

Electronic Supplementary Information

for

Electrochemical C3-methylthiolation of imidazopyridines with dimethyl sulfoxide

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Contents

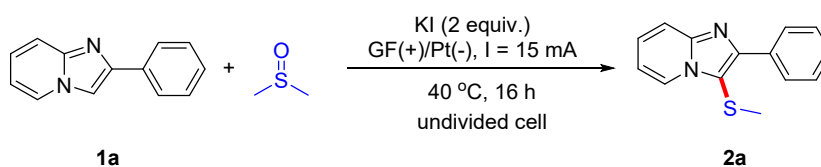
1. General information.....	S2
2. Experimental procedures	S2-S4
3. Mechanistic studies	S4-S9
4. Experimental data for the products 2 and 3	S9-S18
5. References	S18
6. ¹ H and ¹³ C NMR spectra of the products	S19-S47

1 General information

All reagents were obtained from commercial suppliers and used without further purification. Reactions were monitored by thin layer chromatography. Column chromatography was performed using silica gel (300–400 mesh). The NMR spectra were recorded on a Bruker Avance 400 spectrometer at 400 MHz (^1H) and 100 MHz (^{13}C) in CDCl_3 using tetramethylsilane as the internal standard. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, dd = doublet of doublet, dt = doublet of triplet, td = triplet of doublet, q = quartet, m = multiplet. High-resolution mass spectra were obtained with an AB Triple 5600 mass spectrometer by ESI on a TOF mass analyzer. Melting points are uncorrected.

2 Experimental procedures

2.1 General procedure for the electrochemical reactions



In an undivided three-necked flask (25 mL), 2-phenylimidazo[1,2-*a*]pyridine (**1a**, 97.1 mg, 0.5 mmol), KI (166.0 mg, 1.0 mmol), and DMSO (10 mL) were continuously added. The flask was equipped with a graphite felt electrode (30 mm × 10 mm × 2 mm) as the anode and a platinum plate electrode (10 mm × 10 mm × 1 mm) as the cathode (Figure S1). The distance between the electrodes was 10 mm. The reaction mixture was stirred and electrolyzed at a constant current (15 mA) under air at 40 °C for 16 h. After being cooled to room temperature, the resulting solution was diluted with EtOAc (10 mL). The organic layer was washed with water (10 mL). The aqueous phase was re-extracted with EtOAc (10 mL × 2). The combined organic layers were dried over Na_2SO_4 and concentrated in vacuum. Subsequently, the crude residue was purified by silica gel chromatography using petroleum ether/ethyl acetate (5:1, v/v) as eluent to afford the desired product **2a**.

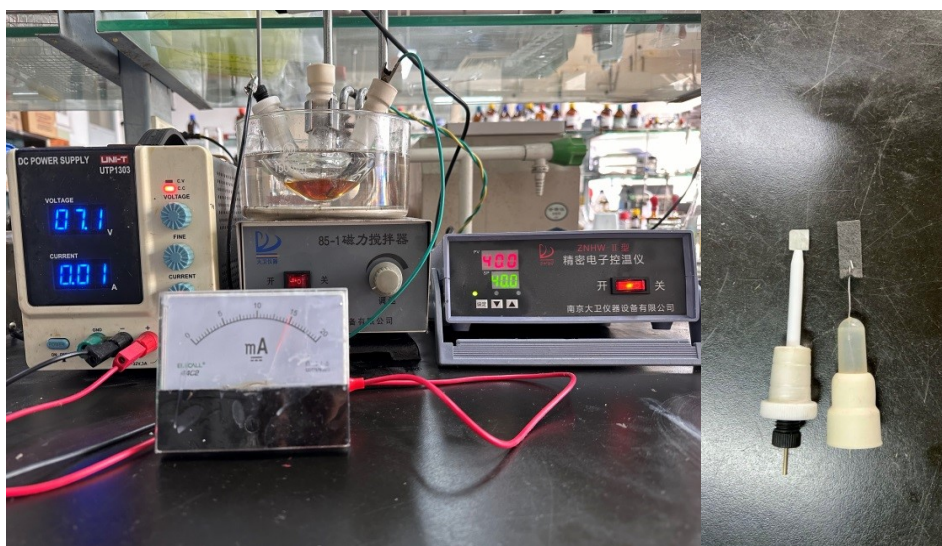
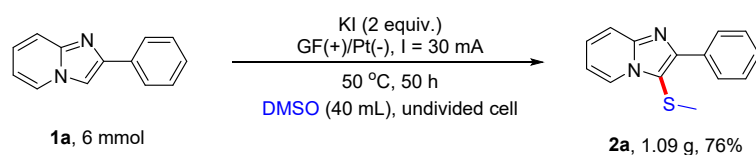


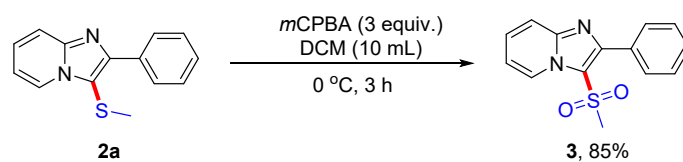
Figure S1. The electrochemical reaction setup.

2.2 Gram-scale synthesis of **2a**



In an undivided three-necked flask (100 mL), 2-phenylimidazo[1,2-*a*]pyridine (**1a**, 1.16 g, 6 mmol), KI (1.99 g, 12 mmol), and DMSO (40 mL) were continuously added. The flask was equipped with a graphite felt electrode as the anode and a platinum plate electrode (15 mm × 15 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current (30 mA) under air at 50 °C for 50 h. After being cooled to room temperature, the resulting solution was diluted with EtOAc (50 mL). The organic layer was washed with water (50 mL). The aqueous phase was re-extracted with EtOAc (50 mL × 2). The combined organic layers were dried over Na₂SO₄ and concentrated in vacuum. Subsequently, the crude residue was purified by silica gel chromatography using petroleum ether/ethyl acetate (5:1, v/v) as eluent to afford the desired product **2a**.

2.3 The transformation of **2a** to **3**



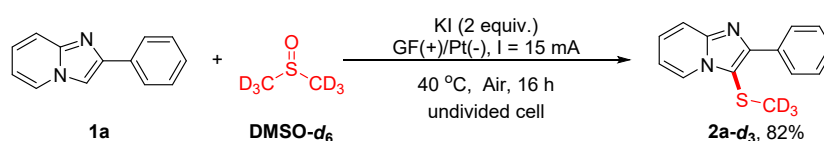
In a Schlenk flask (25 mL), **2a** (0.5 mmol, 120.0 mg), *m*CPBA (1.5 mmol, 258.9 mg) and DCM (10 mL) were added in sequence. After stirring for 3 h at 0 °C, the mixture was quenched with

water, and extracted with ethyl acetate, and the combined organic phases were dried over anhydrous Na₂SO₄, filtered, concentrated in *vacuo*. Subsequently, the crude residue was purified by silica gel chromatography using petroleum ether/ethyl acetate (1:1, v/v) as eluent to afford the desired product **3**.

3 Mechanistic studies

3.1 Control experiments

3.1.1 Deuteration experiments



In an undivided three-necked flask (25 mL), 2-phenylimidazo[1,2-*a*]pyridine (**1a**, 97.1mg, 0.5 mmol), KI (166.0 mg, 1.0 mmol), and dimethyl sulfoxide-*d*₆ (10 mL) were continuously added. The flask was equipped with a graphite felt electrode as the anode and a platinum plate electrode (10 mm × 10 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current (15 mA) under air at 40 °C for 16 h. After being cooled to room temperature, the resulting solution was diluted with EtOAc (10 mL). The organic layer was washed with water (10 mL). The aqueous phase was re-extracted with EtOAc (10 mL × 2). The combined organic layers were dried over Na₂SO₄ and concentrated in vacuum. Subsequently, the crude residue was purified by silica gel chromatography using petroleum ether/ethyl acetate (5:1, v/v) as eluent to afford the desired product **2a-d₃**.

3.1.2 HRMS analysis of the homo-coupling product 1,2-bis(methylsulfinyl)ethane (**4**)

4, HRMS (ESI-TOF) *m/z* [M+H]⁺ calcd for C₄H₁₁O₂S₂⁺, 155.0195; found 155.0198. (Figure S2)

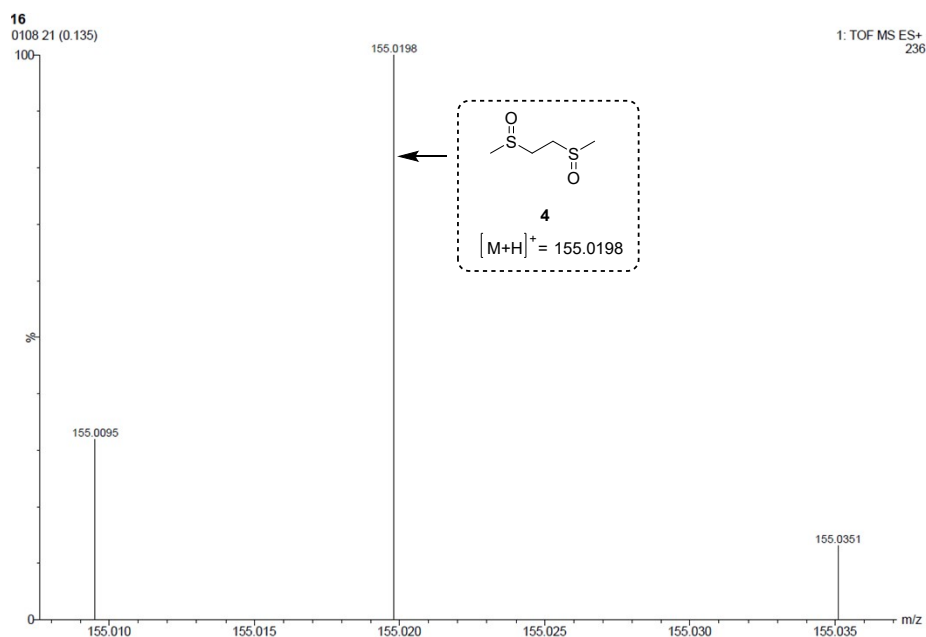
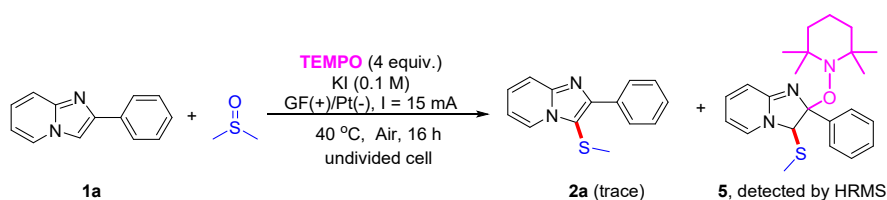


Figure S2. HRMS analysis of the homo-coupling product **4**.

3.1.3 Reaction in the presence of TEMPO



In an undivided three-necked flask (25 mL), 2-phenylimidazo[1,2-*a*]pyridine (**1a**, 97.1mg, 0.5 mmol), KI (166.0 mg, 1.0 mmol), TEMPO (312.5 mg, 2.0 mmol) and DMSO (10 mL) were continuously added. The flask was equipped with a graphite felt electrode as the anode and a platinum plate electrode (10 mm × 10 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current (15 mA) under air at 40 °C for 16 h. The reaction was obviously suppressed by the addition of TEMPO, and a trapping product **5** was detected through the HRMS analysis from the reaction solution (Figure S3).

5, HRMS (ESI-TOF) m/z $[M+H]^+$ calcd for $C_{23}H_{32}N_3OS^+$, 398.2261; found 398.2264.

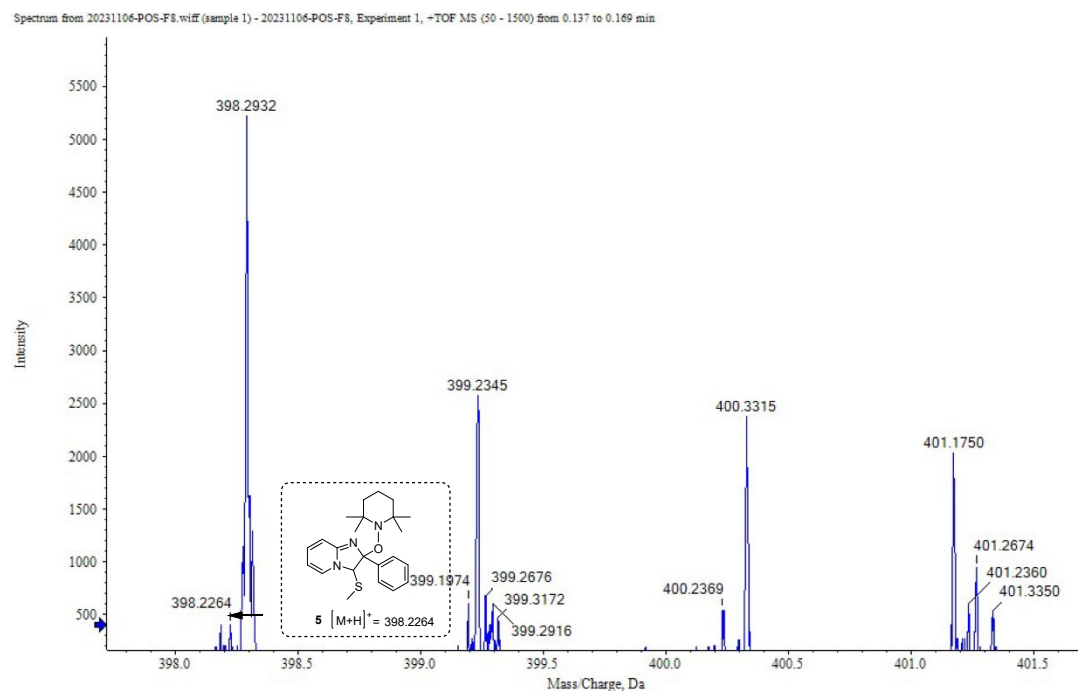
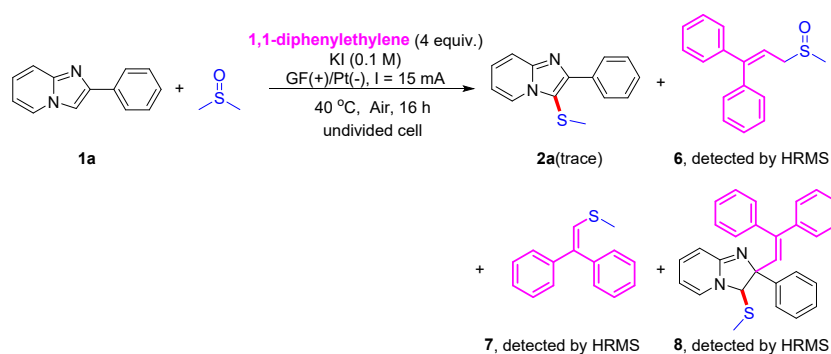


Figure S3. HRMS analysis of the radical-trapping product **5**.

3.1.4 Reaction in the presence of 1,1-diphenylethylene



In an undivided three-necked flask (25 mL), 2-phenylimidazo[1,2-*a*]pyridine (**1a**, 97.1mg, 0.5 mmol), KI (166.0 mg, 1.0 mmol), DMSO (10 mL) and 1,1-diphenylethylene (360.5 mg, 353.1 μ L, 2.0 mmol) were continuously added. The flask was equipped with a graphite felt electrode as the anode and a platinum plate electrode (10 mm \times 10 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current (15 mA) under air at 40 °C for 16 h. The reaction was obviously suppressed by the addition of 1,1-diphenylethylene, and trapping products **6**, **7** and **8** were observed through the HRMS analysis from the reaction solution (Figure S4-S6).

6, HRMS (ESI-TOF) m/z $[M+H]^+$ calcd for $C_{16}H_{17}OS^+$, 257.0095; found 257.0094.

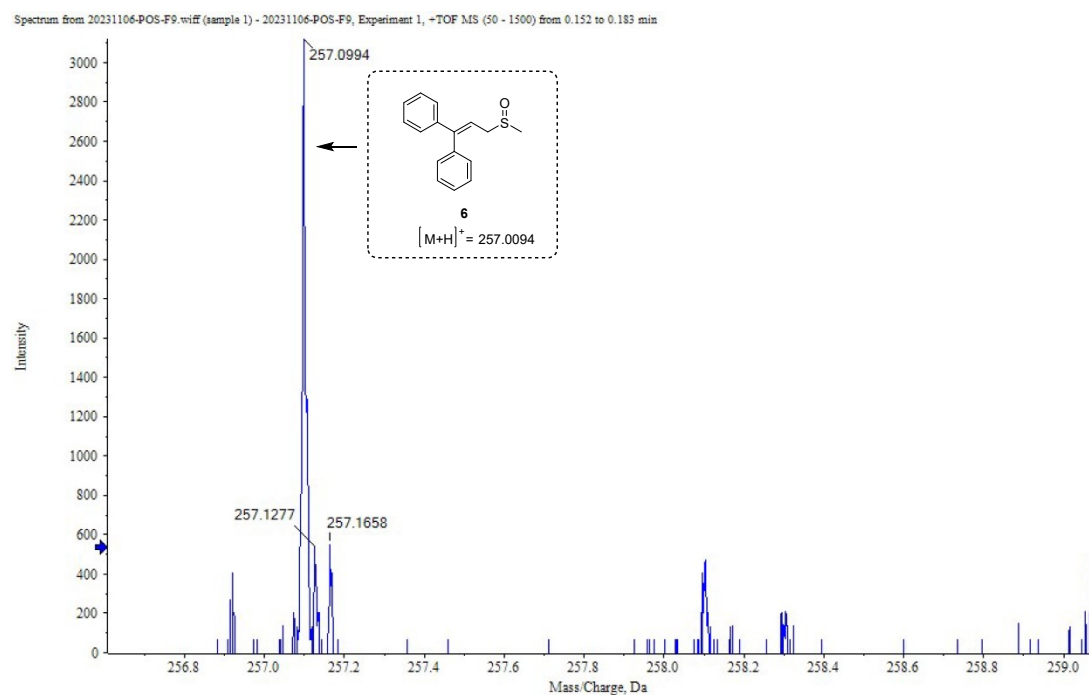


Figure S4. HRMS analysis of the radical-trapping product **6**.

7, HRMS (ESI-TOF) m/z $[M+H]^+$ calcd for $C_{15}H_{15}S^+$, 227.0889; found 227.0876.

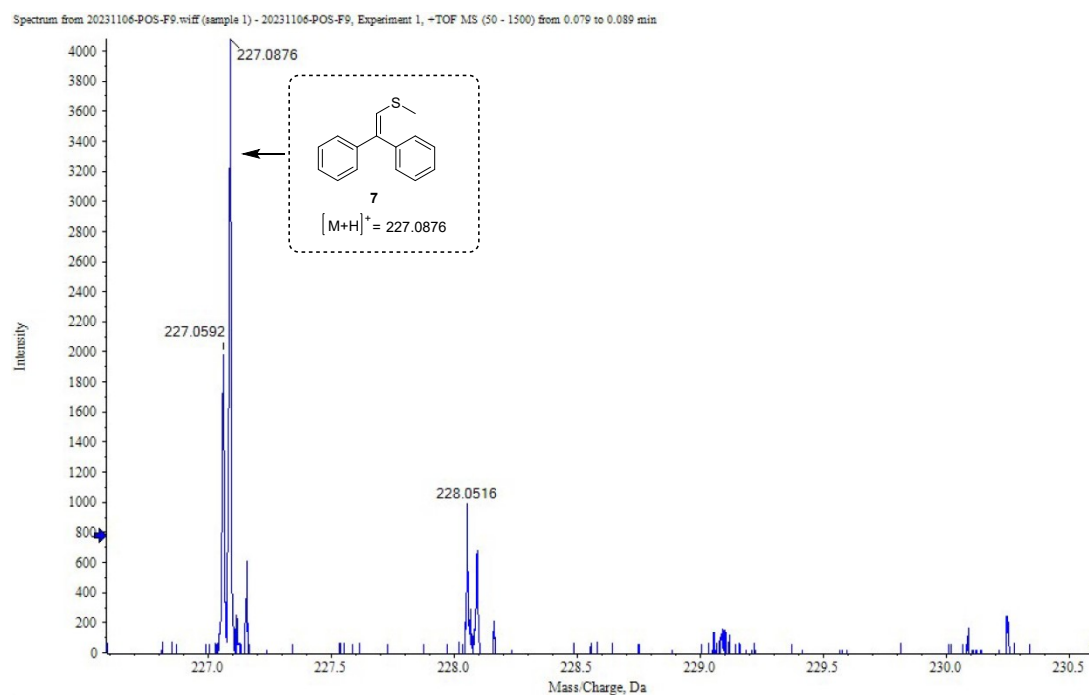


Figure S5. HRMS analysis of the radical-trapping product **7**.

