N
N
Ph
3cq
1H NMR (500 MHz, CDCl3)
1.10
3.19
7.33
1.08
0.99
2.13
2.00
f1 (ppm)

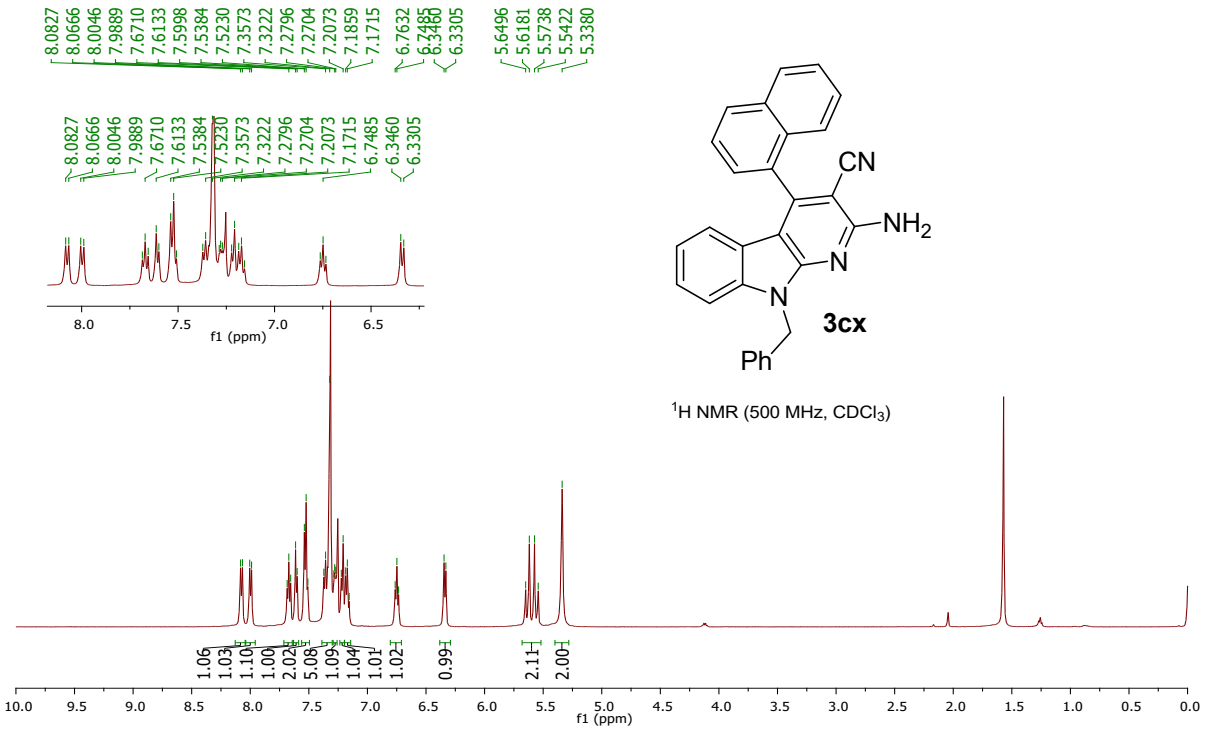

158.6458
153.1143
146.5692
139.4316
136.5724
134.5195
132.6741
130.8662
130.2745
130.1729
128.8007
127.6579
127.4454
127.1048
125.8452
121.2534
120.8844
120.7057
117.3684
109.9366
107.4100
84.7686
45.0906
Cl
CN
NH2
N
N
Ph
3cq
13C NMR (125 MHz, CDCl3)
f1 (ppm)

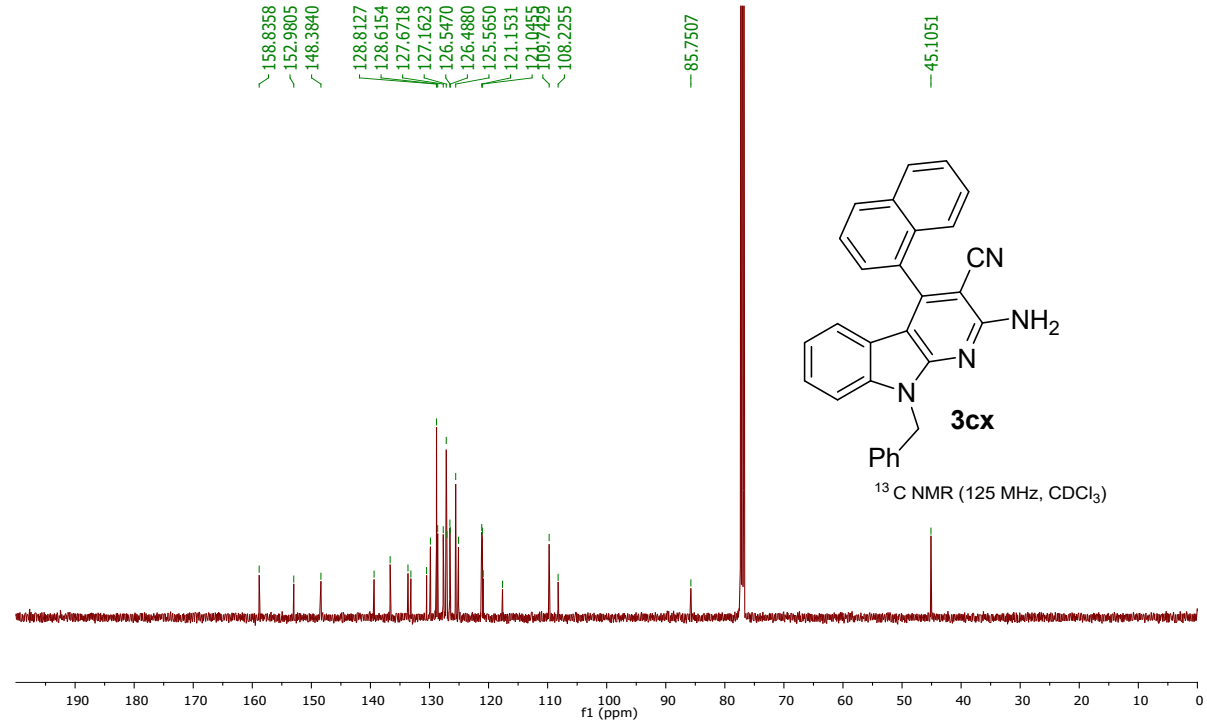


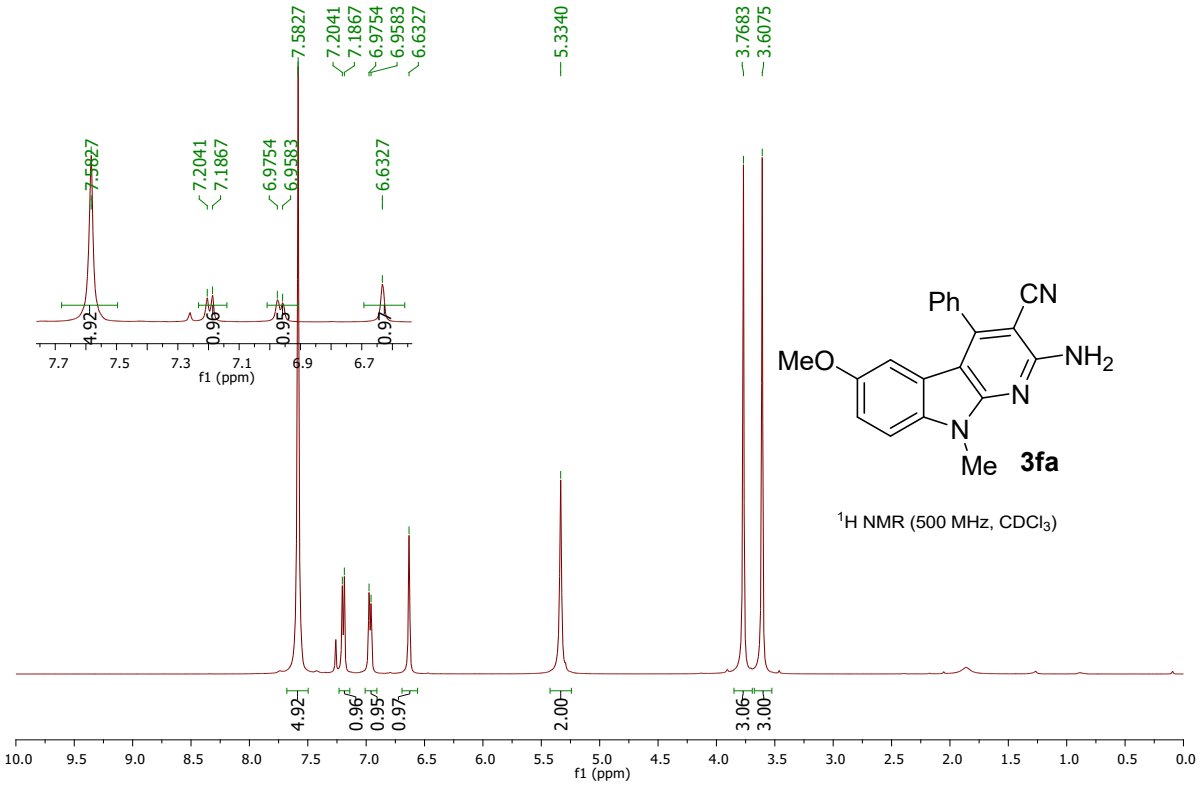
^{1}H NMR (500 MHz, $CDCl_3$)



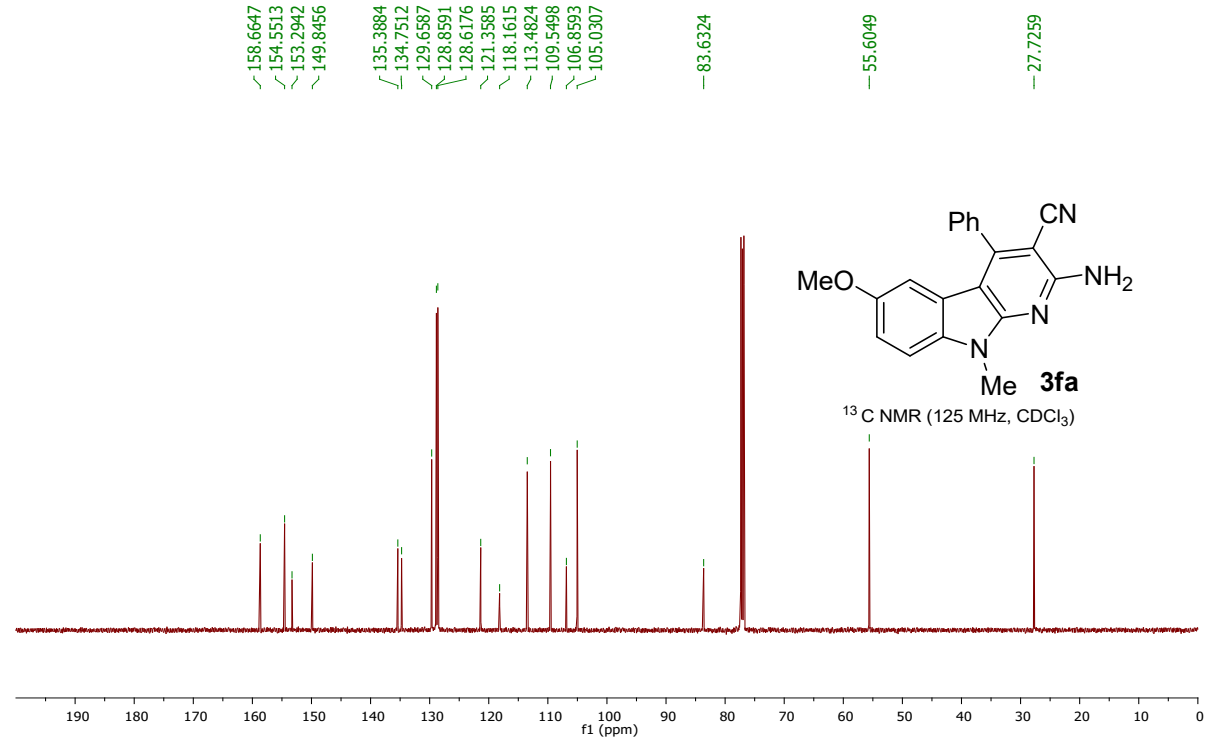
^{13}C NMR (125 MHz, $CDCl_3$)


