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Supporting Information

Metal-Free Electrochemical C3-Sulfonylation of Imidazo[1, 2-a]pyridines

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General information

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). The anodic electrode was graphite rod (ϕ 6 mm) and cathodic electrode was Stainless steel (15 mm×15 mm×0.3 mm). Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 300-400 mesh silica gel in petroleum (boiling point is between 60-90 ℃). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum to the indicated solvent, and they are listed as volume/volume ratios. NMR spectra were recorded on a Bruker spectrometer at 400 MHz (^{1}H NMR), 101 MHz (^{13}C NMR), 376 MHz (^{19}F NMR). All chemical shifts are reported relative to tetramethylsilane and solvent peaks. And all ^{1}H, ^{13}C and ^{19}F NMR data spectra were reported in delta (δ) units, parts per million (ppm) downfield from the internal standard. Coupling constants are reported in Hertz (Hz). High resolution mass spectra (HRMS) were measured with a Bruker UltiMate 3000 & Compact, accurate masses are reported for the molecular ion + hydrogen ($[M+H]^{+}$) or sodium ($[M+Na]^{+}$).

Experimental procedure

General procedure for electrocatalytic synthesis of sulfone

In an undivided three-necked bottle (25 mL) equipped with a stir bar, 2-phenylimidazo[1,2-a]pyridine (**1a**, 0.5 mmol), sodium 4-methylbenzenesulfinate (**2a**, 3 mmol), and $^{n}Bu_4NBF_4$ (0.1 mmol) were combined and added. The bottle was equipped with graphite rod as the anode and Stainless steel as the cathode and was then charged with nitrogen. Under the protection of N_2, MeCN (10 mL) and H_2O (1 mL) were injected respectively into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA at room temperature for 4.3 h. When the reaction was finished, the pure product was obtained by flash column chromatography on silicagel.

Procedure for gram-scale synthesis of sulfone

In an undivided three-necked bottle (100 mL) equipped with a stir bar, 2-phenylimidazo[1,2-a]pyridine (**1a**, 5 mmol), sodium 4-methylbenzenesulfinate (**2a**, 30 mmol), and $^{n}Bu_4NBF_4$ (1 mmol) were combined and added. The bottle was equipped with graphite rod as the anode and Stainless steel as the cathode and was then charged with nitrogen. Under the protection of N_2, MeCN (70 mL) and H_2O (7 mL) were injected respectively into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA at room temperature for 37 h. When the reaction was finished, the pure product was obtained by flash column chromatography on silicagel.

Procedure for cyclic voltammetry (CV)

Cyclic voltammetry was performed in a three-electrode cell connected to a Schlenk line under air at room temperature. The working electrode was a steady glassy carbon disk electrode while the counter electrode was a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. A mixed solvent ($MeCN/H_2O$ = 10/1, 11 mL) containing $^{n}Bu_4NBF_4$ (0.1 mmol) were poured into the electrochemical cell in cyclic voltammetry experiments. The scan rate was 0.10 V/s, ranging from 0.0 V to 2.5 V.

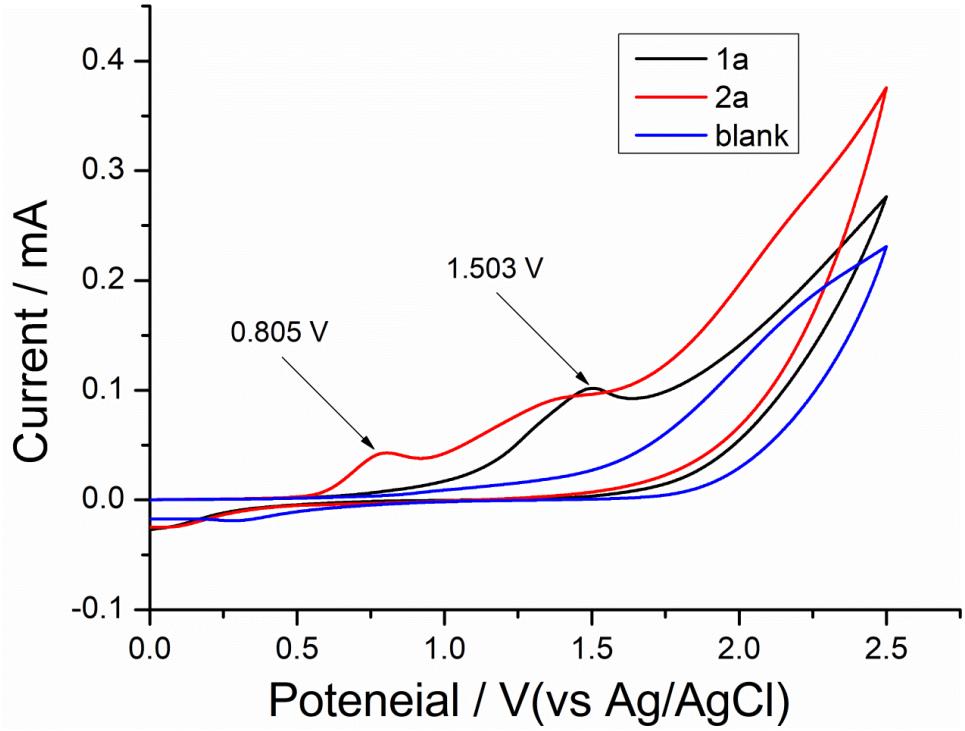
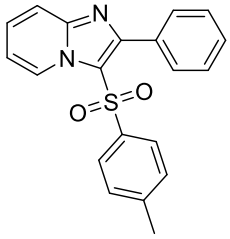


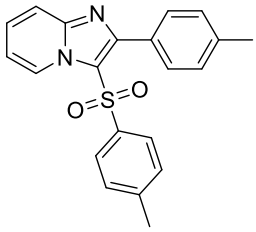
Figure S1. Cyclic voltammograms of related compounds (0.1 mmol) in corresponding solvent containing 0.1 mmol $^{n}Bu_4NBF_4$.