8, HRMS (ESI-TOF) m/z $[M+H]^+$ calcd for $C_{28}H_{25}N_2S^+$, 421.1773; found 421.1772.

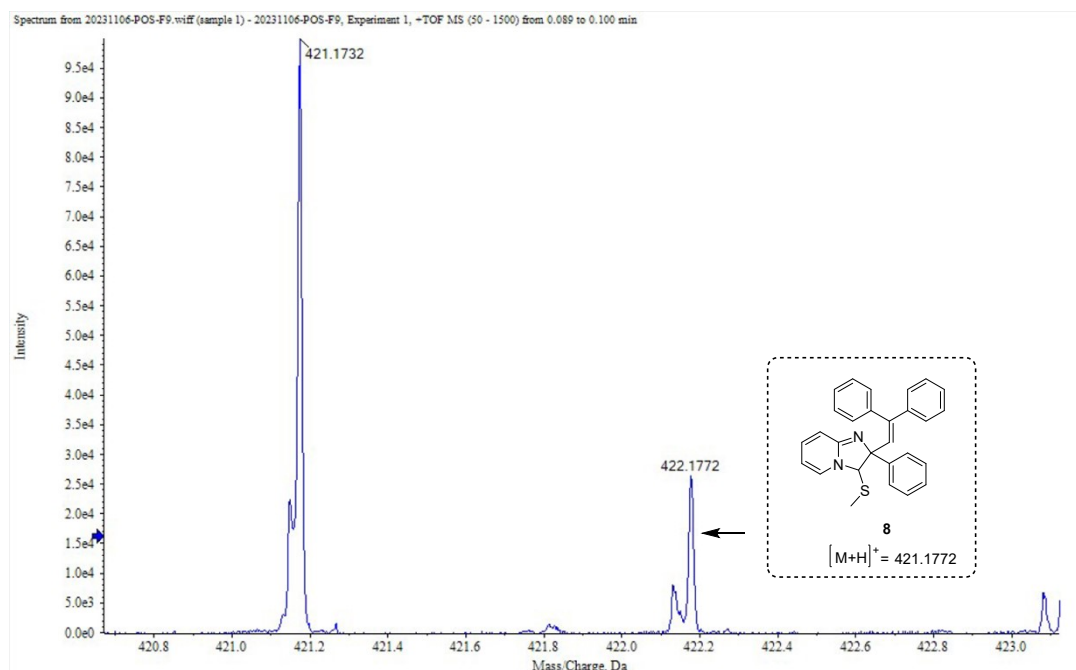


Figure S6. HRMS analysis of the radical-trapping product **8**.

3.2 Cyclic voltammetry analysis

Cyclic voltammetry was performed in a three electrodes cell in a three-necked flask at room temperature. The working electrode was a 3 mm diameter glassy carbon disc electrode, and the counter electrode was a Pt wire. The reference was silver/silver chloride electrode (Ag/AgCl) submerged in saturated aqueous KCl solution. As shown in the Figure S7, DMSO gave an oxidation peak at 1.18 V vs. Ag/AgCl in the range of 0–2.0 V, which indicated that DMSO could be oxidized under the electrochemical conditions (Figure S7).

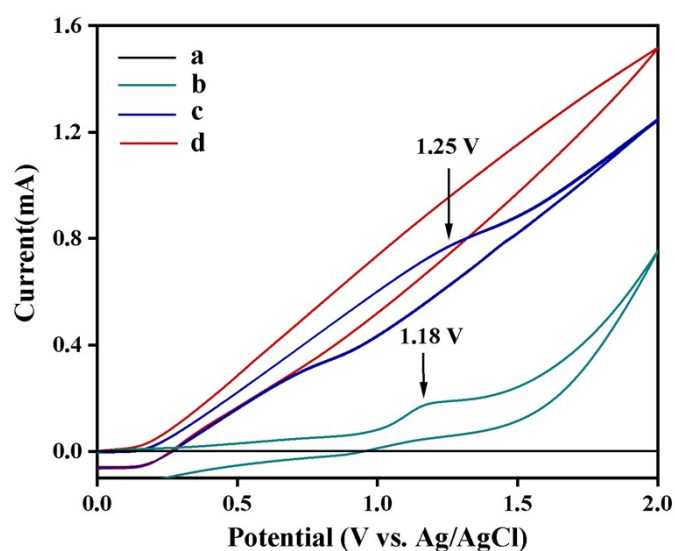
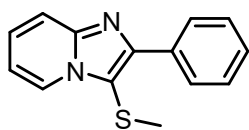


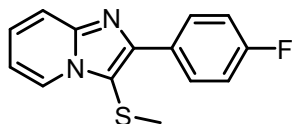
Figure S7 CV scans (scan rate 100 mV s⁻¹) of DMSO (10 mL) at room temperature. (a) Blank experiment (black curve); (b) ^tBu₄NBF₄ (0.02 M) (green curve); (c) KI (0.1 M) (blue curve); (d)

KI (0.1 M) and 2-phenylimidazo[1,2-*a*]pyridine (**1a**) (0.01 M) (red curve).

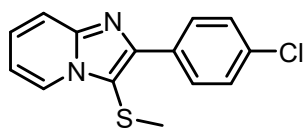
4 Experimental data for the products 2 and 3



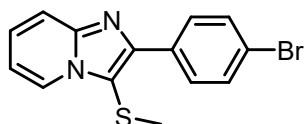
3-(Methylthio)-2-phenylimidazo[1,2-*a*]pyridine (2a).¹ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Brown oil (206.5 mg, 86%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.45 (d, $J = 6.8$ Hz, 1H), 8.28 (d, $J = 7.3$ Hz, 2H), 7.70 (d, $J = 9.0$ Hz, 1H), 7.48 (t, $J = 7.6$ Hz, 2H), 7.38 (t, $J = 7.4$ Hz, 1H), 7.29–7.26 (m, 1H), 6.91 (t, $J = 6.8$ Hz, 1H), 2.22 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 148.43, 146.10, 133.49, 128.42, 128.38, 128.30, 126.29, 124.28, 117.43, 112.97, 111.56, 18.15.



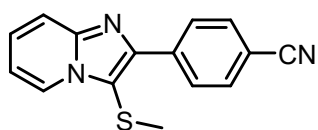
2-(4-Fluorophenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2b).² The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow solid (203.9 mg, 79%), mp 88–90 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.40 (d, $J = 6.8$ Hz, 1H), 8.27–8.23 (m, 2H), 7.64 (d, $J = 9.0$ Hz, 1H), 7.25 (t, $J = 7.9$ Hz, 1H), 7.12 (t, $J = 8.6$ Hz, 2H), 6.89 (t, $J = 6.8$ Hz, 1H), 2.18 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 162.85 (d, $J = 248.0$ Hz), 147.27, 145.92, 130.04 (d, $J = 8.1$ Hz), 129.56 (d, $J = 3.2$ Hz), 126.52, 124.28, 117.26, 115.32 (d, $J = 21.5$ Hz), 113.09, 111.28, 18.05.



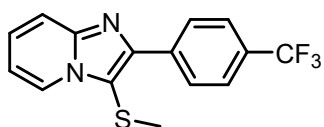
2-(4-Chlorophenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2c).³ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow solid (213.7 mg, 78%), mp 102–104 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.43 (d, $J = 6.9$ Hz, 1H), 8.26 (d, $J = 8.3$ Hz, 2H), 7.64 (d, $J = 9.0$ Hz, 1H), 7.43 (d, $J = 8.3$ Hz, 2H), 7.29–7.25 (m, 1H), 6.91 (t, $J = 6.8$ Hz, 1H), 2.21 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 147.46, 146.27, 134.15, 132.32, 129.44, 128.57, 126.21, 124.25, 117.57, 112.91, 111.53, 18.10.



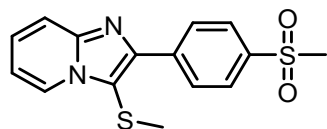
2-(4-Bromophenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2d).¹ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow solid (256.0 mg, 80%), mp 108–110 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.47 (d, *J* = 6.8 Hz, 1H), 8.22 (d, *J* = 8.2 Hz, 2H), 7.67 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.33–7.29 (m, 1H), 6.96 (t, *J* = 6.8 Hz, 1H), 2.26 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 147.57, 146.33, 132.78, 131.55, 129.75, 126.24, 124.28, 122.54, 117.65, 112.94, 111.59, 18.14.



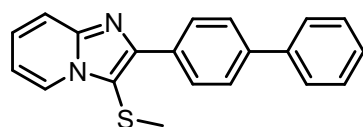
4-(3-(Methylthio)imidazo[1,2-*a*]pyridin-2-yl)benzonitrile (2e).⁴ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow solid (206.8 mg, 78%), mp 143–145 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.53–8.48 (m, 3H), 7.80–7.76 (m, 2H), 7.71 (dt, *J* = 8.8, 1.2 Hz, 1H), 7.39–7.35 (m, 1H), 7.02 (td, *J* = 6.8, 1.2 Hz, 1H), 2.30 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 146.47, 146.35, 138.29, 132.22, 128.54, 126.76, 124.37, 119.08, 117.91, 113.40, 112.98, 111.51, 18.20.



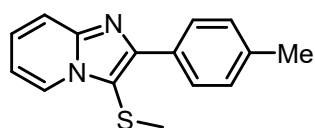
3-(Methylthio)-2-(4-(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyridine (2f). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (219.6 mg, 72%), mp 102–104 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.50–8.44 (m, 3H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.68 (dt, *J* = 9.2, 1.2 Hz, 1H), 7.34–7.30 (m, 1H), 6.96 (td, *J* = 6.8, 1.2 Hz, 1H), 2.26 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 147.09, 146.43, 137.38, 129.89 (q, *J* = 32.4 Hz), 128.34, 126.40, 125.29 (q, *J* = 3.9 Hz), 124.32, 124.31 (q, *J* = 272.1 Hz), 117.81, 113.11, 112.40, 18.14. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₅H₁₂F₃N₂S⁺ 309.0668; Found 309.0663.



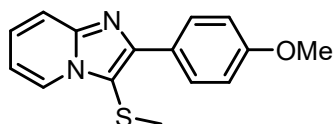
2-(4-(Methylsulfonyl)phenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2g). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (1:1, v/v). Yellow solid (235.4 mg, 74%), mp 129–131 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.57 (d, *J* = 8.1 Hz, 2H), 8.51 (d, *J* = 6.9 Hz, 1H), 8.05 (d, *J* = 8.1 Hz, 2H), 7.70 (d, *J* = 9.0 Hz, 1H), 7.38–7.34 (m, 1H), 7.01 (t, *J* = 6.8 Hz, 1H), 3.12 (s, 3H), 2.29 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 145.72, 145.19, 139.82, 138.19, 129.02, 128.01, 127.55, 124.74, 117.23, 114.19, 113.79, 44.60, 18.35. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₅H₁₅N₂O₂S₂⁺ 318.0497; Found 319.0570.



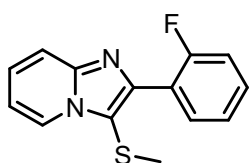
2-([1,1'-Biphenyl]-4-yl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2h). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow oil (240.2 mg, 76%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.82 (s, 1H), 8.52–8.49 (m, 2H), 8.00–7.96 (m, 2H), 7.90–7.88 (m, 1H), 7.74 (dt, *J* = 9.2, 1.2 Hz, 1H), 7.54–7.49 (m, 2H), 7.35–7.31 (m, 1H), 6.96 (td, *J* = 6.8, 1.2 Hz, 1H), 2.29 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 145.79, 143.82, 138.38, 138.24, 130.24, 126.29, 126.08, 124.88, 124.57, 124.56, 123.56, 121.74, 115.07, 110.29, 108.98, 15.68. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₂₀H₁₇N₂S⁺ 317.1107; Found 317.1104.



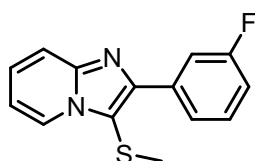
3-(Methylthio)-2-(*p*-tolyl)imidazo[1,2-*a*]pyridine (2i).¹ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (208.4 mg, 82%), mp 112–114 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.46 (dt, *J* = 6.8, 1.2 Hz, 1H), 8.23–8.21 (m, 2H), 7.67 (dt, *J* = 9.2, 1.2 Hz, 1H), 7.32–7.25 (m, 3H), 6.90 (td, *J* = 6.8, 1.2 Hz, 1H), 2.42 (s, 3H), 2.24 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 148.92, 146.29, 138.14, 131.00, 129.14, 128.15, 125.83, 124.20, 117.50, 112.62, 111.00, 21.39, 18.13.



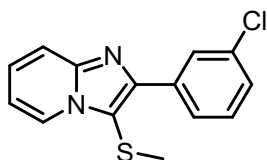
2-(4-Methoxyphenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2j).² The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow oil (183.7 mg, 68%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.47 (d, *J* = 6.8 Hz, 1H), 8.26 (d, *J* = 8.5 Hz, 2H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.32–7.28 (m, 1H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.94 (t, *J* = 6.8 Hz, 1H), 3.87 (s, 3H), 2.25 (d, *J* = 1.6 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 159.86, 148.19, 145.94, 129.59, 126.26, 125.96, 124.23, 117.15, 113.87, 112.87, 110.61, 55.31, 18.11.



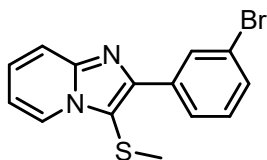
2-(2-Fluorophenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2k).³ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (3:1, v/v). Yellow solid (203.9 mg, 79%), mp 90–92 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.48 (d, *J* = 6.9 Hz, 1H), 7.76–7.70 (m, 2H), 7.46–7.41 (m, 1H), 7.38–7.34 (m, 1H), 7.30–7.26 (m, 1H), 7.25–7.20 (m, 1H), 7.01 (td, *J* = 6.8, 1.1 Hz, 1H), 2.27 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 160.24 (d, *J* = 249.4 Hz), 146.46, 145.39, 132.18 (d, *J* = 3.0 Hz), 130.31 (d, *J* = 8.3 Hz), 126.14, 124.32, 124.03 (d, *J* = 3.6 Hz), 121.79 (d, *J* = 14.2 Hz), 117.86, 115.97 (d, *J* = 22.3 Hz), 113.96, 113.12, 17.89 (d, *J* = 2.5 Hz).



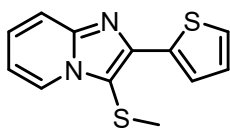
2-(3-Fluorophenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2l). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (10:1, v/v). Yellow solid (188.4 mg, 73%), mp 96–98 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.50 (dt, *J* = 6.8, 1.2 Hz, 1H), 8.16–8.08 (m, 2H), 7.68 (d, *J* = 9.0 Hz, 1H), 7.48–7.43 (m, 1H), 7.35–7.31 (m, 1H), 7.12–7.07 (m, 1H), 6.97 (td, *J* = 6.8, 1.2 Hz, 1H), 2.28 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 162.94 (d, *J* = 244.3 Hz), 147.35, 146.29, 136.05 (d, *J* = 8.2 Hz), 129.86 (d, *J* = 8.2 Hz), 126.24, 124.29, 123.81 (d, *J* = 2.8 Hz), 117.74, 115.08 (d, *J* = 21.2 Hz), 114.99 (d, *J* = 23.2 Hz), 112.97, 111.88, 18.15. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₄H₁₂FN₂S⁺ 259.0700; Found 259.0699.



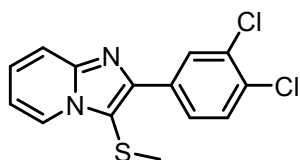
2-(3-Chlorophenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2m). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (208.3 mg, 76%), mp 100–102 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.48 (dt, *J* = 6.8, 1.2 Hz, 1H), 8.34 (t, *J* = 1.9 Hz, 1H), 8.24 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.67 (dt, *J* = 8.8, 1.2 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.38–7.29 (m, 2H), 6.95 (td, *J* = 6.8, 1.2 Hz, 1H), 2.27 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 147.22, 146.32, 135.68, 134.39, 129.64, 128.24, 128.17, 126.26, 126.25, 124.30, 117.73, 112.99, 111.92, 18.17. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₄H₁₂ClN₂S⁺ 275.0404; Found 275.0401.



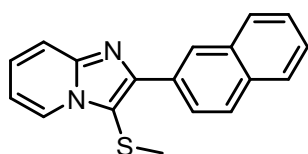
2-(3-Bromophenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2n).⁵ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (222.6 mg, 70%), mp 103–105 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.51–8.49 (m, 2H), 8.30–8.27 (m, 1H), 7.70 (d, *J* = 9.0 Hz, 1H), 7.53 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.38–7.32 (m, 2H), 6.98 (td, *J* = 6.8, 1.1 Hz, 1H), 2.28 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 147.03, 146.27, 135.83, 131.21, 131.09, 129.92, 126.71, 126.37, 124.32, 122.62, 117.71, 113.07, 111.99, 18.19.



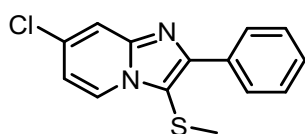
3-(Methylthio)-2-(thiophen-2-yl)imidazo[1,2-*a*]pyridine (2o).⁴ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow oil (182.1 mg, 74%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.43 (dt, *J* = 6.8, 1.2 Hz, 1H), 8.07 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.64 (d, *J* = 9.1 Hz, 1H), 7.40 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.30–7.26 (m, 1H), 7.16 (dd, *J* = 5.2, 4.0 Hz, 1H), 6.91 (td, *J* = 6.8, 1.2 Hz, 1H), 2.29 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 146.39, 144.61, 136.71, 127.66, 126.44, 126.24, 126.20, 124.15, 117.31, 112.82, 110.26, 17.84.



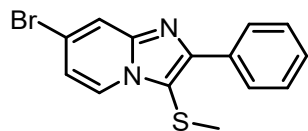
2-(3,4-Dichlorophenyl)-3-(methylthio)imidazo[1,2-*a*]pyridine (2p). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (212.5 mg, 69%), mp 85–87 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.48–8.46 (m, 2H), 8.22 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.66 (dt, *J* = 8.8, 1.2 Hz, 1H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.35–7.31 (m, 1H), 6.97 (td, *J* = 6.8, 1.2 Hz, 1H), 2.27 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 143.79, 143.64, 131.39, 130.04, 129.61, 127.79, 127.30, 124.70, 123.92, 121.75, 115.19, 110.58, 109.46, 15.60. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₄H₁₁Cl₂N₂S⁺ 309.0015; Found 309.0008.



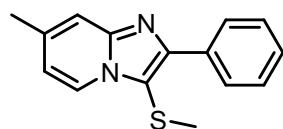
3-(Methylthio)-2-(naphthalen-2-yl)imidazo[1,2-*a*]pyridine (2q).⁴ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow oil (220.5 mg, 76%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.82 (s, 1H), 8.52–8.49 (m, 2H), 8.00–7.96 (m, 2H), 7.90–7.88 (m, 1H), 7.74 (dt, *J* = 9.2, 1.2 Hz, 1H), 7.54–7.49 (m, 2H), 7.35–7.31 (m, 1H), 6.96 (td, *J* = 6.8, 1.2 Hz, 1H), 2.29 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 148.47, 146.32, 133.46, 133.25, 131.12, 128.67, 127.94, 127.66, 127.62, 126.33, 126.27, 126.13, 125.94, 124.32, 117.53, 112.93, 111.90, 18.26.



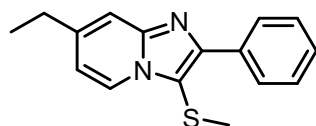
7-Chloro-3-(methylthio)-2-phenylimidazo[1,2-*a*]pyridine (2r). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (197.3 mg, 72%), mp 108–110 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.39 (d, *J* = 7.2 Hz, 1H), 8.29–8.27 (m, 2H), 7.67 (d, *J* = 2.0 Hz, 1H), 7.52–7.48 (m, 2H), 7.43–7.39 (m, 1H), 6.91 (dd, *J* = 7.2, 2.0 Hz, 1H), 2.25 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 149.56, 145.97, 133.40, 132.53, 128.54, 128.47, 128.19, 124.61, 116.46, 114.32, 111.89, 18.24. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₄H₁₂ClN₂S⁺ 275.0405; Found 275.0399.



