Supporting Information

One-pot sequential C–N coupling and cross dehydrogenative couplings: Synthesis of novel azole fused imidazo[1,2-*a*]pyridines

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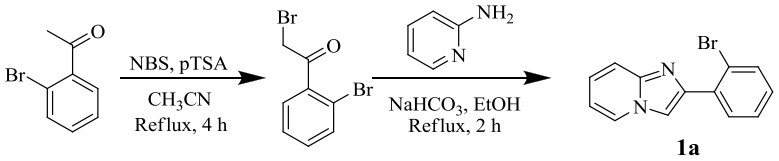
1. General information

All chemicals were obtained from commercial suppliers and used without further purification. Melting points were determined in open capillary tubes on a MPA120-Automated melting point apparatus and are uncorrected. Reactions were monitored by using thin layer chromatography (TLC) on 0.2 mm silica gel F254 plates (Merck). The chemical structures of final products were characterized by nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR) determined on a Bruker NMR spectrometer (300 MHz) or a Varian NMR spectrometer (500 MHz). ^{13}C NMR spectra are fully decoupled. Chemical shifts were reported in parts per million (ppm) using deuterated solvent peak or Tetramethylsilane (internal) as the standard. The chemical structures of final products were confirmed by a high-resolution Biosystems QStar Elite time-of-flight electrospray mass spectrometer.

2. Experimental

*2.1 Preparation of 2-(2-bromophenyl)imidazo[1,2-a]pyridine (**1a**):*



1a

A solution of 2'-bromoacetophenone (5.0 g, 25 mmol), *N*-bromosuccinimide (NBS) (4.5 g, 25 mmol) and *p*-toluenesulphonic acid (7.1 g, 37.5 mmol) in acetonitrile (40 mL) was stirred for 4 h at reflux temperature. After completion of the reaction as indicated by TLC the reaction mass was allowed to cool to ambient temperature and evaporated the volatiles. The residue was diluted with water and the product was extracted into ethyl acetate. Organic layer was dried over anhydrous sodium sulfate and evaporated the volatiles. The crude compound (6.6 gr, 95%, Light brown liquid) was subjected to next step without further purifications.

To a solution of 2-bromo-1-(2-bromophenyl)ethanone (6.5 g, 23.38 mmol) and sodium bicarbonate (2.9 g, 35.07 mmol) in ethanol (65 mL) was added 2-aminopyridine (2.2 g, 23.38 mmol) and reaction mixture was stirred at reflux temperature for 2 h. After completion of the reaction, the reaction mass was allowed to cool to ambient temperature and evaporated the volatiles. The residue was diluted with water and extracted into ethyl acetate. Organic layer was dried over anhydrous sodium sulfate and evaporated the volatiles. The crude compound was purified by column chromatography to get 2-(2-bromophenyl)H-imidazo[1,2-a]pyridine (**1a**) as pale yellow solid.

Similarly, **1b-f** were prepared using 5-bromo-2-aminopyridine, 5-methyl-2-aminopyridine, 6-methyl-2-aminopyridine, 5-fluoro-2-aminopyridine and 5-chloro-2-aminopyridine, respectively.

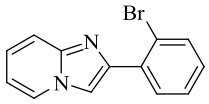
1a: Yield: 4.15 g, (65%); mp 80-81 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (s, 1H), 8.17 – 8.13 (m, 2H), 7.68 – 7.62 (m, 2H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 2H), 6.78 (t, *J* = 6.7 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.5, 143.3, 134.5, 133.6, 131.7, 128.9, 127.5, 125.7, 124.7, 121.5, 117.7, 112.4, 112.0. HRMS calcd for 271.9949, found 272.9788 $[M + H]^+$ and 274.9784 $[M + H + 2]^+$

1d: White solid; Yield 62 %; mp 98-99 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.21 (s, 1H), 8.17 (d, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 6.9 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.49 – 7.36 (m, 2H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.63 (d, *J* = 6.8 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.28,

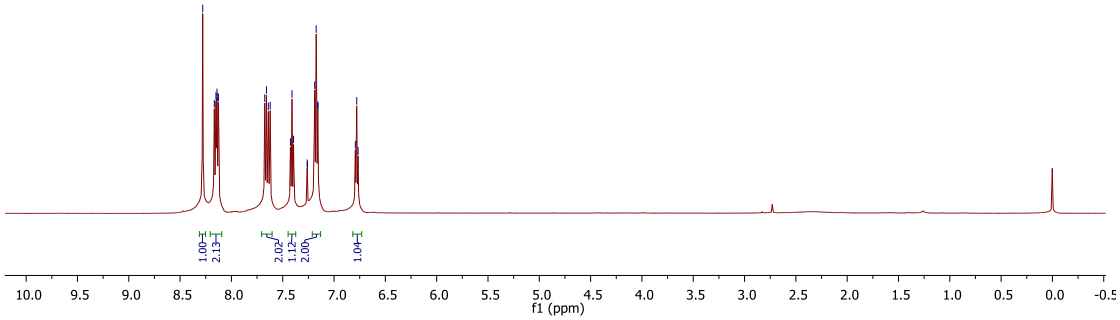
143.27, 136.09, 134.92, 133.96, 132.01, 129.02, 127.77, 125.25, 121.82, 116.27, 115.47, 111.73, 21.58.

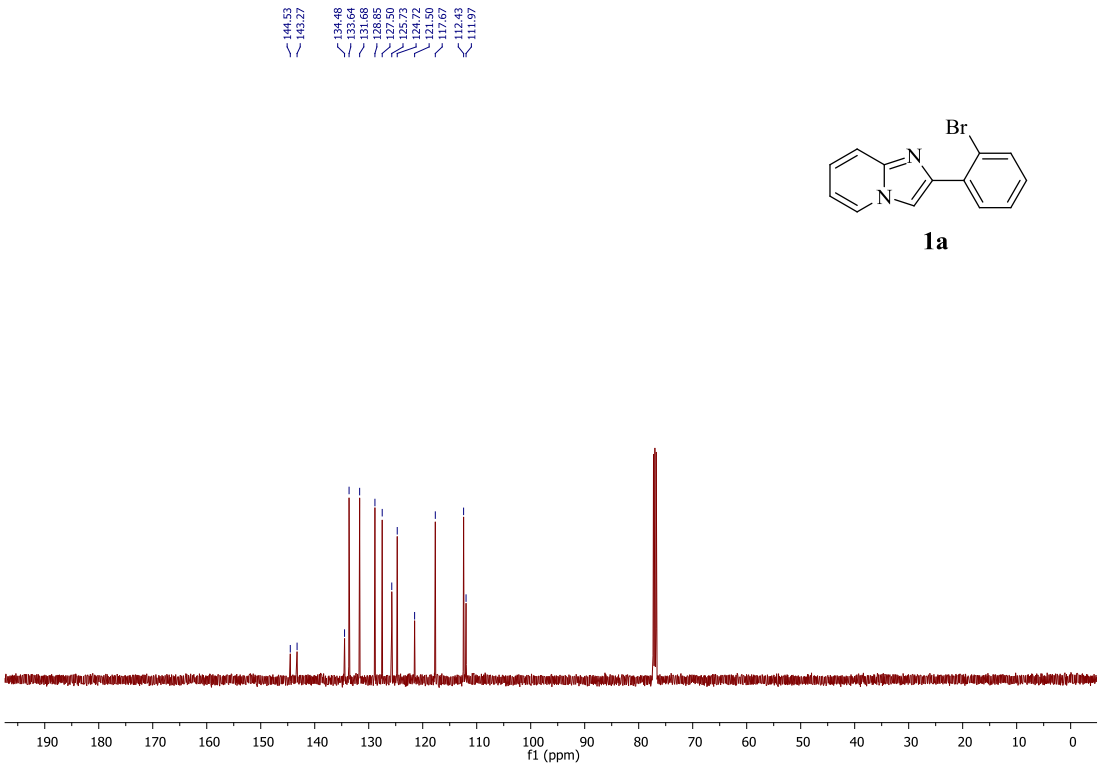
1e: Yield: 56%; mp 109-110 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.18 – 8.06 (m, 2H), 7.76 – 7.61 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.31 – 7.09 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.33, 152.18, 144.93, 142.61, 134.51, 134.02, 131.98, 129.40, 127.85, 121.85, 118.51, 118.39, 117.41, 117.07, 113.59, 112.84, 112.30.

1f: Yield: 63%; mp 118-119 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.28 (s, 1H), 8.23 (s, 1H), 8.15 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.73 – 7.60 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.15 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.64, 143.19, 134.36, 134.04, 132.03, 129.46, 127.85, 126.53, 123.85, 121.87, 121.05, 118.30, 112.63.



1a

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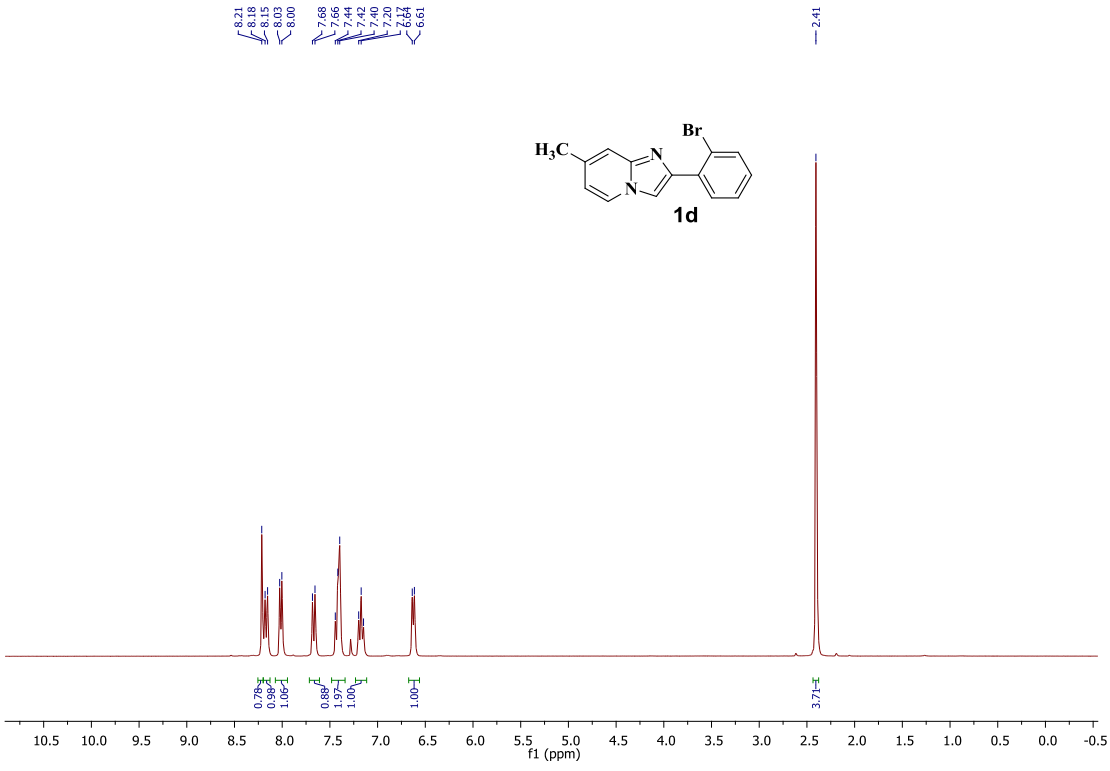
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1.00
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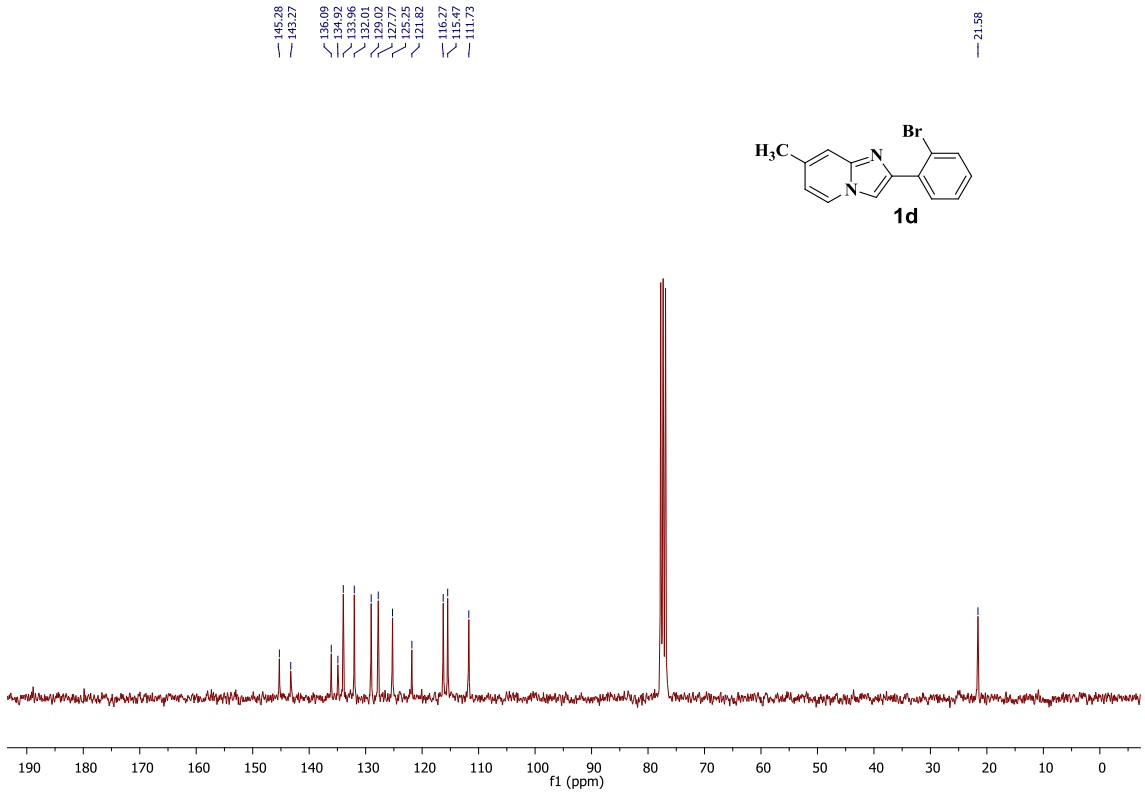
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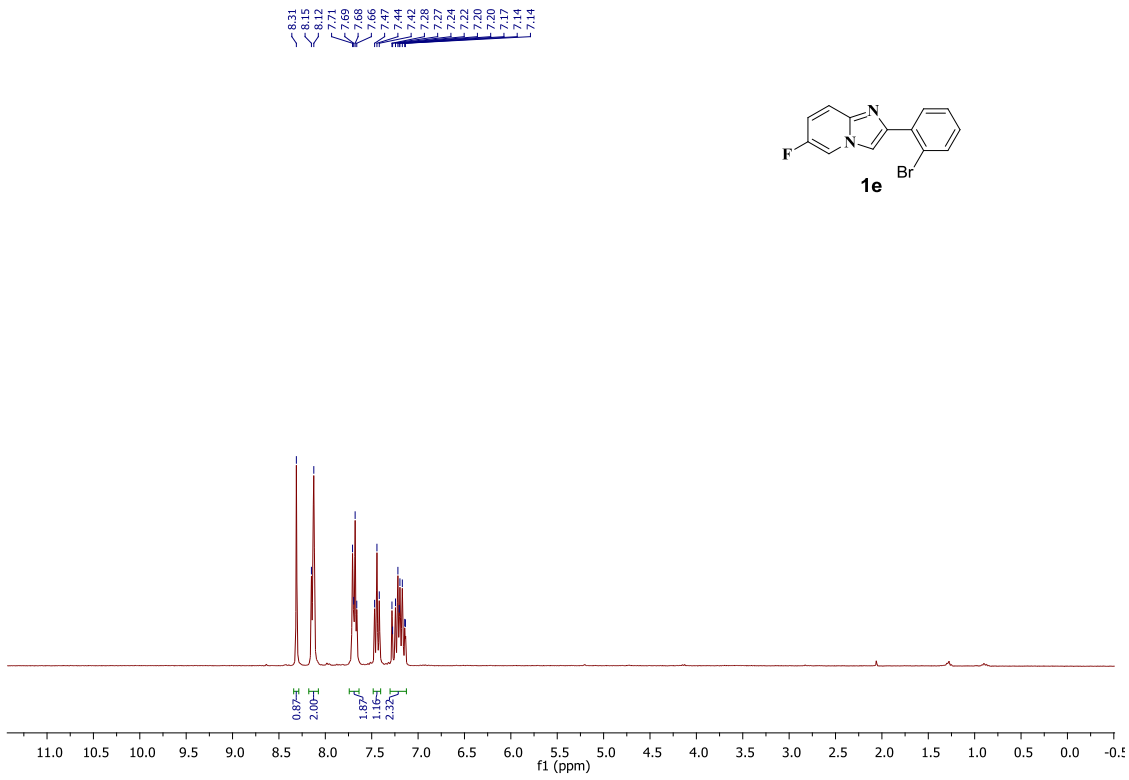
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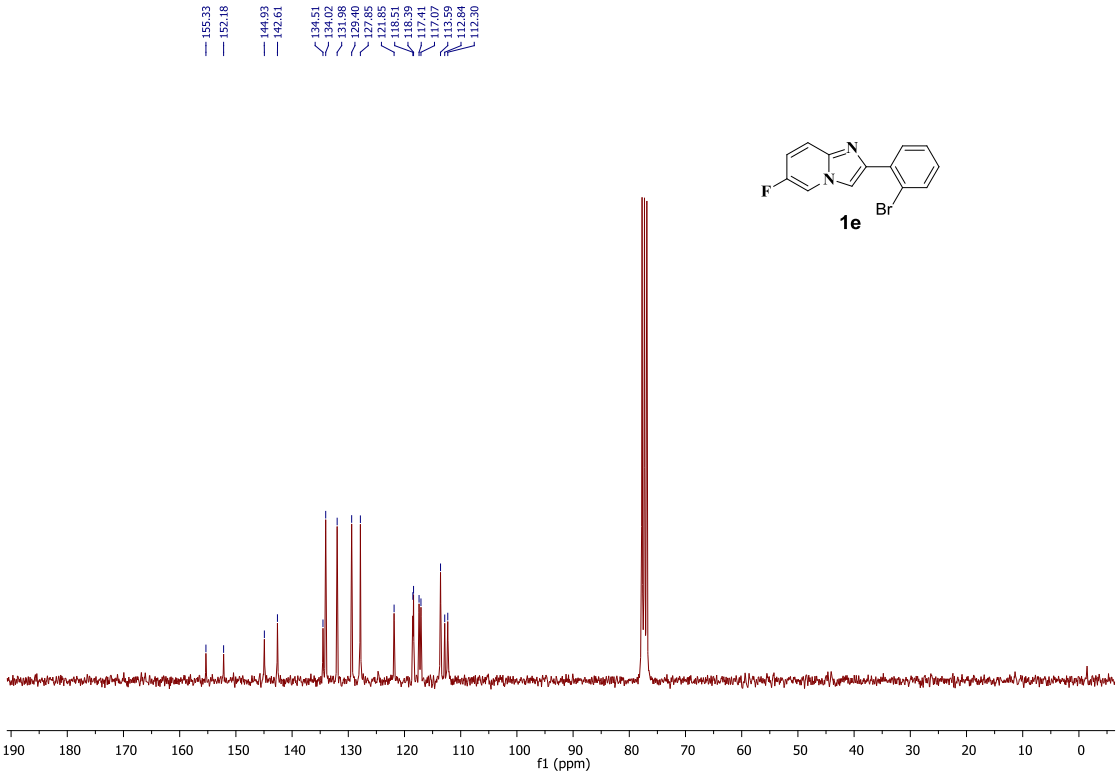
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F
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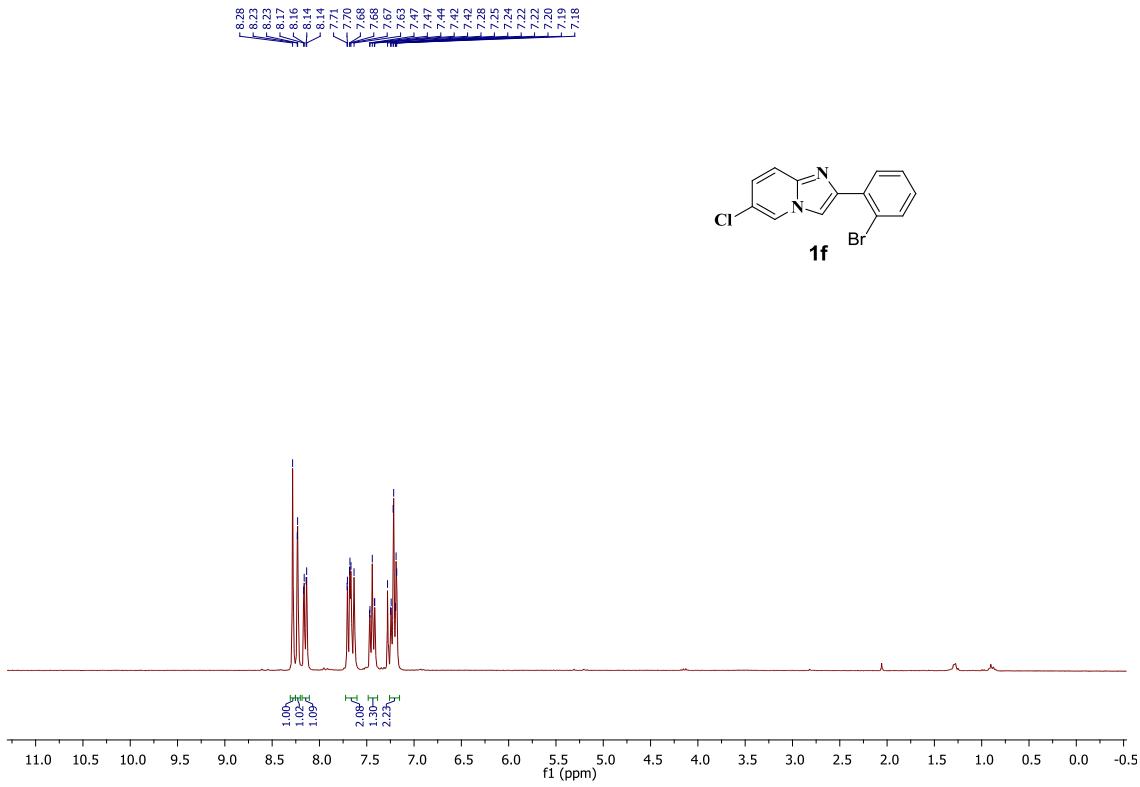
Br
1e
f1 (ppm)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7.22
7.20
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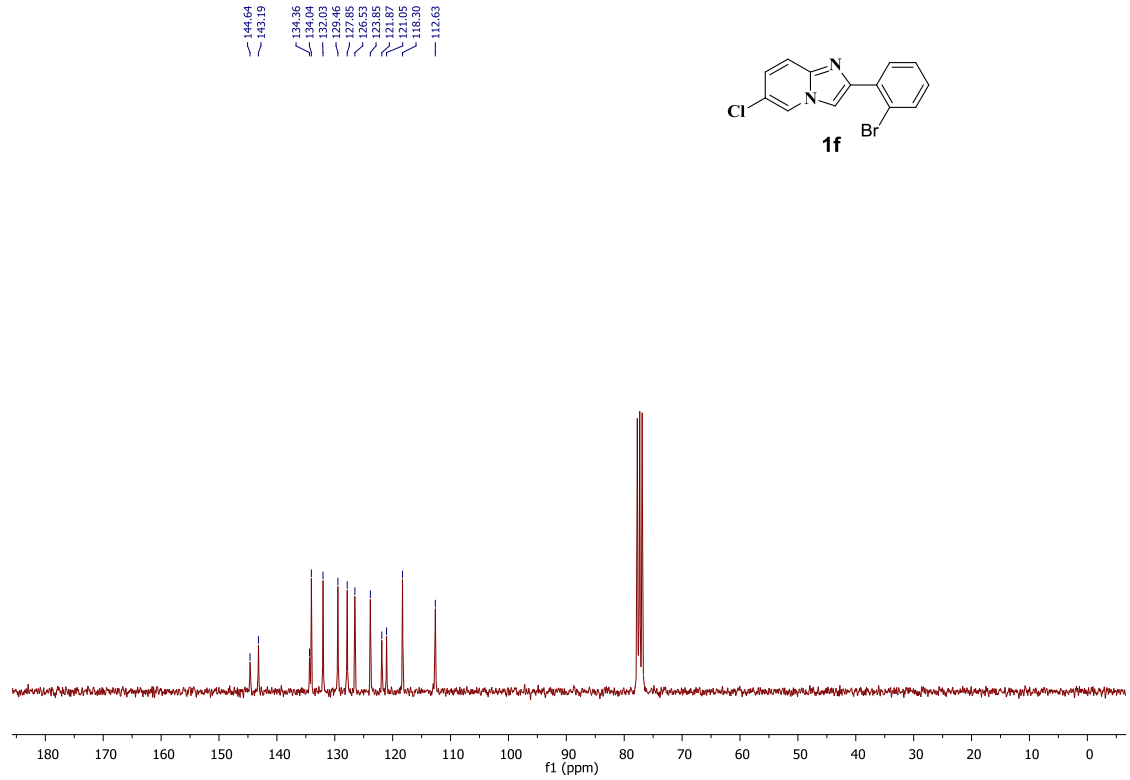
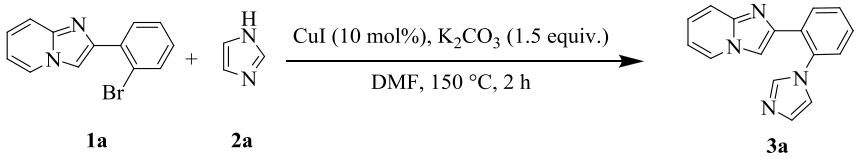