Detailed descriptions for products



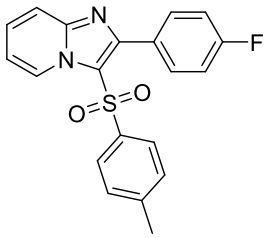
2-Phenyl-3-tosylimidazo[1,2-a]pyridine (3a).[1]

White solid was obtained in 92% isolated yield, 159.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.10 (d, J = 7.0 Hz, 1H), 7.80–7.73 (m, 2H), 7.70 (d, J = 9.0 Hz, 1H), 7.53 (d, J = 8.3 Hz, 2H), 7.49–7.38 (m, 4H), 7.13 (d, J = 8.1 Hz, 2H), 7.06–7.01 (m, 1H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.67, 146.47, 144.29, 138.92, 132.59, 130.41, 129.58, 129.19, 128.36, 127.66, 126.68, 126.27, 117.85, 117.65, 114.47, 21.40.



2-(P-tolyl)-3-tosylimidazo[1,2-a]pyridine (3b).

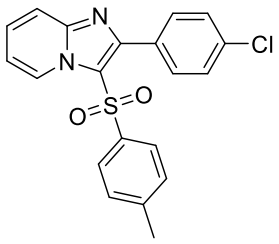
White solid was obtained in 93% isolated yield, 168.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (d, J = 6.8 Hz, 1H), 7.86–7.62 (m, 3H), 7.54 (d, J = 8.4 Hz, 2H), 7.51–7.38 (m, 1H), 7.37–7.23 (m, 2H), 7.15 (d, J = 8.0 Hz, 2H), 7.13–6.95 (m, 1H), 2.44 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.89, 146.49, 144.24, 139.22, 138.92, 130.32, 129.59, 128.43, 128.34, 126.63, 126.25, 117.77, 117.31, 114.38, 21.44, 21.41. HRMS (ESI) m/z: [M+H]+ Calcd for $C_{21}H_{19}N_2O_2S^+$; 363.1162, found 363.1172.



2-(4-Fluorophenyl)-3-tosylimidazo[1,2-a]pyridine (3c).

White solid was obtained in 54% isolated yield, 98.0 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15–9.11 (m, 1H), 7.76–7.66 (m, 3H), 7.55–7.43 (m, 5H), 7.42–7.34 (m, 1H), 7.15 (d, J = 8.0 Hz, 2H), 2.34 (s, 3H).

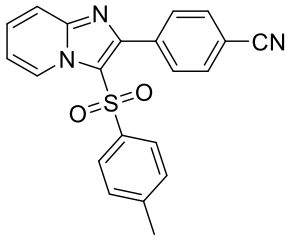
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.88 (d, $J_{C\text{-}F}$ = 240.0 Hz), 153.25 (d, $J_{C\text{-}F}$ = 2.5 Hz), 144.66, 143.96, 138.58, 132.26, 130.34, 129.71, 129.42, 127.81, 126.37, 120.23 (d, $J_{C\text{-}F}$ = 25.2 Hz), 118.29 (d, $J_{C\text{-}F}$ = 8.9 Hz), 114.43, 114.00, 21.52. ^{19}F NMR (376 MHz, $CDCl_3$) δ -135.33.HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{16}FN_2O_2S^+$; 367.0911, found 367.0905.



3d

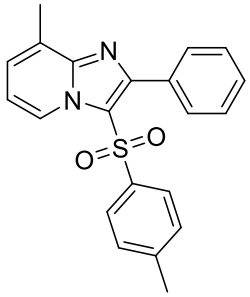
2-(4-Chlorophenyl)-3-tosylimidazo[1,2-a]pyridine (3d).

White solid was obtained in 75% NMR quantitative yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (d, J = 6.8 Hz, 1H), 7.80–7.69 (m, 3H), 7.54 (d, J = 8.4 Hz, 2H), 7.48–7.43 (m, 3H), 7.17 (d, J = 8.0 Hz, 2H), 7.10–7.05 (m, 1H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.32, 146.51, 144.61, 138.73, 135.58, 131.88, 130.98, 129.78, 128.69, 128.05, 126.72, 126.29, 117.93, 117.82, 114.76, 21.52. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{16}ClN_2O_2S^+$; 383.0616, found 383.0608.



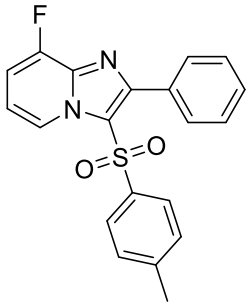
4-(3-Tosylimidazo[1,2-a]pyridin-2-yl)benzonitrile (3e).

White solid was obtained in 92% isolated yield, 171.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (d, J = 7.2 Hz, 1H), 7.92 (d, J = 8.4 Hz, 2H), 7.85–7.69 (m, 3H), 7.65–7.44 (m, 3H), 7.19 (d, J = 8.4 Hz, 2H), 7.16–7.07 (m, 1H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.23, 146.66, 144.87, 138.50, 137.24, 131.48, 131.29, 129.89, 128.92, 126.66, 126.27, 118.65, 118.35, 118.14, 115.08, 112.90, 21.50. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{16}N_3O_2S^+$; 374.0958, found 374.0965.



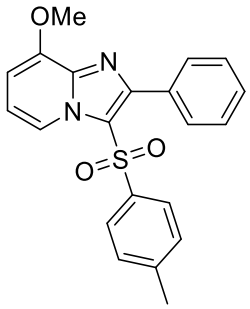
8-Methyl-2-phenyl-3-tosylimidazo[1,2-a]pyridine (3f).

White solid was obtained in 87% isolated yield, 157.9 mg.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 (d, J = 6.8 Hz, 1H), 7.85–7.68 (m, 2H), 7.52 (d, J = 8.4 Hz, 2H), 7.50–7.39 (m, 3H), 7.21 (d, J = 7.2 Hz, 1H), 7.12 (d, J = 8.4 Hz, 2H), 6.93 (t, J = 7.0 Hz, 1H), 2.62 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.09, 146.70, 144.15, 138.98, 132.85, 130.47, 129.53, 129.04, 127.93, 127.63, 127.18, 126.27, 124.28, 117.92, 114.48, 21.38, 16.97. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{19}N_2O_2S^+$; 363.1162, found 363.1157.



8-Fluoro-2-phenyl-3-tosylimidazo[1,2-a]pyridine (3g).