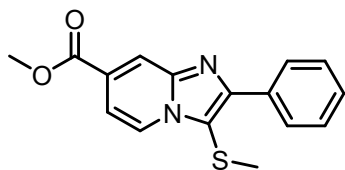
7-Bromo-3-(methylthio)-2-phenylimidazo[1,2-*a*]pyridine (2s). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (10:1, v/v). Yellow solid (232.1 mg, 73%), mp 98–100 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.37 (d, *J* = 7.2 Hz, 1H), 8.30–8.27 (m, 2H), 7.89 (d, *J* = 1.8 Hz, 1H), 7.53–7.49 (m, 2H), 7.45–7.41 (m, 1H), 7.08 (dd, *J* = 7.2, 2.0 Hz, 1H), 2.28 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 149.10, 146.10, 133.05, 128.69, 128.53, 128.25, 124.65, 120.28, 119.73, 116.88, 112.14, 18.22. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₄H₁₂BrN₂S⁺ 318.9900; Found 318.9903.



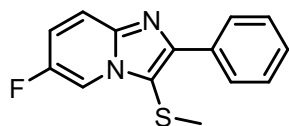
7-Methyl-3-(methylthio)-2-phenylimidazo[1,2-*a*]pyridine (2t).⁴ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (203.3 mg, 80%), mp 116–118 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.38 (d, *J* = 7.0 Hz, 1H), 8.31–8.29 (m, 2H), 7.52–7.46 (m, 3H), 7.42–7.38 (m, 1H), 6.80 (dd, *J* = 7.2, 2.0 Hz, 1H), 2.47 (s, 3H), 2.28 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 148.48, 146.62, 137.28, 133.81, 128.37, 128.22, 128.20, 123.46, 116.08, 115.45, 110.70, 21.39, 18.32.



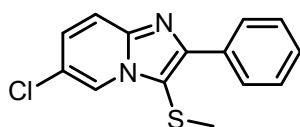
7-Ethyl-3-(methylthio)-2-phenylimidazo[1,2-*a*]pyridine (2u).³ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (10:1, v/v). Yellow oil (211.8 mg, 79%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.38 (d, *J* = 7.0 Hz, 1H), 8.31–8.29 (m, 2H), 7.51–7.47 (m, 3H), 7.41–7.37 (m, 1H), 6.81 (dd, *J* = 6.8, 1.6 Hz, 1H), 2.75 (q, *J* = 7.5 Hz, 2H), 2.26 (s, 3H), 1.32 (t, *J* = 7.6 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 148.63, 146.81, 143.28, 133.97, 128.35, 128.19, 128.14, 123.61, 114.66, 114.40, 110.66, 28.42, 18.33, 14.44.



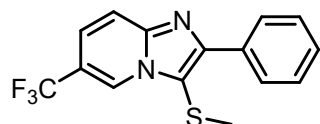
Methyl 3-(methylthio)-2-phenylimidazo[1,2-*a*]pyridine-7-carboxylate (2v). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (199.7 mg, 67%), mp 112–114 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.55 (dd, *J* = 7.2, 1.2 Hz, 1H), 8.44 (t, *J* = 1.2 Hz, 1H), 8.34–8.31 (m, 2H), 7.58 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.55–7.51 (m, 2H), 7.47–7.43 (m, 1H), 4.01 (s, 3H), 2.32 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 165.51, 144.98, 132.94, 128.86, 128.58, 128.34, 127.58, 124.00, 119.87, 113.76, 112.27, 52.73, 18.08. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₆H₁₅N₂O₂S⁺ 299.0849; Found 299.0831.



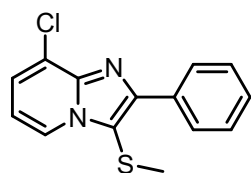
6-Fluoro-3-(methylthio)-2-phenylimidazo[1,2-*a*]pyridine (2w).⁴ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (10:1, v/v). Yellow solid (191.0 mg, 74%), mp 135–137 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.42–8.40 (m, 1H), 8.30–8.27 (m, 2H), 7.66–7.62 (m, 1H), 7.52–7.47 (m, 2H), 7.42–7.38 (m, 1H), 7.23–7.18 (m, 1H), 2.26 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 153.79 (d, *J* = 237.6 Hz), 150.02 (d, *J* = 2.4 Hz), 143.85, 133.58, 128.45, 128.44, 128.10, 118.15 (d, *J* = 8.7 Hz), 117.78 (d, *J* = 25.6 Hz), 112.91, 111.11 (d, *J* = 41.5 Hz), 18.03.



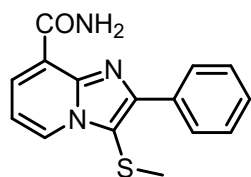
6-Chloro-3-(methylthio)-2-phenylimidazo[1,2-*a*]pyridine (2x).⁴ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (194.6 mg, 71%), mp 164–166 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.54 (dd, *J* = 2.0, 0.8 Hz, 1H), 8.31–8.29 (m, 2H), 7.64 (dd, *J* = 9.6, 0.8 Hz, 1H), 7.53–7.49 (m, 2H), 7.44–7.40 (m, 1H), 7.28 (dd, *J* = 9.2, 2.0 Hz, 1H), 2.30 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 149.58, 144.60, 133.33, 128.58, 128.50, 128.18, 127.37, 122.31, 121.32, 118.01, 112.24, 18.23.



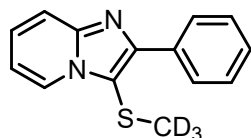
3-(Methylthio)-2-phenyl-6-(trifluoromethyl)imidazo[1,2-*a*]pyridine (2y).⁴ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (215.6 mg, 70%), mp 140–142 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.86 (s, 1H), 8.35–8.32 (m, 2H), 7.79 (d, *J* = 9.3 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 2H), 7.48–7.43 (m, 2H), 2.32 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 150.45, 146.05, 133.03, 128.86, 128.56, 123.63 (q, *J* = 271.2 Hz), 123.32 (q, *J* = 5.5 Hz), 121.89 (q, *J* = 2.9 Hz), 118.30, 117.26 (q, *J* = 34.3 Hz), 113.35, 18.34.



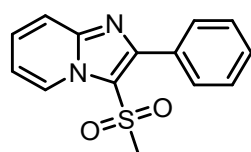
8-Chloro-3-(methylthio)-2-phenylimidazo[1,2-*a*]pyridine (2z).⁴ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow solid (205.5 mg, 75%), mp 110–112 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.40 (dd, *J* = 6.8, 0.8 Hz, 1H), 8.34–8.32 (m, 2H), 7.52–7.48 (m, 2H), 7.41 (t, *J* = 7.3 Hz, 1H), 7.35 (dd, *J* = 7.2, 1.2 Hz, 1H), 6.86 (t, *J* = 7.1 Hz, 1H), 2.25 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 149.48, 143.55, 133.39, 128.80, 128.52, 128.39, 124.85, 123.38, 123.07, 113.40, 112.30, 18.22.



3-(Methylthio)-2-phenylimidazo[1,2-*a*]pyridine-8-carboxamide (2aa). The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (1:1, v/v). Yellow solid (164.2 mg, 58%), mp 182–184 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 10.16 (s, 1H), 8.68 (d, *J* = 6.7 Hz, 1H), 8.37–8.33 (m, 3H), 7.56–7.51 (m, 2H), 7.48–7.44 (m, 1H), 7.15 (t, *J* = 7.0 Hz, 1H), 6.11 (s, 1H), 2.32 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 164.96, 148.12, 144.35, 133.00, 129.89, 128.82, 128.54, 128.30, 127.28, 120.75, 112.62, 18.29. HRMS (ESI) *m/z*: [M + H]⁺ Calcd for C₁₅H₁₄N₃OS⁺ 284.0852; Found 284.0856.



3-((Methyl-*d*₃)thio)-2-phenylimidazo[1,2-*a*]pyridine (2a-*d*₃).² The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (5:1, v/v). Yellow oil (199.3 mg, 82%). ¹H NMR (400 MHz, CDCl₃) δ (ppm) 8.51 (d, *J* = 6.8 Hz, 1H), 8.33–8.30 (m, 2H), 7.71 (d, *J* = 9.0 Hz, 1H), 7.53–7.49 (m, 2H), 7.44–7.39 (m, 1H), 7.35–7.31 (m, 1H), 6.99–6.95 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 148.69, 146.25, 133.69, 128.42, 128.34, 128.28, 126.07, 124.29, 117.61, 112.83, 112.67.



3-(Methylsulfonyl)-2-phenylimidazo[1,2-*a*]pyridine (3).⁶ The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (1:1, v/v). Yellow solid (231.3 mg, 85 %), mp 185–187 °C. ¹H NMR (400 MHz, CDCl₃) δ (ppm) 9.08 (d, *J* = 6.8 Hz, 1H), 7.83 (d, *J* = 6.8 Hz, 2H), 7.79 (d, *J* = 9.0 Hz, 1H), 7.52–7.43 (m, 4H), 7.02 (t, *J* = 6.8 Hz, 1H), 3.15 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm) 148.86, 147.57, 132.24, 129.29, 129.24, 128.72, 127.72, 126.90, 118.33, 116.09, 113.79, 37.96.

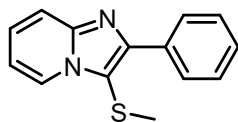
5 References

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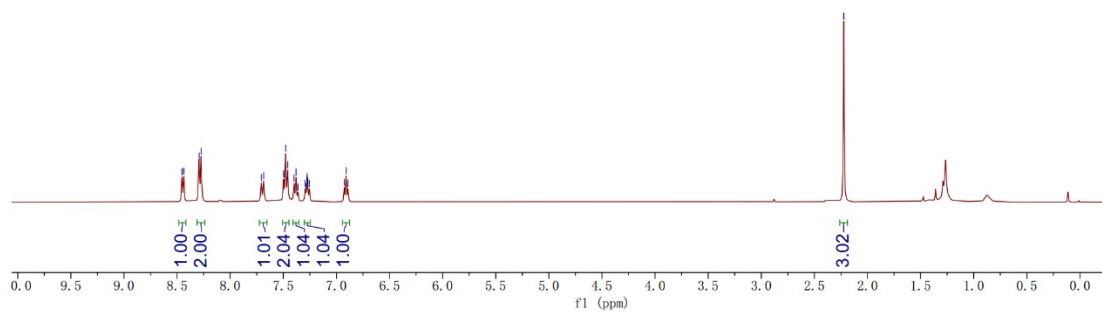
6 ^1H and ^{13}C NMR spectra of the products 2 and 3

8.454
8.437
8.292
8.274
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7.685
7.497
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7.459
7.399
7.380
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6.926
6.909
6.892

-2.223

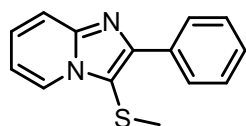


2a (^1H NMR) (400 MHz, CDCl_3)

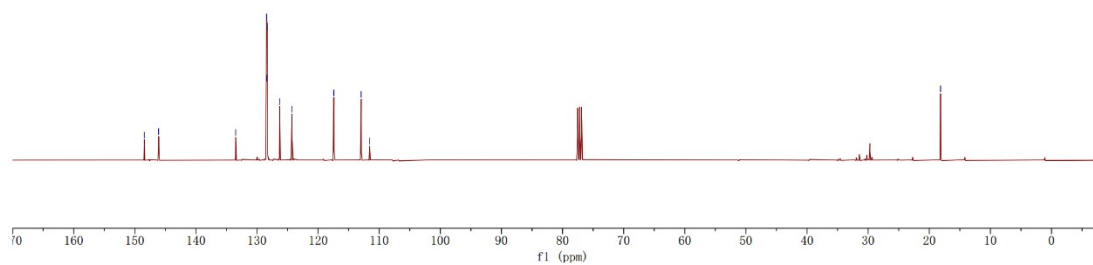


148.434
146.102
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128.423
128.383
128.304
126.292
124.277
117.428
112.966
111.562

-18.151

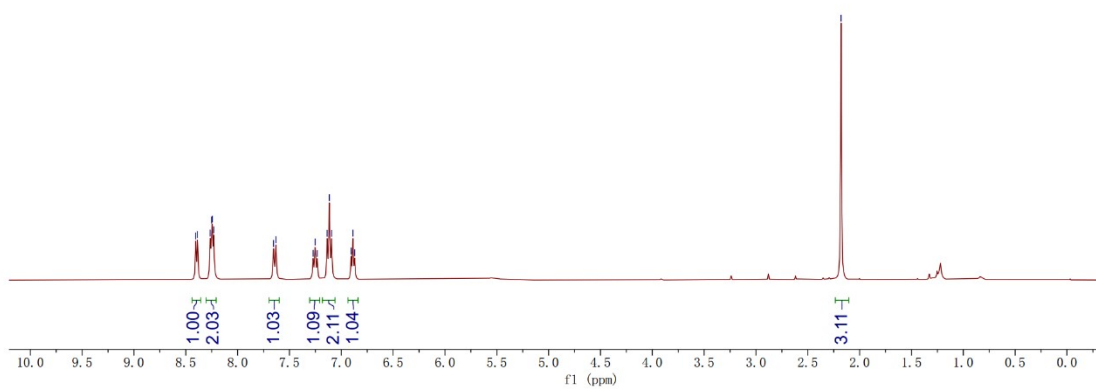
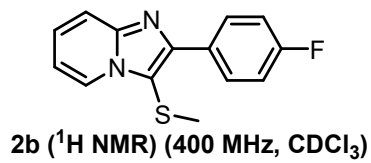


2a (^{13}C NMR) (100 MHz, CDCl_3)



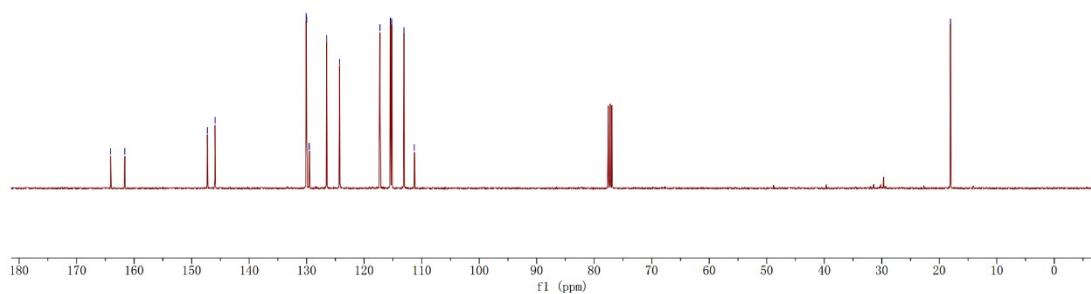
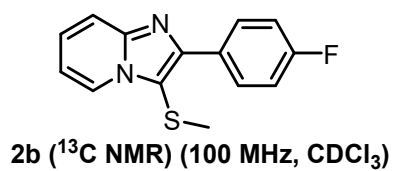
8.404
8.387
8.265
8.252
8.244
8.230
7.654
7.631
7.272
7.252
7.232
7.137
7.115
7.094
6.905
6.888
6.871

-2.179



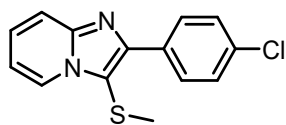
164.086
161.621
147.266
145.919
130.079
129.998
129.575
129.543
126.519
124.280
117.261
115.430
115.216
113.088
111.279

-18.046

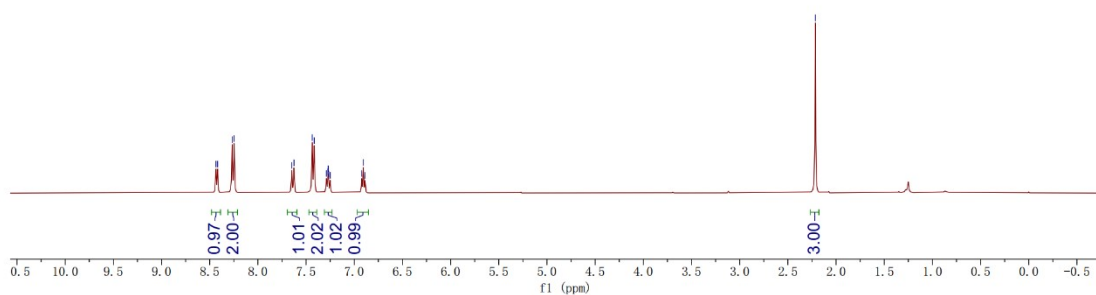


8.435
8.418
8.267
8.247
7.648
7.625
7.436
7.415
7.289
7.274
7.270
7.265
7.250
6.922
6.905
6.888

-2.215

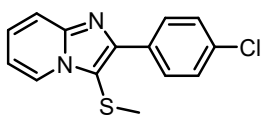


2c (¹H NMR) (400 MHz, CDCl₃)

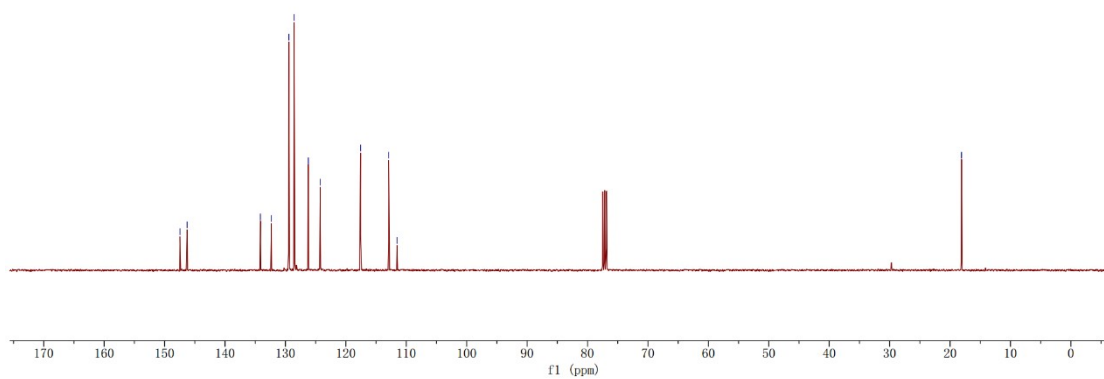


147.457
146.273
134.146
132.321
129.443
128.566
126.210
124.246
117.570
112.911
111.532

-18.104

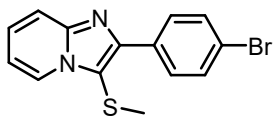


2c (¹³C NMR) (100 MHz, CDCl₃)

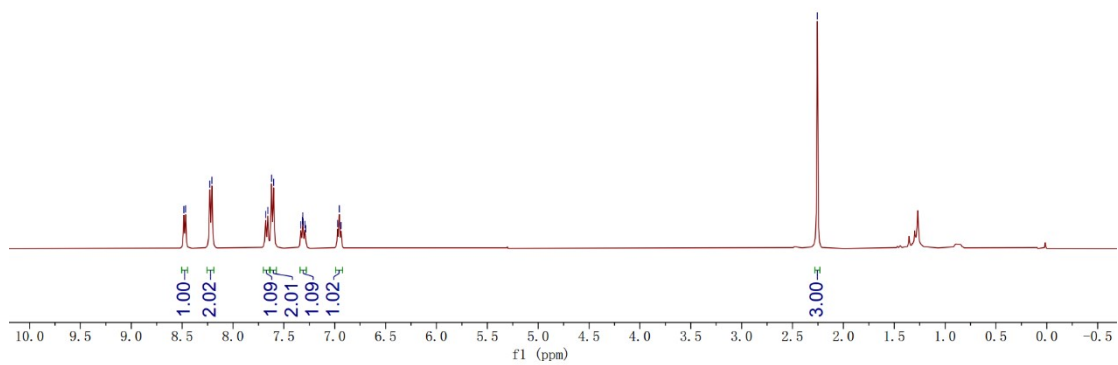


8.483
8.466
8.228
8.207
7.680
7.658
7.621
7.601
7.333
7.318
7.314
7.309
7.294
7.285
6.972
6.955
6.938

-2.256

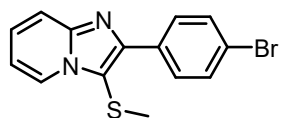


2d (^1H NMR) (400 MHz, CDCl_3)