*2.2 Preparation of 2-(2-(1H-imidazol-1-yl)phenyl)imidazo[1,2-a]pyridine (**3a**):*

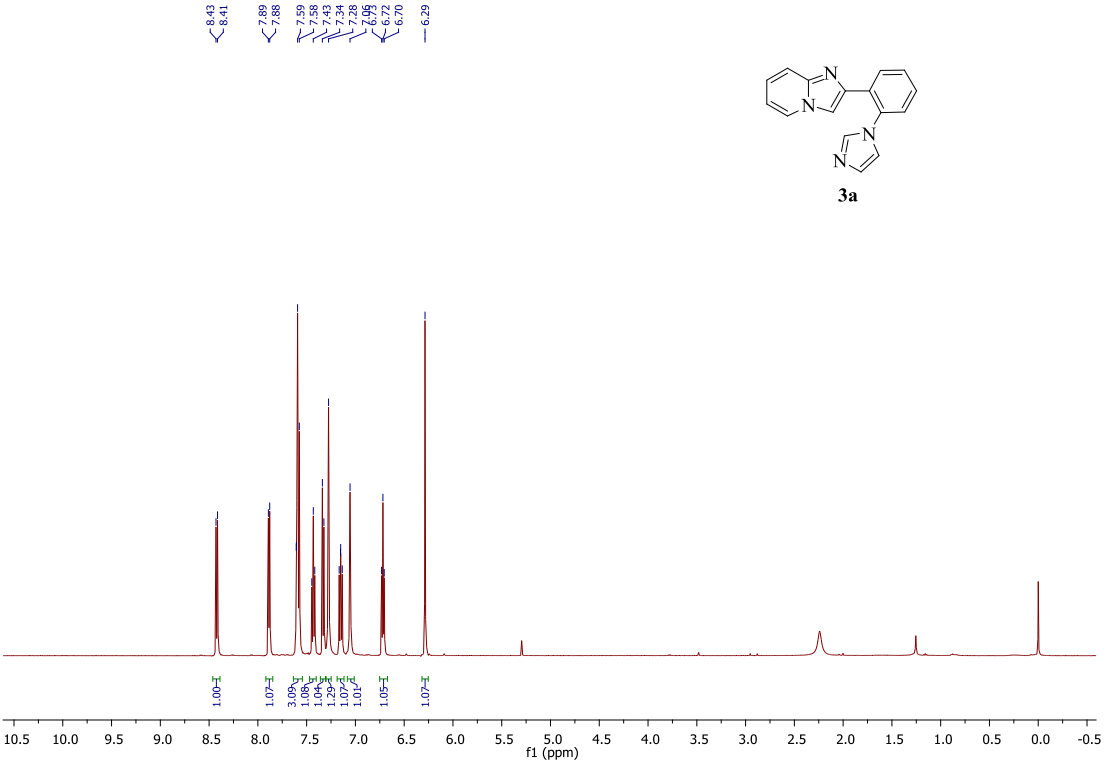


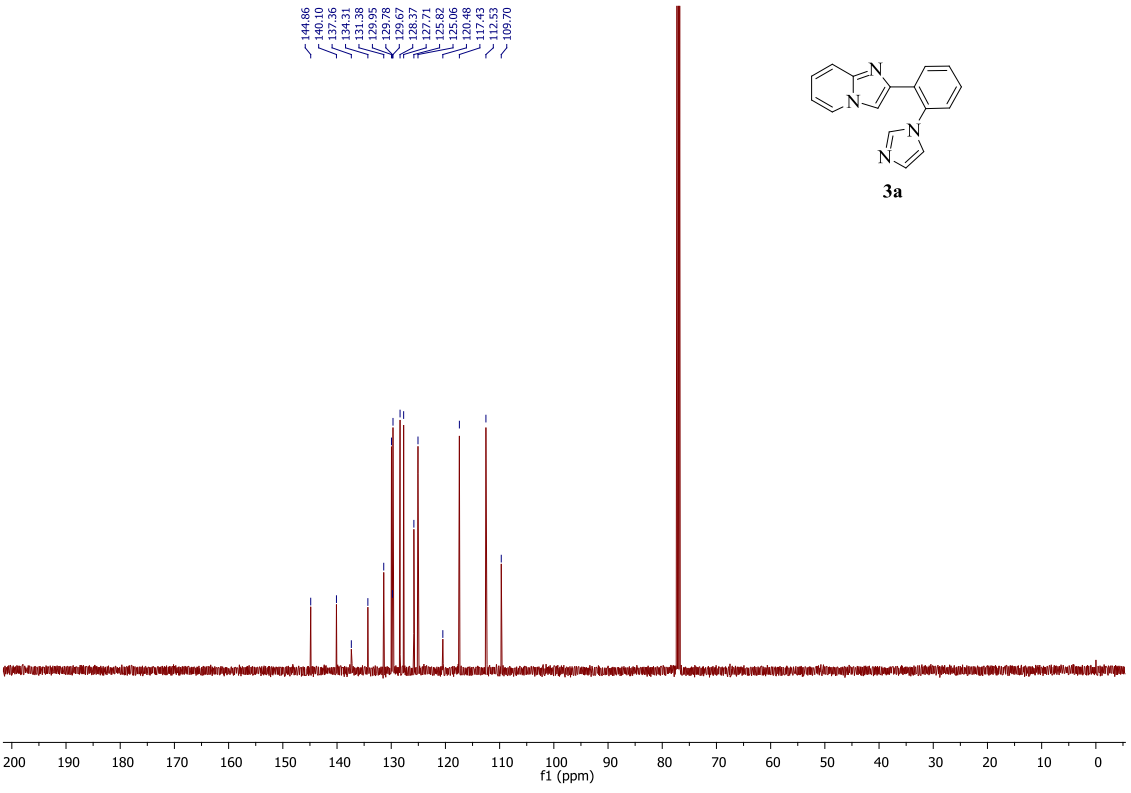
1a **2a** **3a**

To a solution of **1a** (0.27 g, 1 mmol) in DMF (3 mL) was added CuI (0.019 g, 0.1 mmol), K_2CO_3 (0.2 g, 1.5 mmol) and purged the solution with N_2 then stirred for 2 h at 150 °C. The reaction mass was cooled to room temperature, diluted with water and extracted into ethyl acetate. Organic layer was dried over anhydrous Na_2SO_4 and evaporated the volatiles. The crude compound was purified by column chromatography (EtOAc/hexanes) to get 2-(2-(1H-imidazol-1-yl)phenyl)imidazo[1,2-a]pyridine (**3a**) as off-white solid.

Compound 3a: Yield: 240 mg, (92%); mp 149-151 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (dd, J = 7.9, 1.4 Hz, 1H), 7.89 (dt, J = 6.8, 1.1 Hz, 1H), 7.65 – 7.55 (m, 3H), 7.44 (td, J = 7.6, 1.5 Hz, 1H), 7.34 (dd, J = 7.8, 1.2 Hz, 1H), 7.29 (s, 1H), 7.18 – 7.14 (m, 1H), 7.06 (s, 1H), 6.73 (td, J = 6.8, 1.1 Hz, 1H), 6.29 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144 .86, 140.10, 137.36, 134.31,

131.38, 129.95, 129.78, 129.67, 128.37, 127.71, 125.82, 125.06, 120.48, 117.43, 112.53, 109.70; HRMS calcd for 260.1062, found 261.0903 $[M + H]^+$





2.3 Spectroscopic data for 4a-p:

4a: Yield: 75%; mp 217-218 °C, ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.35 (d, *J* = 6.2 Hz, 1H), 8.65 (d, *J* = 7.4 Hz, 1H), 8.05 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 9.1 Hz, 1H), 7.69 – 7.55 (m, 2H), 7.54 – 7.44 (m, 1H), 7.11 (t, *J* = 6.4 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.59, 139.87, 137.17, 132.27, 131.58, 128.72, 127.81, 127.68, 125.47, 125.08, 119.50, 117.61, 115.95, 113.98, 113.04, 111.67; HRMS (ESI) calcd for $C_{16}H_{11}N_4^+$ 259.0978, found 259.0956 $[M + H]^+$.

4b: Yield: 68%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.62 (d, *J* = 6.6 Hz, 1H), 8.76 (d, *J* = 7.7 Hz, 1H), 8.67 (d, *J* = 8.5 Hz, 1H), 8.41 (d, *J* = 8.1 Hz, 1H), 8.03 (d, *J* = 7.9 Hz, 1H), 7.91 (d, *J* = 9.0 Hz, 1H), 7.78 (t, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.52 (m, 3H), 7.18 (t, *J* = 6.7 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.54, 145.34, 142.45, 141.69, 135.04, 131.34, 129.14, 128.31, 128.16, 124.89, 124.56, 124.12, 122.56, 120.00, 119.23, 117.30, 115.94, 113.62, 113.21; HRMS (ESI) calcd for $C_{20}H_{13}N_4^+$ 309.1135, found 309.1126 [M + H]+.