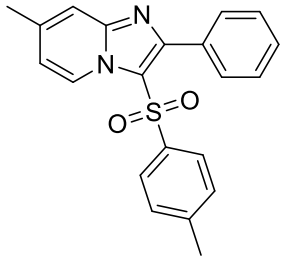
White solid was obtained in 71% isolated yield, 130.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, J = 6.8 Hz, 1H), 8.19–7.68 (m, 2H), 7.60–7.36 (m, 4H), 7.25–7.09 (m, 2H), 7.08–6.91 (m, 1H), 2.34 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 152.58, 151.13 (d, $J_{C\text{-}F}$ = 255.8 Hz), 144.71, 138.49, 132.03, 130.59, 129.71, 129.51, 127.77, 126.47, 123.08 (d, $J_{C\text{-}F}$ = 5.4 Hz), 119.63, 113.67 (d, $J_{C\text{-}F}$ = 6.3 Hz), 111.09 (d, $J_{C\text{-}F}$ = 15.8 Hz), 21.54.^{19}F NMR (376 MHz, $CDCl_3$) δ -127.72. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{16}FN_2O_2S^+$; 367.0911, found 367.0902.



8-Methoxy-2-phenyl-3-tosylimidazo[1,2-a]pyridine (3h).

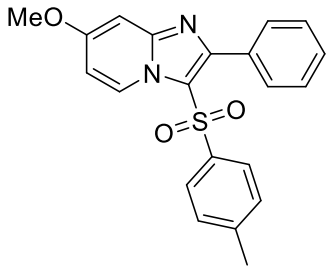
White solid was obtained in 51% NMR quantitative yield. ^{1}H NMR (400 MHz, DMSO-D^6) δ 8.54 (d, J = 6.8 Hz, 1H), 7.71–7.67 (m, 2H), 7.64 (d, J = 8.4 Hz, 2H), 7.52–7.45 (m, 3H), 7.33 (d, J = 8.0 Hz, 2H), 7.15 (t, J = 7.4 Hz, 1H), 7.04 (d, J = 8.0 Hz, 1H), 3.95 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, DMSO-D^6) δ 151.15, 148.88, 145.14, 140.84, 138.62, 133.23, 130.76, 130.62, 129.54, 128.09, 126.57,

119.16, 117.92, 116.11, 106.74, 56.68, 21.44. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{19}N_2O_3S^+$; 379.1111, found 379.1102.



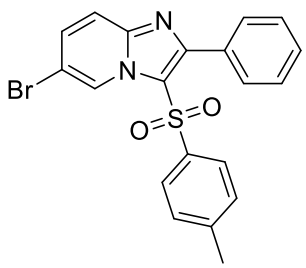
7-Methyl-2-phenyl-3-tosylimidazo[1,2-a]pyridine (3i).

White solid was obtained in 93% isolated yield, 168.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, J = 7.2 Hz, 1H), 7.83–7.68 (m, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.48–7.40 (m, 4H), 7.12 (d, J = 8.4 Hz, 2H), 6.93–6.77 (m, 1H), 2.43 (s, 3H), 2.31 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 152.82, 146.97, 144.13, 139.95, 139.12, 132.69, 130.40, 129.55, 129.14, 127.64, 126.20, 125.80, 117.03, 116.96, 116.36, 21.40, 21.25. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{19}N_2O_2S^+$; 363.1162, found 363.1167.



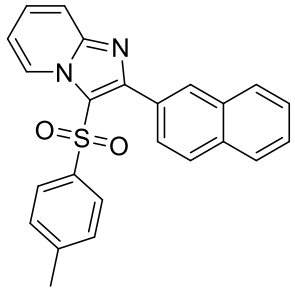
7-Methoxy-2-phenyl-3-tosylimidazo[1,2-a]pyridine (3j).

White solid was obtained in 94% isolated yield, 179.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, J = 7.6 Hz, 1H), 7.88–7.63 (m, 2H), 7.55–7.40 (m, 5H), 7.12 (d, J = 8.0 Hz, 2H), 6.95 (d, J = 2.4 Hz, 1H), 6.78–6.64 (m, 1H), 3.86 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.13, 152.90, 148.47, 143.96, 139.01, 132.51, 130.21, 129.45, 129.03, 127.50, 126.90, 125.97, 116.18, 108.85, 95.19, 55.60, 21.24. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{19}N_2O_3S^+$; 379.1111, found 379.1101.



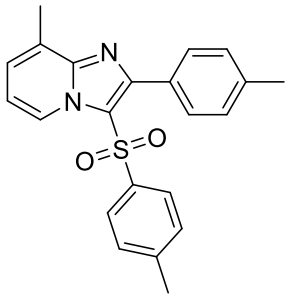
6-Bromo-2-phenyl-3-tosylimidazo[1,2-a]pyridine (3k).

White solid was obtained in 43% NMR quantitative yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.31 (d, J = 0.8 Hz, 1H), 7.84–7.66 (m, 2H), 7.60 (d, J = 9.6 Hz, 1H), 7.56–7.42 (m, 6H), 7.15 (d, J = 8.4 Hz, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.87, 144.85, 144.67, 138.63, 132.14, 131.87, 130.39, 129.71, 129.48, 127.82, 126.86, 126.42, 118.44, 118.35, 109.38, 21.53. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{16}BrN_2O_2S^+$; 427.0110, found 427.0115.



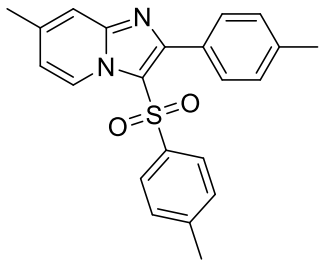
2-(Naphthalen-2-yl)-3-tosylimidazo[1,2-a]pyridine (3l).

White solid was obtained in 61% isolated yield, 121.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 (d, J = 7.2 Hz, 1H), 8.27 (s, 1H), 8.02–7.84 (m, 4H), 7.74 (d, J = 8.8 Hz, 1H), 7.67–7.50 (m, 4H), 7.52–7.41 (m, 1H), 7.22–6.96 (m, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.63, 146.64, 144.39, 138.97, 133.59, 132.67, 130.46, 130.01, 129.62, 128.67, 128.48, 127.73, 127.67, 127.29, 126.84, 126.74, 126.38, 126.17, 118.00, 117.95, 114.56, 21.44. HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{24}H_{18}N_2NaO_2S^+$; 421.0981, found 421.0976.