8.0827
8.0666
8.0046
7.9889
7.6710
7.6133
7.5998
7.5384
7.5230
7.3573
7.3222
7.2796
7.2704
7.2073
7.1859
7.1715
6.7632
6.7485
6.3460
6.3305
5.6496
5.6181
5.5738
5.5422
5.3380
f1 (ppm)
CN
NH2
N
N
Ph
3cx
1H NMR (500 MHz, CDCl3)
1.06
1.03
1.10
1.00
2.02
5.08
1.09
1.04
1.01
1.02
0.99
2.11
2.00
f1 (ppm)

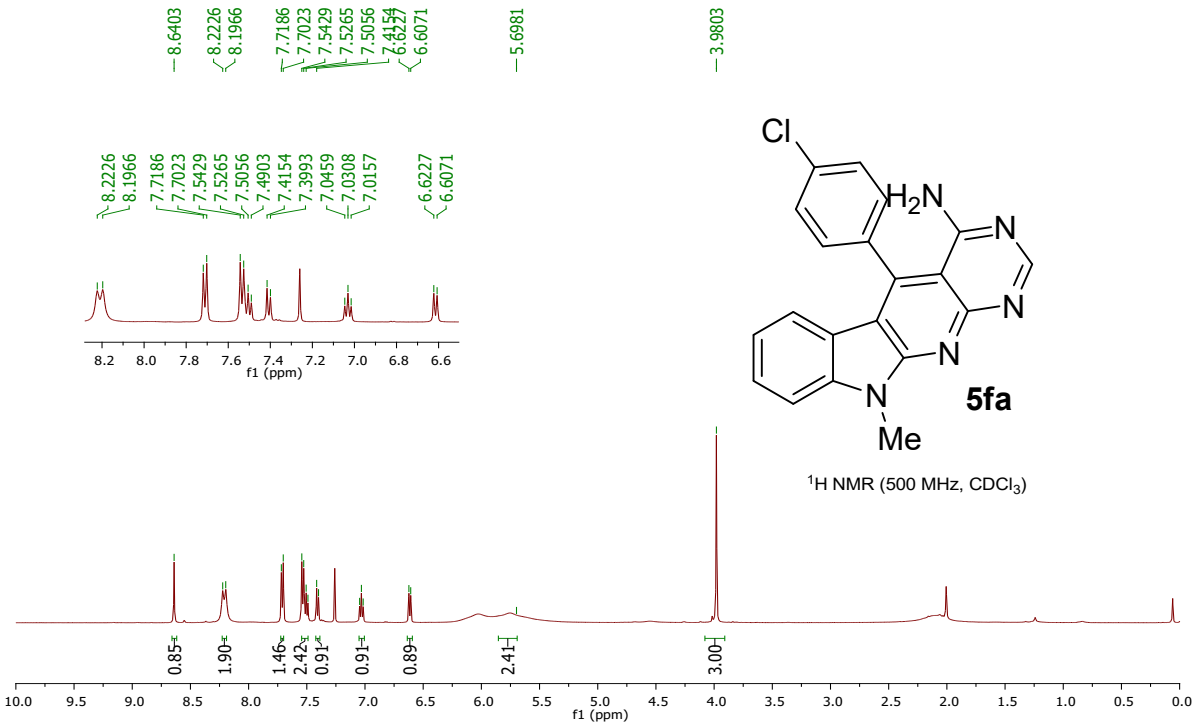

158.8358
152.9805
148.3840
128.8127
128.6154
127.6718
127.1623
126.5470
126.4880
125.5650
121.1531
109.7429
108.2255
85.7507
45.1051
CN
NH2
N
N
Ph
3cx
13C NMR (125 MHz, CDCl3)
f1 (ppm)



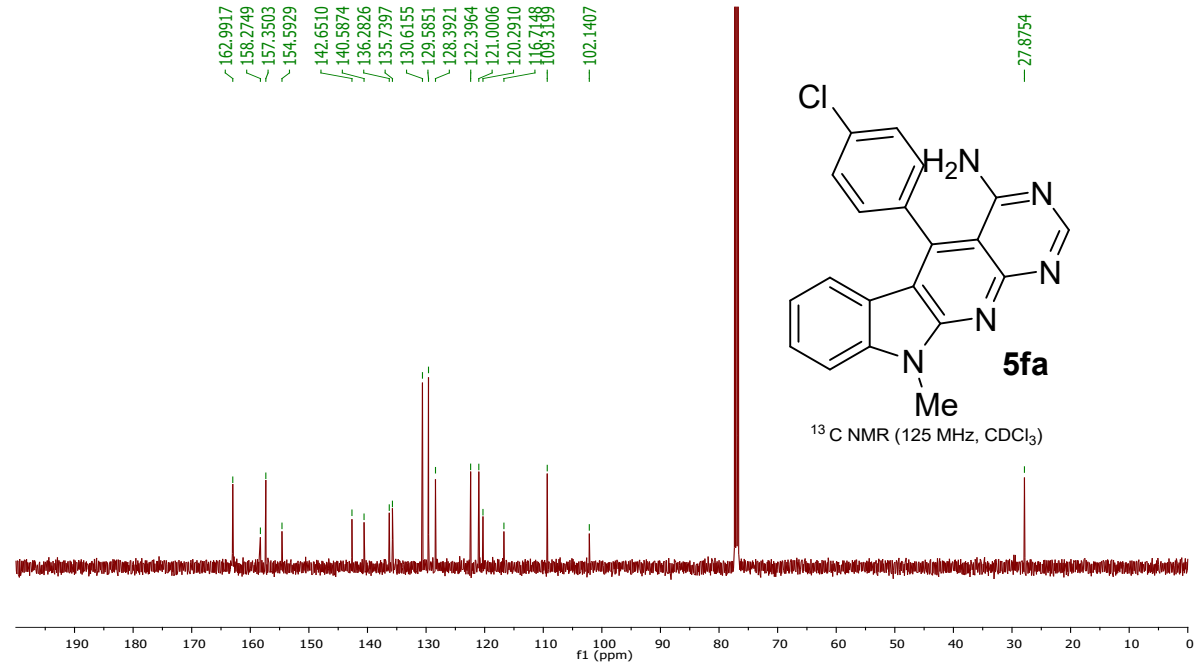
^{1}H NMR (500 MHz, $CDCl_3$)



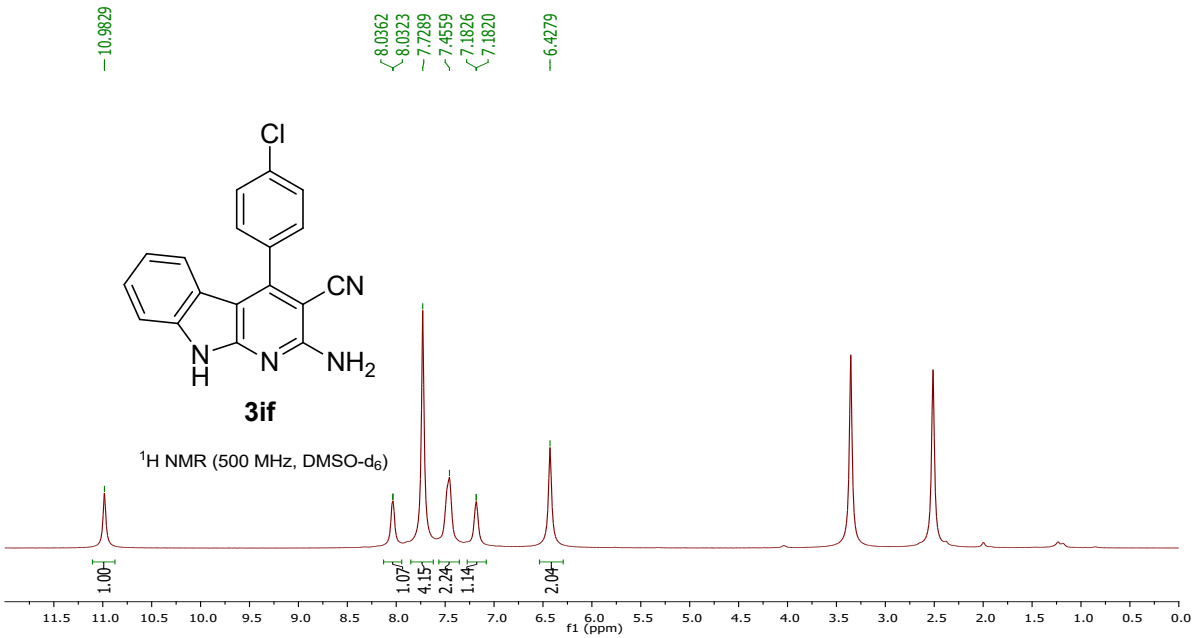
^{13}C NMR (125 MHz, $CDCl_3$)