4c: Yield: 78%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.24 (d, *J* = 6.4 Hz, 1H), 8.73 (d, *J* = 7.6 Hz, 1H), 8.59 (d, *J* = 8.2 Hz, 1H), 8.44 (s, 1H), 7.94 (d, *J* = 9.1 Hz, 1H), 7.81 (t, *J* = 7.5 Hz, 1H), 7.71 (t, *J* = 7.3 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 6.6 Hz, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.34, 148.32, 142.02, 141.80, 132.57, 129.38, 128.55, 127.29, 126.12, 124.15, 118.37, 117.63, 116.68, 113.31; HRMS (ESI) calcd for $C_{15}H_{10}N_5^+$ 260.0931, found 260.0938 $[M + H]^+$.

4d: Yield: 76%; mp 197-198 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.26 (d, *J* = 6.5 Hz, 1H), 8.58 (d, *J* = 7.5 Hz, 1H), 7.79 (t, *J* = 8.8 Hz, 2H), 7.68 (s, 1H), 7.62 – 7.36 (m, 3H), 7.03 (t, *J* = 6.5 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.95, 140.92, 139.09, 136.03, 131.49, 130.59, 128.24, 127.47, 127.33, 124.63, 124.40, 118.50, 117.05, 115.46, 112.58, 108.09, 14.38; HRMS (ESI) calcd for $C_{17}H_{13}N_4^+$ 273.1135, found 273.1129 $[M + H]^+$.

4e: Yield: 72%; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.16 (d, *J* = 6.9 Hz, 1H), 8.63 (d, *J* = 7.8 Hz, 1H), 8.03 (s, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.59 (m, 4H), 6.90 (d, *J* = 6.8 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.67, 139.40, 138.85, 136.85, 131.67, 131.18, 128.17, 126.35, 125.04, 124.49, 119.06, 115.63, 115.61, 115.39, 113.28, 111.25, 21.90; HRMS (ESI) calcd for $C_{17}H_{13}N_4^+$ 273.1135, found 273.1118 $[M + H]^+$.

4f: Yield: 71%; mp 242-244 °C, ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.24 (d, *J* = 6.7 Hz, 1H), 8.54 (d, *J* = 7.7 Hz, 1H), 8.44 (d, *J* = 8.4 Hz, 1H), 8.21 (d, *J* = 8.1 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.51 (s, 1H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 6.7 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.70, 145.06,

142.15, 141.33, 139.63, 134.57, 130.98, 128.67, 126.91, 124.49, 124.19, 123.79, 122.14, 119.61, 118.92, 115.62, 115.56, 115.53, 113.39, 112.08, 21.94; HRMS (ESI) calcd for $C_{21}H_{15}N_4^+$ 323.1291, found 323.1303 [M + H]+.

4g: Yield: 72%; mp 221-222 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.96 (d, *J* = 6.9 Hz, 1H), 8.61 (d, *J* = 7.9 Hz, 1H), 8.51 (d, *J* = 8.3 Hz, 1H), 8.36 (s, 1H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.56 (s, 1H), 6.92 (d, *J* = 6.9 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.21, 148.67, 141.95, 141.60, 140.10, 132.30, 129.12, 126.15, 125.94, 124.01, 118.26, 116.53, 115.87, 111.46, 21.94; HRMS (ESI) calcd for $C_{16}H_{12}N_5^+$ 274.1087, found 274.1106 [M + H]+.

4h: Yield: 75%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.14 (d, *J* = 6.9 Hz, 1H), 8.61 (d, *J* = 7.8 Hz, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.72 (s, 1H), 7.65 – 7.47 (m, 3H), 6.87 (d, *J* = 6.9 Hz, 1H), 2.52 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.54, 140.88, 139.23, 138.72, 136.27, 131.48, 128.07, 126.53, 124.57, 124.41, 118.71, 115.49, 115.19, 113.05, 107.98, 21.89, 14.43; HRMS (ESI) calcd for $C_{18}H_{15}N_4^+$ 287.1291, found 287.1288 [M + H]+.

4i: Yield: 62%; mp 190-191 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.04 (s, 1H), 8.59 (d, *J* = 7.2 Hz, 1H), 8.00 (s, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 9.2 Hz, 1H), 7.63 – 7.48 (m, 3H), 7.33 – 7.24 (m, 1H), 2.46 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.20, 139.17, 136.76, 131.58, 131.08, 130.68, 128.19, 125.08, 124.84, 124.43, 122.81, 118.97, 116.38, 115.59, 113.20, 111.33, 18.19; HRMS (ESI) calcd for $C_{17}H_{13}N_4^+$ 273.1135, found 273.1145 $[M + H]^+$.

4j: Yield: 66%; mp 234-235 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.35 (s, 1H), 8.70 (d, *J* = 7.7 Hz, 1H), 8.62 (d, *J* = 8.5 Hz, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.83 – 7.69 (m, 2H), 7.62 – 7.32 (m, 5H), 2.54 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.53, 145.21, 142.21, 134.79, 131.52, 131.22, 128.91, 125.69, 124.65, 124.47, 124.00, 123.27, 122.42, 119.80, 119.20, 116.47, 115.85, 113.57, 18.33; HRMS (ESI) calcd for $C_{21}H_{15}N_4^+$ 323.1291, found 323.1278 $[M + H]^+$.

4k: Yield: 64%; mp 196-198 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.02 (s, 1H), 8.72 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.60 (d, *J* = 8.2 Hz, 1H), 8.44 (s, 1H), 7.87 – 7.76 (m, 2H), 7.74 – 7.66 (m, 1H), 7.43 (dd, *J* = 9.3, 1.6 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.28, 147.46, 141.94, 132.46, 131.91, 129.29, 129.16, 126.17, 124.90, 124.08, 123.56, 118.50, 116.90, 116.71, 18.25; HRMS (ESI) calcd for $C_{16}H_{12}N_5^+$ 274.1087, found 274.1104 $[M + H]^+$.

4l: Yield: 76%; mp 212-214 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.11 (s, 1H), 8.67 (s, 1H), 8.43 (d, *J* = 7.7 Hz, 1H), 8.37 (d, *J* = 8.3 Hz, 1H), 7.94 (dd, *J* = 9.3, 4.5 Hz, 1H), 7.78 – 7.52 (m,

4H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 145.18, 140.42, 136.08, 132.39, 131.69, 129.72, 126.23, 124.55, 120.58, 120.24, 119.10, 118.83, 118.71, 117.59, 114.71, 114.44, 114.05, 113.89; HRMS (ESI) calcd for $C_{16}H_{10}FN_4^+$ 277.0884, found 277.0872 $[M + H]^+$.

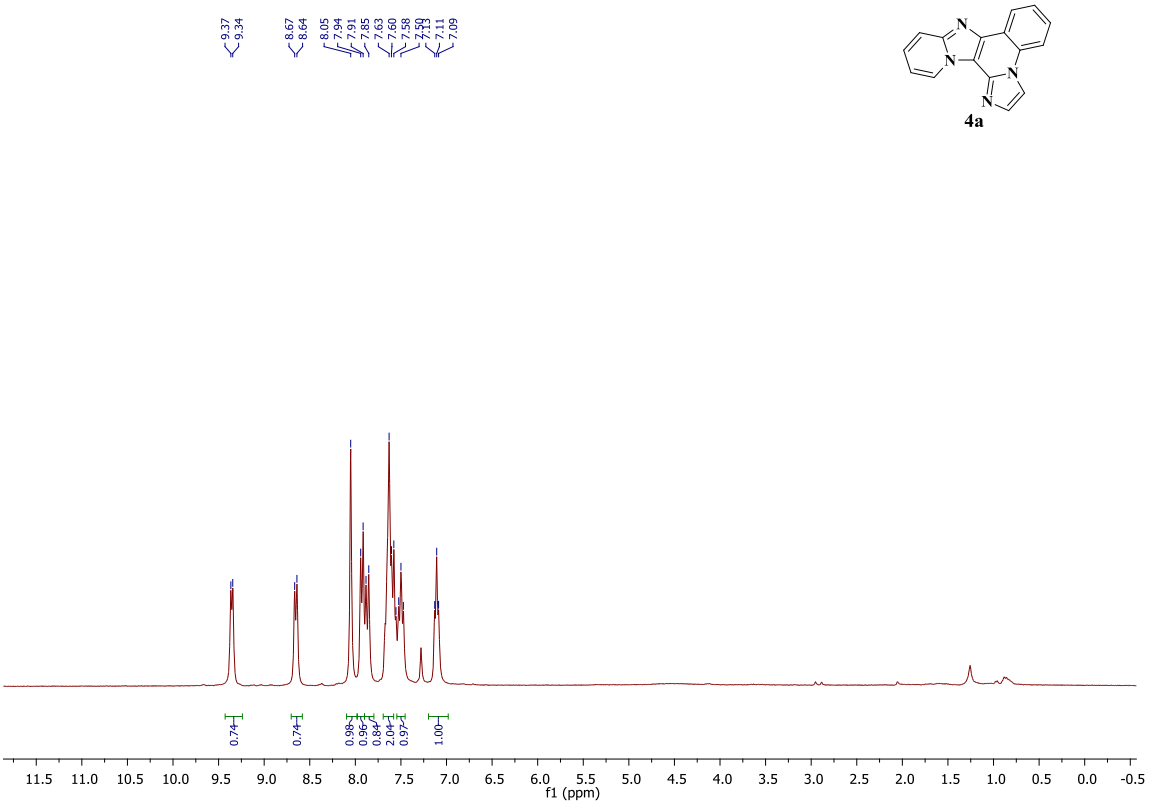
4m: Yield: 62%; mp 228-229 °C; ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.14 (s, 1H), 8.63 (s, 1H), 8.44 (d, *J* = 7.7 Hz, 1H), 8.36 (d, *J* = 8.3 Hz, 1H), 7.88 (d, *J* = 9.6 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.66 – 7.48 (m, 3H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 145.60, 139.88, 136.16, 132.49, 132.10, 129.74, 129.19, 126.16, 125.04, 124.63, 120.74, 118.93, 118.73, 117.57, 114.01; HRMS (ESI) calcd for $C_{16}H_{10}ClN_4^+$ 293.0589, found 293.0591 $[M + H]^+$.

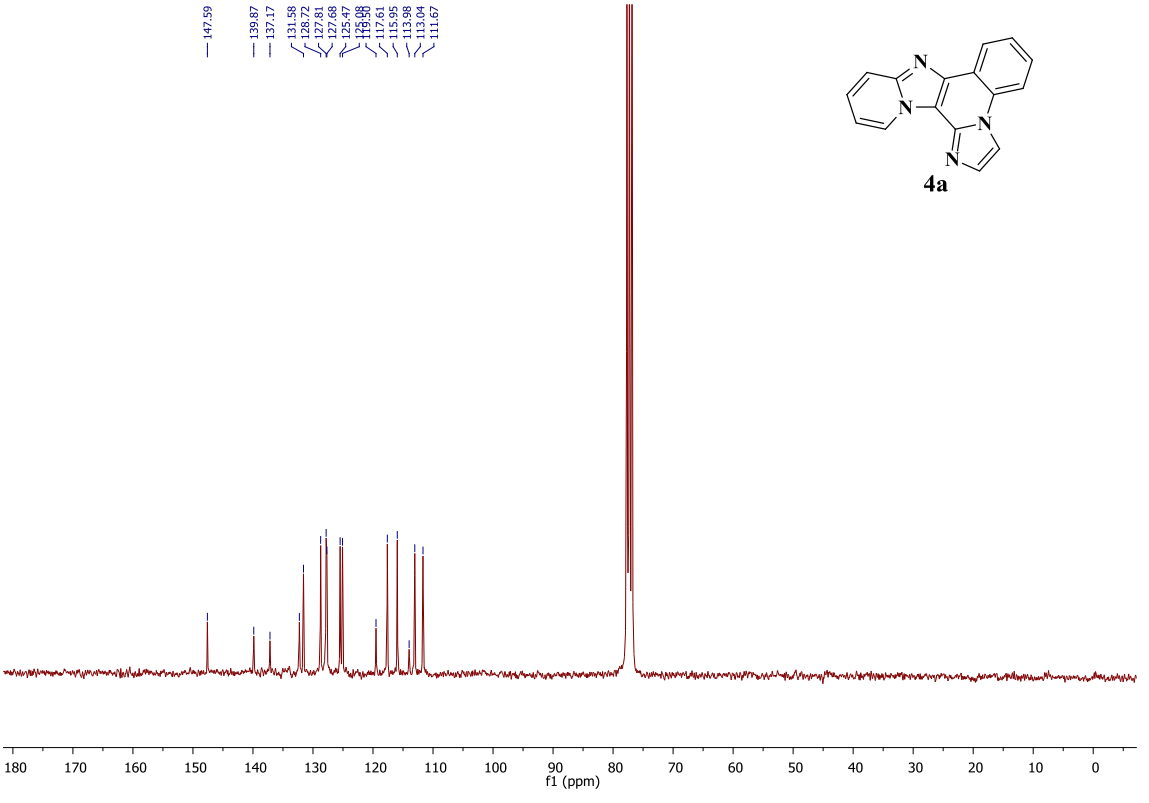
4n: Yield: 71%; mp 264-266 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.60 (s, 1H), 8.73 (d, *J* = 7.2 Hz, 1H), 8.65 (d, *J* = 8.5 Hz, 1H), 8.40 (d, *J* = 7.5 Hz, 1H), 8.05 (d, *J* = 7.3 Hz, 1H), 7.92 (dd, *J* = 9.6, 4.7 Hz, 1H), 7.80 (t, *J* = 7.9 Hz, 1H), 7.66 – 7.46 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.08, 135.18, 131.39, 129.69, 125.17, 124.98, 124.58, 123.20, 120.86, 120.52, 120.35, 119.05, 117.75, 117.64, 116.19, 115.69, 115.14, 113.82 HRMS (ESI) calcd for $C_{20}H_{12}FN_4^+$ 327.1041, found 327.1065 $[M + H]^+$.

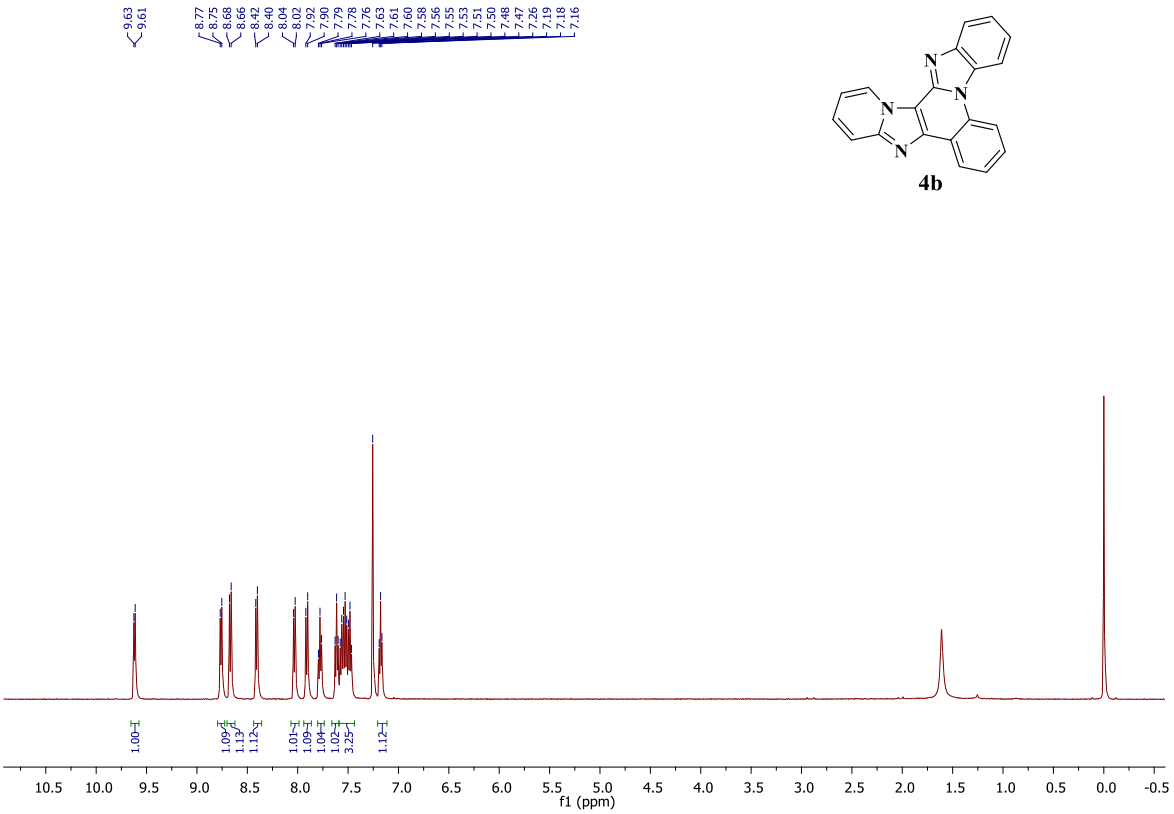
4o: Yield: 64%; mp > 270 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.04 (d, *J* = 8.5 Hz, 1H), 9.52 (d, *J* = 6.7 Hz, 1H), 8.68 (d, *J* = 7.8 Hz, 1H), 8.56 (d, *J* = 4.7 Hz, 1H), 8.20 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 9.1 Hz, 1H), 7.80 (t, *J* = 7.8 Hz, 1H), 7.67 – 7.55 (m, 2H), 7.45 (dd, *J* = 8.0, 4.8 Hz, 1H), 7.20 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.68, 146.68, 143.24, 142.73, 141.79, 137.37, 134.82, 130.09, 129.21, 128.50, 126.66, 125.55, 124.55, 119.97, 118.82, 118.50, 117.49, 114.00, 112.38; HRMS (ESI) calcd for $C_{19}H_{12}N_5^+$ 310.1087, found 310.1095 $[M + H]^+$.