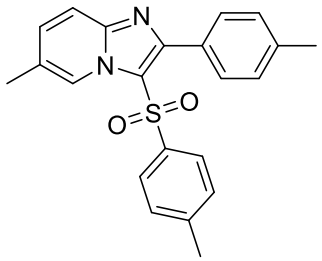
8-Methyl-2-(p-tolyl)-3-tosylimidazo[1,2-a]pyridine (3m).

White solid was obtained in 76% isolated yield, 143.7 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (d, J = 7.2 Hz, 1H), 7.65 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8.4 Hz, 2H), 7.27 (d, J = 7.6 Hz, 2H), 7.22–7.16 (m, 1H), 7.13 (d, J = 8.4 Hz, 2H), 6.92 (t, J = 7.0 Hz, 1H), 2.61 (s, 3H), 2.42 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.26, 146.67, 144.05, 138.97, 138.93, 130.33, 129.90, 129.49, 128.33, 127.79, 127.09, 126.20, 124.18, 117.56, 114.34, 21.36, 21.34, 16.94. HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{22}H_{20}N_2NaO_2S^+$; 399.1138, found 399.1136.



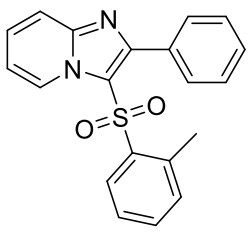
7-Methyl-2-(p-tolyl)-3-tosylimidazo[1,2-a]pyridine (3n).

White solid was obtained in 86% isolated yield, 161.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, J = 7.2 Hz, 1H), 7.65 (d, J = 8.0 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.44 (d, J = 0.4 Hz, 1H), 7.26 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.4 Hz, 2H), 6.88–6.83 (m, 1H), 2.43 (s, 6H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.09, 147.01, 144.08, 139.89, 139.17, 130.32, 129.75, 129.58, 128.43, 126.20, 125.79, 116.93, 116.65, 116.33, 21.46, 21.44, 21.31. HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{22}H_{20}N_2NaO_2S^+$; 399.1138, found 399.1145.



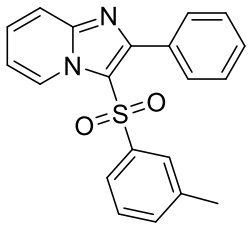
6-Methyl-2-(p-tolyl)-3-tosylimidazo[1,2-a]pyridine (3o).

White solid was obtained in 71% isolated yield, 133.5 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (s, 1H), 7.63 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 9.2 Hz, 1H), 7.54 (d, J = 8.4 Hz, 2H), 7.27 (d, J = 18.0 Hz,2H), 7.15 (d, J = 8.4 Hz, 2H), 2.43 (s, 3H), 2.41 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.63, 147.44, 145.46, 144.15, 139.10, 139.06, 131.39, 130.27, 129.69, 129.57, 128.39, 126.20, 124.43, 124.38, 116.97, 116.85, 21.44, 21.39, 18.53. HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{22}H_{20}N_2NaO_2S^+$; 399.1138, found 399.1128.



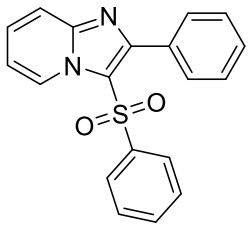
2-Phenyl-3-(o-tolylsulfonyl)imidazo[1,2-a]pyridine (4a).

White solid was obtained in 71% isolated yield, 49.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (d, J = 6.8 Hz, 1H), 7.92–7.69 (m, 2H), 7.70–7.57 (m, 2H), 7.47 (d, J = 1.2 Hz, 1H), 7.40–7.23 (m, 4H), 7.18–6.96 (m, 3H), 2.09 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.78, 146.35, 139.06, 137.68, 133.22, 132.48, 132.19, 130.35, 129.16, 128.77, 128.37, 127.68, 127.00, 125.67, 117.92, 116.70, 114.46, 19.19. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{17}N_2O_2S^+$; 349.1005, found 349.1002.



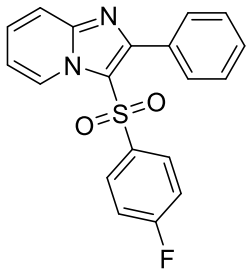
2-Phenyl-3-(m-tolylsulfonyl)imidazo[1,2-a]pyridine (4b).

White solid was obtained in 93% isolated yield, 64.7 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (d, J = 7.2 Hz, 1H), 7.87–7.62 (m, 3H), 7.53–7.40 (m, 5H), 7.37 (s, 1H), 7.35–7.14 (m, 2H), 7.13–6.99 (m, 1H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.88, 146.54, 141.68, 139.24, 134.07, 132.58, 130.42, 129.27, 128.80, 128.44, 127.71, 126.81, 126.69, 123.35, 117.90, 117.58, 114.53, 21.14. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{17}N_2O_2S^+$; 349.1005, found 349.0097.



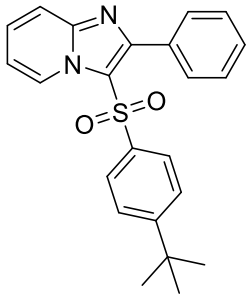
2-Phenyl-3-(phenylsulfonyl)imidazo[1,2-a]pyridine (4c).[1]

White solid was obtained in 87% isolated yield, 58.3 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (d, J = 7.2 Hz, 1H), 7.78–7.69 (m, 3H), 7.63 (d, J = 7.6 Hz, 2H), 7.55–7.42 (m, 5H), 7.34 (t, J = 7.8 Hz, 2H), 7.06 (t, J = 6.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.06, 146.64, 141.86, 133.30, 132.50, 130.45, 129.33, 129.00, 128.54, 127.76, 126.78, 126.26, 117.96, 117.35, 114.61.