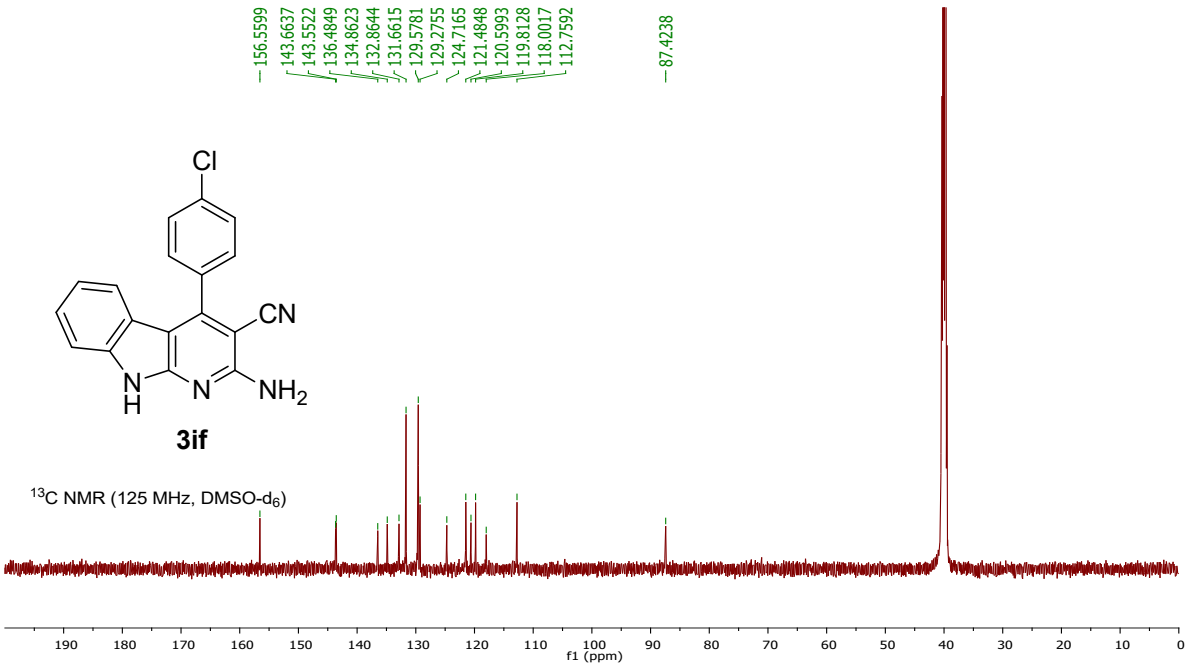


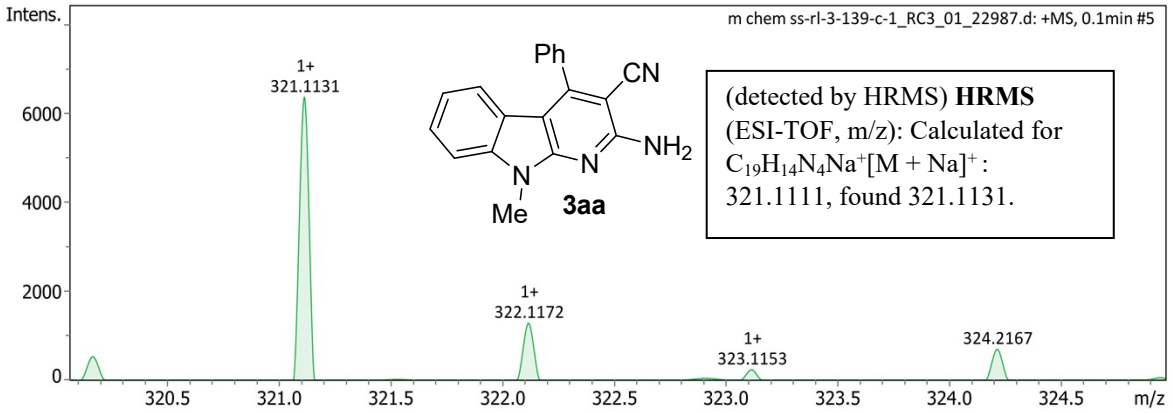
^{1}H NMR (500 MHz, $CDCl_3$)



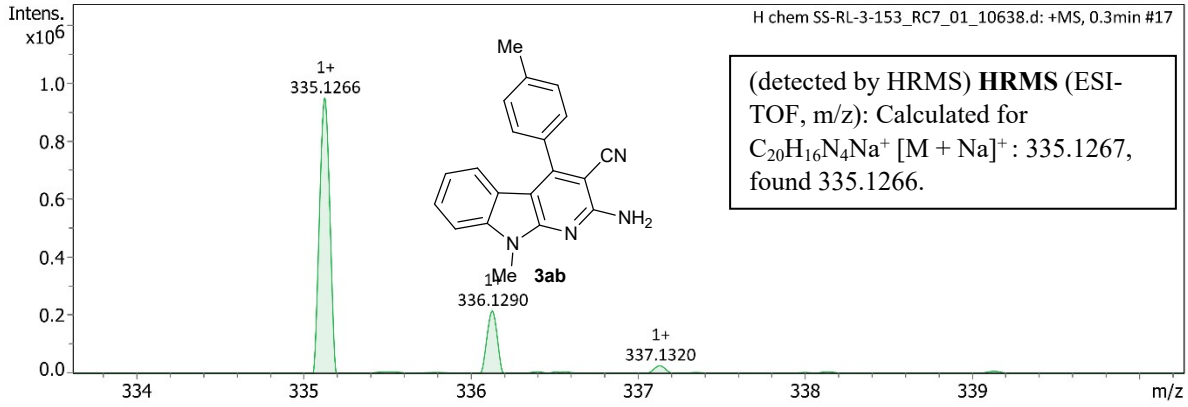
^{13}C NMR (125 MHz, $CDCl_3$)


10.9829
8.0362
8.0323
7.7289
7.4559
7.1826
7.1820
6.4279
Cl
CN
N
H
N
NH2
3if
1H NMR (500 MHz, DMSO-d6)
1.00
1.07
4.15
2.24
1.14
2.04
f1 (ppm)

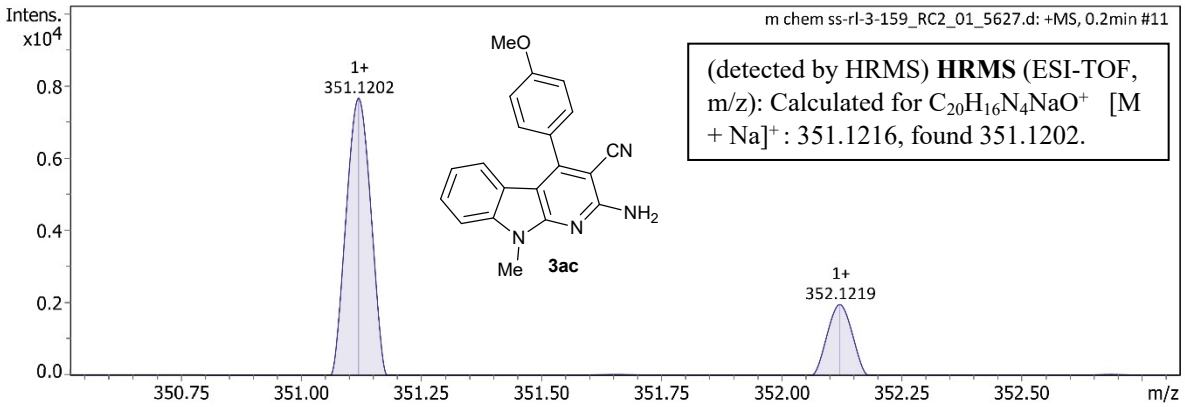

156.5599
143.6637
143.5522
136.4849
134.8623
132.8644
131.6615
129.5781
129.2755
124.7165
121.4848
120.5993
119.8128
118.0017
112.7592
87.4238
Cl
CN
N
H
N
NH2
3if
13C NMR (125 MHz, DMSO-d6)
f1 (ppm)



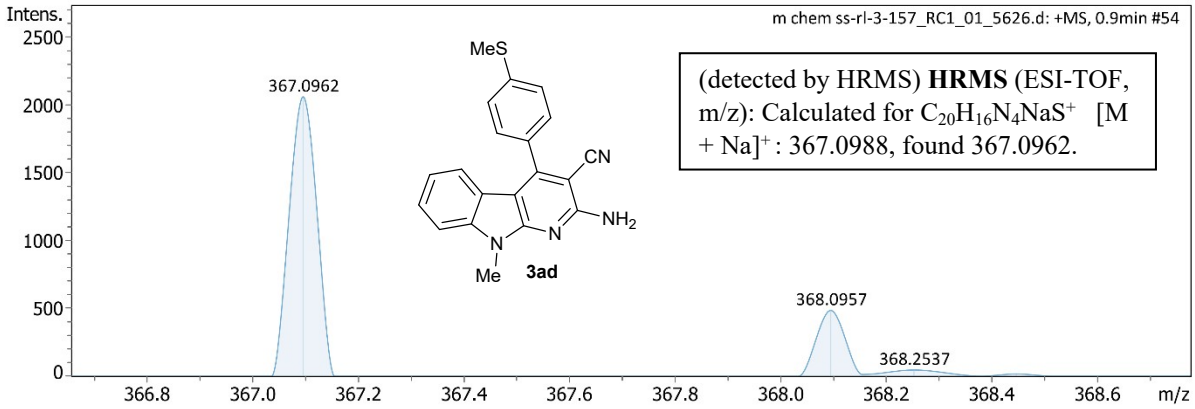
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{14}N_4Na^+$[M + Na]$^+$: 321.1111, found 321.1131.



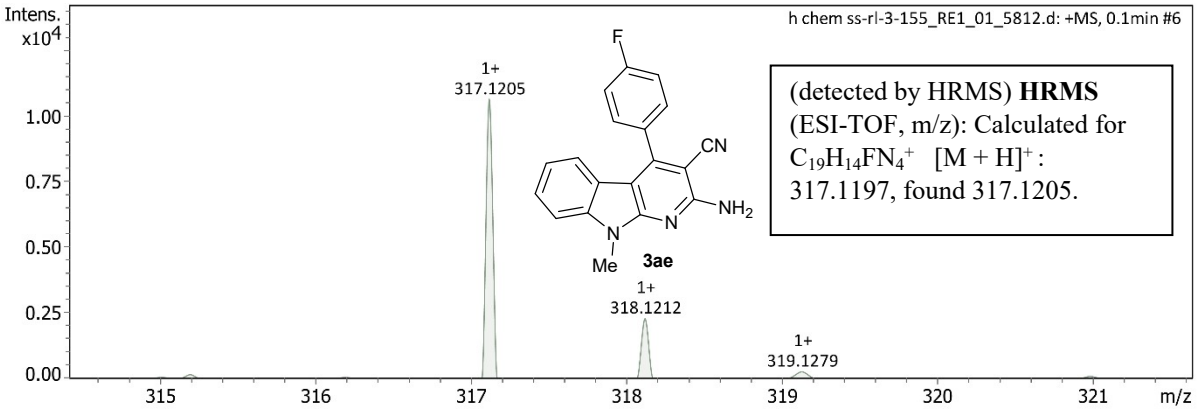
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{20}H_{16}N_4Na^+$ [M + Na]$^+$: 335.1267, found 335.1266.