4p: Pale yellow solid; Yield 78%; mp 238-240 °C; ^{1}H NMR (300 MHz, CDCl3) δ 9.16 (s, 1H), 8.68 (d, *J* = 7.5 Hz, 1H), 8.59 (d, *J* = 8.1 Hz, 1H), 8.45 (s, 1H), 7.99 – 7.87 (m, 1H), 7.82 (t, *J* = 7.4 Hz, 1H), 7.71 (t, *J* = 7.1 Hz, 1H), 7.52 (t, *J* = 8.3 Hz, 1H); ^{13}C NMR (75 MHz, CDCl3) δ 155.38, 152.80, 152.19, 146.09, 142.90, 141.87, 133.07, 129.94, 126.59, 124.52, 121.16, 120.82, 118.61, 118.42, 118.31, 117.13, 114.82, 114.27, 113.37; HRMS (ESI) calcd for $C_{15}H_9FN_5^+$ 278.0836, found 278.0841 $[M + H]^+$.

3. Copy of ^{1}H NMR and ^{13}C NMR spectra of 4a-p.



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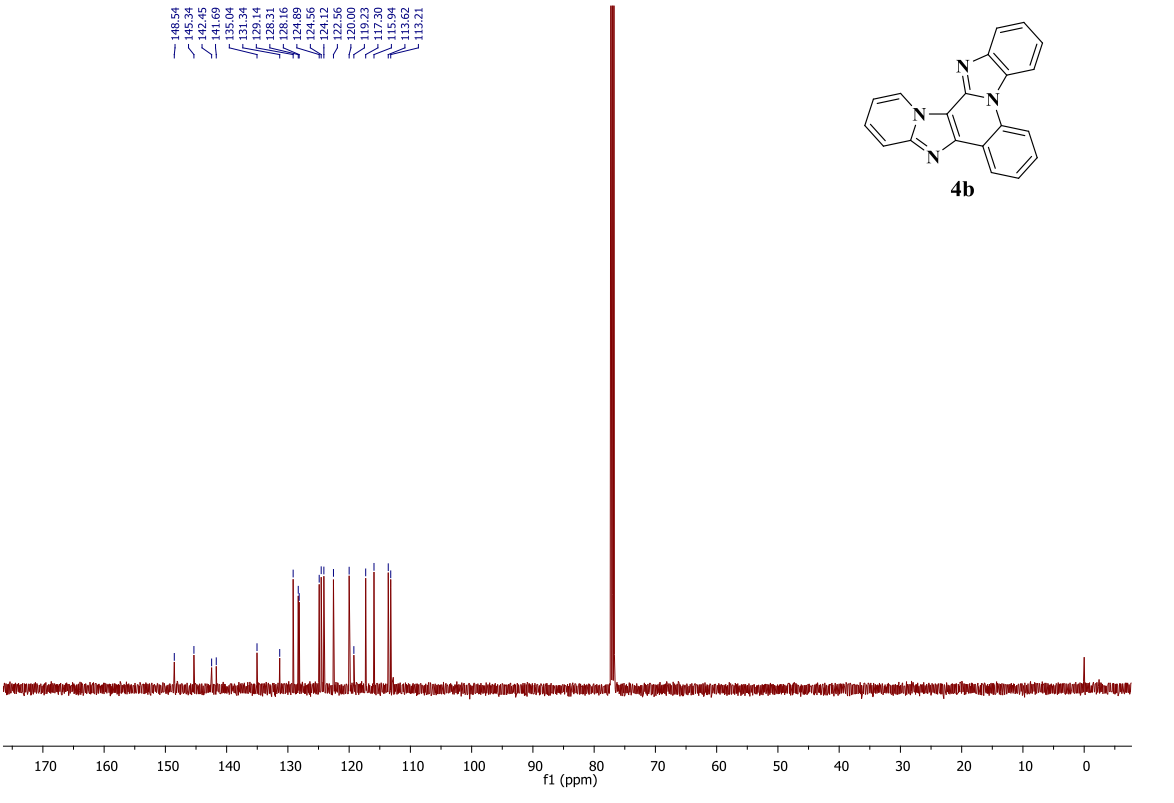
7.79
7.78
7.76
7.63
7.61
7.60
7.58
7.56
7.55
7.53
7.51
7.50
7.48
7.47
7.26
7.19
7.18
7.16
1.00
1.09
1.13
1.12
1.01
1.09
1.04
1.02
3.25
1.12
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
4b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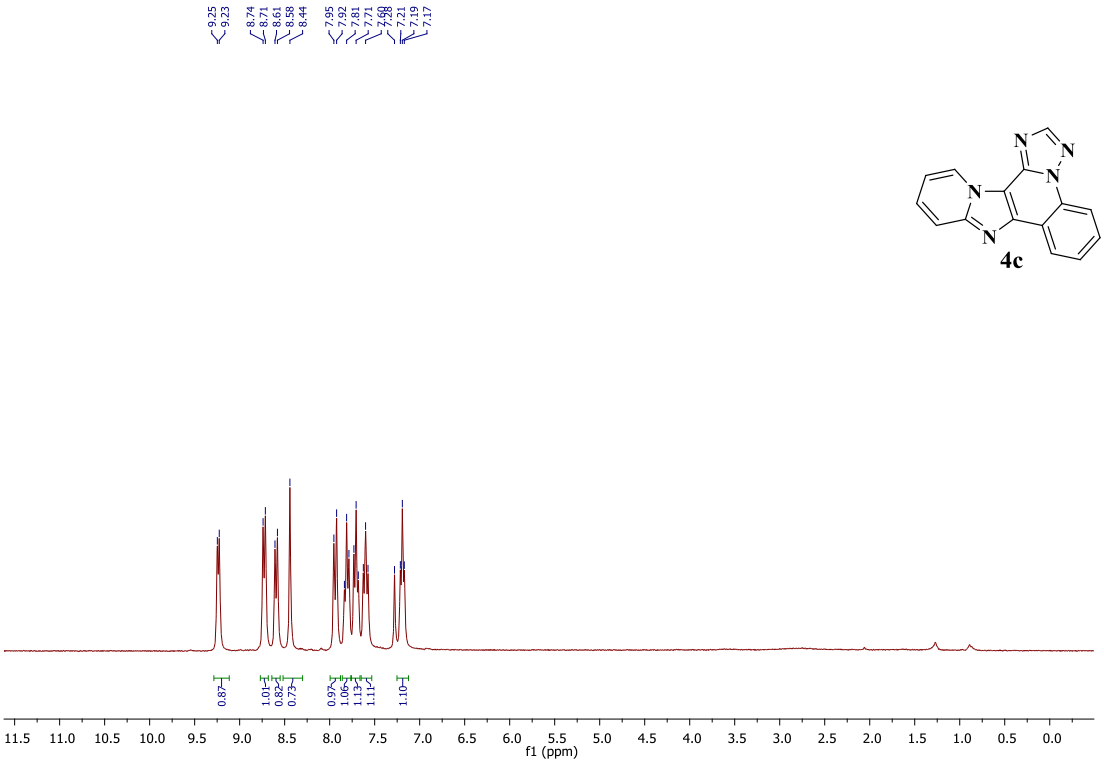
129.14
128.31
128.16
124.89
124.56
124.12
122.56
120.00
119.23
117.30
115.94
113.62
113.21
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
4b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7.81
7.71
7.68
7.66
7.21
7.19
7.17
4c
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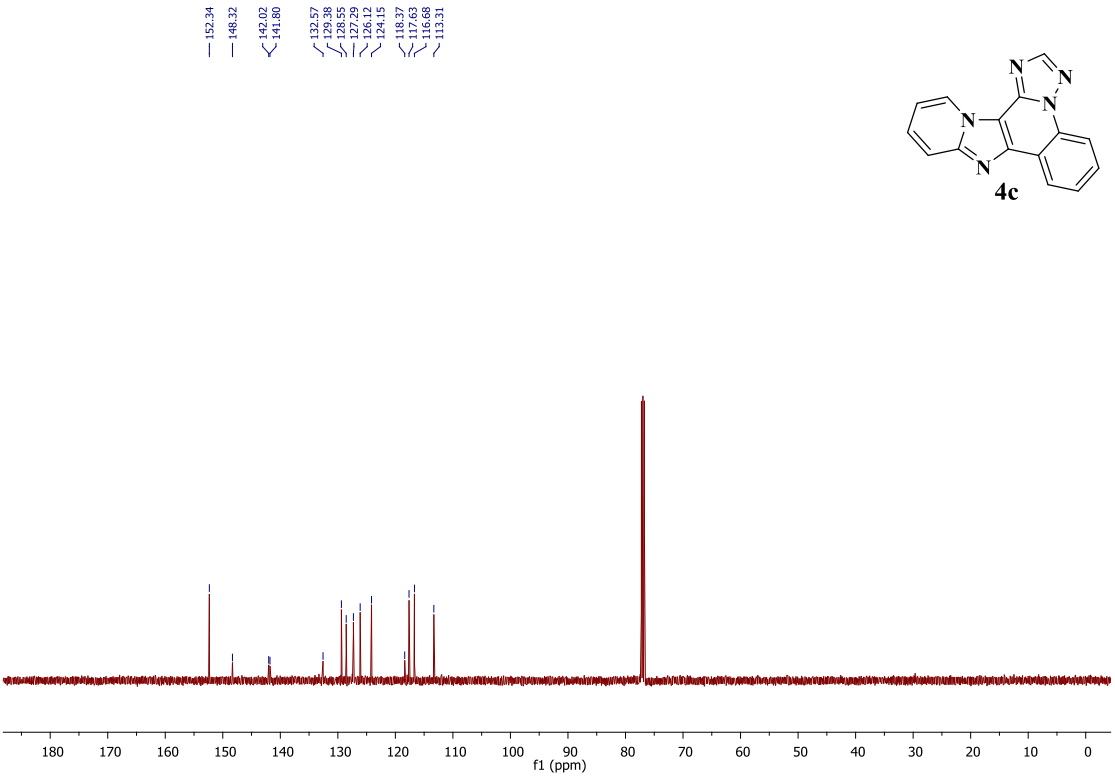
0.97
1.06
1.13
1.11
1.10
f1 (ppm)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127.29
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124.15
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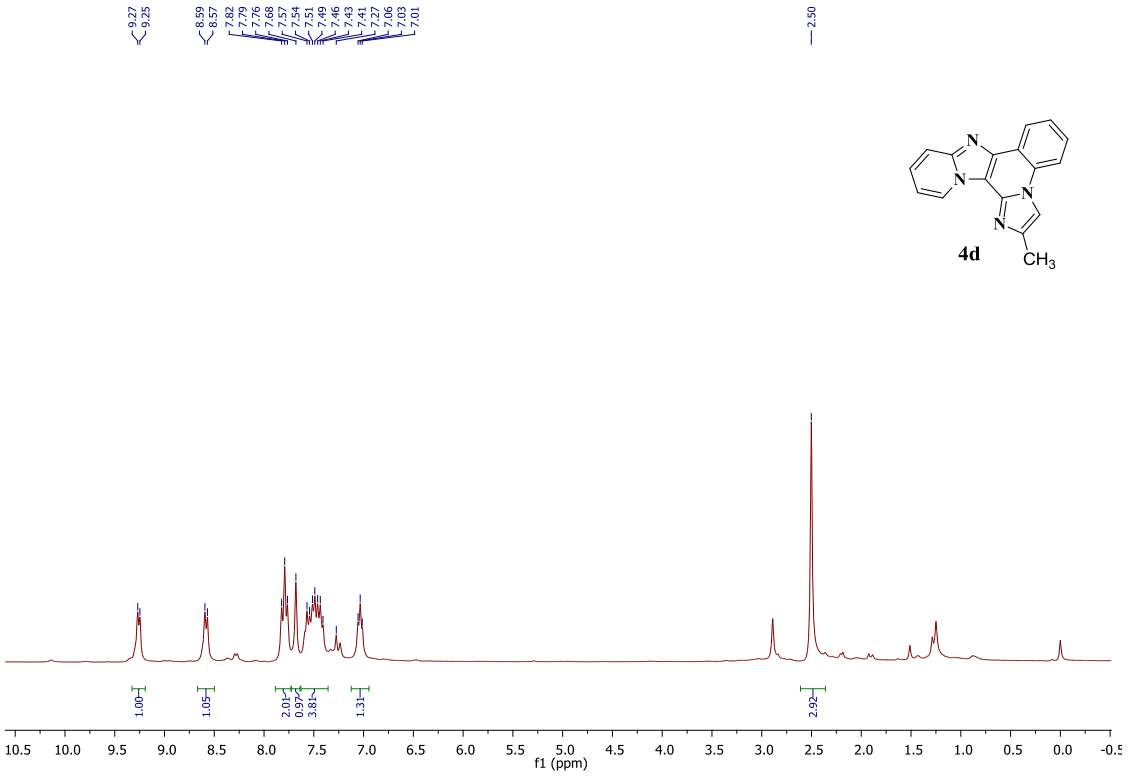
117.63
116.68
113.31
4c
f1 (ppm)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7.51
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7.46
7.43
7.41
7.27
7.06
7.03
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2.50
4d
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1.05
2.01
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3.81
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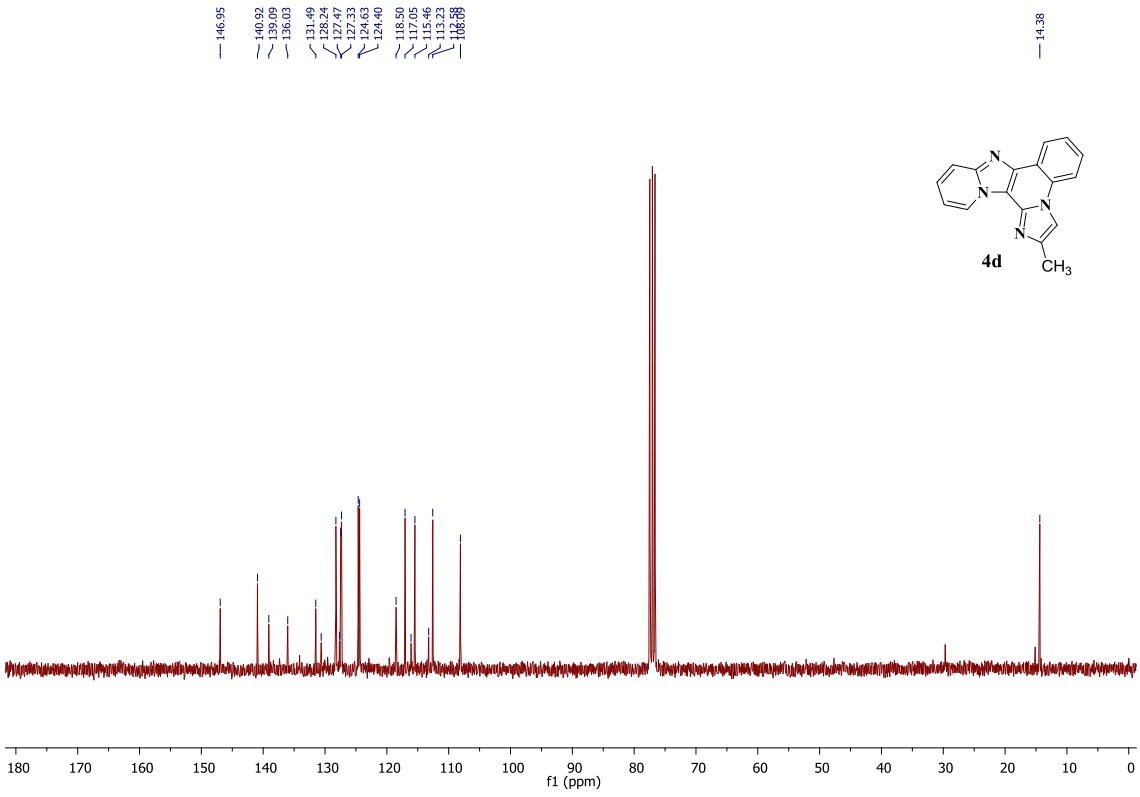
2.92
f1 (ppm)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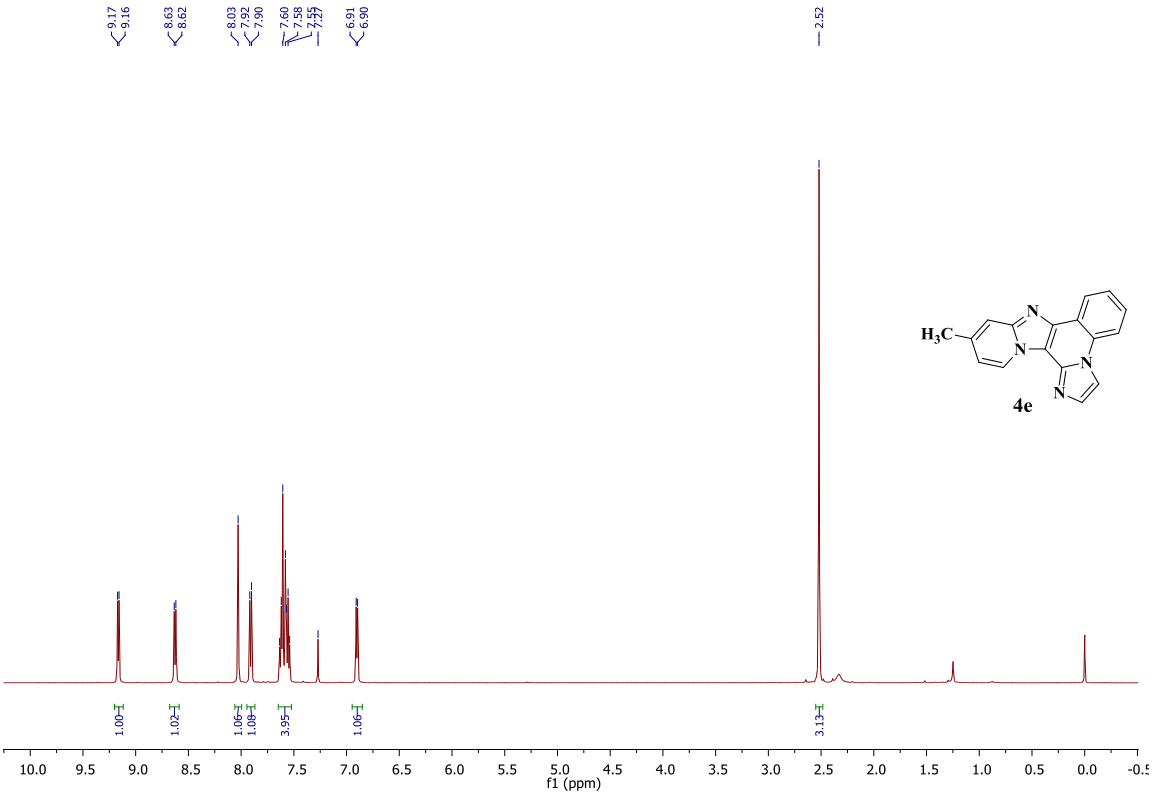
118.50
117.05
115.46
113.23
14.38
4d
f1 (ppm)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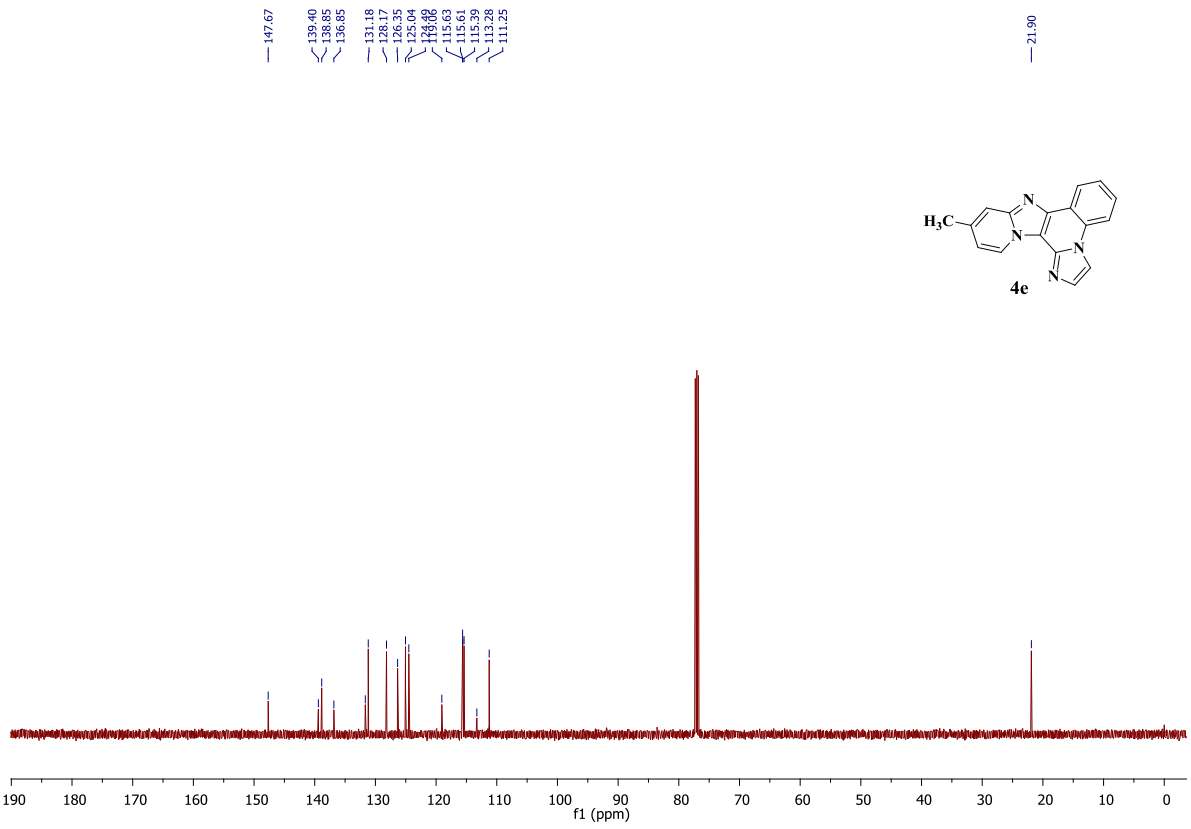
7.58
7.55
7.27
6.91
6.90
2.52
1.00
1.02
1.06
1.08
3.95
1.06
3.13
f1 (ppm)