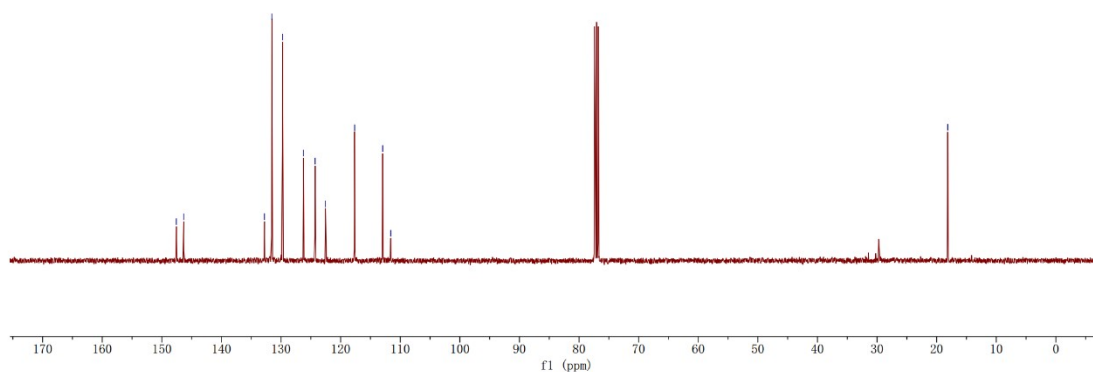


147.570
146.334
132.783
131.550
129.754
126.236
124.281
122.541
117.650
112.944
111.594

-18.140

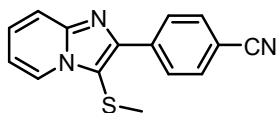


2d (^{13}C NMR) (100 MHz, CDCl_3)

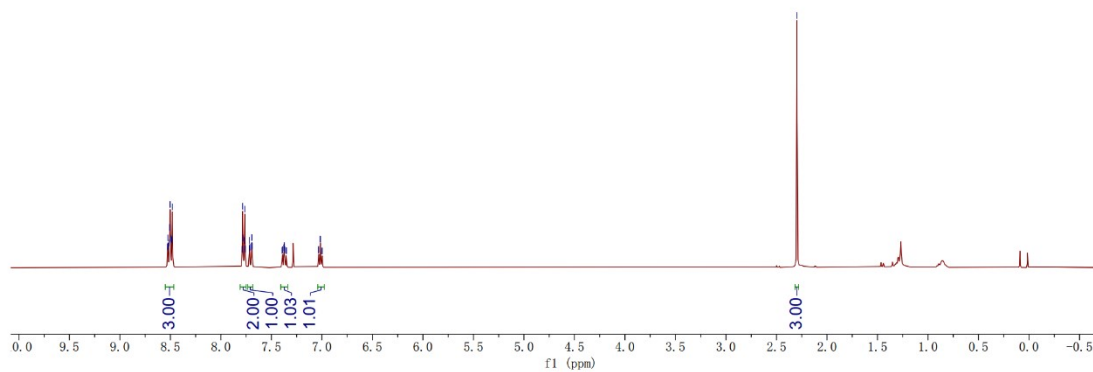


8.528
8.525
8.522
8.511
8.508
8.503
8.498
8.486
8.481
7.790
7.785
7.781
7.768
7.764
7.759
7.719
7.716
7.714
7.697
7.694
7.691
7.393
7.390
7.376
7.373
7.371
7.367
7.354
7.351
7.035
7.032
7.018
7.015
7.001
6.998

2.297

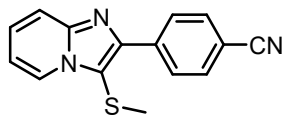


2e (^1H NMR) (400 MHz, CDCl_3)

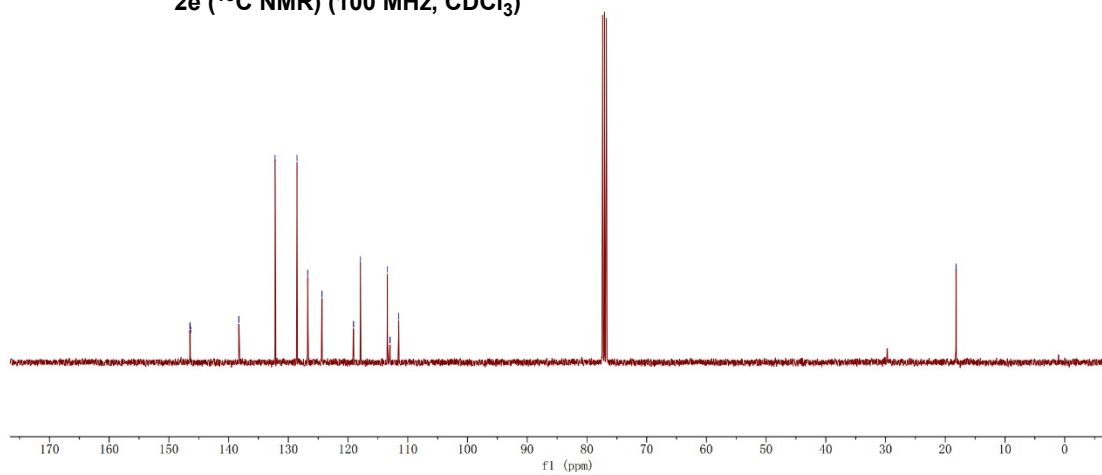


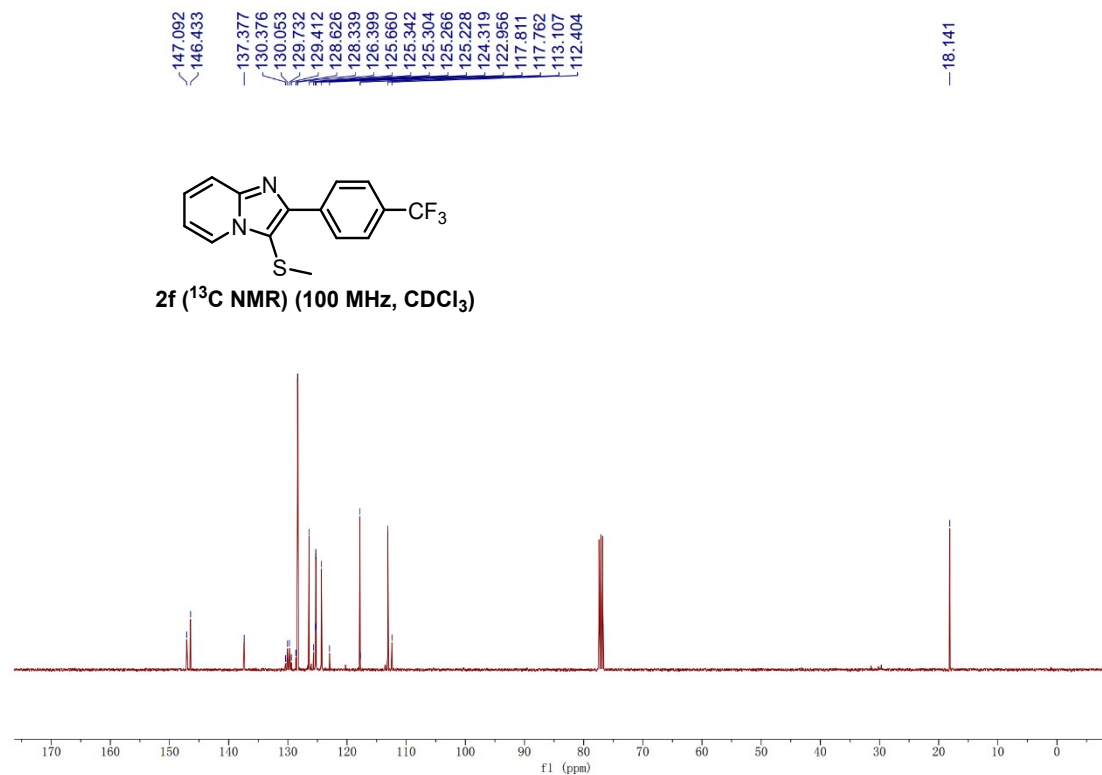
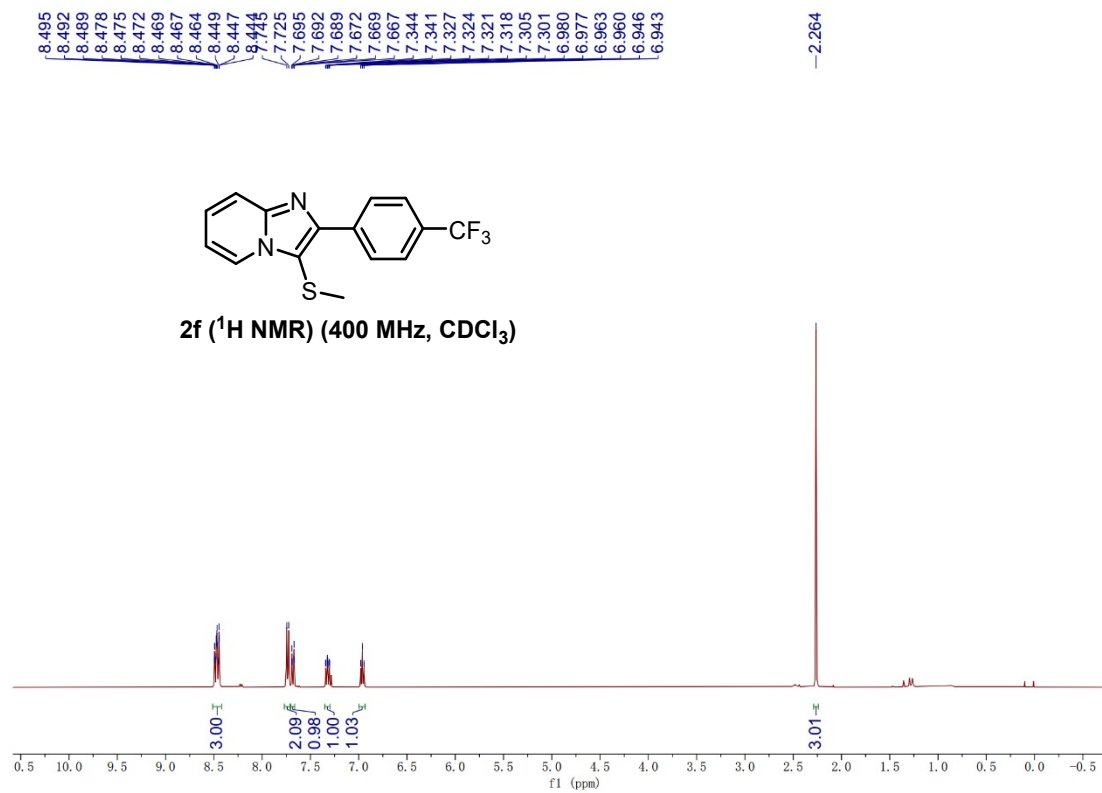
146.469
146.349
138.285
132.222
128.544
126.758
124.374
119.078
117.910
113.395
112.976
111.508

18.204



2e (^{13}C NMR) (100 MHz, CDCl_3)

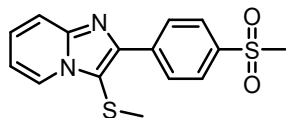




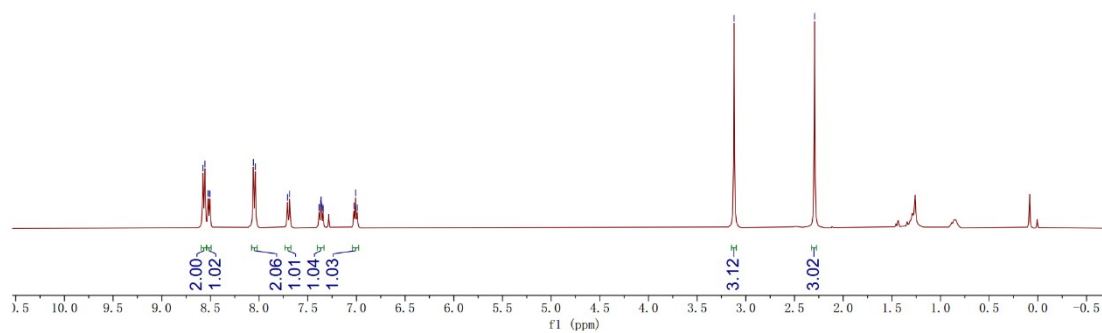
8.577
8.556
8.523
8.506
8.059
8.039
7.708
7.686
7.384
7.381
7.367
7.363
7.358
7.344
7.341
7.026
7.009
6.992

— 3.121

— 2.293



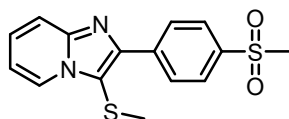
2g (¹H NMR) (400 MHz, CDCl₃)



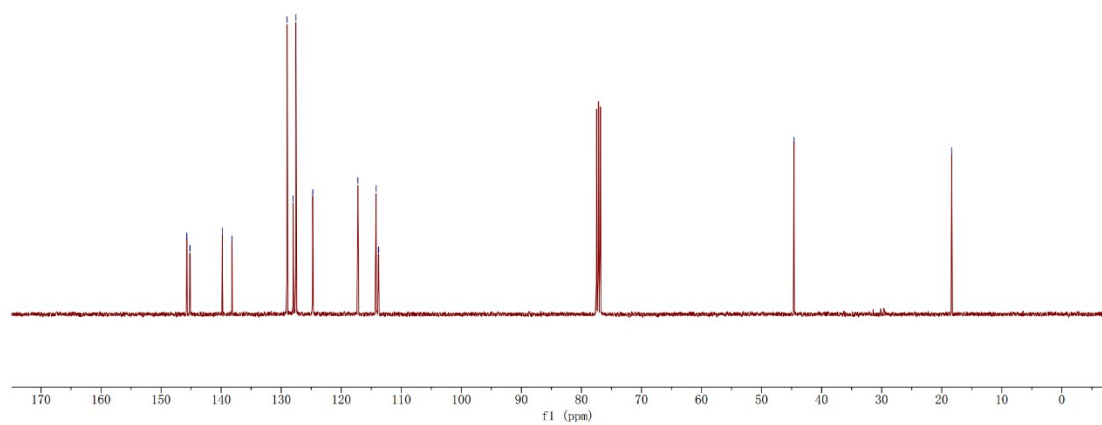
145.720
145.193
139.821
138.189
129.018
128.007
127.545
124.738
117.231
114.191
113.788

— 44.603

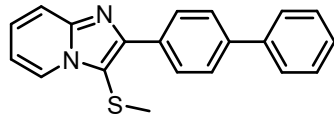
— 18.353



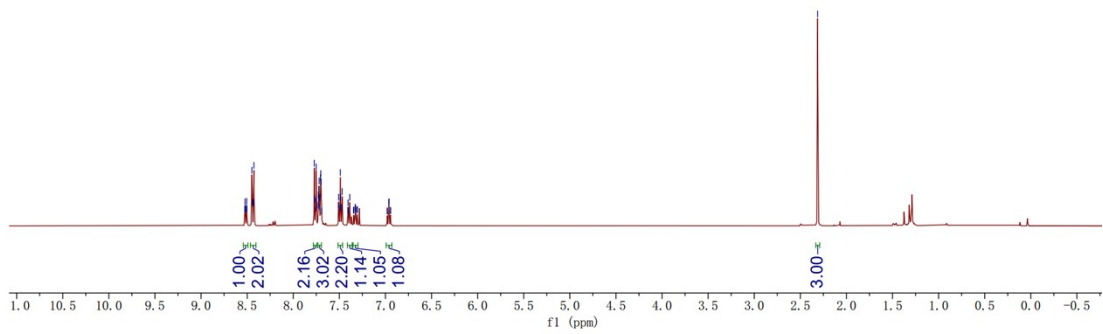
2g (¹³C NMR) (100 MHz, CDCl₃)



8.526
8.523
8.520
8.508
8.505
8.503
8.448
8.443
8.432
8.427
8.422
7.772
7.767
7.756
7.751
7.746
7.731
7.728
7.725
7.722
7.719
7.714
7.708
7.705
7.701
7.698
7.693
7.510
7.508
7.494
7.490
7.486
7.474
7.470
7.408
7.405
7.402
7.387
7.346
7.343
7.330
7.326
7.324
7.321
7.307
7.304
6.981
6.978
6.964
6.961
6.947
6.944
2.312

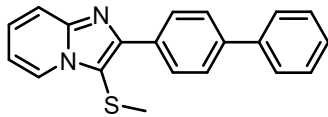


2h (¹H NMR) (400 MHz, CDCl₃)

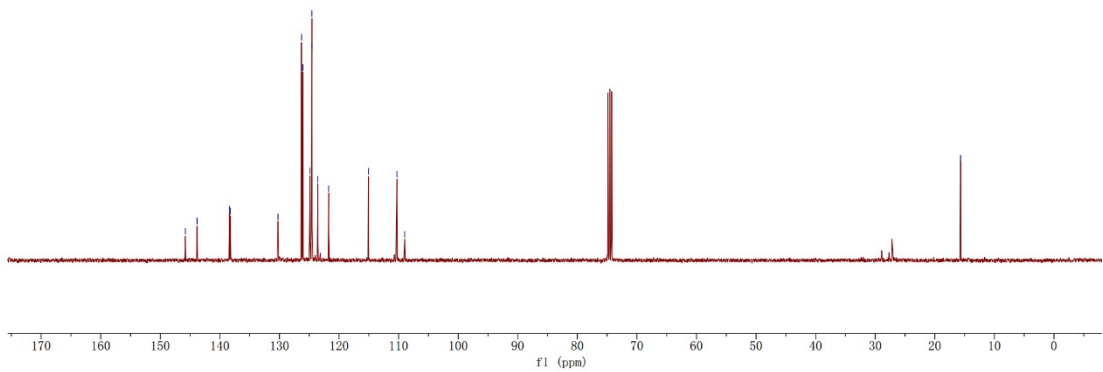


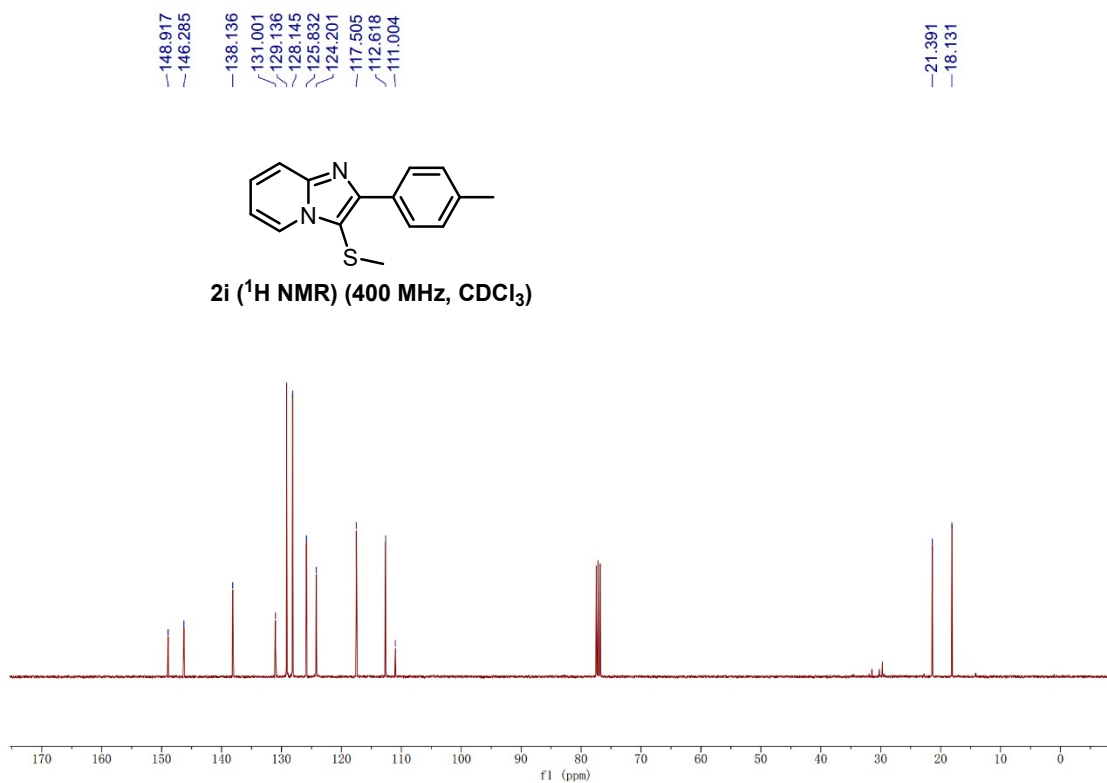
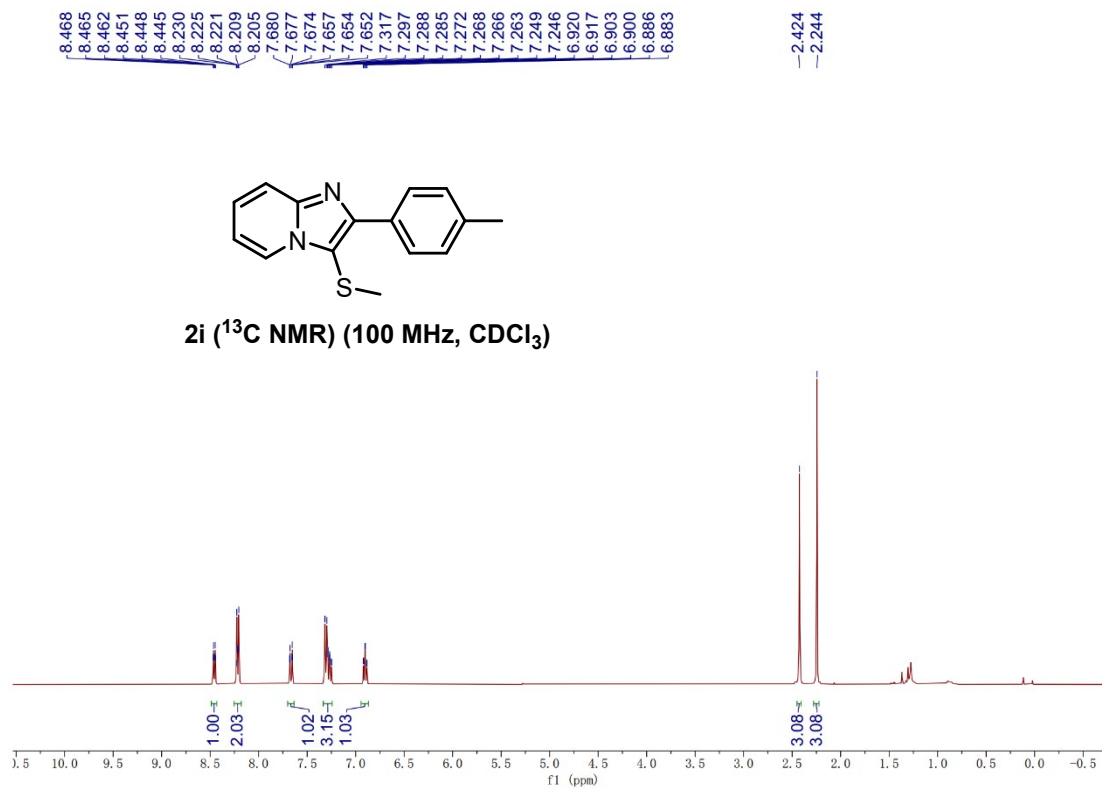
145.792
143.819
138.383
138.241
130.240
126.287
126.076
124.876
124.569
124.555
123.560
121.740
115.066
110.290
108.981