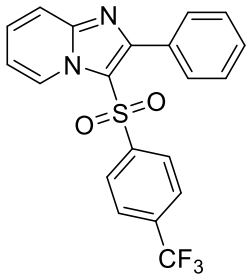
3-((4-Fluorophenyl)sulfonyl)-2-phenylimidazo[1,2-a]pyridine (4d).[1]

White solid was obtained in 87% isolated yield, 70.0 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (d, J = 7.2 Hz, 1H), 7.77–7.69 (m, 3H), 7.67–7.58 (m, 2H), 7.54–7.44 (m, 4H), 7.13–7.06 (m, 1H), 7.04–6.97 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.28 (d, $J_{C\text{-}F}$ = 256.3 Hz), 152.82, 146.51, 137.75 (d, $J_{C\text{-}F}$ = 3.1 Hz), 132.20, 130.35, 129.40, 129.08 (d, $J_{C\text{-}F}$ = 9.6 Hz), 128.72, 127.76, 126.63, 117.90, 117.23, 116.20 (d, $J_{C\text{-}F}$ = 22.7 Hz), 114.77. ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.54.



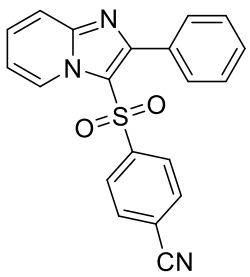
3-((4-(Tert-butyl)phenyl)sulfonyl)-2-phenylimidazo[1,2-a]pyridine (4e).

White solid was obtained in 58% isolated yield, 45.4 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (d, J = 6.8 Hz, 1H), 7.82–7.67 (m, 3H), 7.58 (d, J = 8.8 Hz, 2H), 7.52–7.42 (m, 4H), 7.35 (d, J = 8.4 Hz, 2H), 7.06 (t, J = 6.8 Hz, 1H), 1.25 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.24, 152.69, 146.50, 138.78, 132.61, 130.44, 129.22, 128.39, 127.71, 126.83, 126.22, 126.02, 117.90, 117.76, 114.50, 35.10, 30.89. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{23}N_2O_2S^+$; 391.1475, found 391.1465.



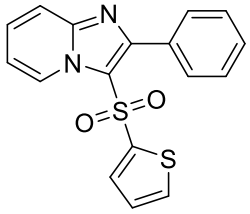
2-Phenyl-3-((4-(trifluoromethyl)phenyl)sulfonyl)imidazo[1,2-a]pyridine (4f).[1]

White solid was obtained in 79% NMR quantitative yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (d, J = 6.8 Hz, 1H), 7.82–7.67 (m, 5H), 7.59 (d, J = 8.4 Hz, 2H), 7.55–7.43 (m, 4H), 7.12 (t, J = 7.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.77, 146.95, 145.24, 134.80 (d, $J_{C\text{-}F}$ = 33.1 Hz), 132.13, 130.44, 129.64, 129.07, 127.91, 126.77, 126.14 (d, $J_{C\text{-}F}$ = 3.7 Hz), 122.93 (d, $J_{C\text{-}F}$ = 273.1 Hz), 118.16, 116.50, 115.02. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.24.



4-((2-Phenylimidazo[1,2-a]pyridin-3-yl)sulfonyl)benzonitrile (4g).

White solid was obtained in 66% isolated yield, 47.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (d, J = 7.2 Hz, 1H), 7.76 (d, J = 8.8 Hz, 1H), 7.72–7.57 (m, 6H), 7.57–7.43 (m, 4H), 7.13 (t, J = 7.0 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 154.04, 147.07, 145.73, 132.72, 132.00, 130.39, 129.74, 129.22, 127.95, 126.77, 126.74, 118.21, 116.99, 116.80, 116.07, 115.13. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{14}N_3O_2S^+$; 360.0801, found 360.0795.



2-Phenyl-3-(thiophen-2-ylsulfonyl)imidazo[1,2-a]pyridine (4h).

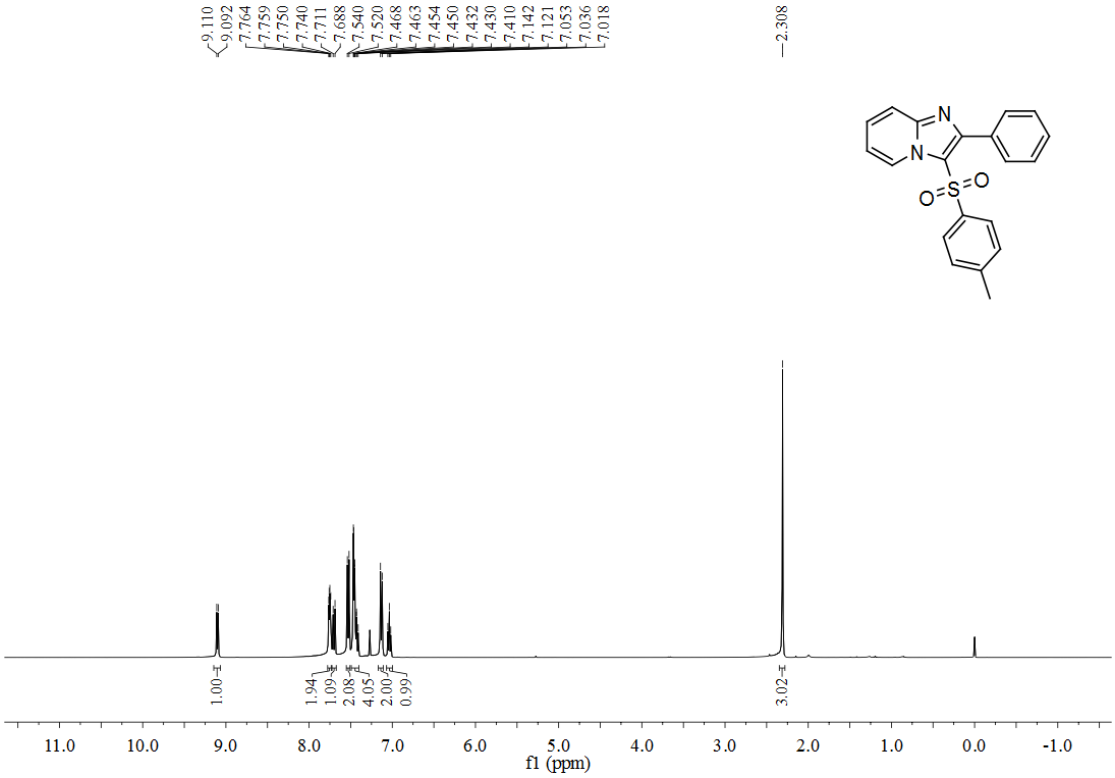
White solid was obtained in 69% NMR quantitative yield. ^{1}H NMR (400 MHz, DMSO-D^6) δ 8.99 (d, J = 6.8 Hz, 1H), 8.03 (d, J = 4.8 Hz, 1H), 7.91 (d, J = 2.8 Hz, 1H), 7.86 (d, J = 8.8 Hz, 1H), 7.79–7.62 (m, 3H), 7.55–7.48 (m, 3H), 7.33 (t, J = 7.0 Hz, 1H), 7.21–7.13 (m, 1H). ^{13}C NMR (101 MHz, DMSO-D^6) δ 152.08, 146.78, 142.52, 136.12, 133.83, 133.11, 130.70, 130.29, 129.68, 128.78, 128.17, 127.27, 118.16, 117.29, 116.21. HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{17}H_{12}N_2NaO_2S_2^+$; 363.0232, found 363.0232.