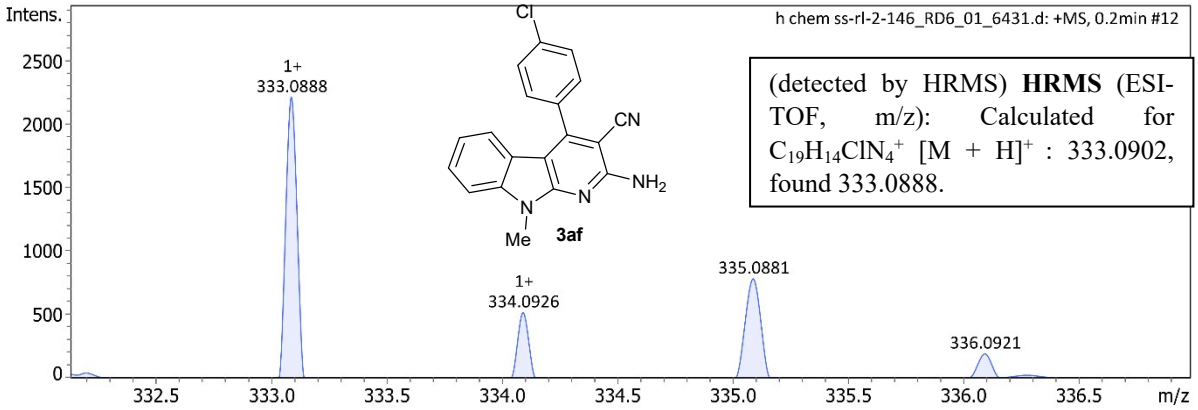
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{20}H_{16}N_4NaO^+$ [M + Na]$^+$: 351.1216, found 351.1202.



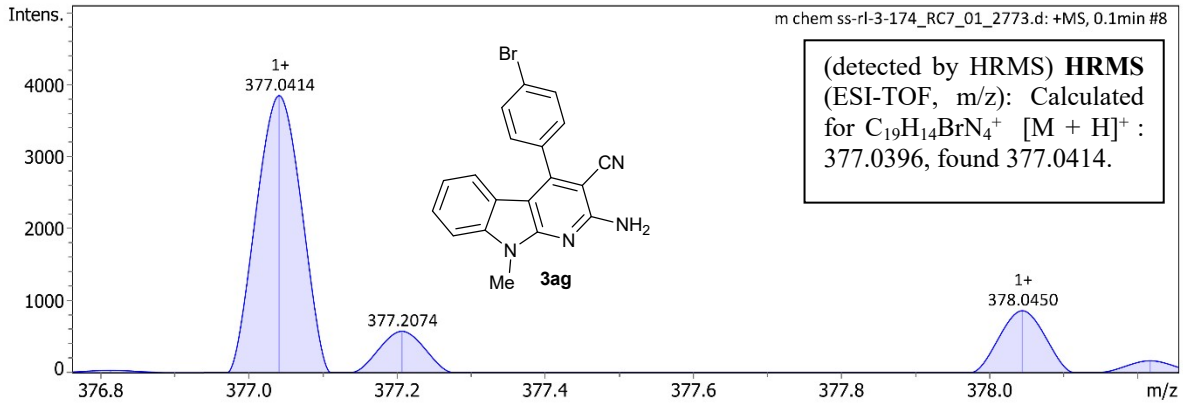
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{20}H_{16}N_4NaS^+$ $[M + Na]^+$: 367.0988, found 367.0962.



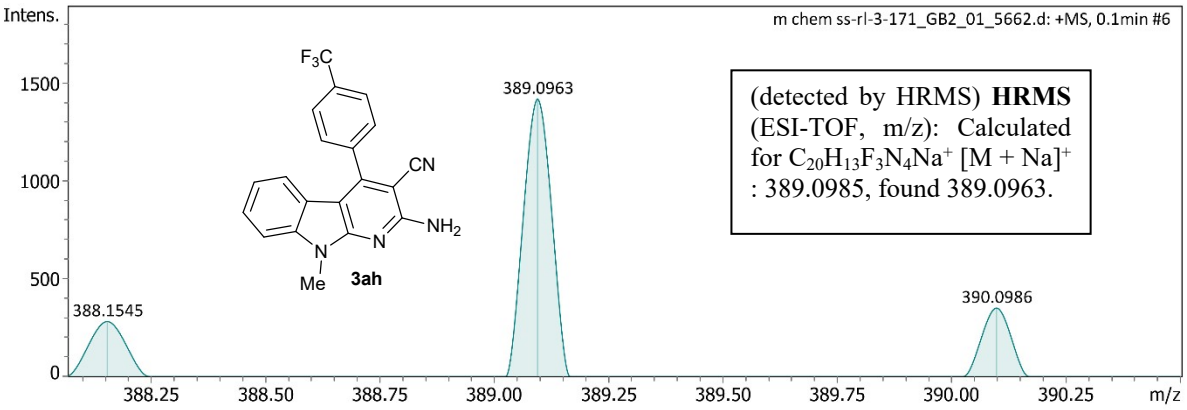
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{14}FN_4^+$ $[M + H]^+$: 317.1197, found 317.1205.



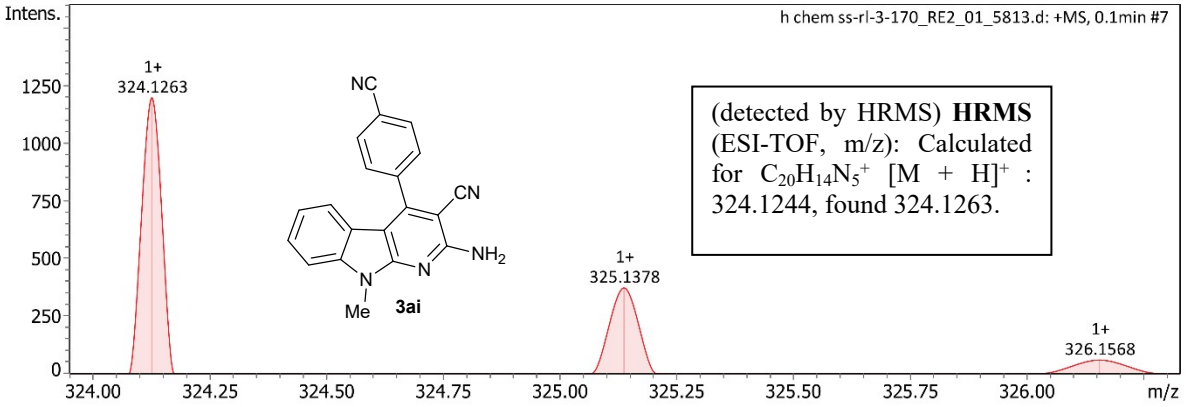
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{14}ClN_4^+$ $[M + H]^+$: 333.0902, found 333.0888.



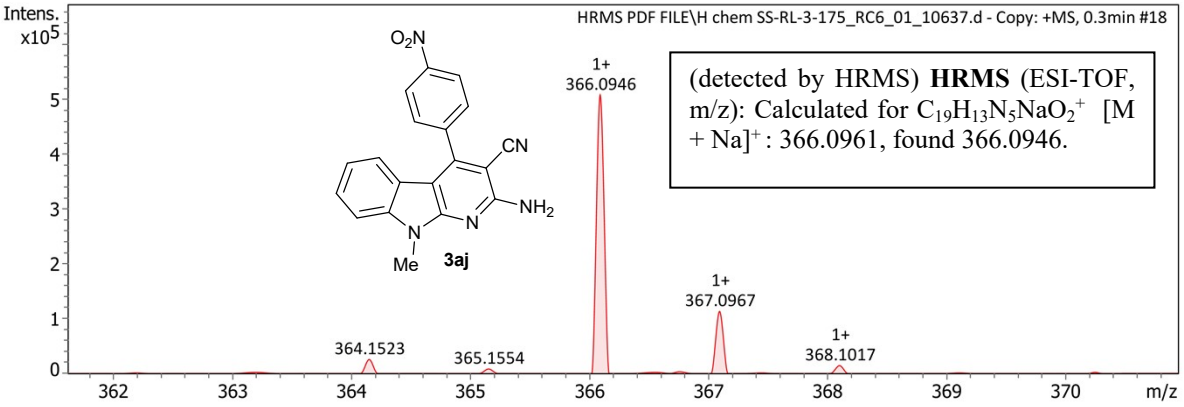
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{14}BrN_4^+$ $[M + H]^+$: 377.0396, found 377.0414.



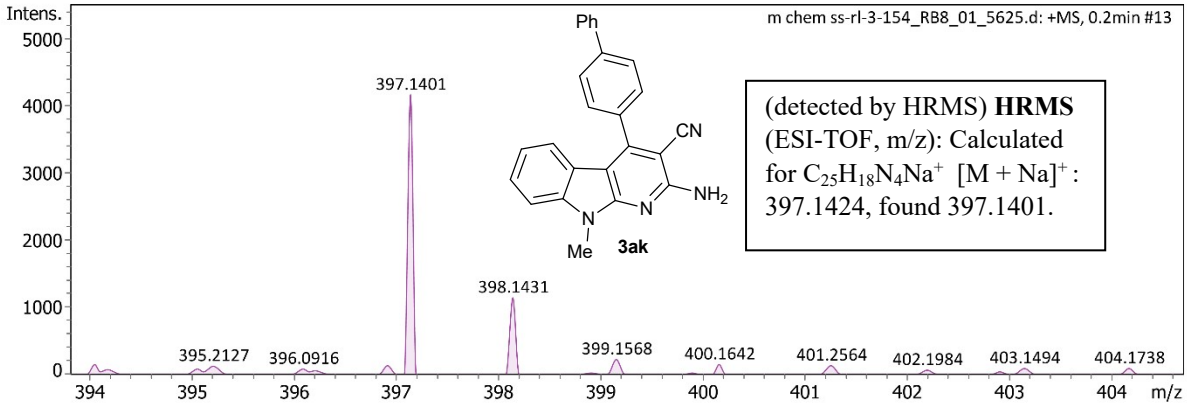
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{20}H_{13}F_3N_4Na^+$ $[M + Na]^+$: 389.0985, found 389.0963.



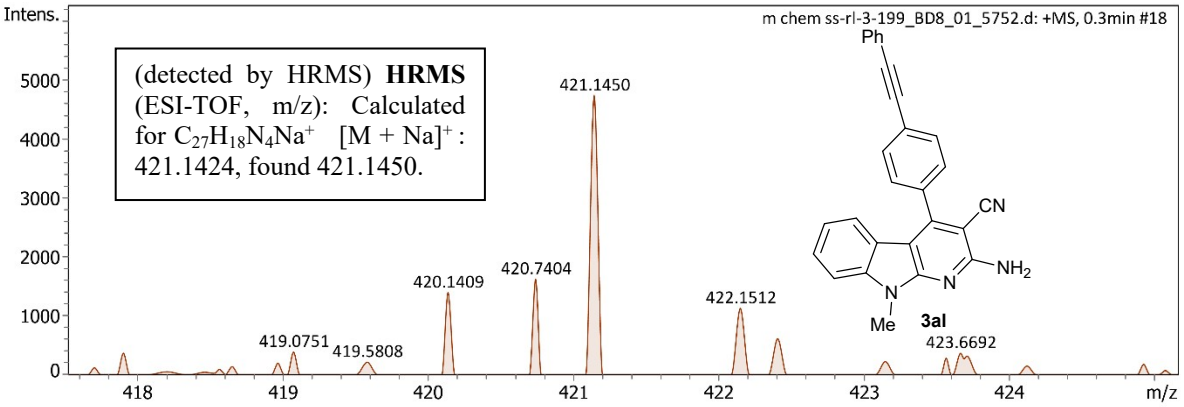
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{20}H_{14}N_5^+$ $[M + H]^+$: 324.1244, found 324.1263.