—15.677



2h (¹³C NMR) (100 MHz, CDCl₃)

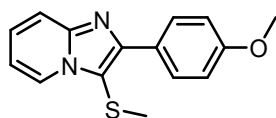




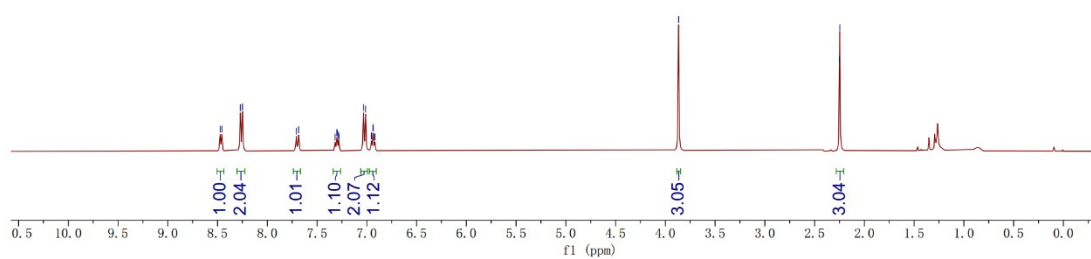
8.474
8.457
8.271
8.250
7.708
7.686
7.319
7.302
7.287
7.285
7.279
7.034
7.013
6.954
6.937
6.920

3.867

2.250
2.247



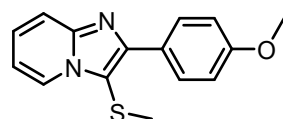
2j (¹H NMR) (400 MHz, CDCl₃)



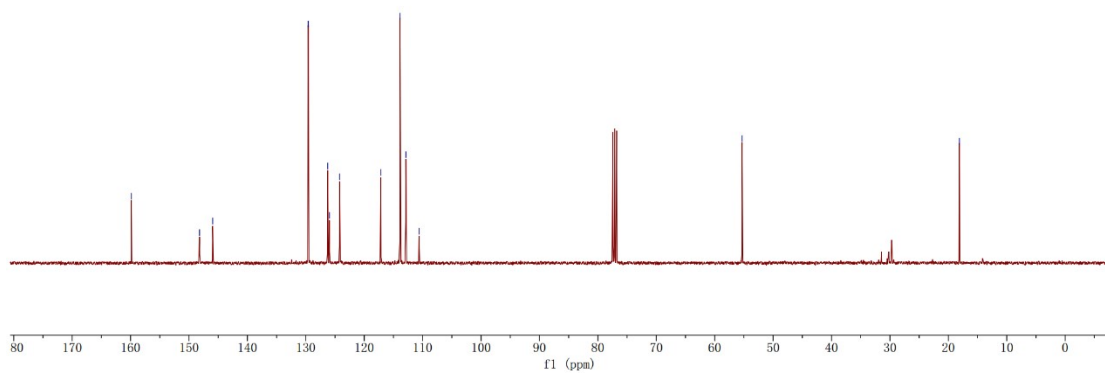
159.860
148.194
145.941
129.586
126.255
125.955
124.227
117.151
113.870
112.868
110.614

55.312

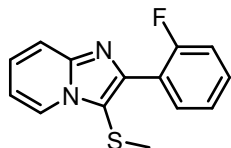
18.106



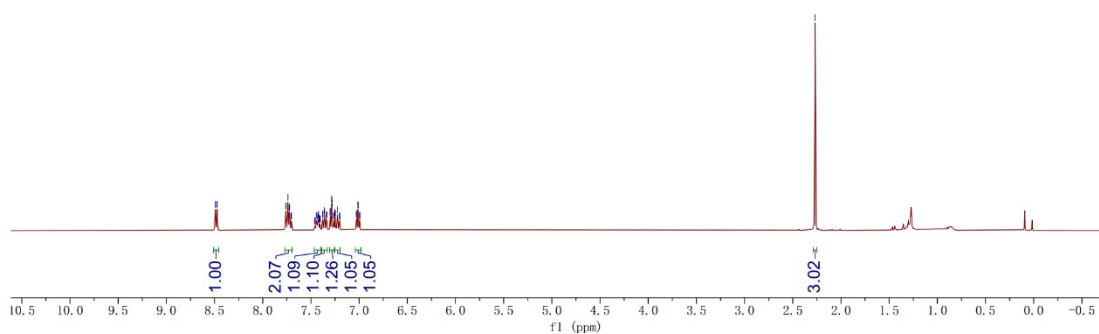
2j (¹³C NMR) (100 MHz, CDCl₃)



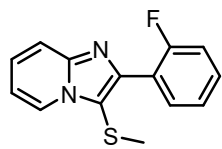
8.491
8.474
7.760
7.738
7.725
7.720
7.706
7.702
7.461
7.457
7.443
7.430
7.422
7.418
7.418
7.409
7.405
7.379
7.376
7.362
7.359
7.340
7.337
7.301
7.298
7.285
7.279
7.264
7.261
7.250
7.248
7.225
7.204
7.201
7.029
7.026
7.012
7.009
6.995
6.992
2.268



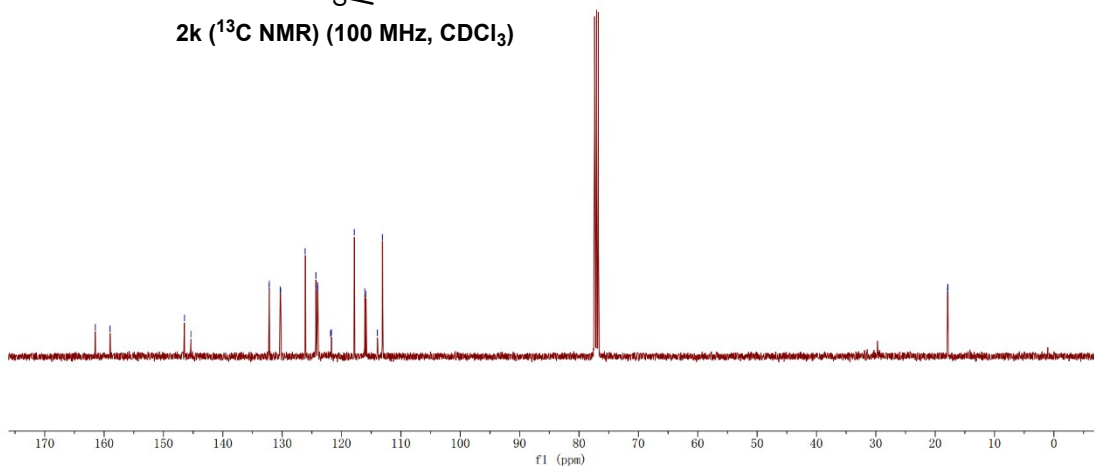
2k (^1H NMR) (400 MHz, CDCl_3)

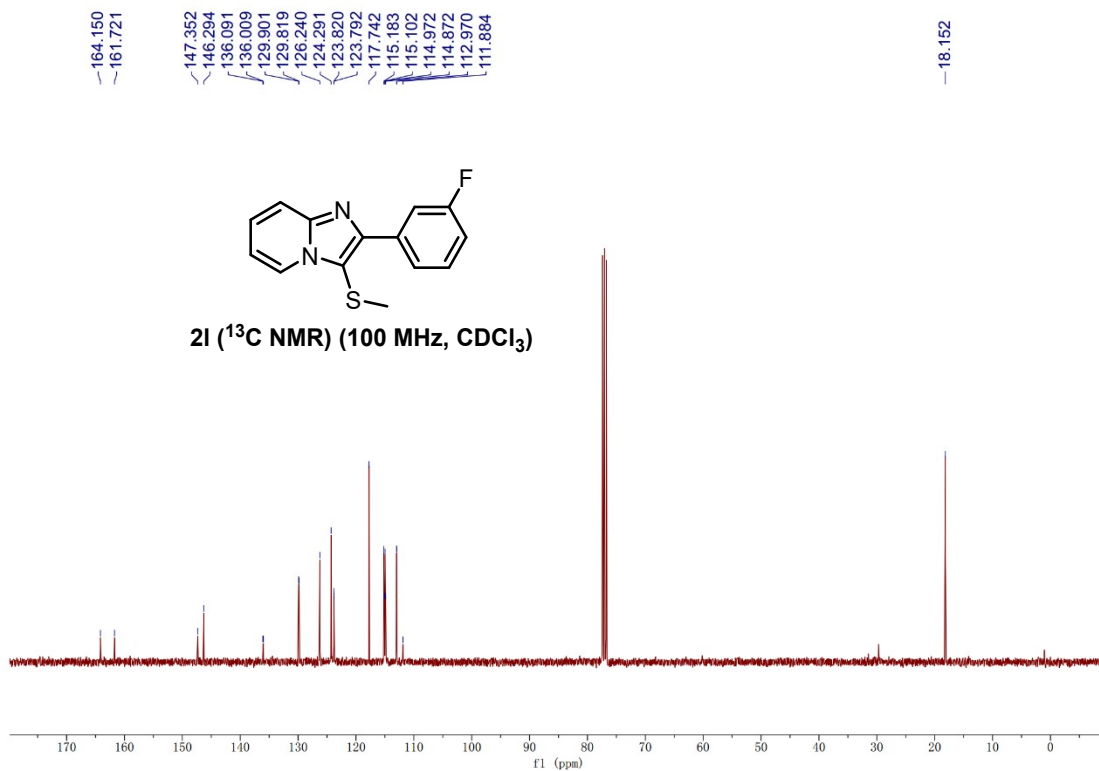
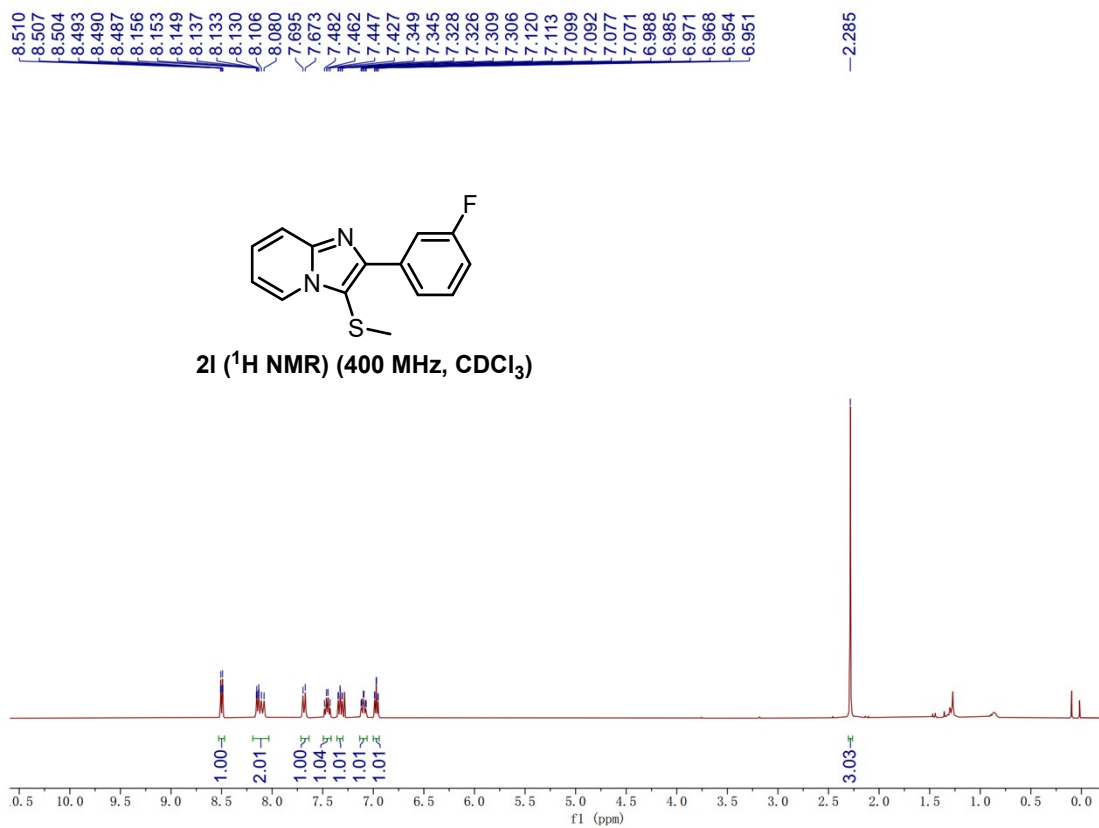


161.478
158.999
146.461
145.388
132.198
132.168
130.355
130.273
126.136
124.324
124.051
124.015
121.861
121.720
117.862
116.081
115.859
113.959
113.118
17.904
17.879

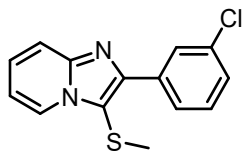


2k (^{13}C NMR) (100 MHz, CDCl_3)

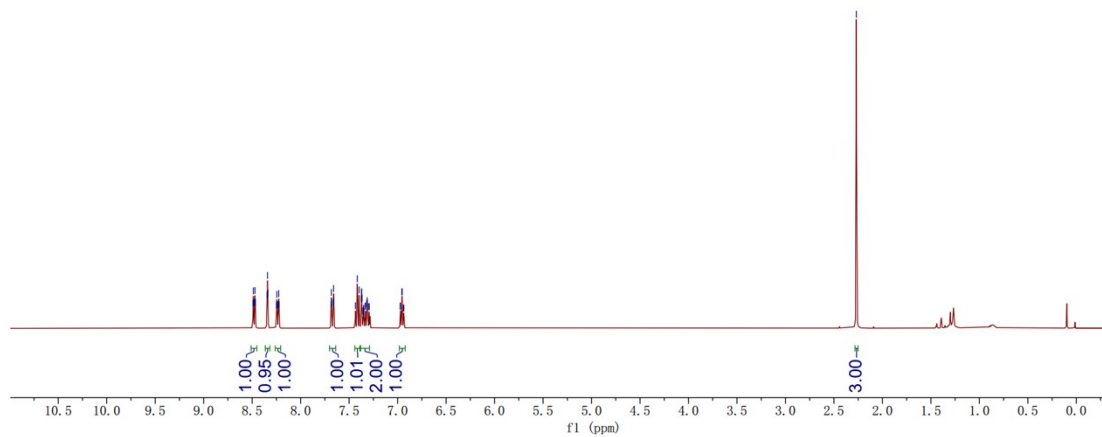




8.491
8.488
8.485
8.474
8.471
8.468
8.347
8.342
8.337
8.249
8.245
8.242
8.230
8.226
8.223
7.686
7.683
7.680
7.664
7.661
7.658
7.435
7.416
7.396
7.375
7.372
7.370
7.367
7.356
7.352
7.350
7.347
7.345
7.335
7.332
7.318
7.315
7.313
7.309
7.296
7.292
6.970
6.966
6.953
6.939
6.936
2.269

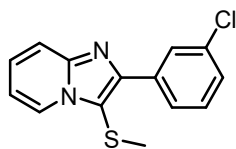


2m (¹H NMR) (400 MHz, CDCl₃)

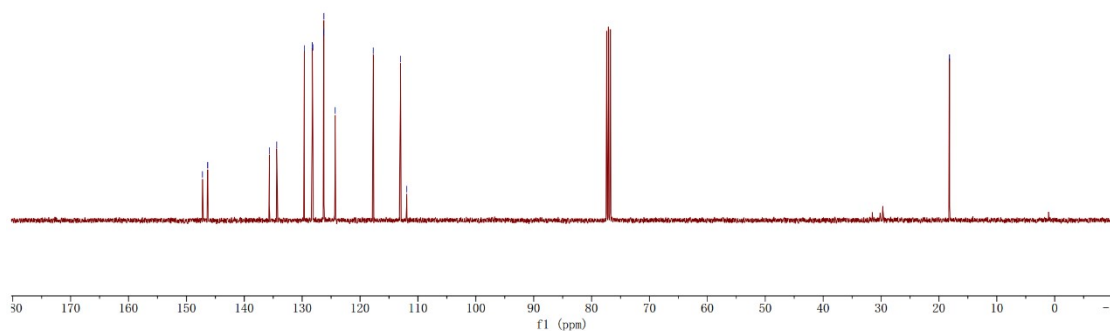


147.225
146.323
135.675
134.389
129.641
128.245
128.173
126.262
126.247
124.297
117.726
112.988
111.919

18.174

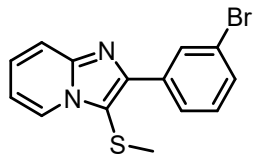


2m (¹³C NMR) (100 MHz, CDCl₃)

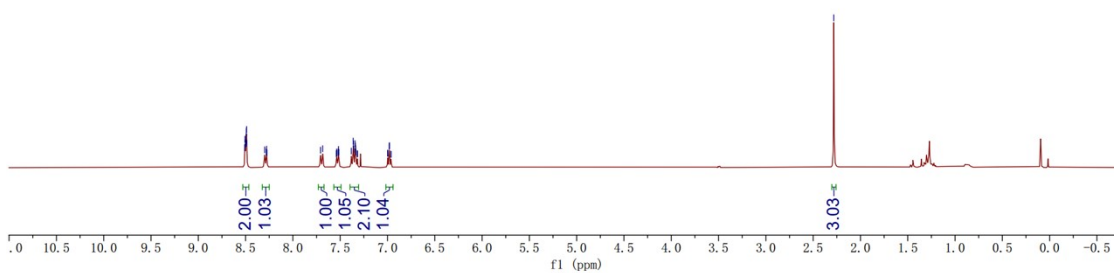


8.509
8.506
8.503
8.499
8.496
8.492
8.489
8.486
8.297
8.281
8.278
8.274
7.707
7.685
7.541
7.537
7.534
7.522
7.518
7.514
7.382
7.363
7.360
7.356
7.343
7.339
7.337
7.334
7.320
7.317
6.999
6.996
6.982
6.979
6.965
6.962

-2.281

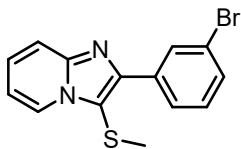


2n (¹H NMR) (400 MHz, CDCl₃)