H3C
N
N
N
N

4e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21.90
f1 (ppm)

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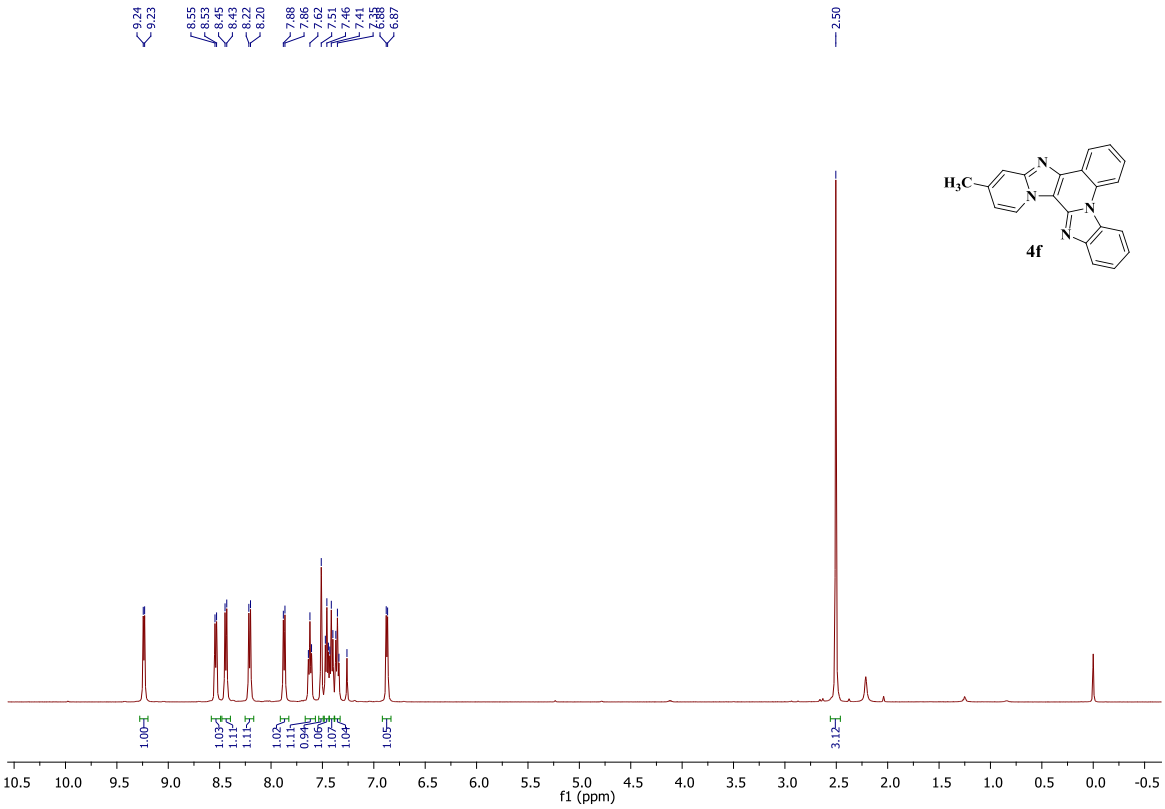
N
N

4e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7.46
7.41
7.35
6.88
6.87
2.50
1.00
1.03
1.11
1.11
1.02
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1.07
1.04
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f1 (ppm)

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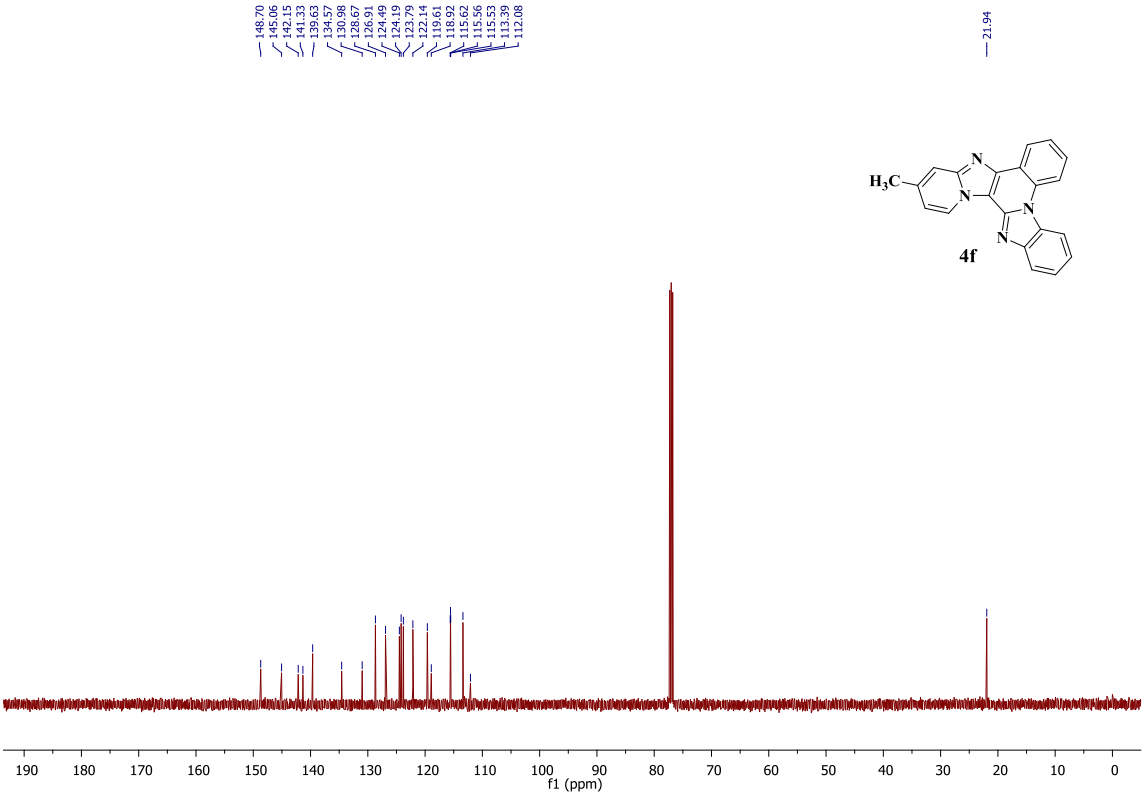
N
N

4f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134.57
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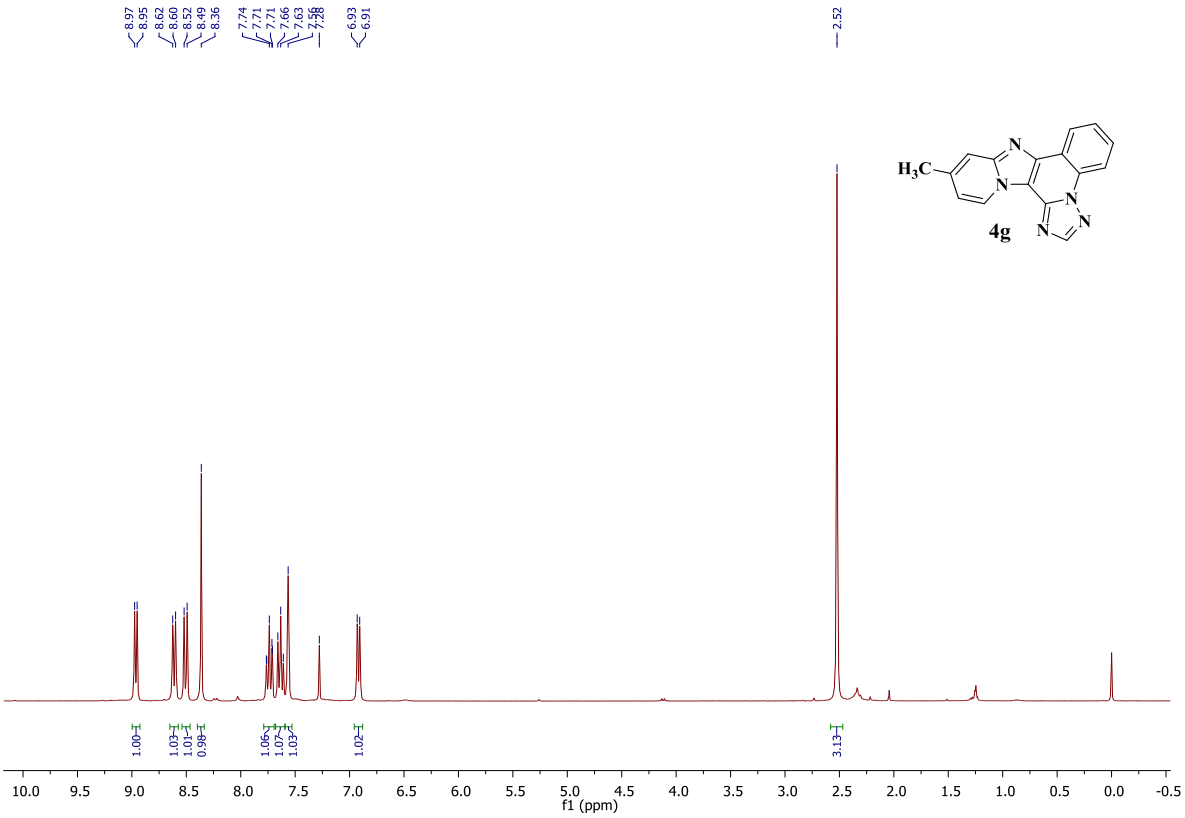
128.67
126.91
124.49
124.19
123.79
122.14
119.61
118.92
115.62
115.56
115.53
113.39
112.08
21.94
f1 (ppm)