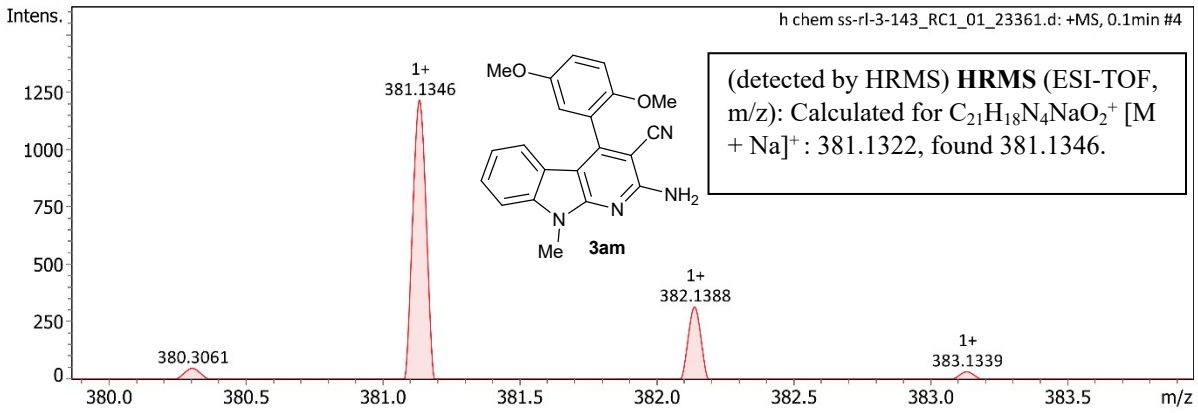
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{13}N_5NaO_2^+$ $[M + Na]^+$: 366.0961, found 366.0946.



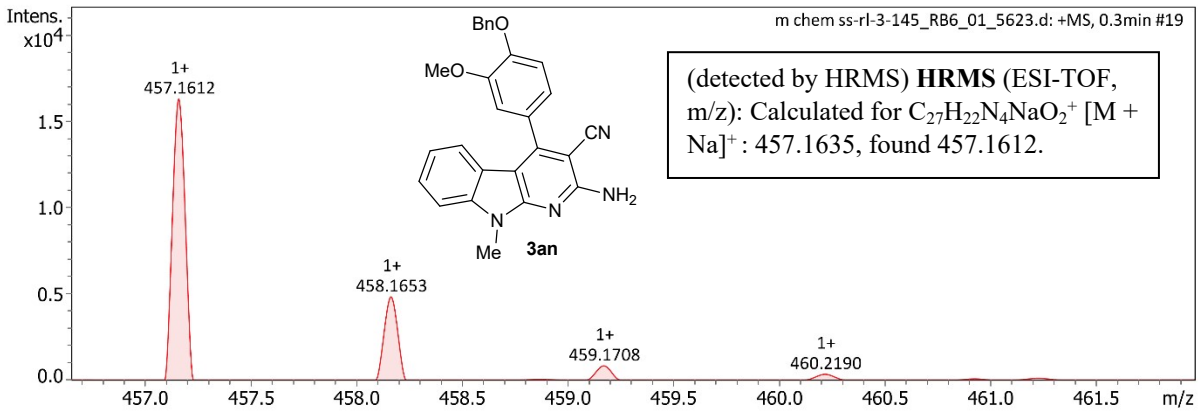
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{25}H_{18}N_4Na^+$ $[M + Na]^+$: 397.1424, found 397.1401.



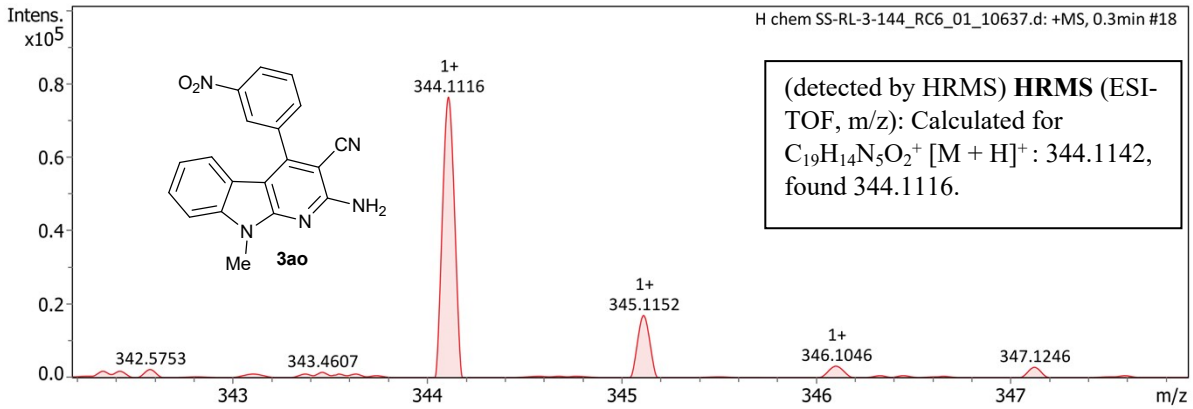
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{27}H_{18}N_4Na^+$ $[M + Na]^+$: 421.1424, found 421.1450.



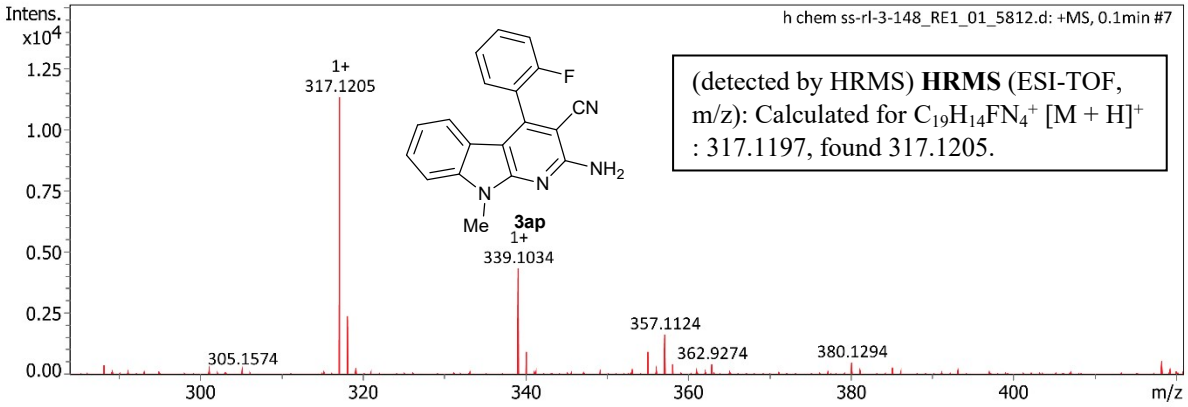
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{21}H_{18}N_4NaO_2^+$ [M + Na]$^+$: 381.1322, found 381.1346.

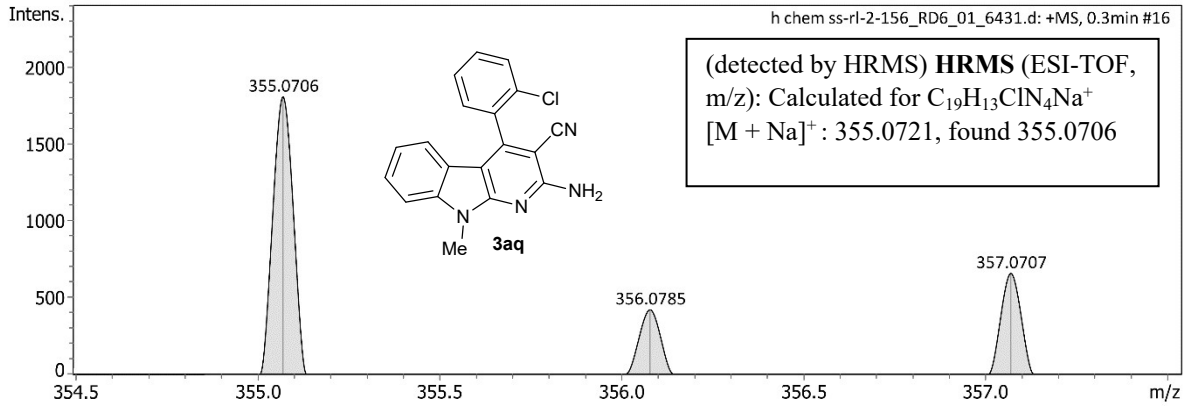


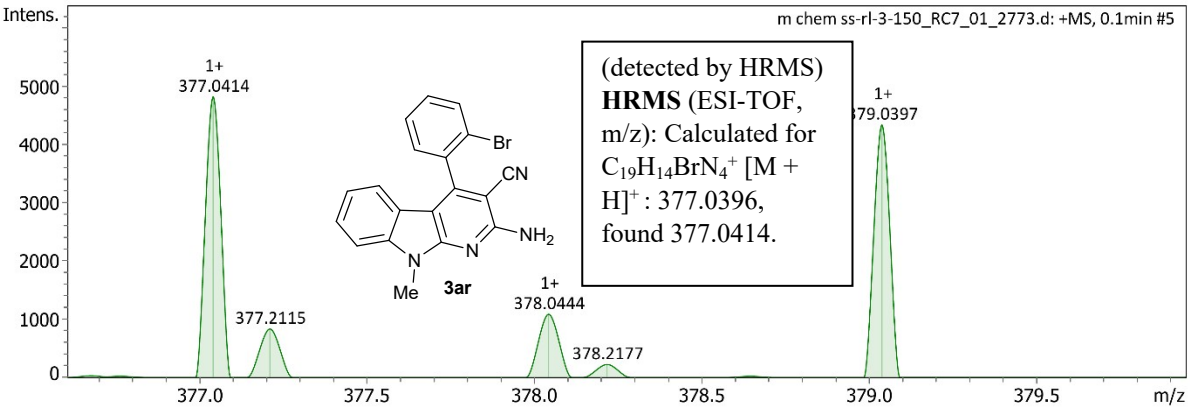
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{27}H_{22}N_4NaO_2^+$ [M + Na]$^+$: 457.1635, found 457.1612.