References:

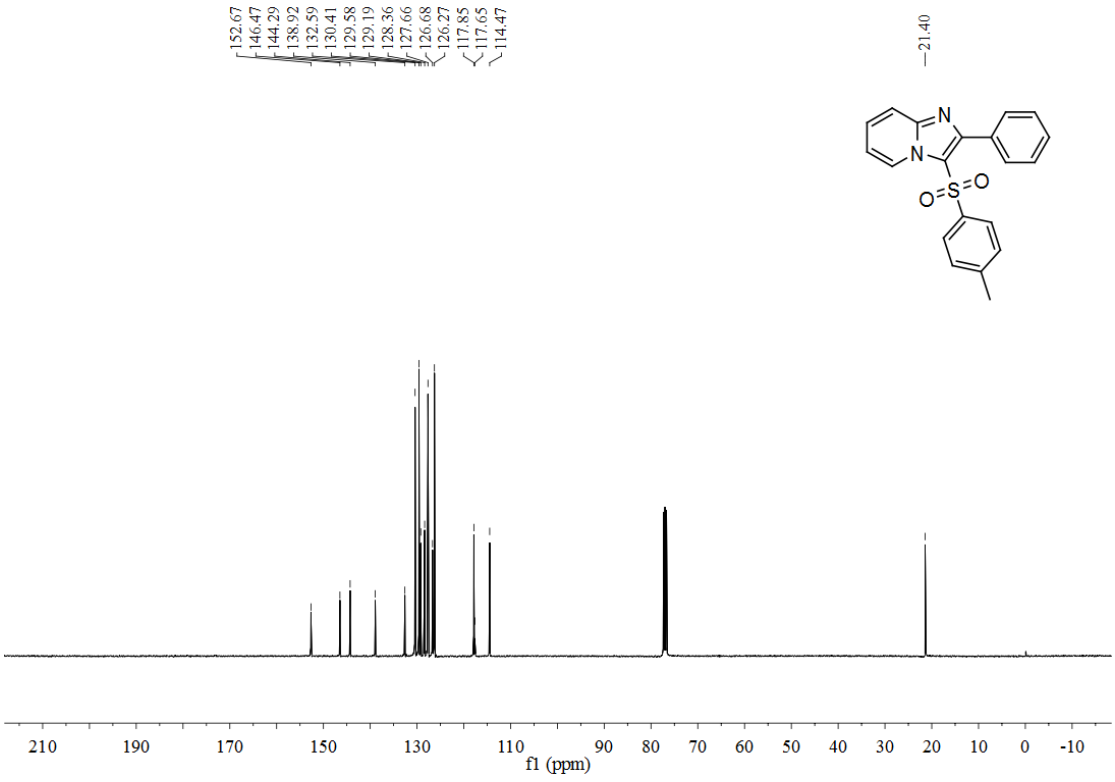
1. Yu-Jing Guo, Shuai Lu, Lu-Lu Tian, En-Ling Huang, Xin-Qi Hao, Xinju Zhu,* Tian Shao,*and Mao-Ping Song, Iodine-Mediated Difunctionalization of Imidazopyridines with Sodium Sulfinates Synthesis of Sulfones and Sulfides. *J. Org. Chem.* 2018, **83**, 338−349

Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra

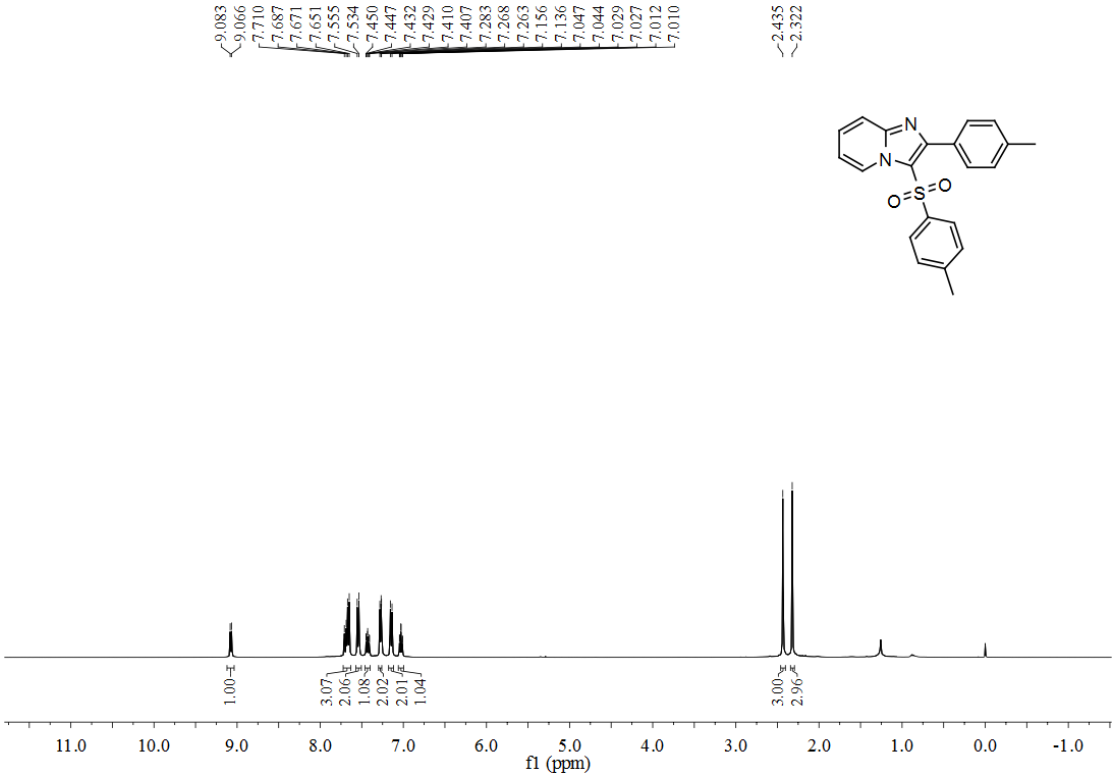
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3a