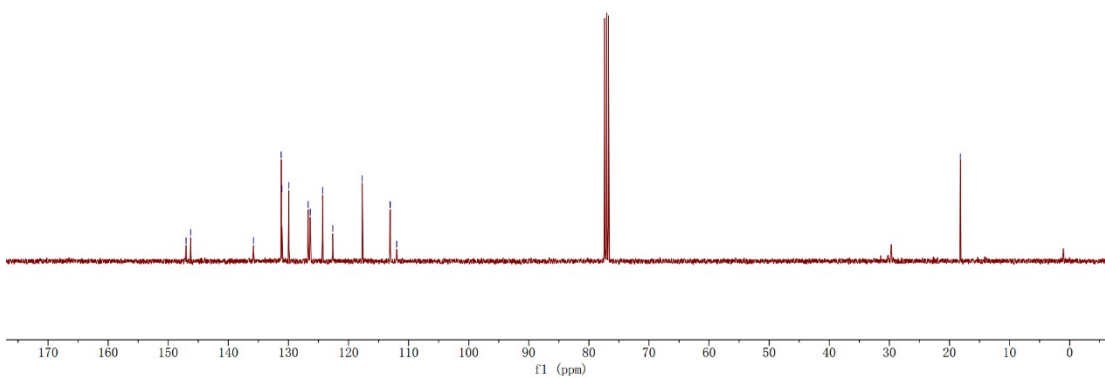


147.033
146.268
135.825
131.212
131.089
129.924
126.714
126.368
124.319
122.616
117.713
113.067
111.989

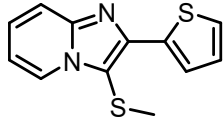
-18.188



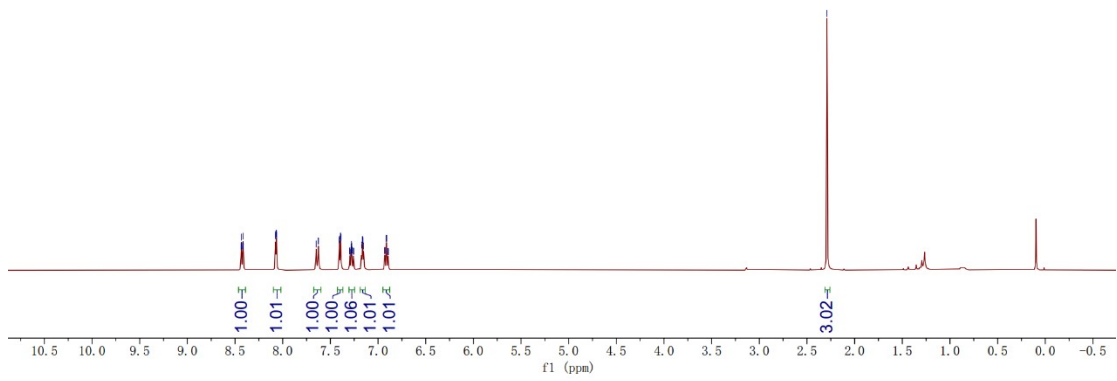
2n (¹³C NMR) (100 MHz, CDCl₃)



8.437
8.434
8.431
8.420
8.417
8.414
8.076
8.073
8.067
8.064
7.649
7.626
7.406
7.403
7.393
7.390
7.298
7.295
7.285
7.281
7.278
7.276
7.272
7.259
7.256
7.173
7.163
7.160
7.151
6.930
6.927
6.913
6.910
6.896
6.893
-2.290

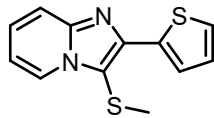


2o (¹H NMR) (400 MHz, CDCl₃)

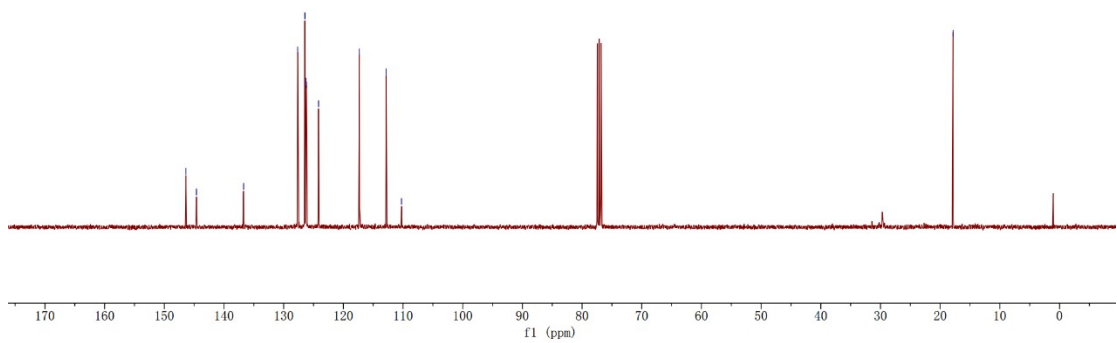


146.385
144.611
136.711
127.655
126.444
126.244
126.195
124.153
117.313
112.823
110.257

17.838

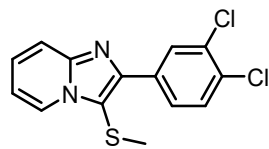


2o (¹³C NMR) (100 MHz, CDCl₃)

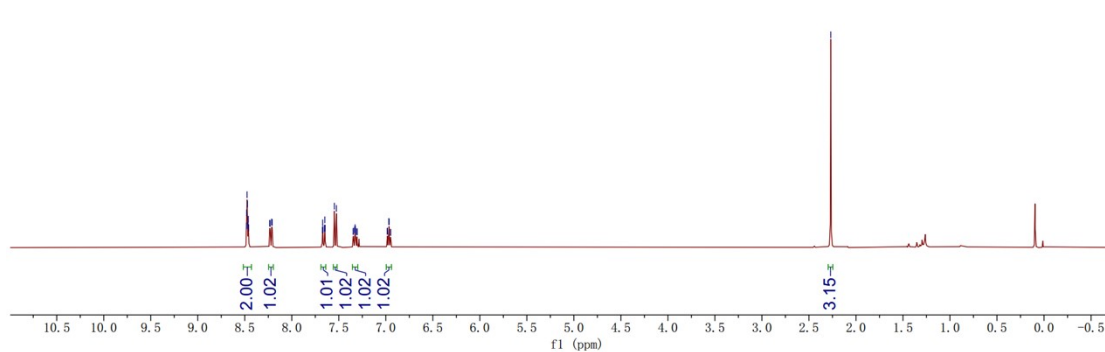


8.482
8.479
8.476
8.471
8.465
8.459
8.235
8.230
8.214
8.209
7.674
7.671
7.669
7.652
7.649
7.646
7.547
7.526
7.347
7.344
7.331
7.327
7.325
7.321
7.308
7.305
6.985
6.983
6.968
6.965
6.951
6.949

-2.268

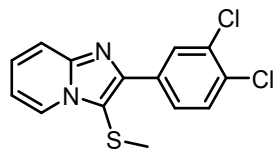


2p (¹H NMR) (400 MHz, CDCl₃)

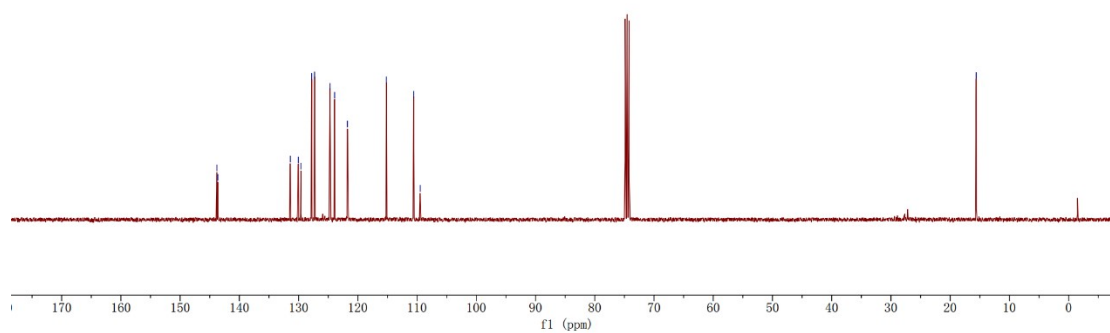


143.791
143.639
131.395
130.042
129.614
127.793
127.301
124.689
123.916
121.752
115.186
110.580
109.465

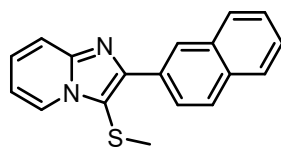
-15.604



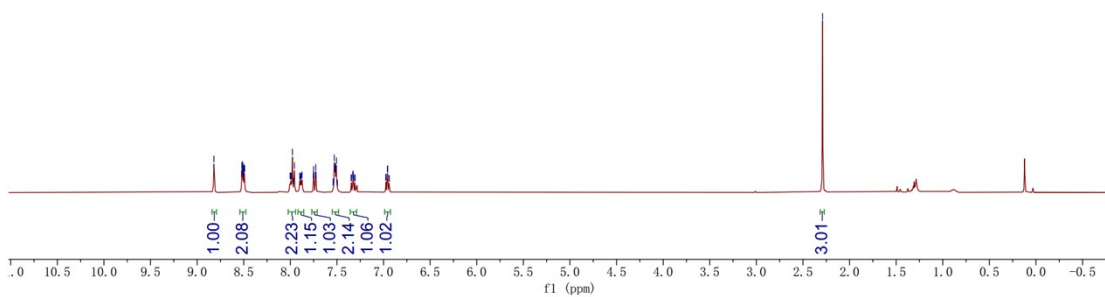
2p (¹³C NMR) (100 MHz, CDCl₃)



8.820
8.523
8.520
8.516
8.511
8.506
8.503
8.500
8.494
8.490
8.003
7.995
7.991
7.978
7.964
7.956
7.899
7.893
7.887
7.883
7.875
7.753
7.750
7.747
7.730
7.727
7.724
7.724
7.541
7.536
7.529
7.523
7.519
7.516
7.511
7.506
7.494
7.494
7.348
7.344
7.331
7.328
7.325
7.322
7.309
7.305
6.976
6.973
6.959
6.956
6.942
6.939
2.289

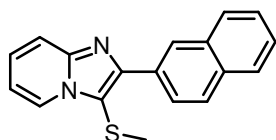


2q (¹H NMR) (400 MHz, CDCl₃)

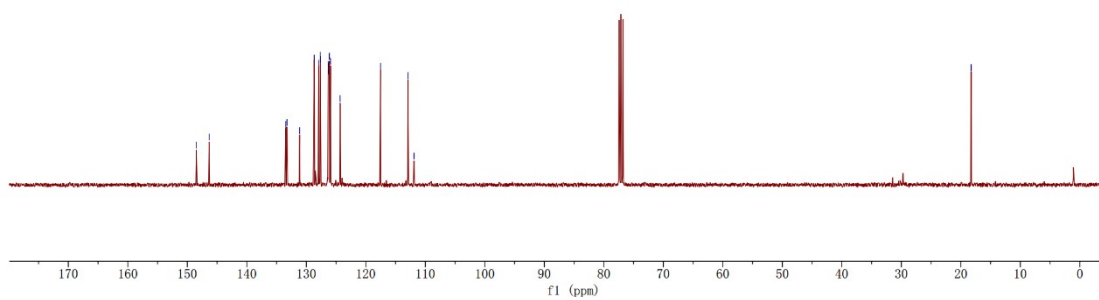


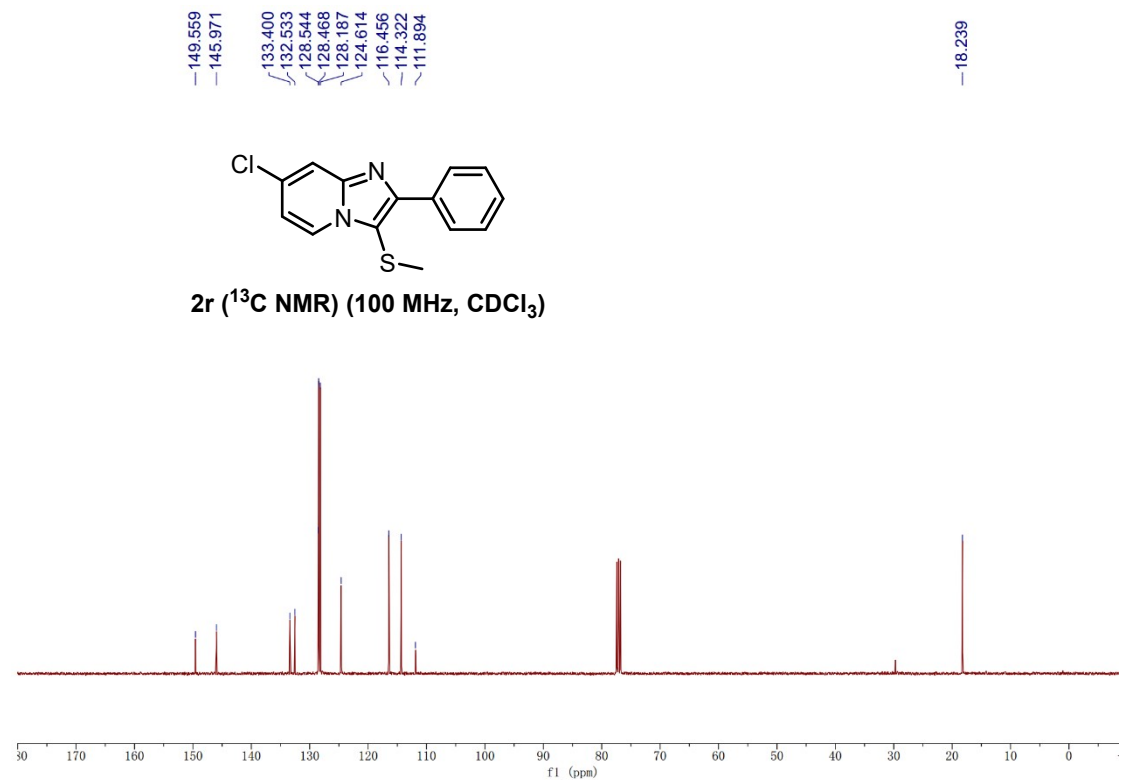
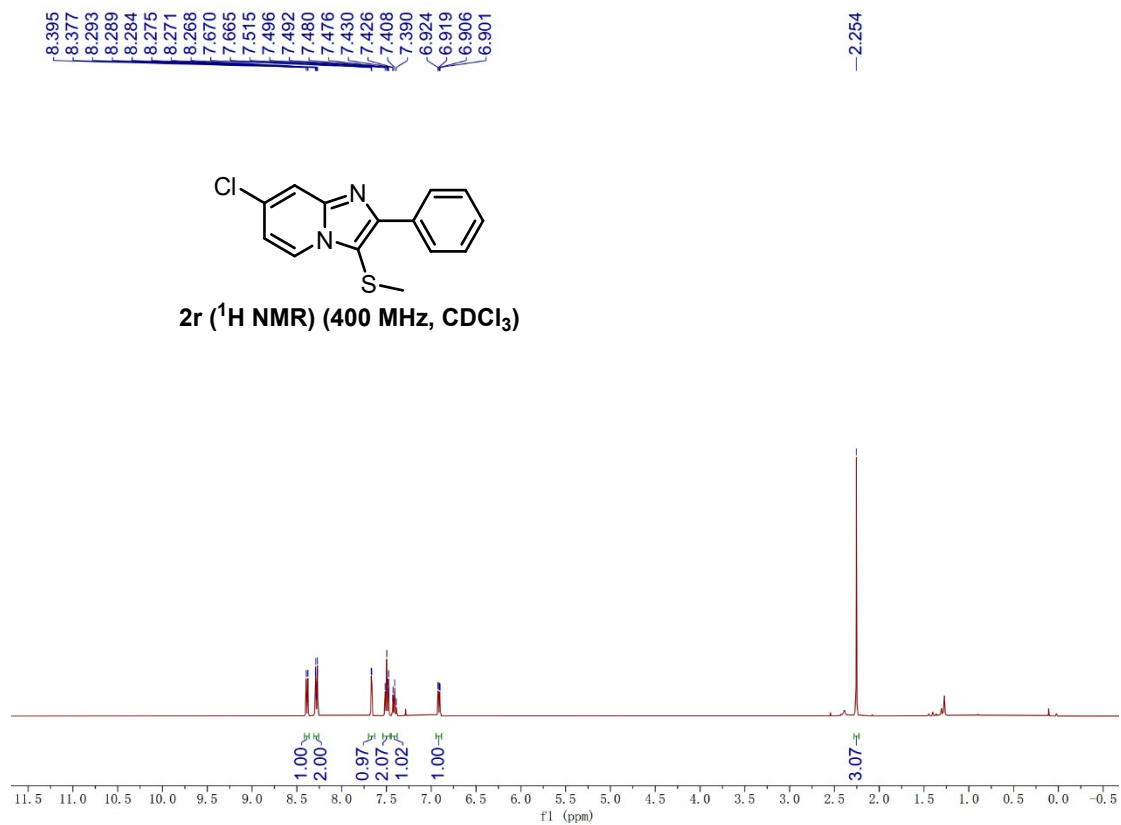
148.475
146.324
133.456
133.250
131.122
128.669
127.936
127.661
127.622
126.327
126.265
126.134
125.941
124.322
117.528
112.928
111.899

18.264



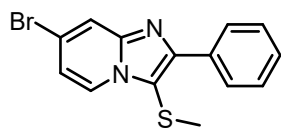
2q (¹³C NMR) (100 MHz, CDCl₃)



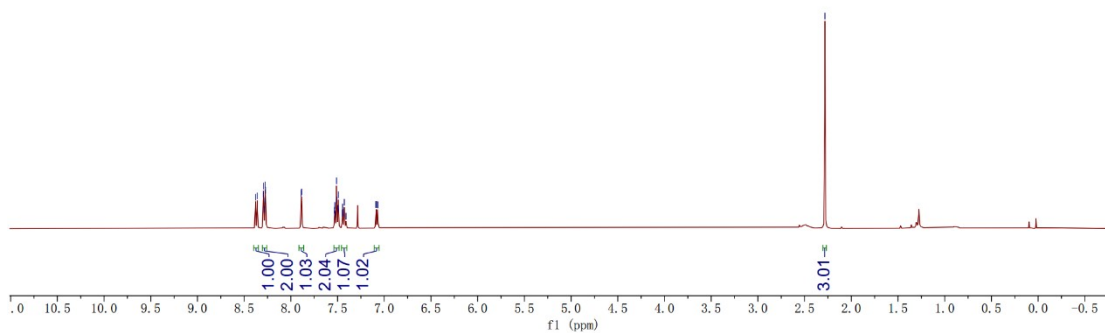


8.379
8.361
8.295
8.292
8.287
8.278
8.274
8.271
7.889
7.885
7.532
7.529
7.525
7.511
7.507
7.496
7.492
7.449
7.446
7.443
7.428
7.409
7.091
7.086
7.073
7.068

— 2.282

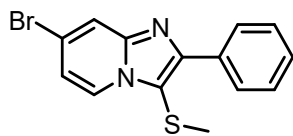


2s (^1H NMR) (400 MHz, CDCl_3)

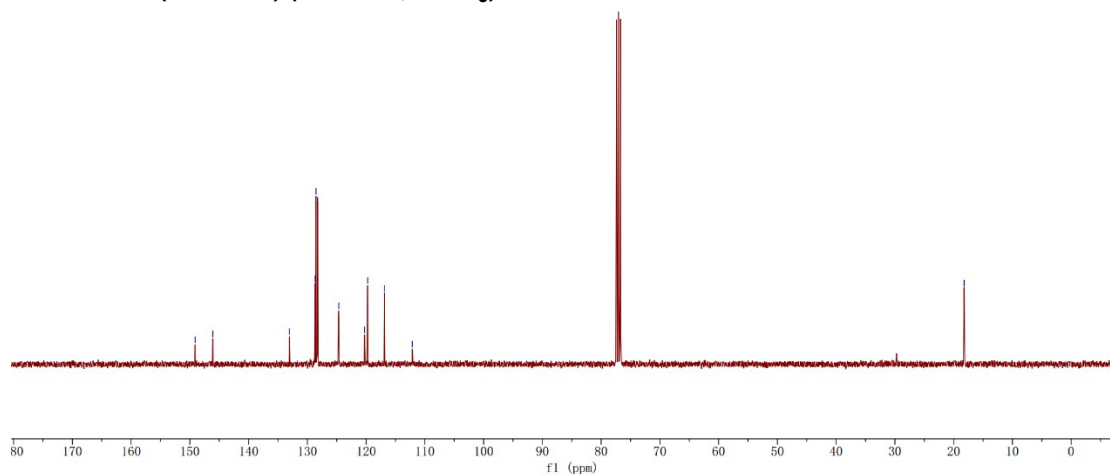


149.100
146.098
133.050
128.686
128.526
128.253
124.647
120.275
119.732
116.883
112.138