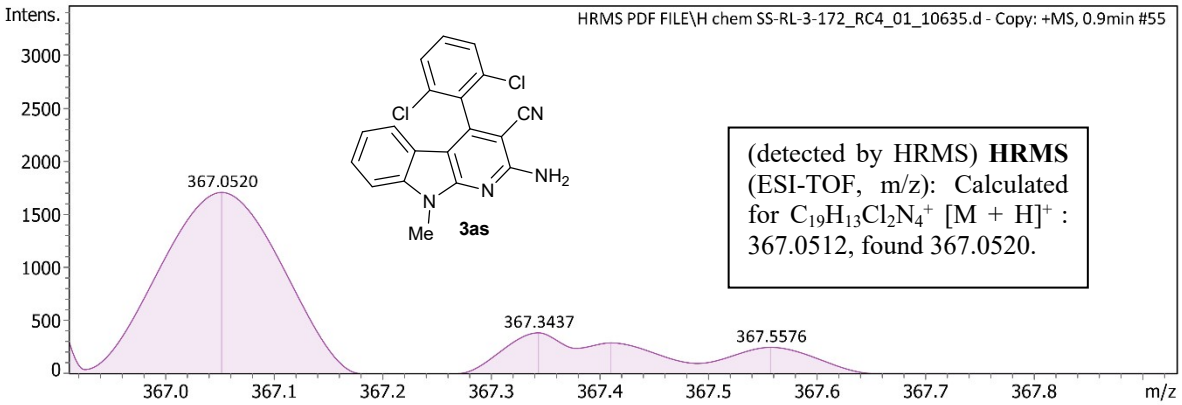


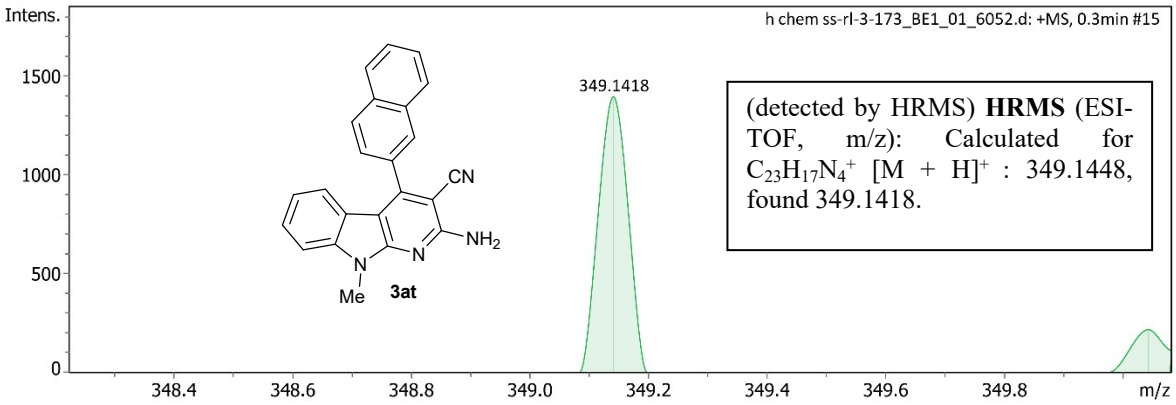
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{14}N_5O_2^+$ [M + H]$^+$: 344.1142, found 344.1116.

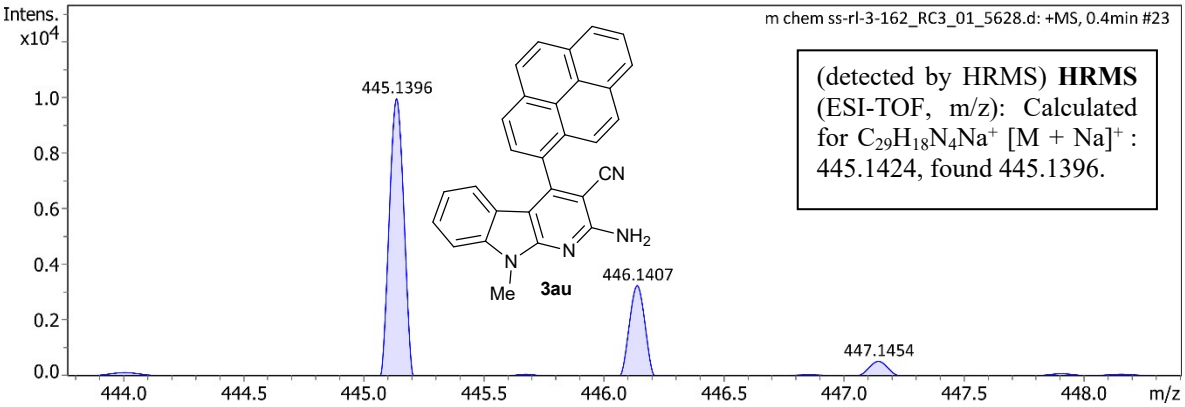

h chem ss-rl-3-148_RE1_01_5812.d: +MS, 0.1min #7
Intens.
x10^4
1.25
1.00
0.75
0.50
0.25
0.00
1+
317.1205
1+
339.1034
305.1574
357.1124
362.9274
380.1294
F
CN
NH2
N
N
Me
3ap
300
320
340
360
380
400
m/z
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{14}FN_4^+$ [M + H]$^+$: 317.1197, found 317.1205.

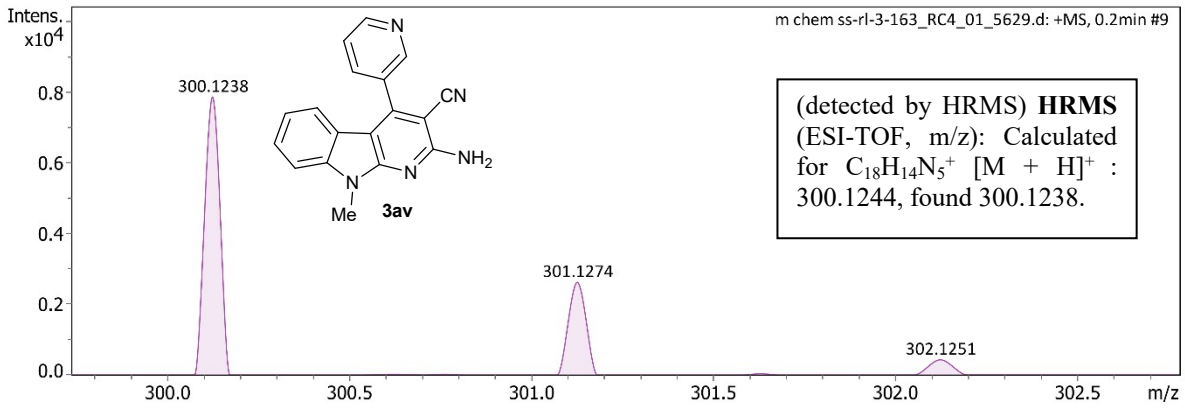

h chem ss-rl-2-156_RD6_01_6431.d: +MS, 0.3min #16
Intens.
2000
1500
1000
500
0
355.0706
356.0785
357.0707
Cl
CN
NH2
N
N
Me
3aq
354.5
355.0
355.5
356.0
356.5
357.0
m/z
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{13}ClN_4Na^+$ [M + Na]$^+$: 355.0721, found 355.0706


m chem ss-rl-3-150_RC7_01_2773.d: +MS, 0.1min #5
Intens.
5000
4000
3000
2000
1000
0
1+
377.0414
377.2115
1+
378.0444
378.2177
1+
379.0397
Br
CN
NH2
N
N
Me
3ar
377.0
377.5
378.0
378.5
379.0
379.5
m/z
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{14}BrN_4^+$ [M + H]$^+$: 377.0396, found 377.0414.

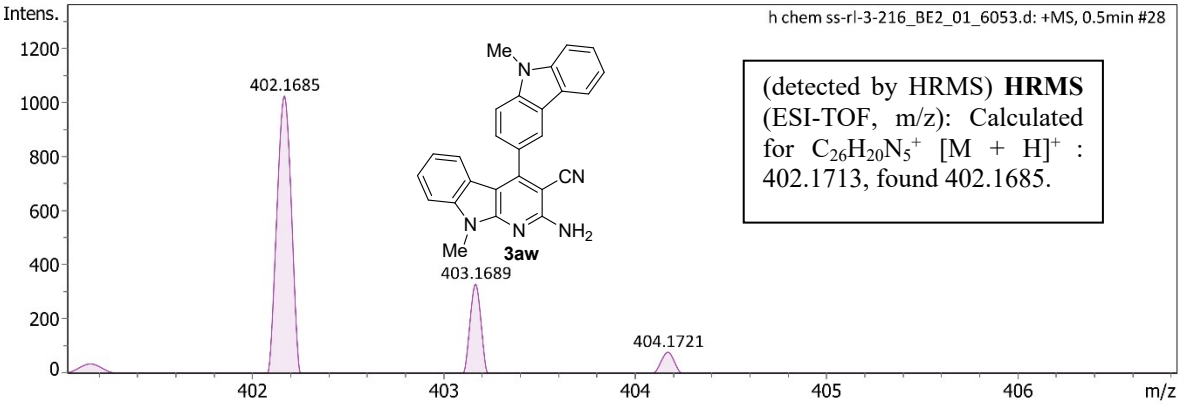

Intens.
HRMS PDF FILE\H chem SS-RL-3-172_RC4_01_10635.d - Copy: +MS, 0.9min #55
Cl
Cl
CN
NH2
N
N
Me
3as
367.0520
367.3437
367.5576
(detected by HRMS) HRMS (ESI-TOF, m/z): Calculated for C19H13Cl2N4+ [M + H]+ : 367.0512, found 367.0520.
m/z


Intens.
h chem ss-rl-3-173_BE1_01_6052.d: +MS, 0.3min #15
CN
NH2
N
N
Me
3at
349.1418
(detected by HRMS) HRMS (ESI-TOF, m/z): Calculated for C23H17N4+ [M + H]+ : 349.1448, found 349.1418.
m/z

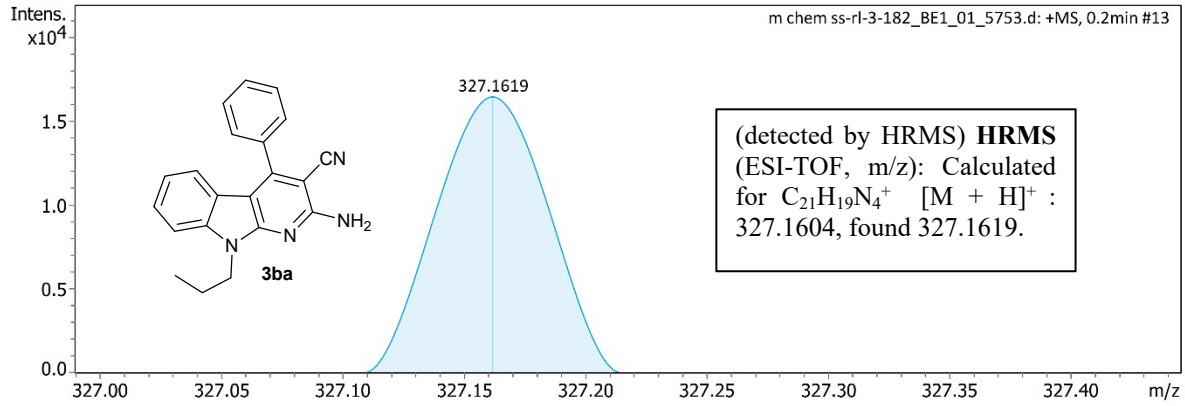

Intens.
x10^4
m chem ss-rl-3-162_RC3_01_5628.d: +MS, 0.4min #23
CN
NH2
N
N
Me
3au
445.1396
446.1407
447.1454
(detected by HRMS) HRMS (ESI-TOF, m/z): Calculated for C29H18N4Na+ [M + Na]+ : 445.1424, found 445.1396.
m/z



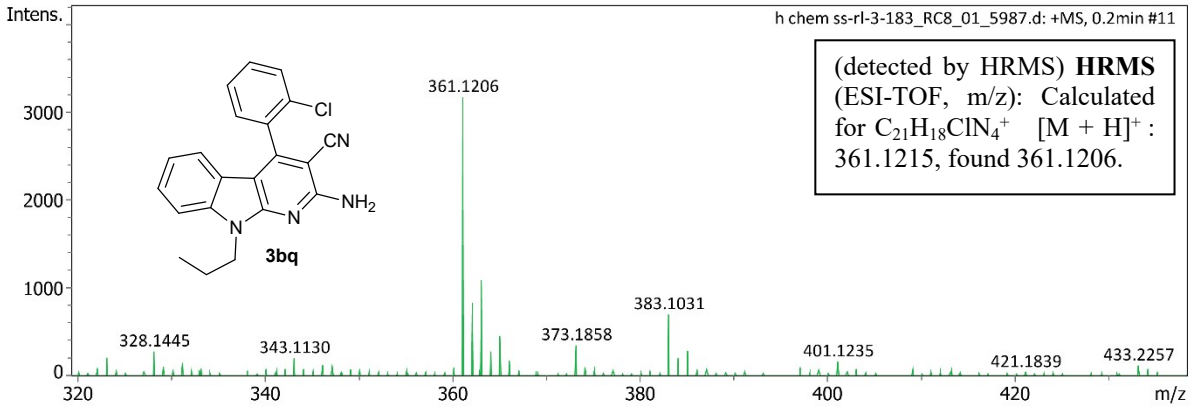
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{18}H_{14}N_5^+$ $[M + H]^+$: 300.1244, found 300.1238.