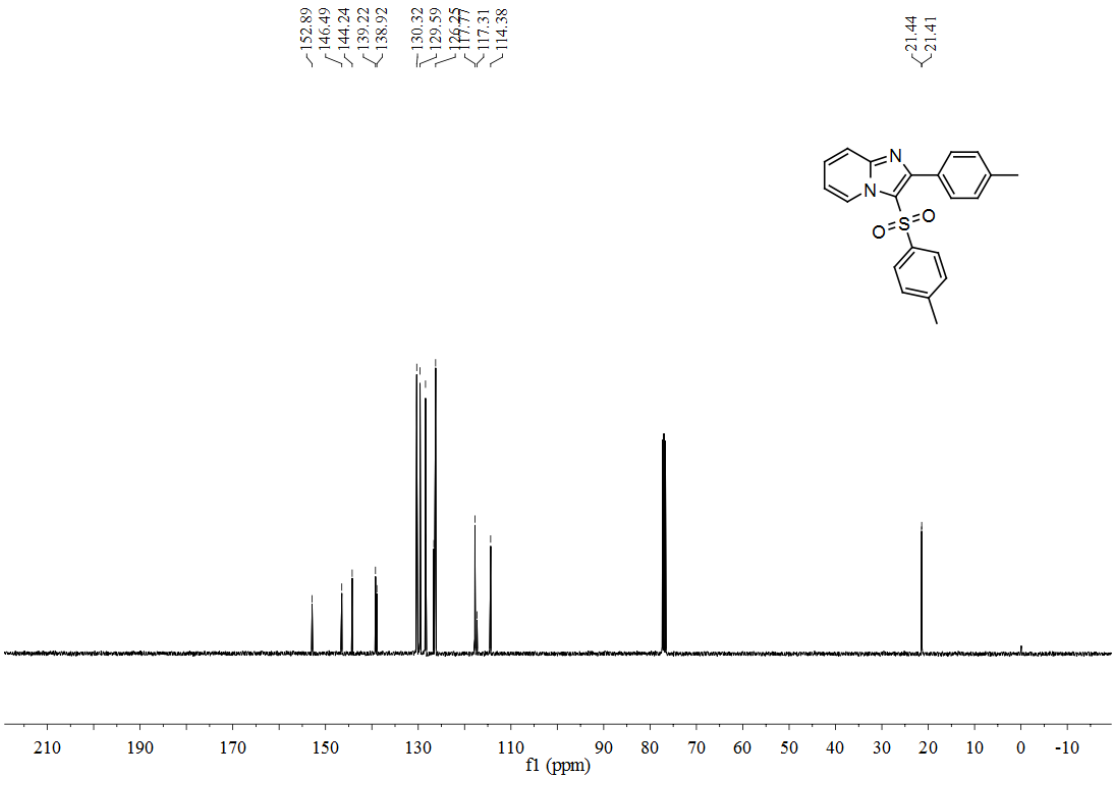
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3a



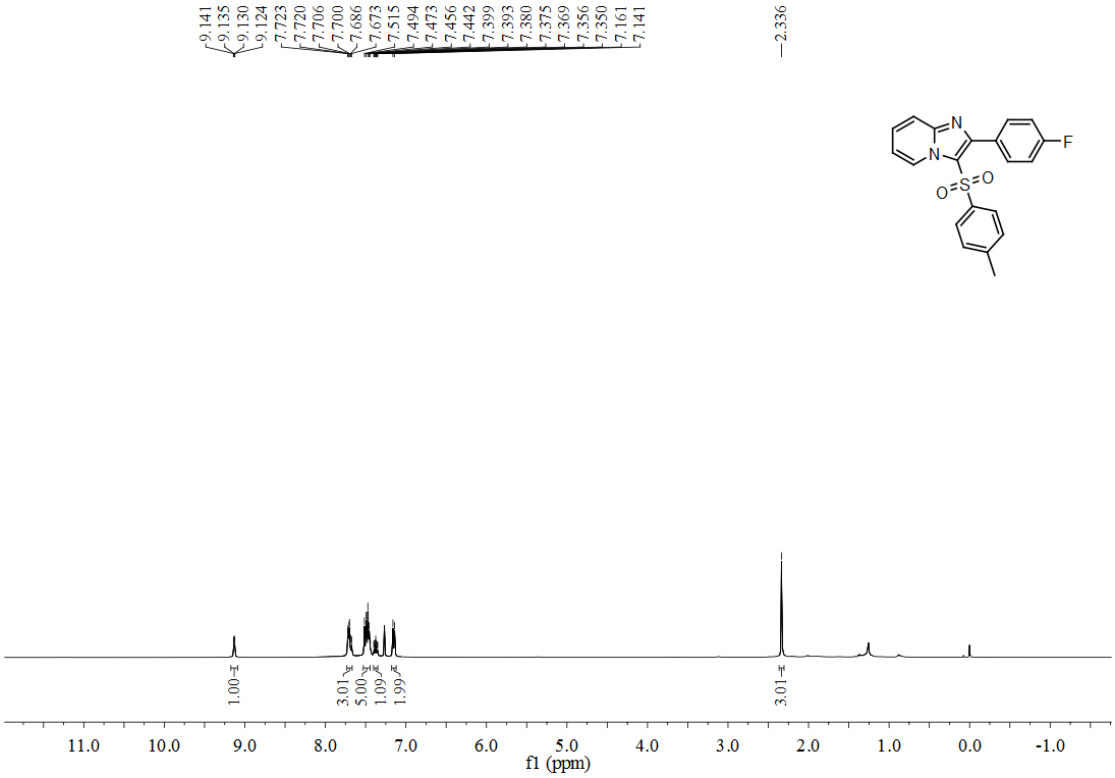
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3b