— 18.217

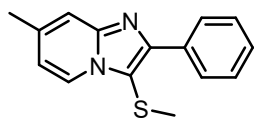


2s (^{13}C NMR) (100 MHz, CDCl_3)

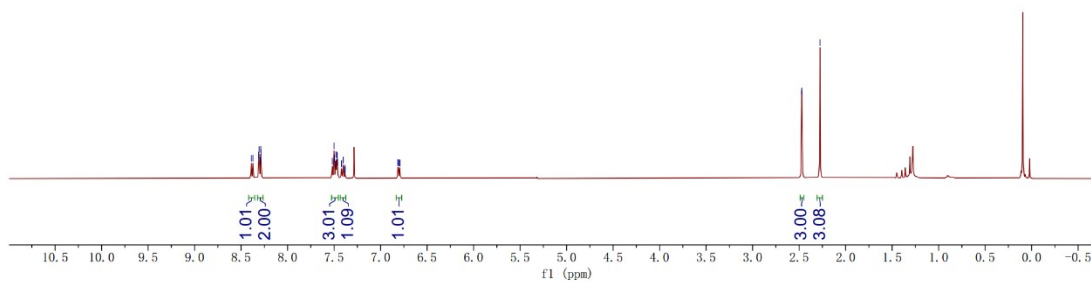


8.390
8.373
8.310
8.307
8.293
8.289
8.286
7.519
7.501
7.497
7.485
7.481
7.469
7.466
7.463
7.421
7.402
7.387
7.384
7.381
6.815
6.810
6.797
6.793

-2.472
-2.276

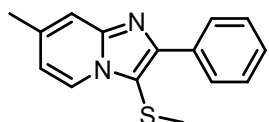


2t (¹H NMR) (400 MHz, CDCl₃)

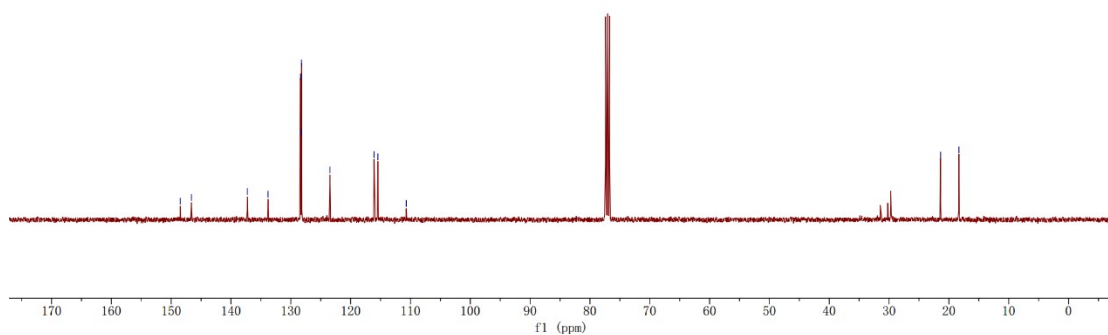


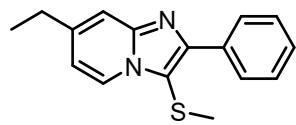
148.481
146.617
137.278
133.811
128.370
128.217
128.198
123.458
116.078
115.445
110.703

-21.387
-18.322

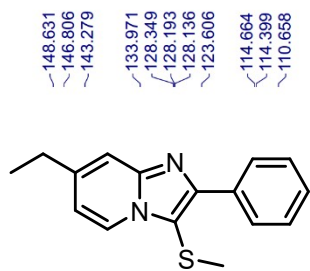
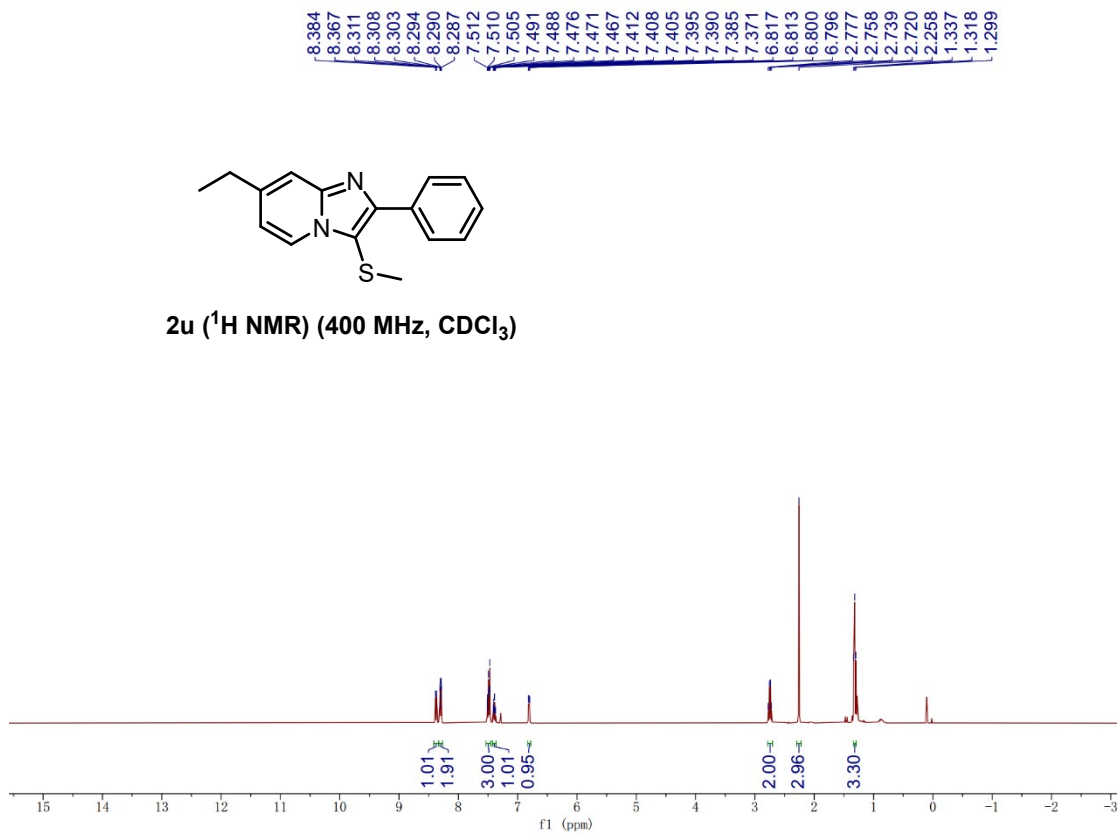


2t (¹³C NMR) (100 MHz, CDCl₃)

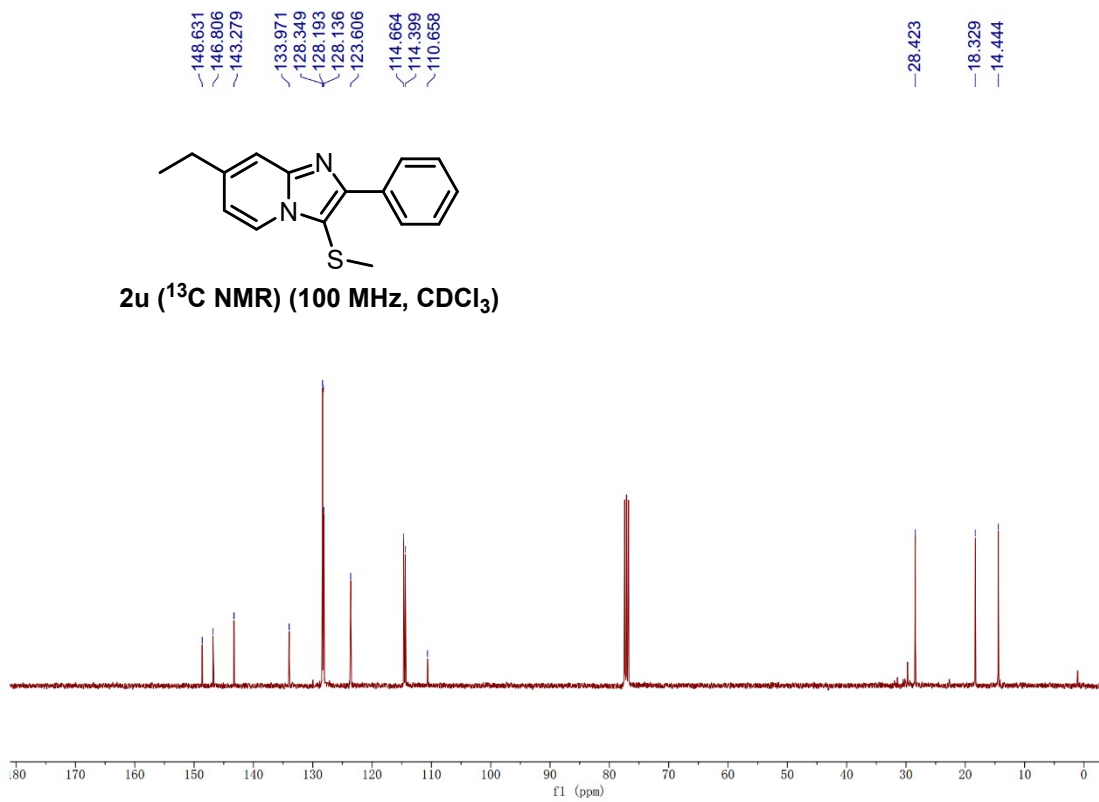




2u (¹H NMR) (400 MHz, CDCl₃)

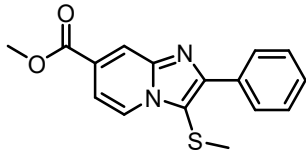


2u (¹³C NMR) (100 MHz, CDCl₃)

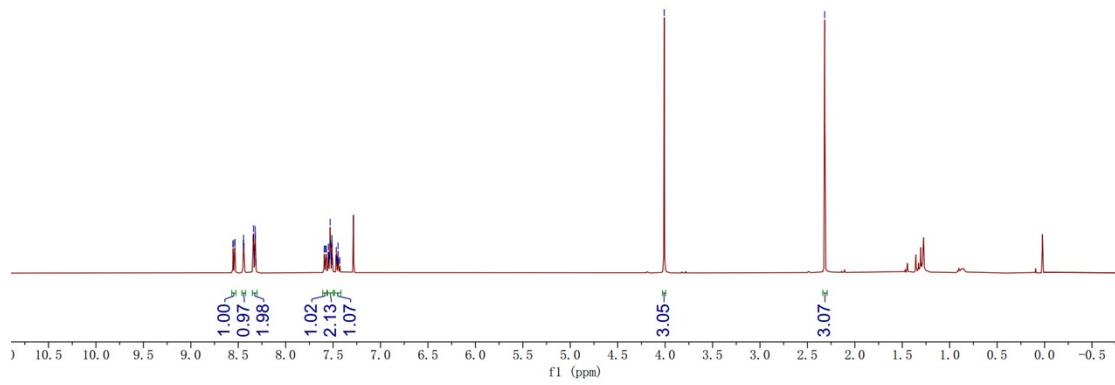


8.556
8.553
8.538
8.535
8.446
8.443
8.440
8.343
8.339
8.334
8.325
8.322
8.319
8.314
7.593
7.589
7.575
7.571
7.554
7.552
7.549
7.545
7.536
7.531
7.527
7.515
7.512
7.510
7.507
7.470
7.466
7.463
7.453
7.448
7.442
7.430
4.010

-2.317



2v (¹H NMR) (400 MHz, CDCl₃)



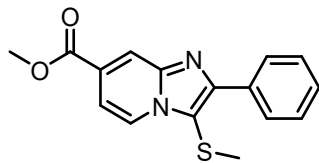
-165.508

-144.977

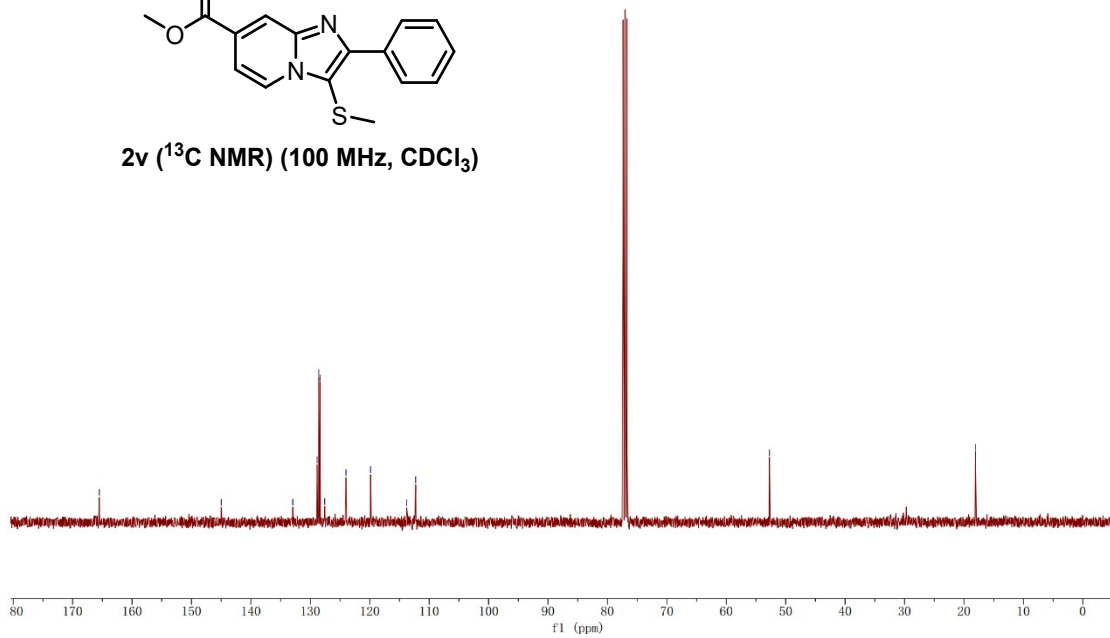
132.945
128.861
128.576
128.339
127.579
124.000
119.866
113.764
112.271

-52.730

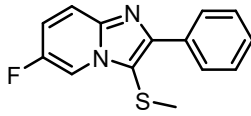
-18.076



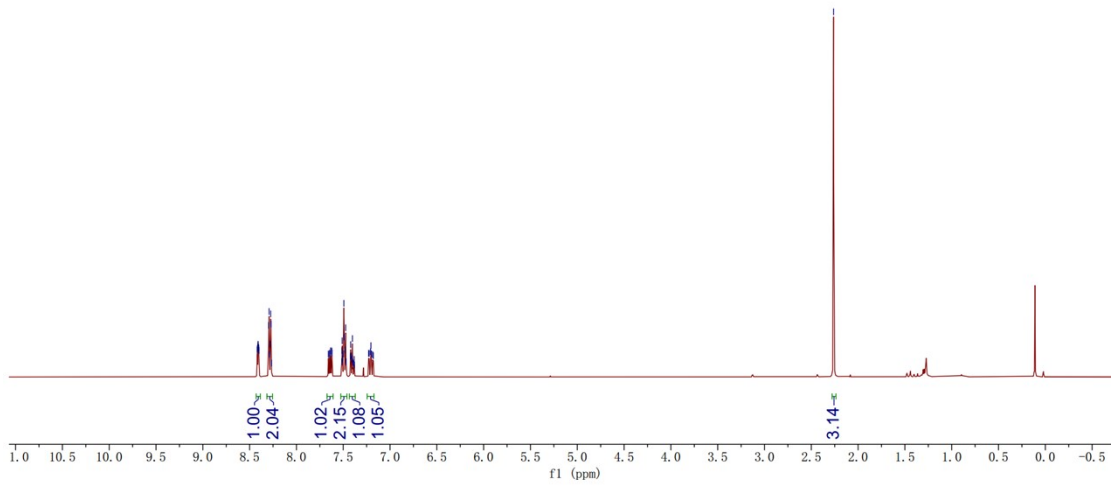
2v (¹³C NMR) (100 MHz, CDCl₃)



8.419
8.417
8.413
8.410
8.408
8.406
8.402
8.400
8.296
8.292
8.287
8.279
8.275
8.272
6.267
7.659
7.657
7.646
7.644
7.635
7.633
7.622
7.620
7.516
7.514
7.511
7.507
7.498
7.493
7.490
7.478
7.474
7.469
7.424
7.420
7.417
7.407
7.402
7.396
7.387
7.383
7.380
7.229
7.223
7.209
7.204
7.198
7.185
7.179
2.262

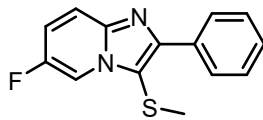


2w (¹H NMR) (400 MHz, CDCl₃)

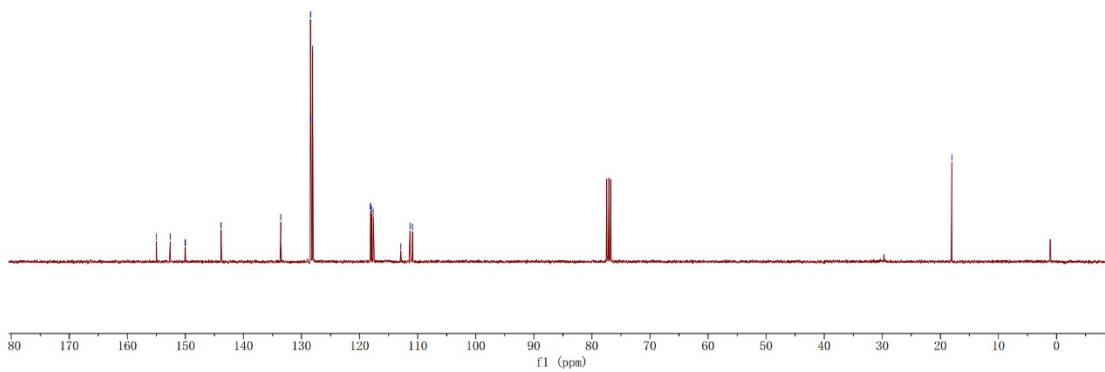


154.972
152.610
150.032
150.008
143.855
133.582
128.453
128.439
128.096
118.190
118.103
117.910
117.655
112.907
111.318
110.905

18.028

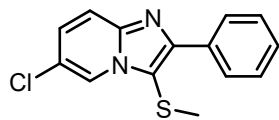


2w (¹³C NMR) (100 MHz, CDCl₃)

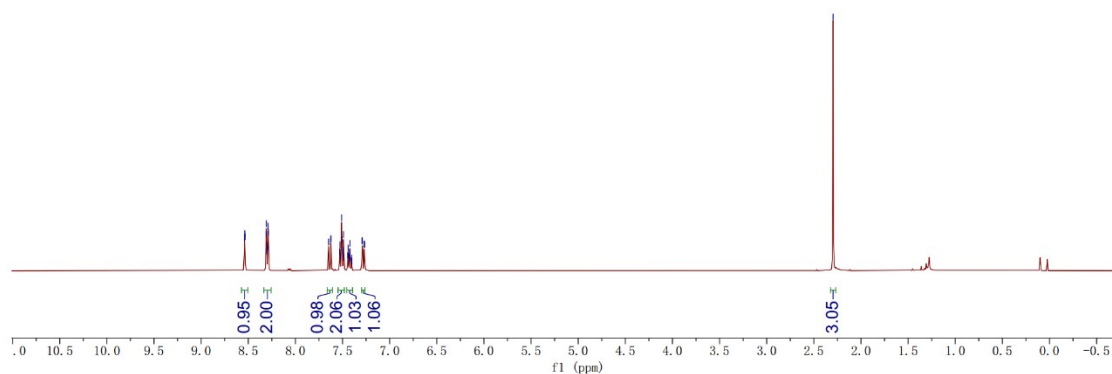


8.541
8.539
8.536
8.534
8.312
8.308
8.303
8.294
8.290
8.287
7.648
7.646
7.624
7.622
7.530
7.527
7.523
7.509
7.506
7.494
7.490
7.485
7.444
7.441
7.437
7.428
7.424
7.422
7.407
7.404
7.401
7.294
7.289
7.271
7.266