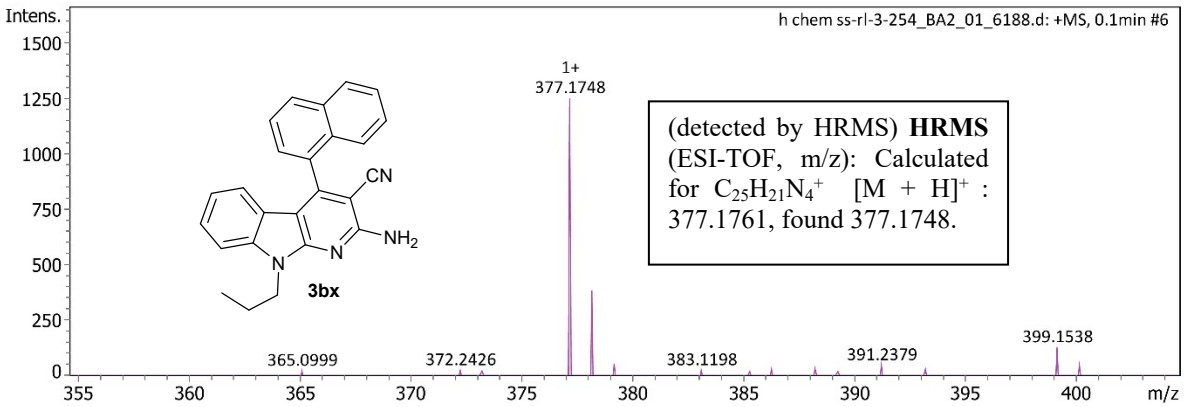
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{26}H_{20}N_5^+$ $[M + H]^+$: 402.1713, found 402.1685.



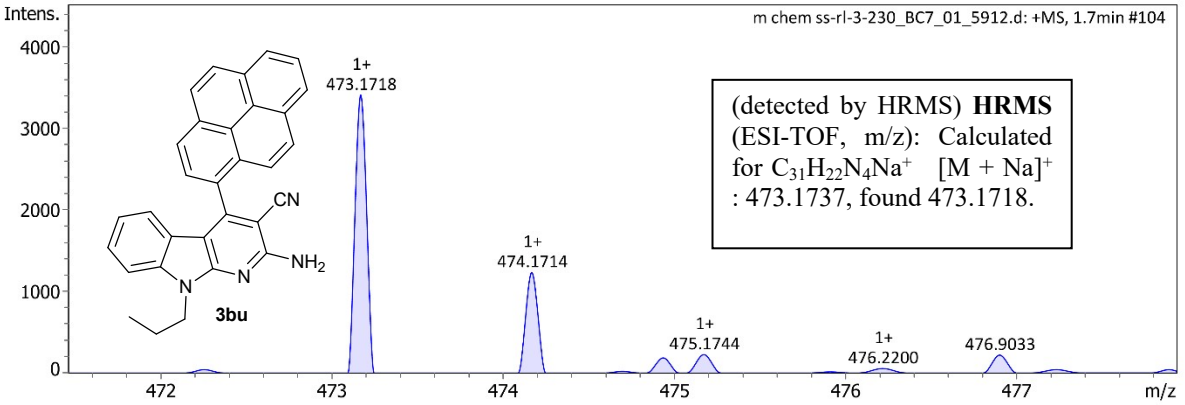
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{21}H_{19}N_4^+$ $[M + H]^+$: 327.1604, found 327.1619.



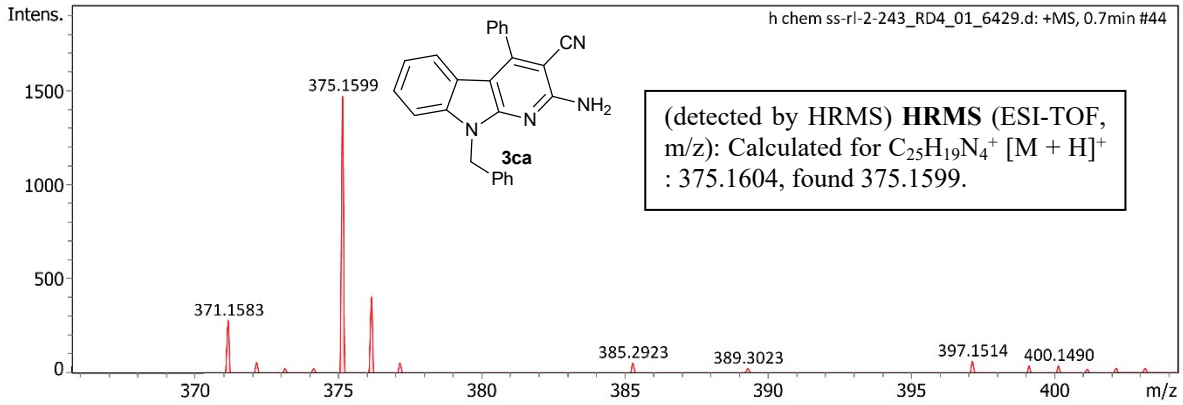
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{21}H_{18}ClN_4^+$ $[M + H]^+$: 361.1215, found 361.1206.

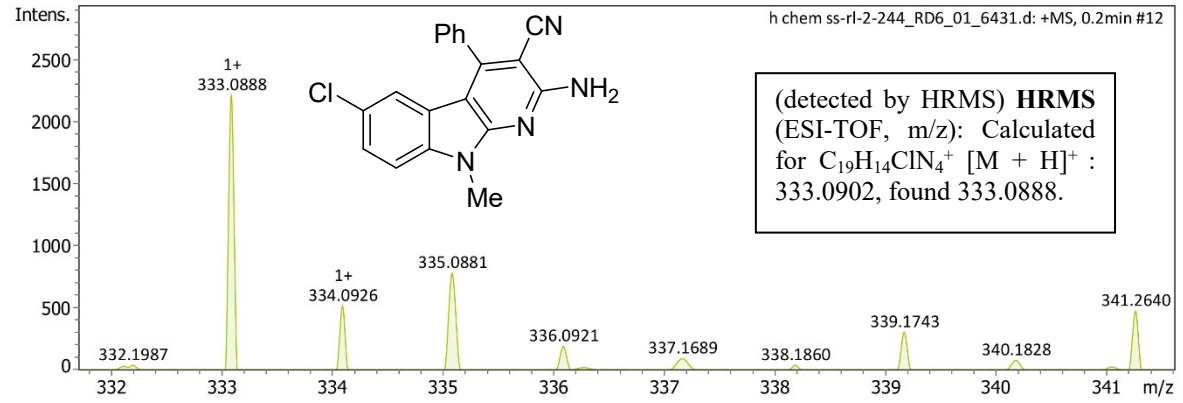


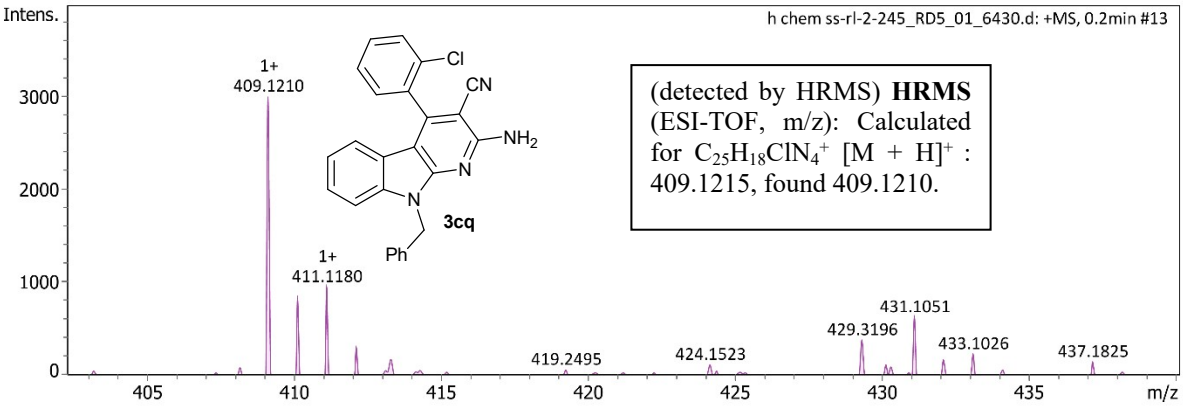
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{25}H_{21}N_4^+$ $[M + H]^+$: 377.1761, found 377.1748.