H3C
N
N
N
N

4f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8.49
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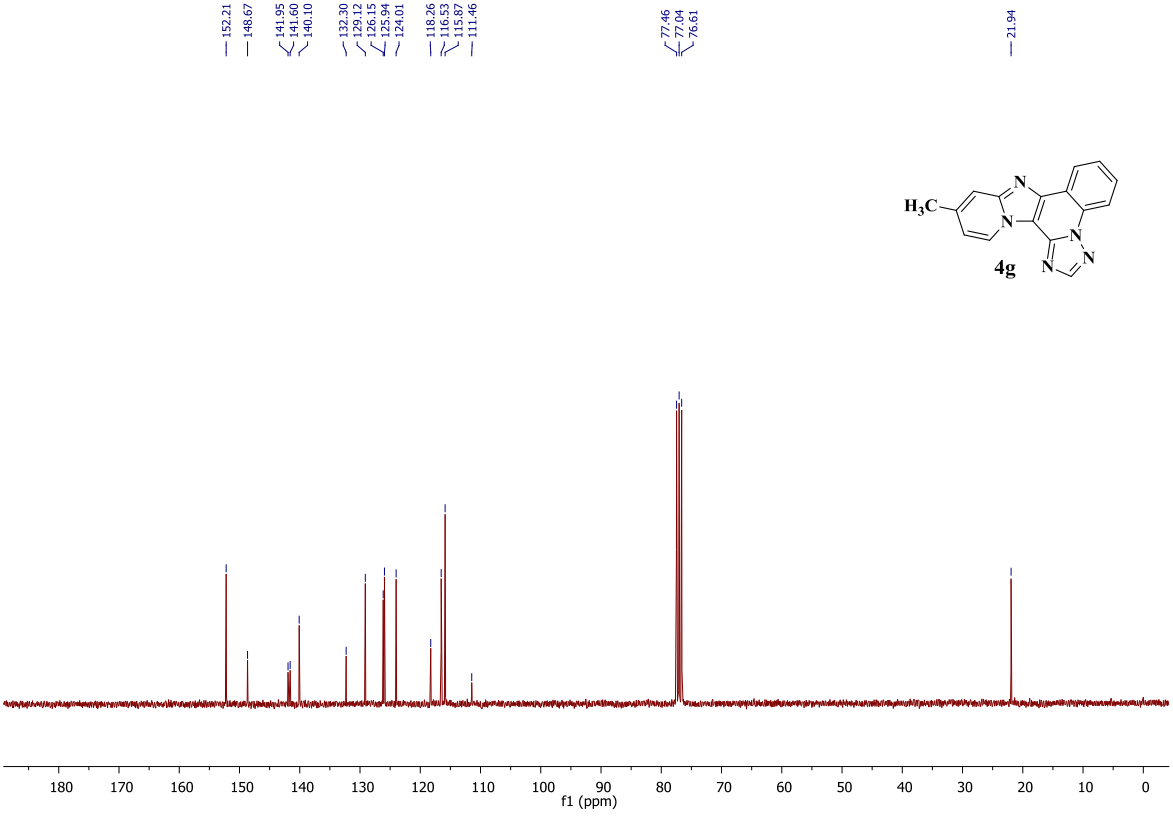
7.71
7.66
7.63
7.56
7.28
6.93
6.91
2.52
1.00
1.03
1.01
0.98
1.06
1.07
1.03
1.02
3.13
H3C
N
N
N
N
N
4g
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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124.01
118.26
116.53
115.87
111.46
77.46
77.04
76.61
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H3C
N
N
N
N
N
4g
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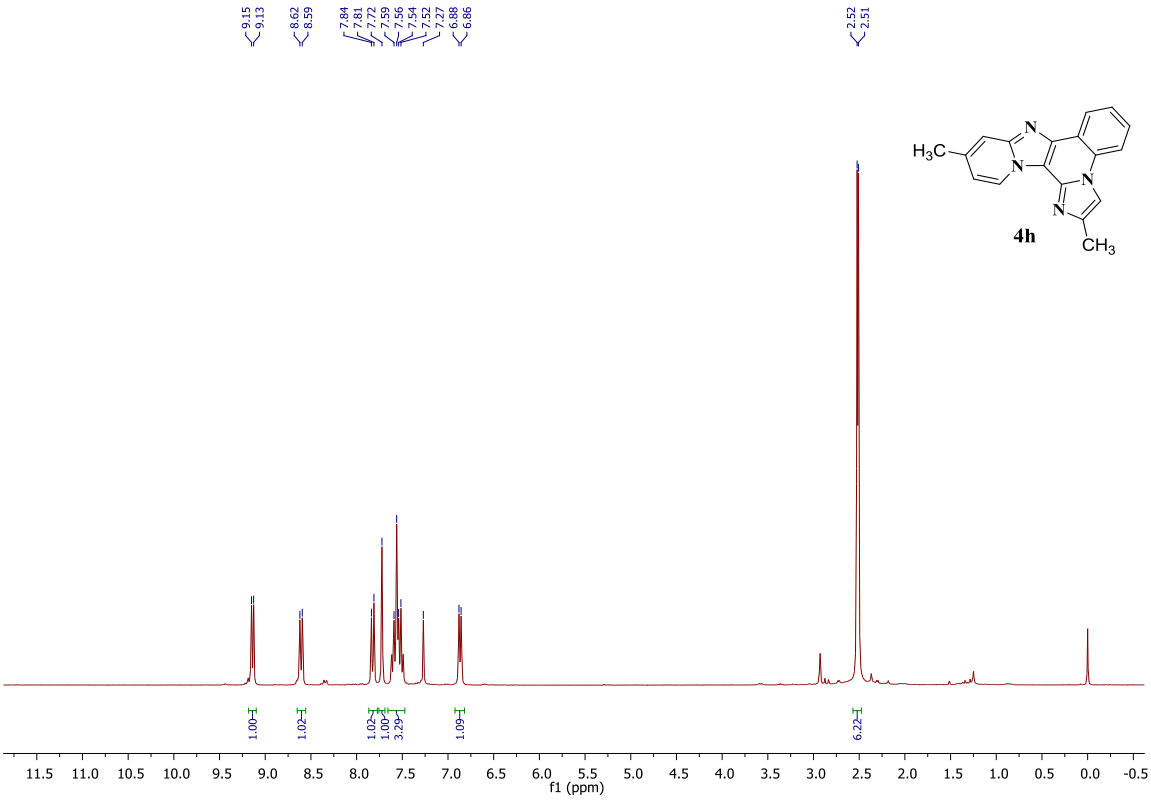
f1 (ppm)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7.54
7.52
7.27
6.88
6.86
2.52
2.51
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4h
CH3
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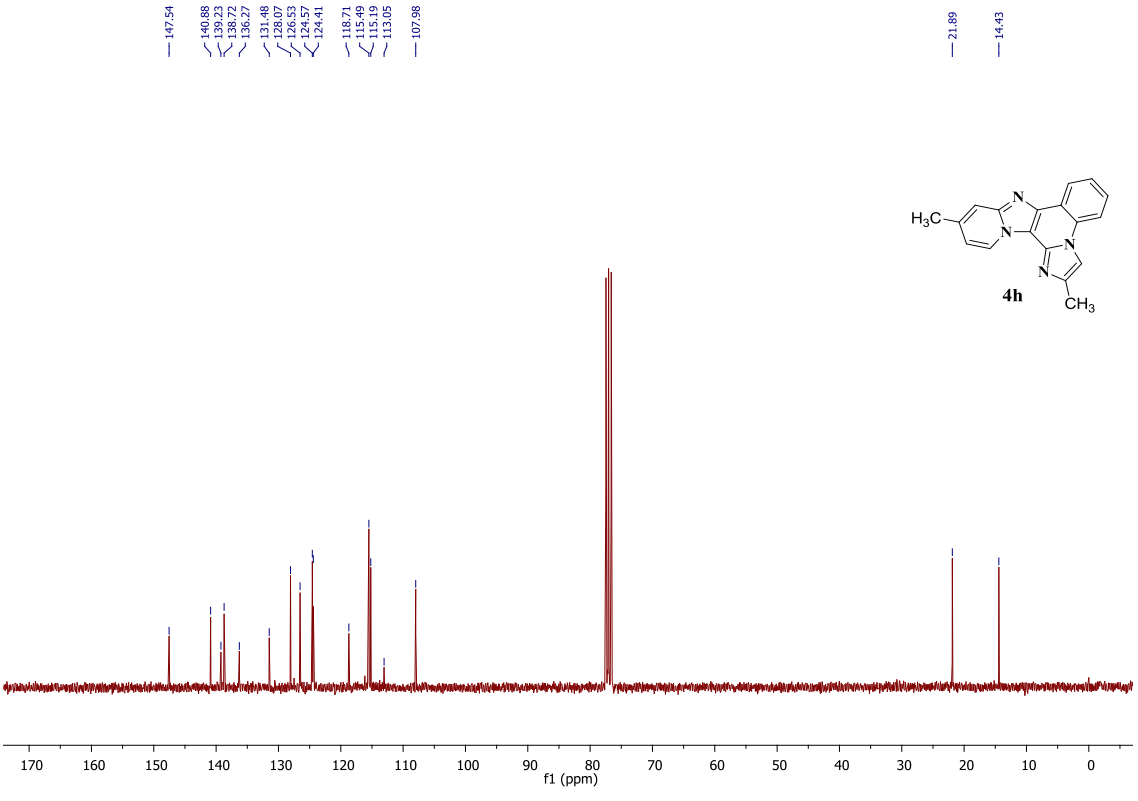
1.02
1.02
1.00
3.29
1.09
6.22
f1 (ppm)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126.53
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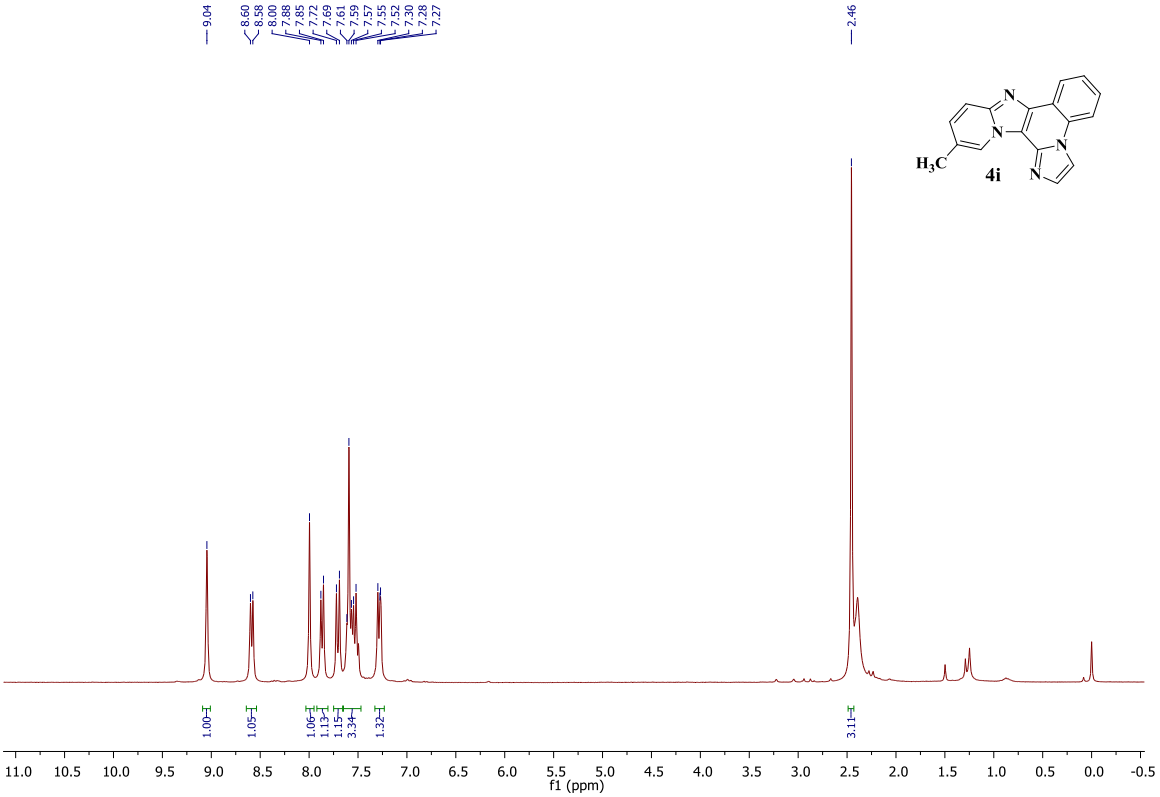
21.89
14.43
H3C
4h
CH3
f1 (ppm)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7.52
7.30
7.28
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1.06
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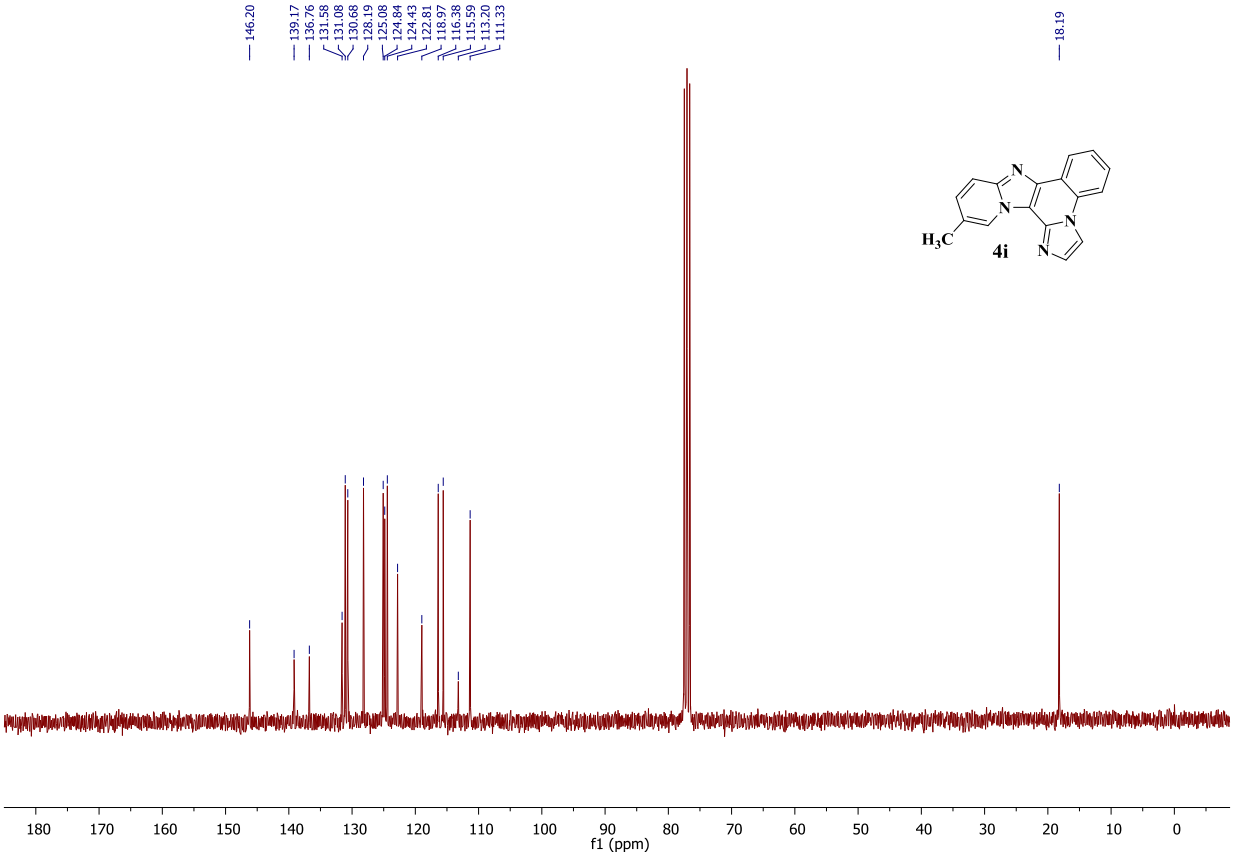
1.15
3.34
1.32
3.11
f1 (ppm)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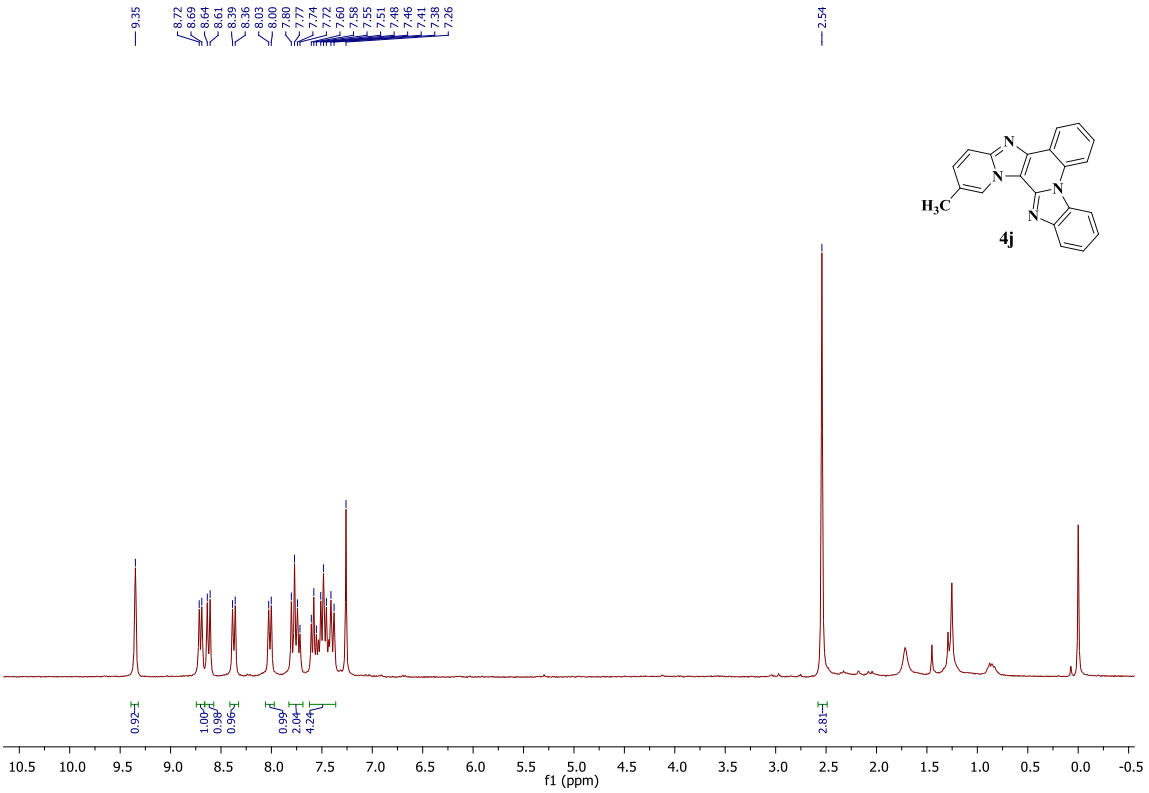
111.33
18.19
f1 (ppm)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7.46
7.41
7.38
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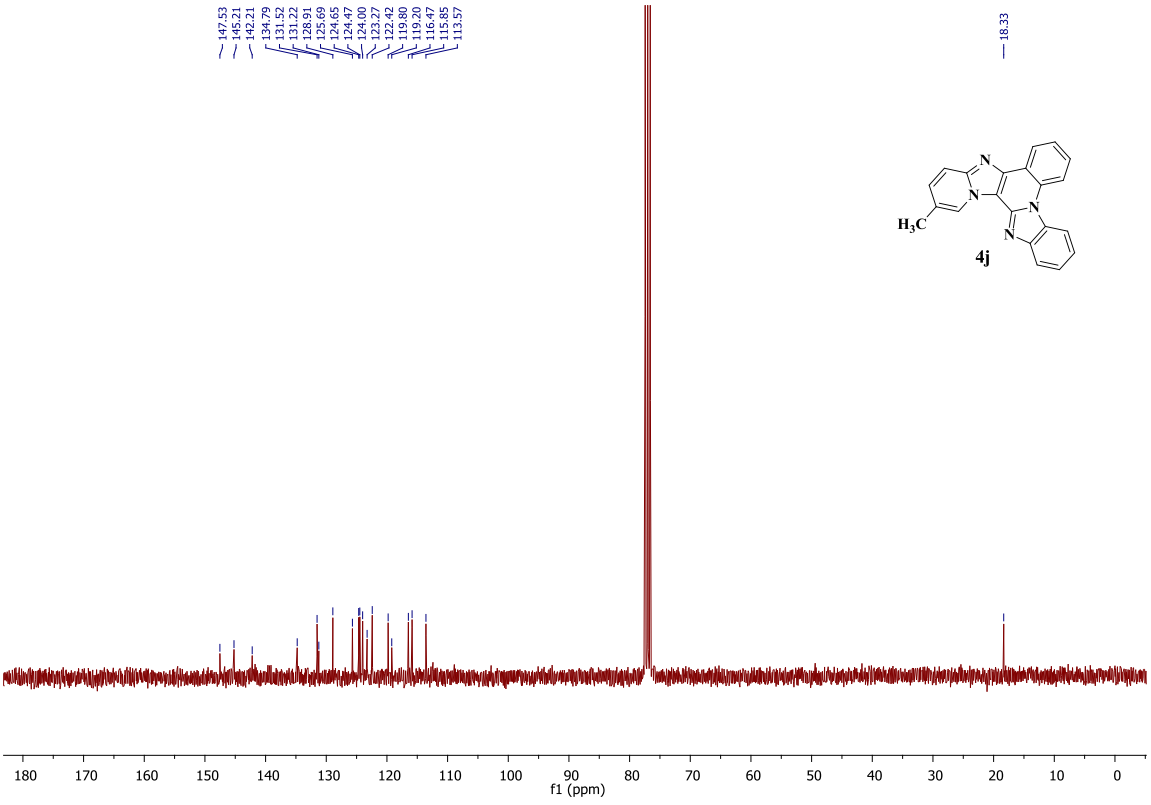
f1 (ppm)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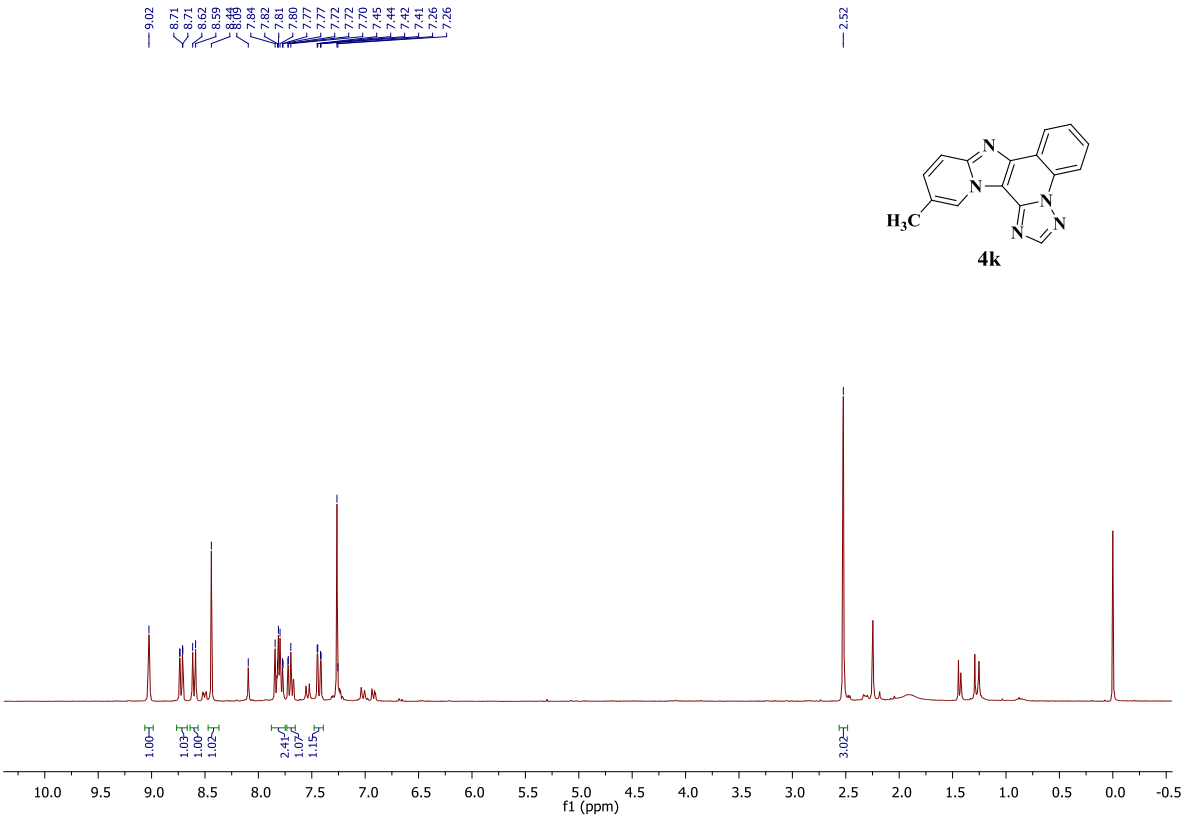
18.33
4j
f1 (ppm)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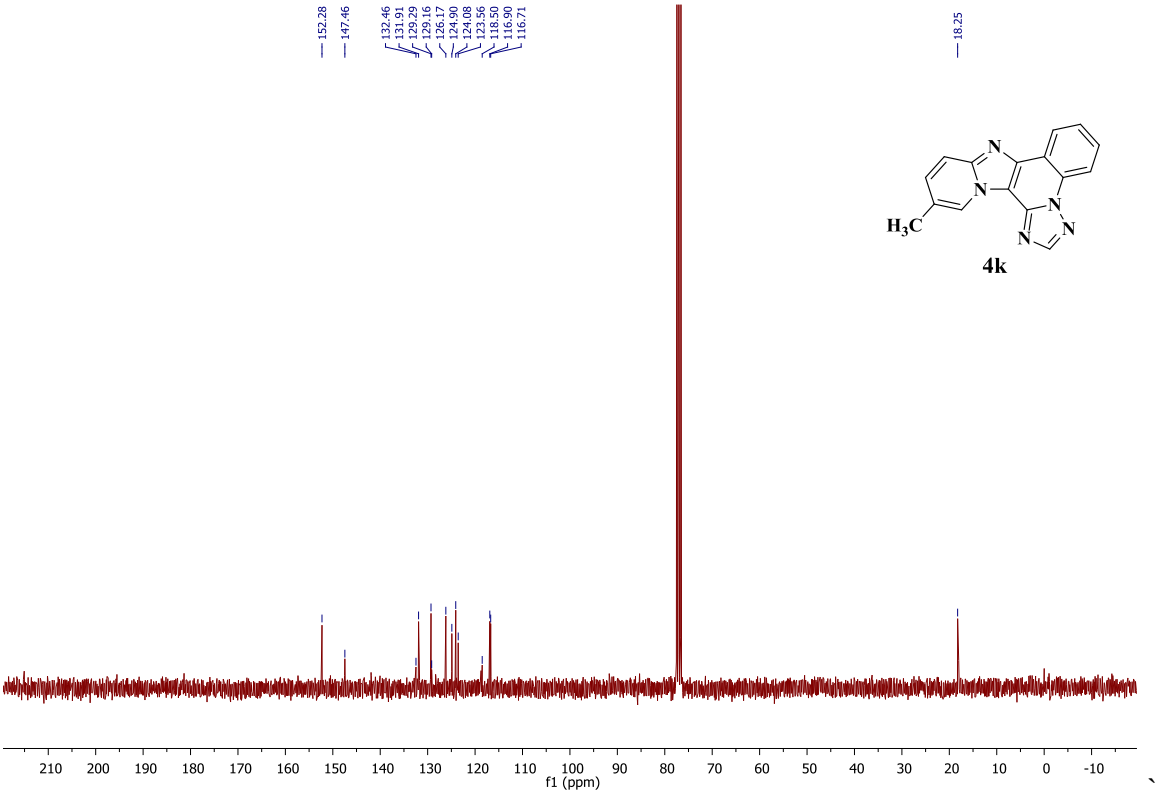
2.52
1.00
1.03
1.00
1.02
2.41
1.07
1.15
3.02
f1 (ppm)