-2.296

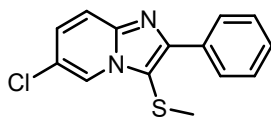


2x (¹H NMR) (400 MHz, CDCl₃)

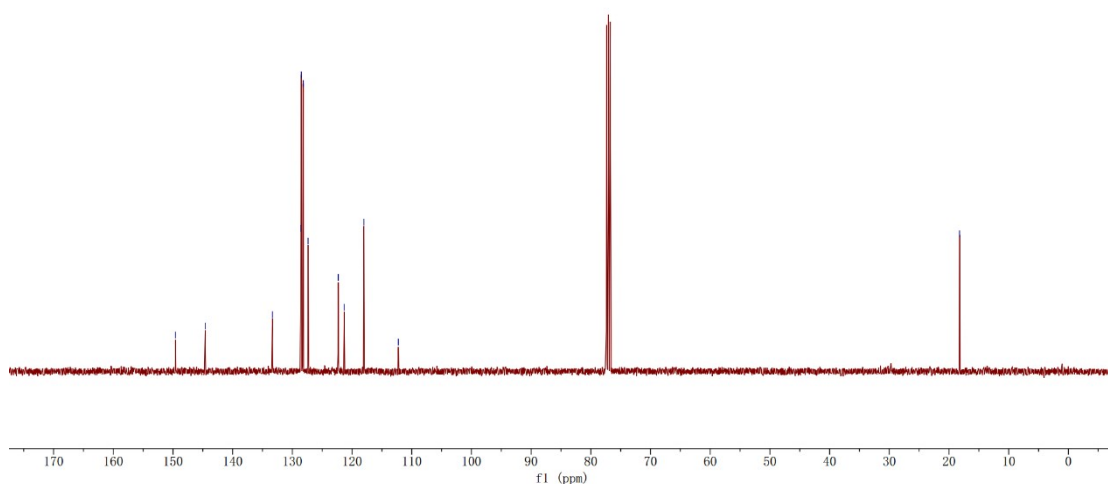


-149.579
-144.597
133.334
128.583
128.496
128.180
127.365
122.310
121.318
118.012
112.244

-18.232

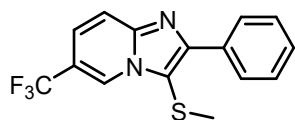


2x (¹³C NMR) (100 MHz, CDCl₃)

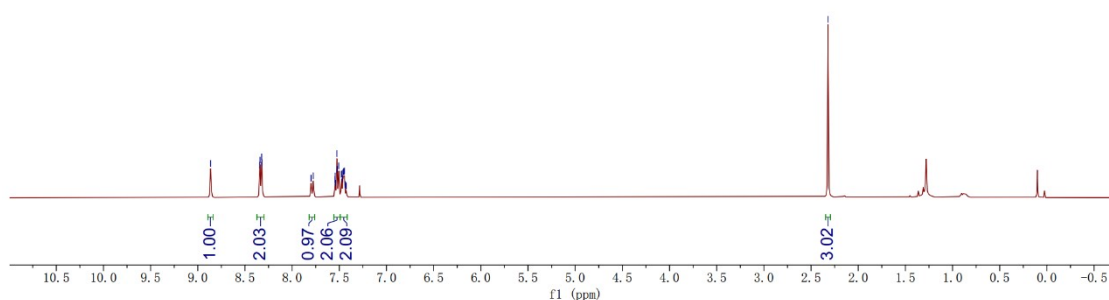


8.864
8.345
8.340
8.323
8.320
7.800
7.776
7.546
7.544
7.539
7.526
7.522
7.507
7.480
7.475
7.466
7.463
7.457
7.451
7.444
7.438
7.429
7.426

2.320

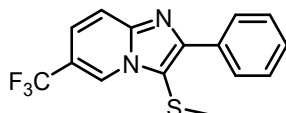


2y (¹H NMR) (400 MHz, CDCl₃)

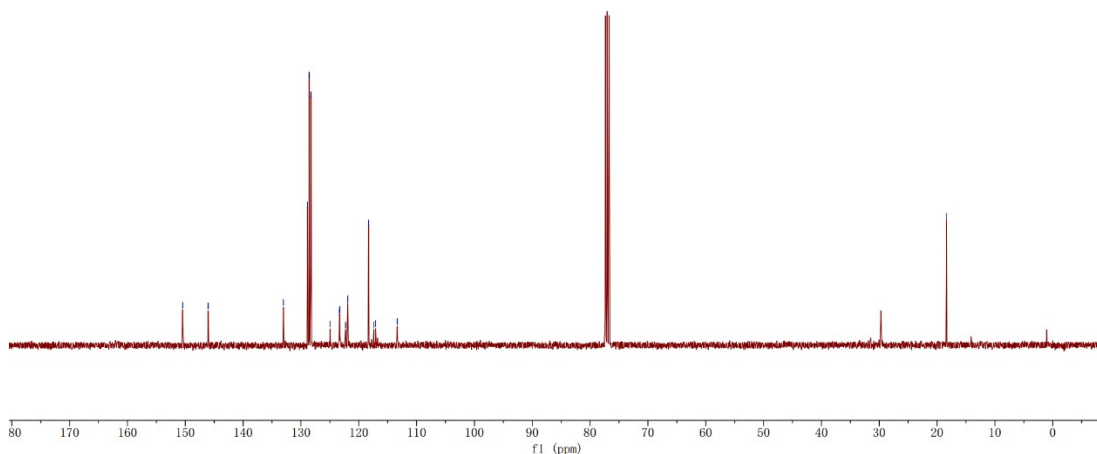


150.450
146.047
133.031
128.864
128.565
128.270
124.977
123.349
123.294
122.281
121.905
121.877
118.302
117.433
117.093
113.345

18.342

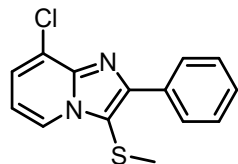


2y (¹³C NMR) (100 MHz, CDCl₃)

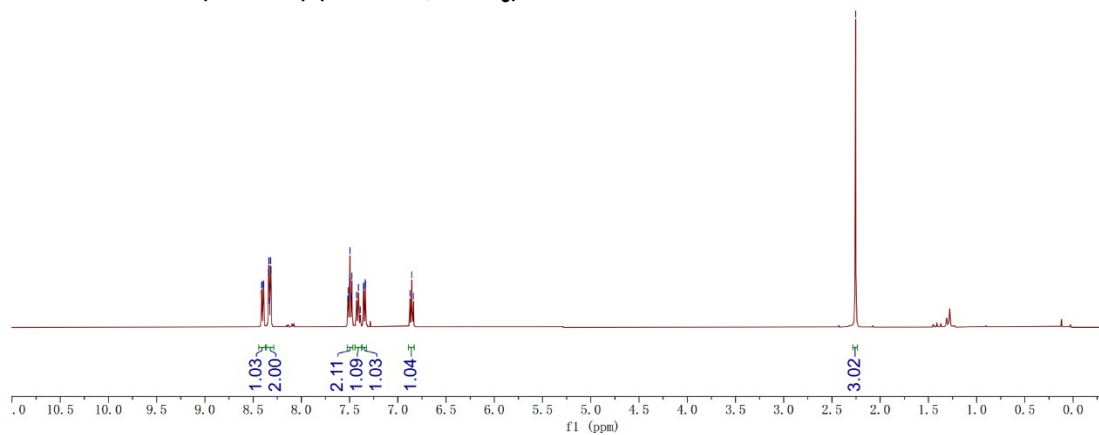


8.411
8.409
8.394
8.392
8.340
8.336
8.332
8.323
8.319
8.316
7.517
7.515
7.497
7.493
7.481
7.477
7.427
7.409
7.390
7.357
7.354
7.339
7.336
6.874
6.857
6.839

-2.255

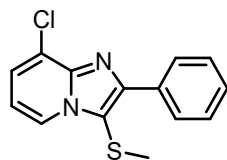


2z (^1H NMR) (400 MHz, CDCl_3)

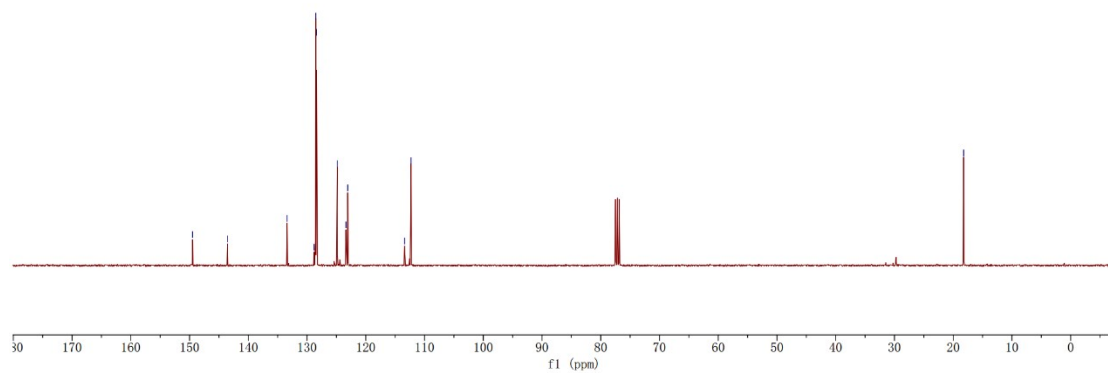


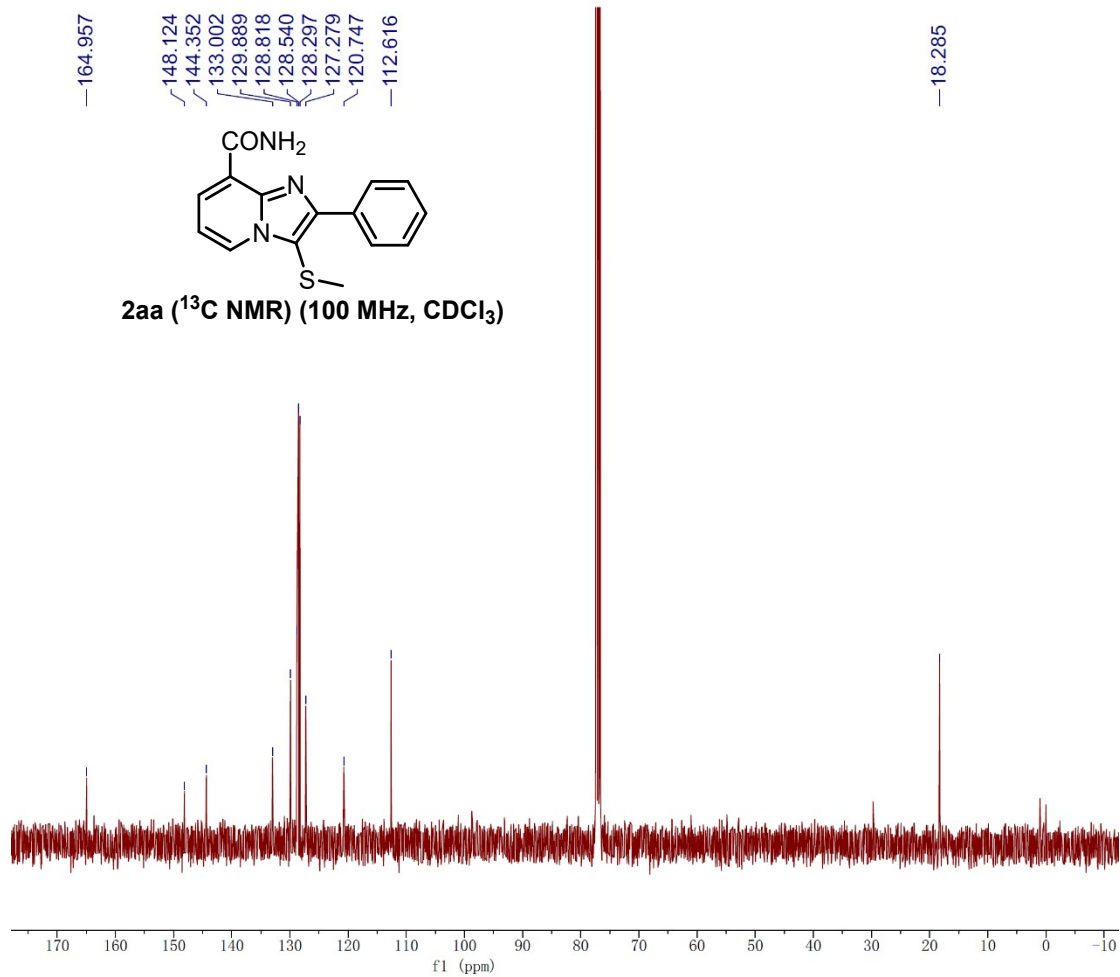
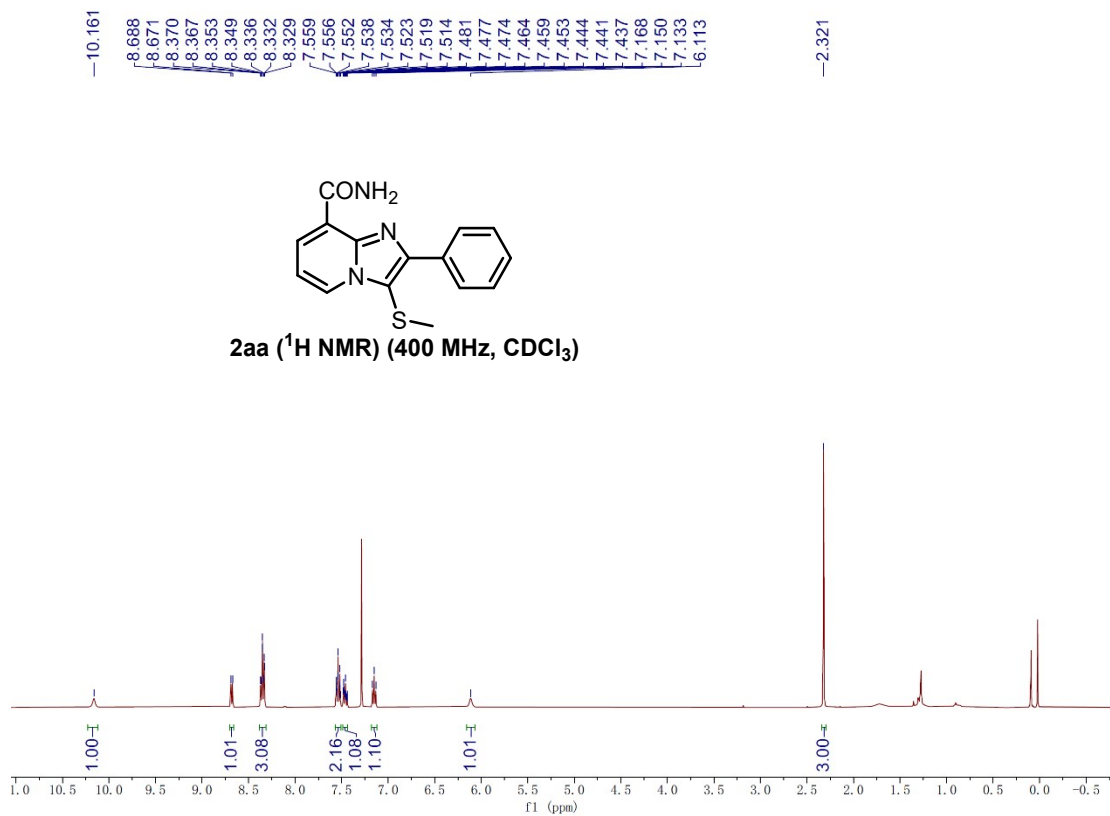
149.485
143.551
133.393
128.796
128.516
128.387
124.852
123.376
123.075
113.403
112.296

-18.221

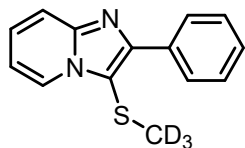


2z (^{13}C NMR) (100 MHz, CDCl_3)

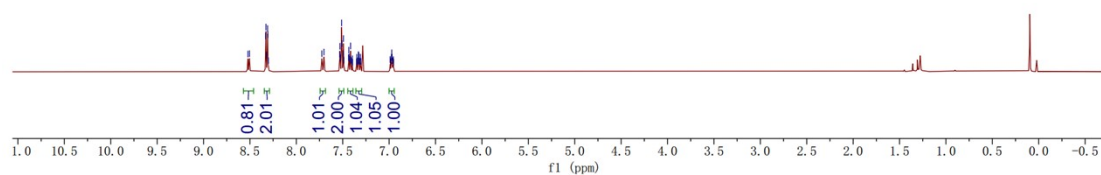




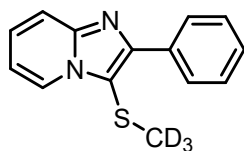
8.522
8.505
8.331
8.327
8.323
8.310
8.307
8.302
7.725
7.702
7.532
7.530
7.526
7.512
7.508
7.496
7.492
7.488
7.437
7.434
7.431
7.421
7.416
7.410
7.400
7.397
7.394
7.351
7.348
7.345
7.335
7.331
7.327
7.325
7.322
7.312
7.309
7.305
6.989
6.986
6.976
6.972
6.969
6.959
6.955
6.952



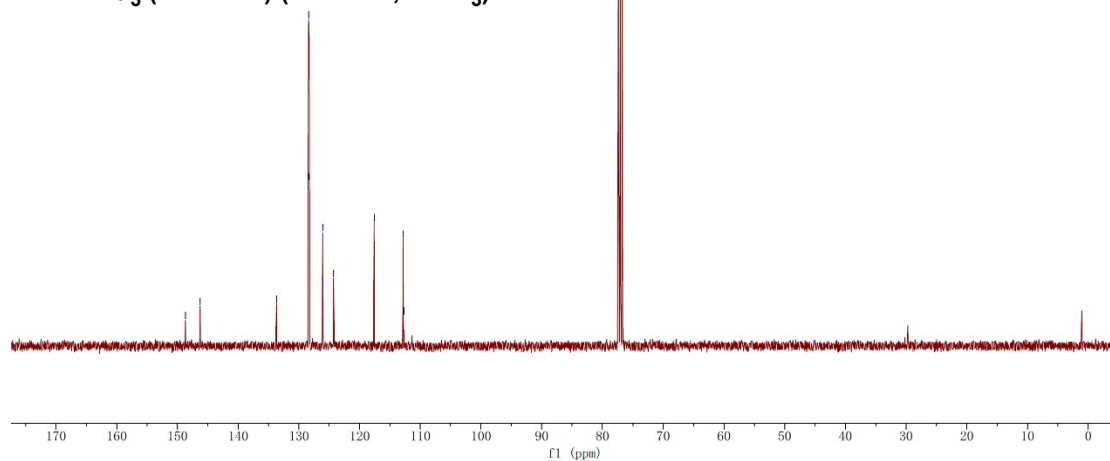
2a-d₃ (¹H NMR) (400 MHz, CDCl₃)



148.689
146.246
133.687
128.420
128.337
128.285
126.069
124.287
117.606
112.829
112.675

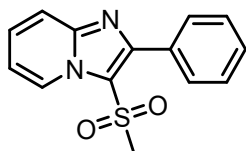


2a-d₃ (¹³C NMR) (100 MHz, CDCl₃)

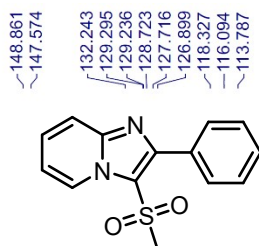
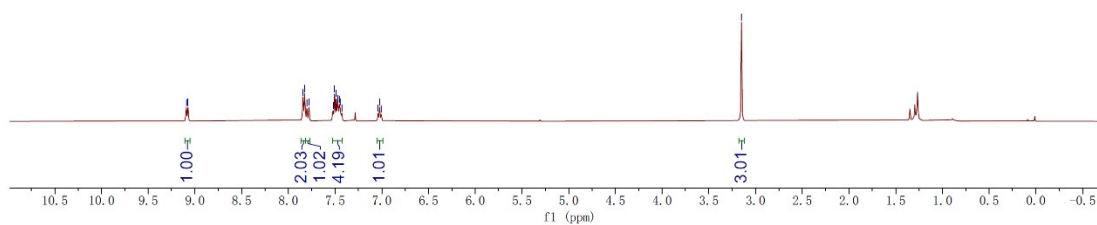


9.092
9.075
7.843
7.826
7.803
7.780
7.522
7.505
7.486
7.472
7.467
7.454
7.446
7.427
7.040
7.023
7.006

—3.151



3 (¹H NMR) (400 MHz, CDCl₃)



3 (¹³C NMR) (100 MHz, CDCl₃)