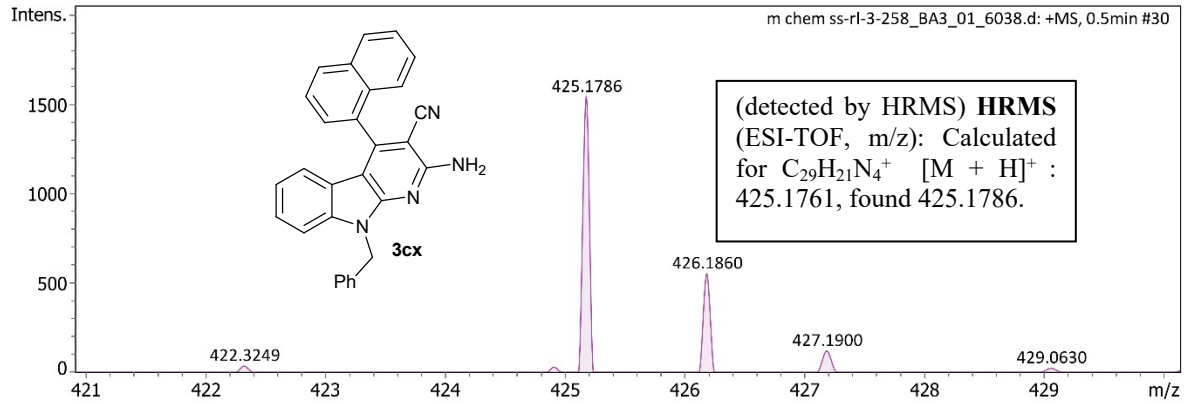


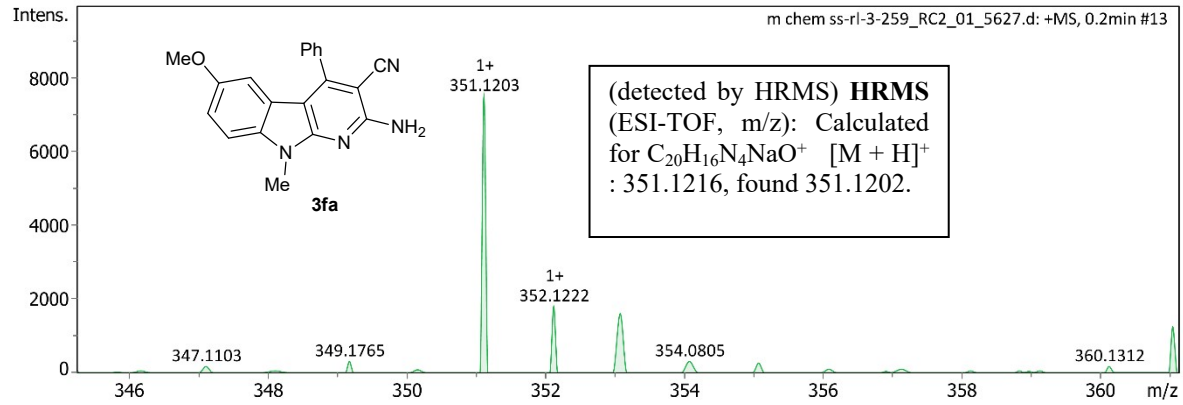
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{31}H_{22}N_4Na^+$ $[M + Na]^+$: 473.1737, found 473.1718.

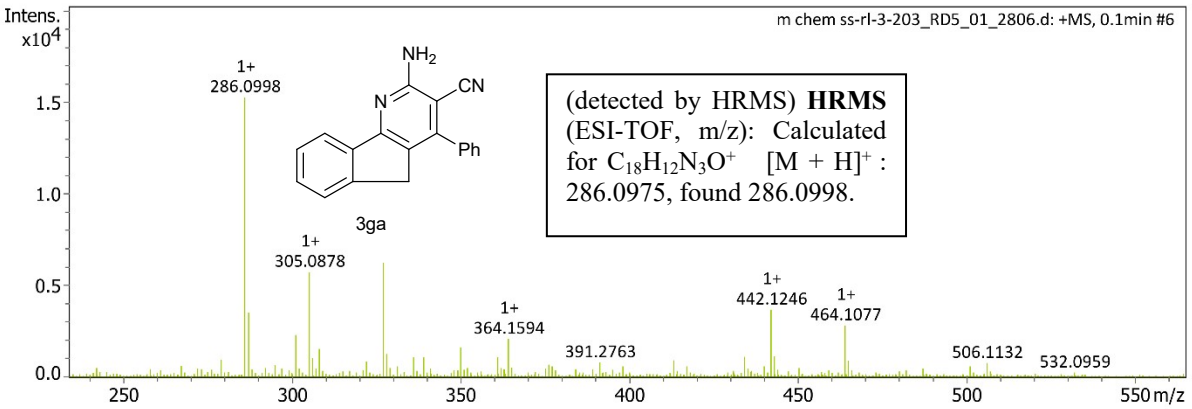

Intens.
h chem ss-rl-2-243_RD4_01_6429.d: +MS, 0.7min #44
1500
1000
500
0
375.1599
371.1583
385.2923
389.3023
397.1514
400.1490
370
375
380
385
390
395
400
m/z
Ph
CN
NH2
N
N
3ca
Ph
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{25}H_{19}N_4^+$ [M + H]$^+$: 375.1604, found 375.1599.


Intens.
h chem ss-rl-2-244_RD6_01_6431.d: +MS, 0.2min #12
2500
2000
1500
1000
500
0
1+
333.0888
1+
334.0926
335.0881
332.1987
336.0921
337.1689
338.1860
339.1743
340.1828
341.2640
332
333
334
335
336
337
338
339
340
341
m/z
Ph
CN
Cl
NH2
N
N
Me
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{19}H_{14}ClN_4^+$ [M + H]$^+$: 333.0902, found 333.0888.

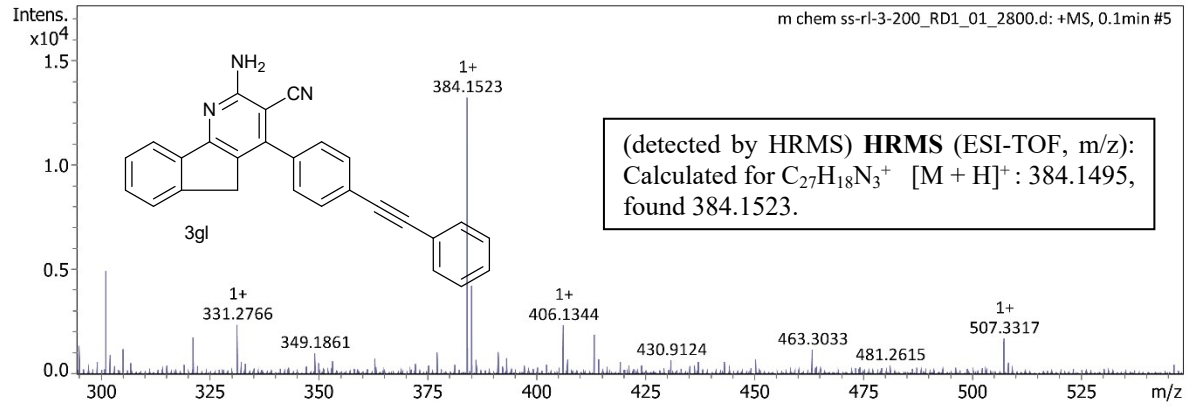

Intens.
h chem ss-rl-2-245_RD5_01_6430.d: +MS, 0.2min #13
1+
409.1210
1+
411.1180
Cl
CN
NH2
N
N
Ph
3cq
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{25}H_{18}ClN_4^+$ $[M + H]^+$: 409.1215, found 409.1210.
419.2495
424.1523
429.3196
431.1051
433.1026
437.1825
m/z


Intens.
m chem ss-rl-3-258_BA3_01_6038.d: +MS, 0.5min #30
CN
NH2
N
N
Ph
3cx
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{29}H_{21}N_4^+$ $[M + H]^+$: 425.1761, found 425.1786.
422.3249
425.1786
426.1860
427.1900
429.0630
m/z

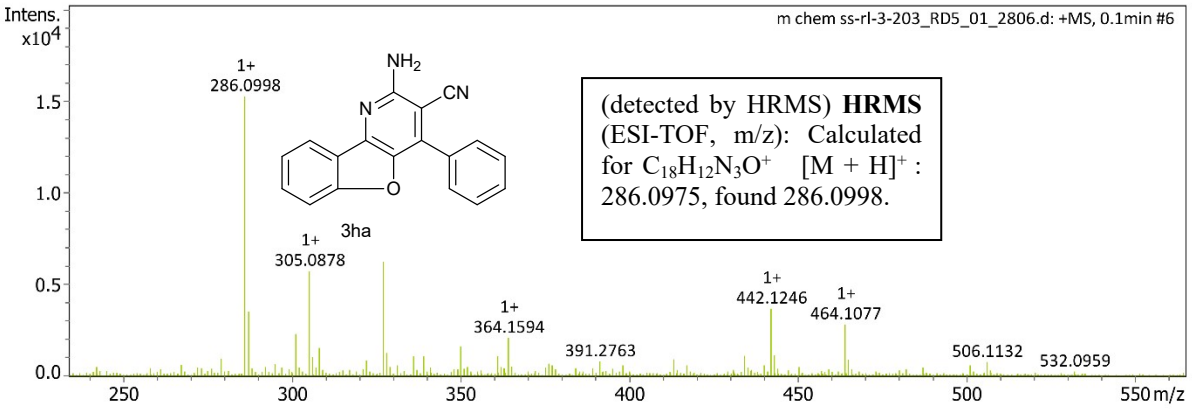

Intens.
m chem ss-rl-3-259_RC2_01_5627.d: +MS, 0.2min #13
MeO
Ph
CN
NH2
N
N
Me
3fa
1+
351.1203
1+
352.1222
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{20}H_{16}N_4NaO^+$ $[M + H]^+$: 351.1216, found 351.1202.
347.1103
349.1765
354.0805
360.1312
m/z



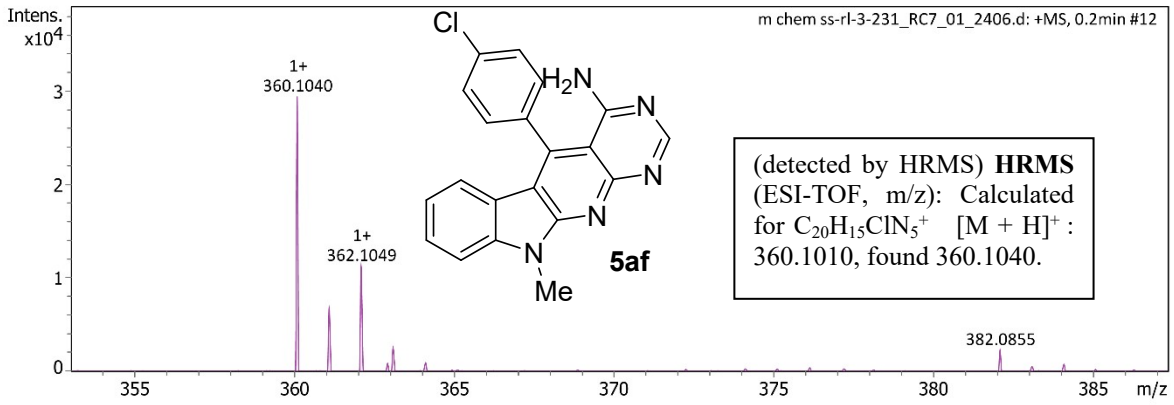
(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{18}H_{12}N_3O^+$ $[M + H]^+$: 286.0975, found 286.0998.



(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{27}H_{18}N_3^+$ $[M + H]^+$: 384.1495, found 384.1523.



(detected by HRMS) **HRMS** (ESI-TOF, m/z): Calculated for $C_{18}H_{12}N_3O^+$ $[M + H]^+$: 286.0975, found 286.0998.


Intens.
x10^4
m chem ss-rl-3-231_RC7_01_2406.d: +MS, 0.2min #12
1+
360.1040
1+
362.1049
382.0855
Cl
H2N
N
N
N
N
Me
5af
(detected by HRMS) HRMS (ESI-TOF, m/z): Calculated for C20H15ClN5+ [M + H]+ : 360.1010, found 360.1040.
m/z