N
N
N
N
N
H3C

4k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116.71
18.25
f1 (ppm)

N
N
N
N
N
H3C

4k


9.11
8.67
8.45
8.42
8.39
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7.93
7.91
7.76
7.74
7.71
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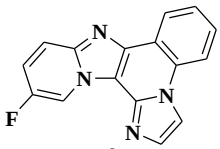
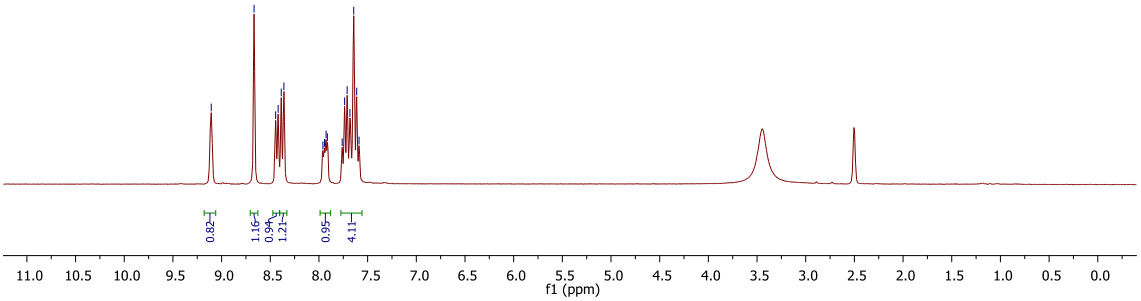
7.61
7.59


N
N
N
N
F

4l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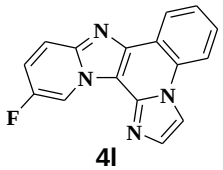
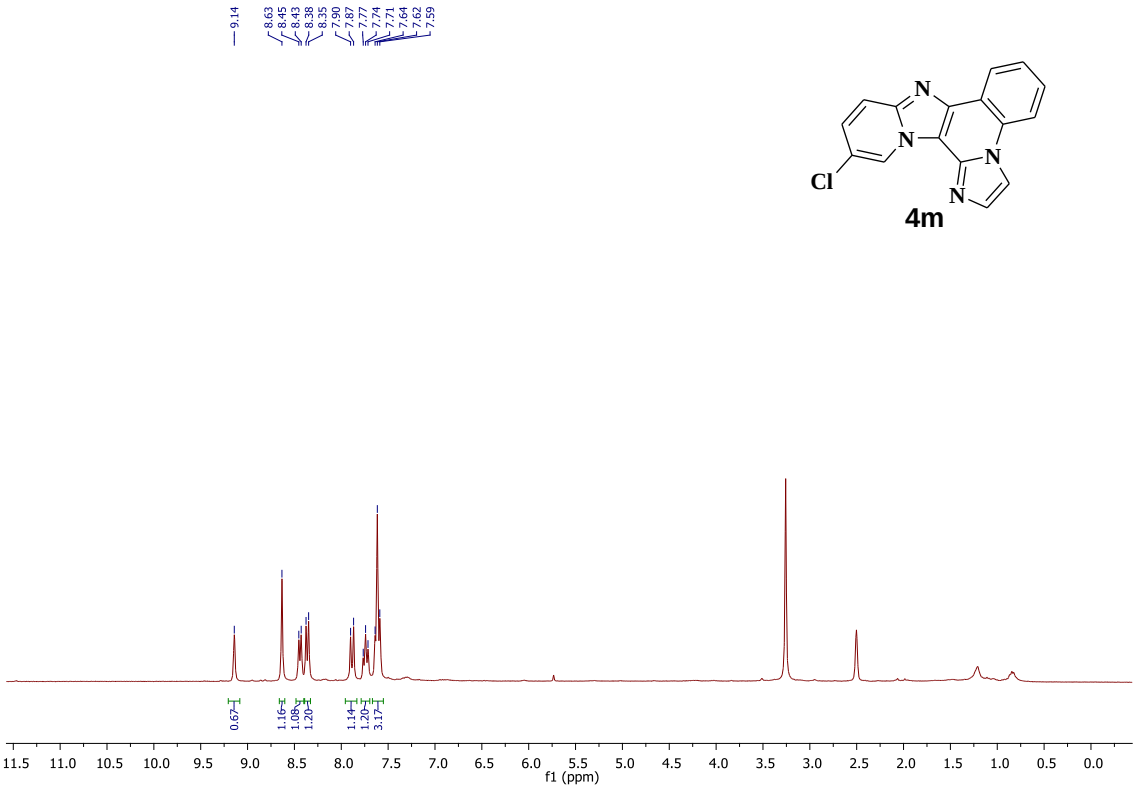
1.21
0.95
4.11
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

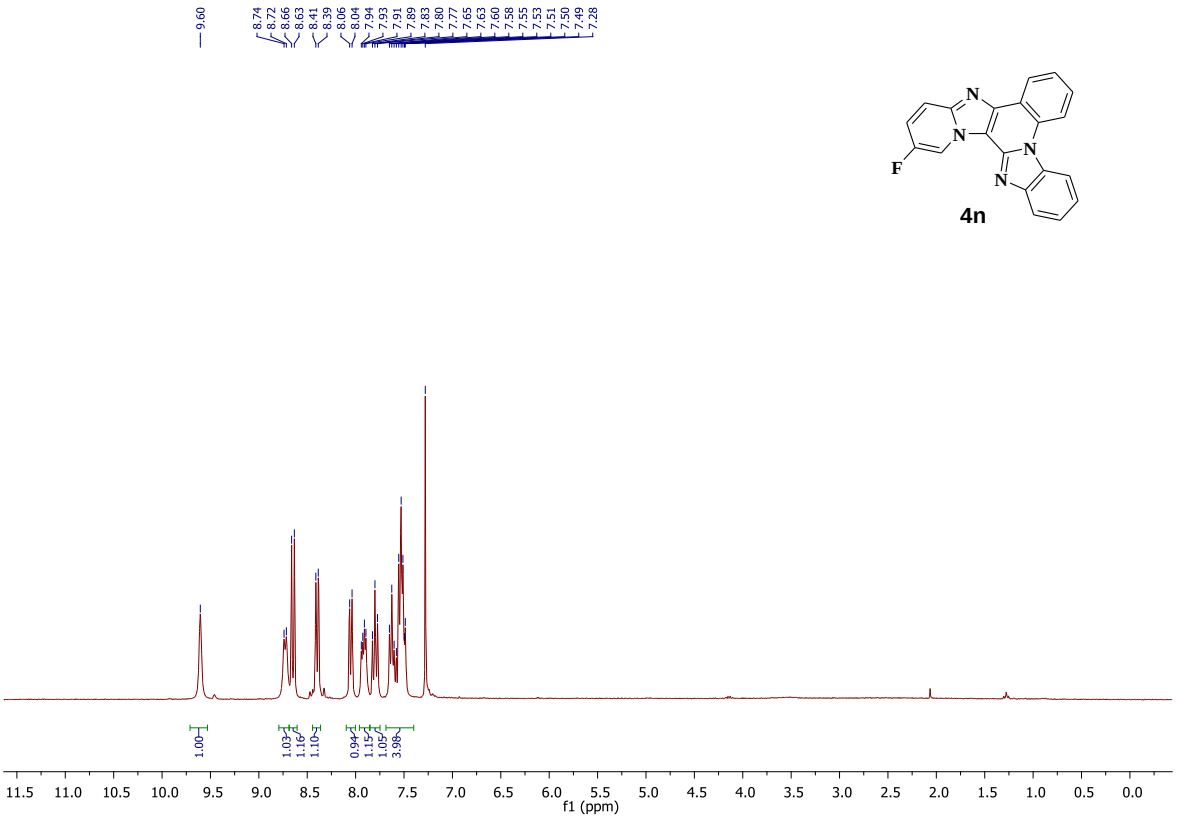

145.18
140.42
136.08
132.39
131.69
129.72
126.23
124.55
120.58
120.24
119.10
118.83
118.71
117.59
114.71
114.44
114.05
113.89

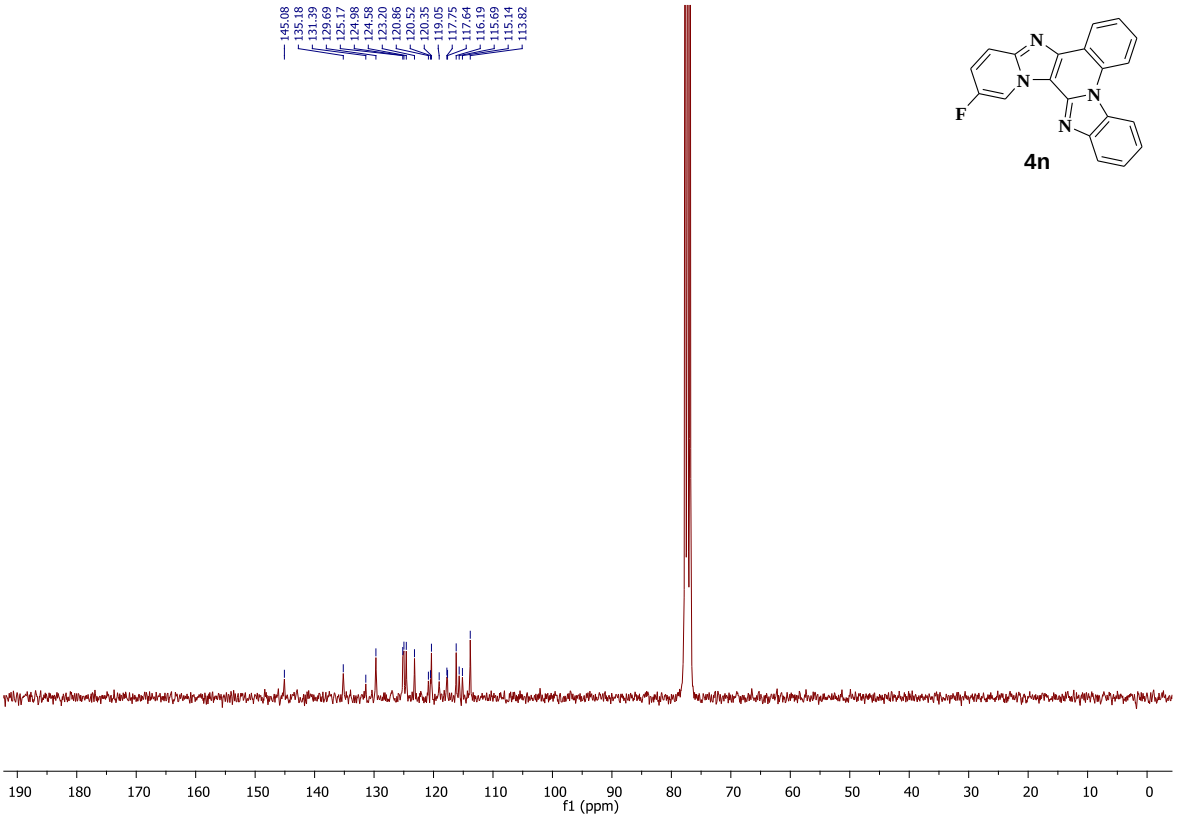

N
N
N
N
F

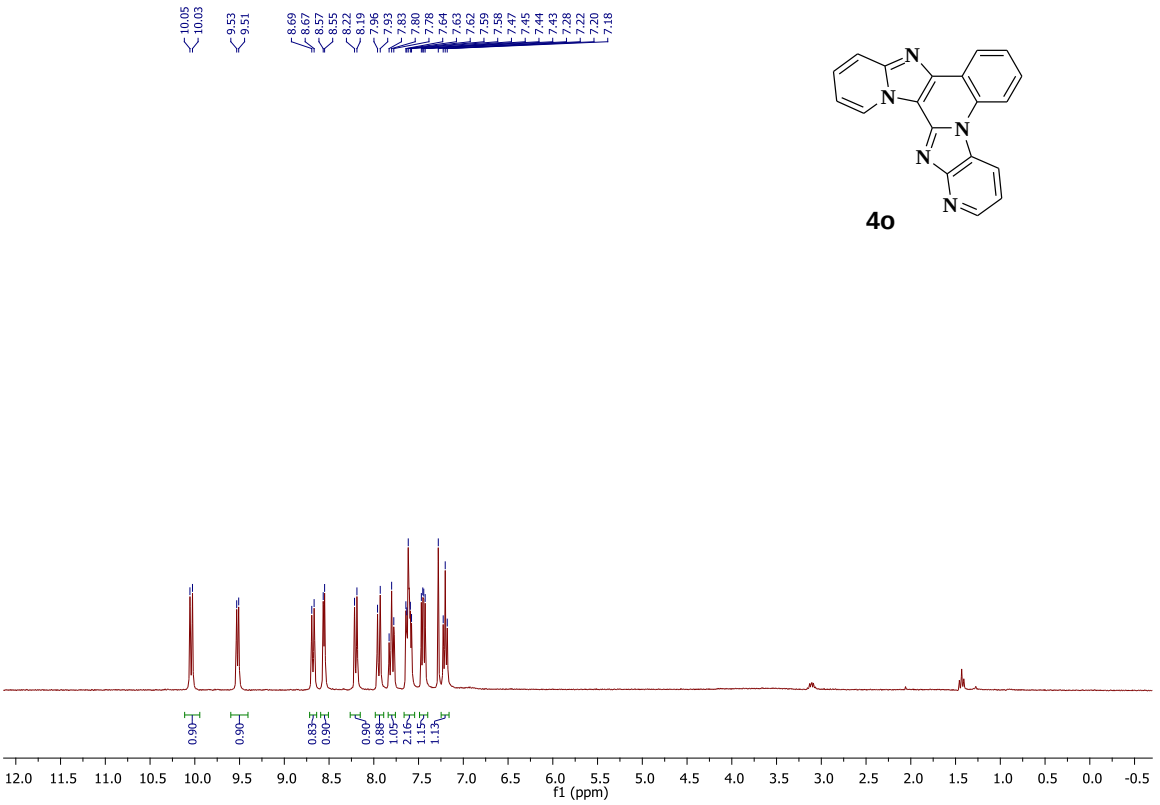
4l

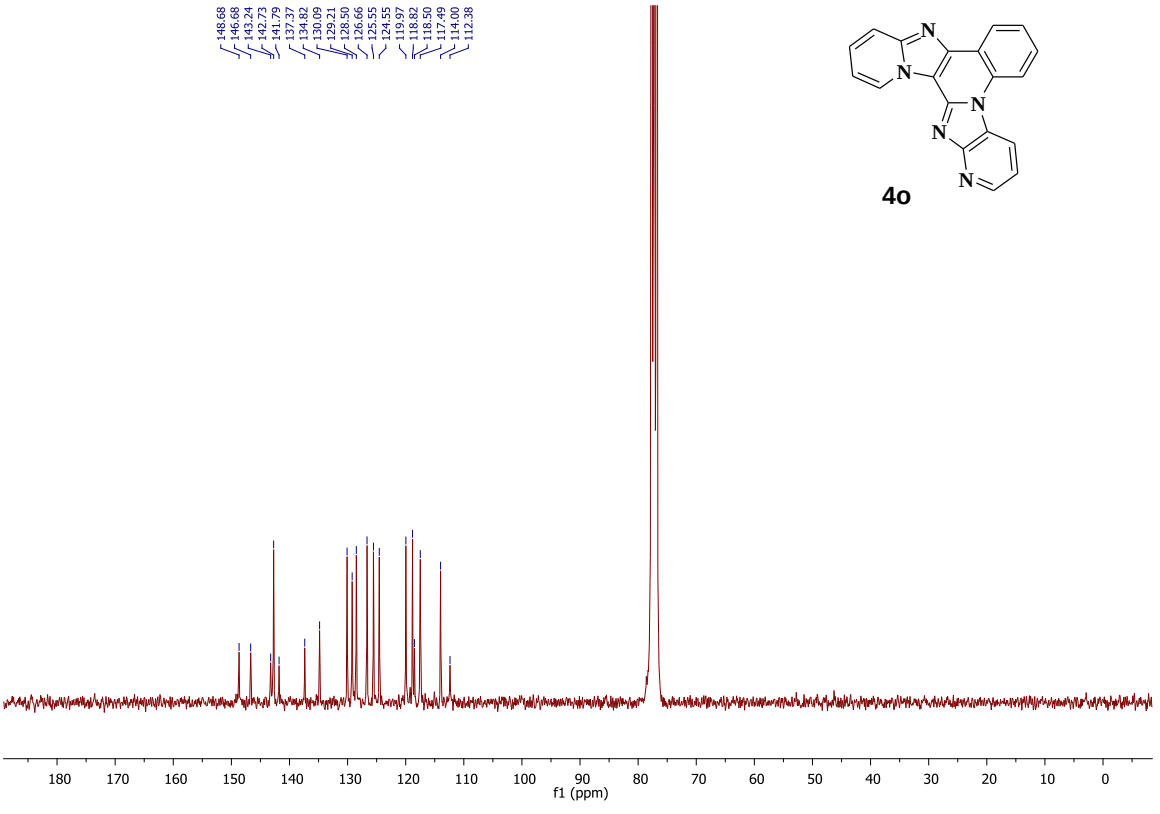
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

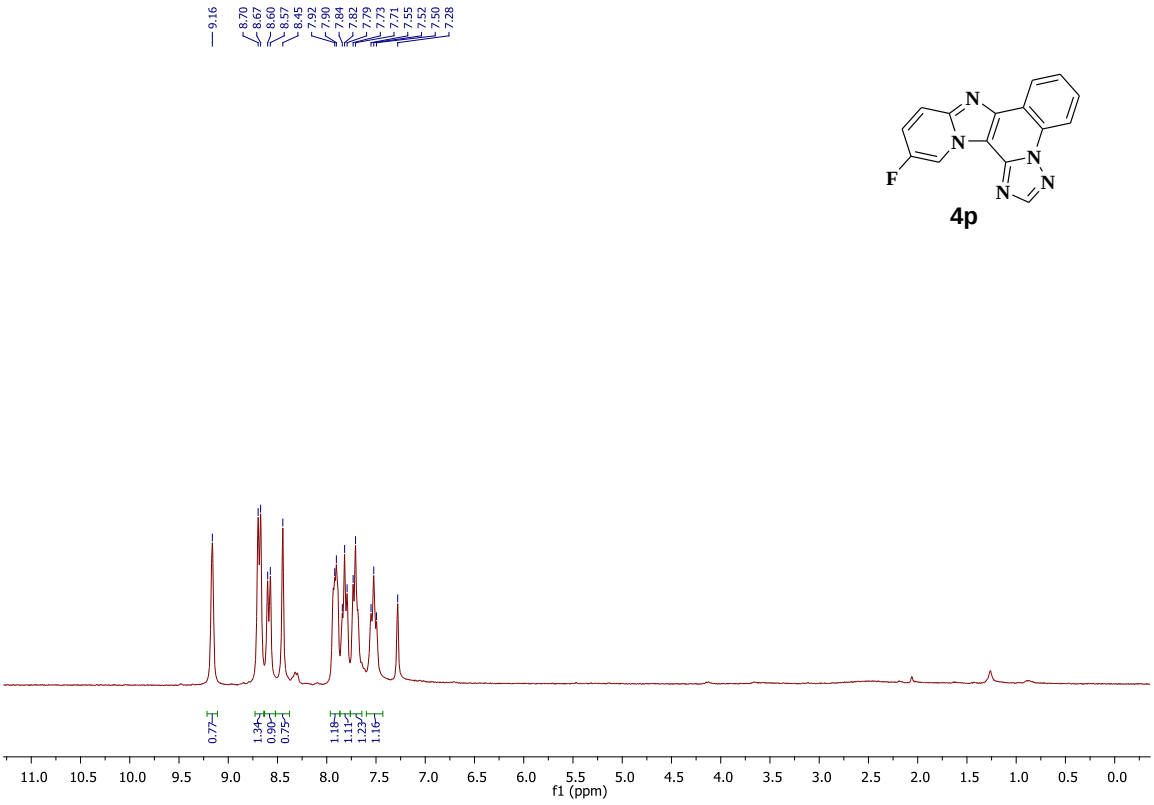

9.14
8.63
8.45
8.43
8.38
8.35
7.90
7.87
7.77
7.74
7.71
7.64
7.62
7.59
N
N
N
N
Cl
4m
0.67
1.16
1.08
1.20
1.14
1.20
3.17
f1 (ppm)
145.60
139.88
136.16
132.49
132.10
129.74
129.19
126.16
125.04
124.63
120.74
118.93
118.73
117.57
114.01
N
N
N
N
Cl
4m
f1 (ppm)

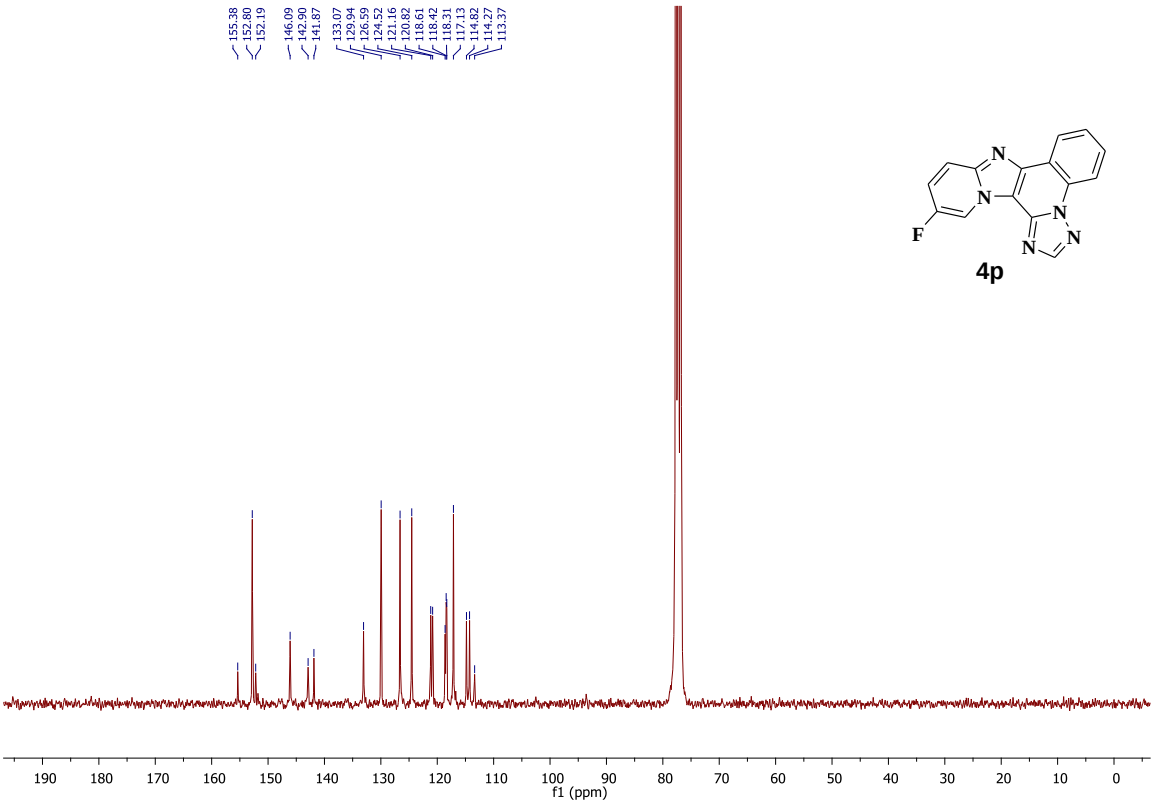

9.60
8.74
8.72
8.66
8.63
8.41
8.39
8.06
8.04
7.94
7.93
7.91
7.89
7.83
7.80
7.77
7.65
7.63
7.60
7.58
7.55
7.53
7.51
7.50
7.49
7.28
F
4n
1.00
1.03
1.16
1.10
0.94
1.15
1.05
3.98
f1 (ppm)


145.08
135.18
131.39
129.69
125.17
124.98
124.58
123.20
120.86
120.52
120.35
119.05
117.75
117.64
116.19
115.69
115.14
113.82
F
4n
f1 (ppm)


10.05
10.03
9.53
9.51
8.69
8.67
8.57
8.55
8.22
8.19
7.96
7.93
7.83
7.80
7.78
7.64
7.63
7.62
7.59
7.58
7.47
7.45
7.44
7.43
7.28
7.22
7.20
7.18
4o
0.90
0.90
0.83
0.90
0.90
0.88
1.05
2.16
1.15
1.13
f1 (ppm)


148.68
146.68
143.24
142.73
141.79
137.37
134.82
130.09
129.21
128.50
126.66
125.55
124.55
119.97
118.82
118.50
117.49
114.00
112.38
4o
f1 (ppm)


9.16
8.70
8.67
8.60
8.57
8.45
7.92
7.90
7.84
7.82
7.79
7.73
7.71
7.55
7.52
7.50
7.28
F
4p
0.77
1.34
0.90
0.75
1.10
1.11
1.23
1.16
f1 (ppm)


155.38
152.80
152.19
146.09
142.90
141.87
133.07
129.94
126.59
124.52
121.16
120.82
118.61
118.42
118.31
117.13
114.82
114.27
113.37
F
4p
f1 (ppm)