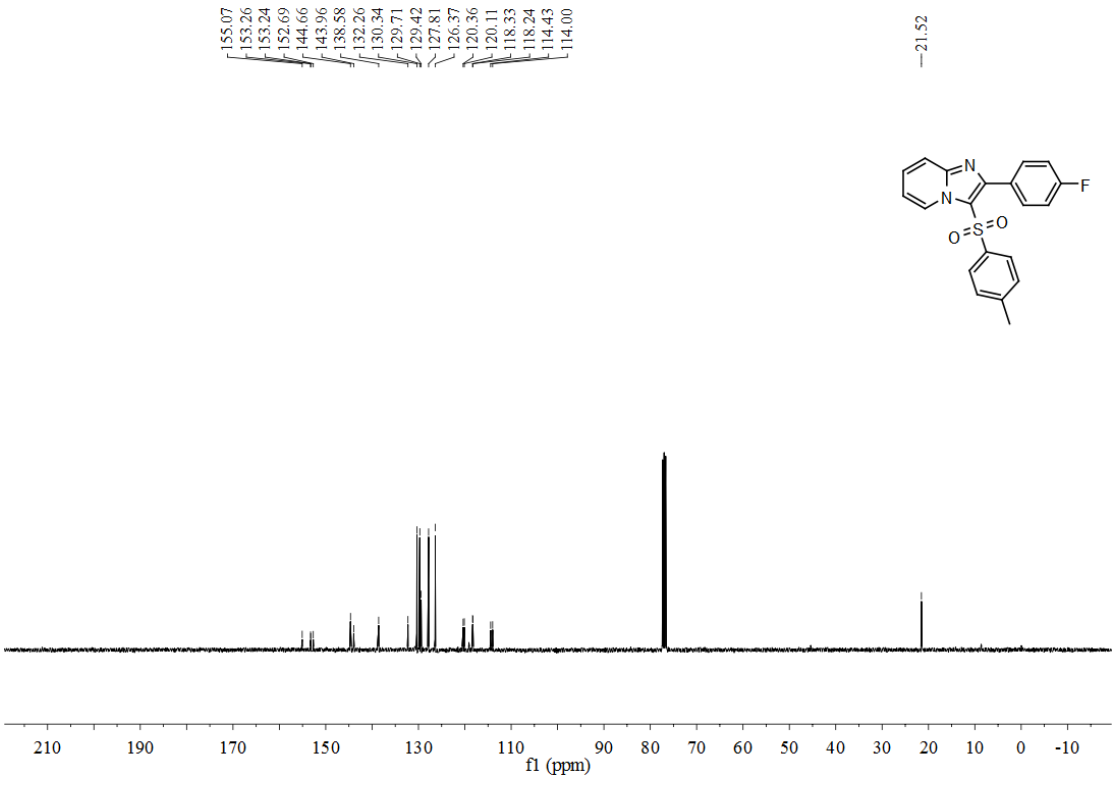
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3b



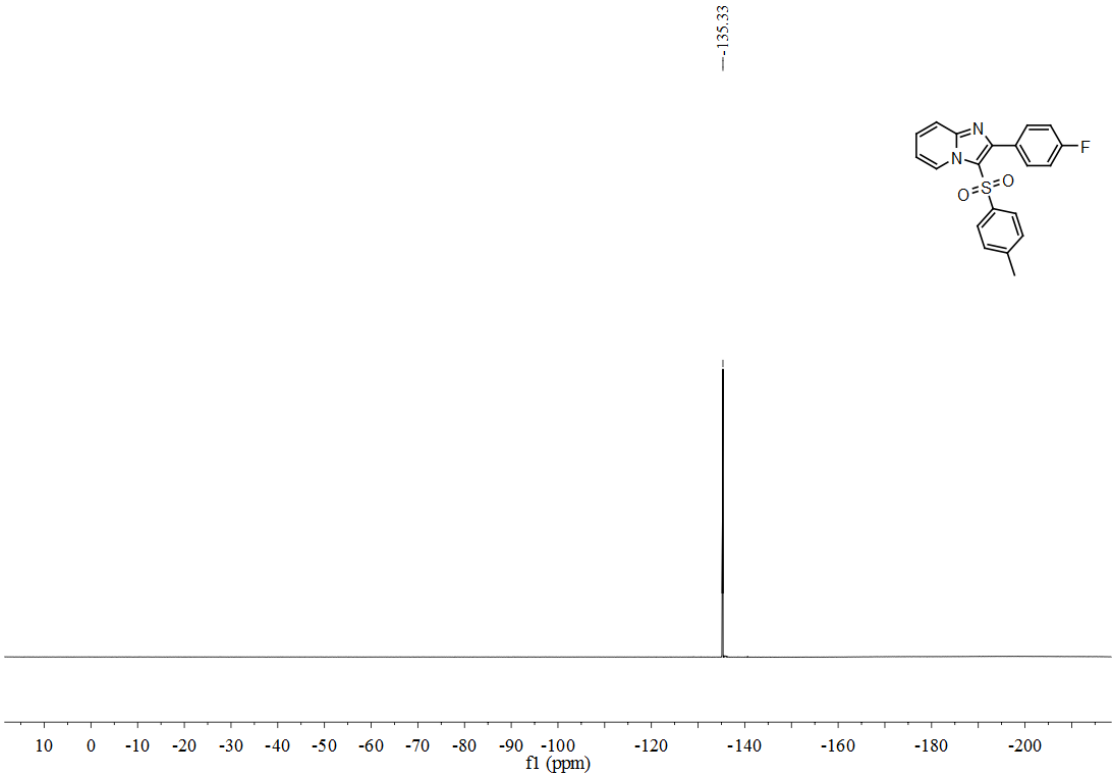
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3c



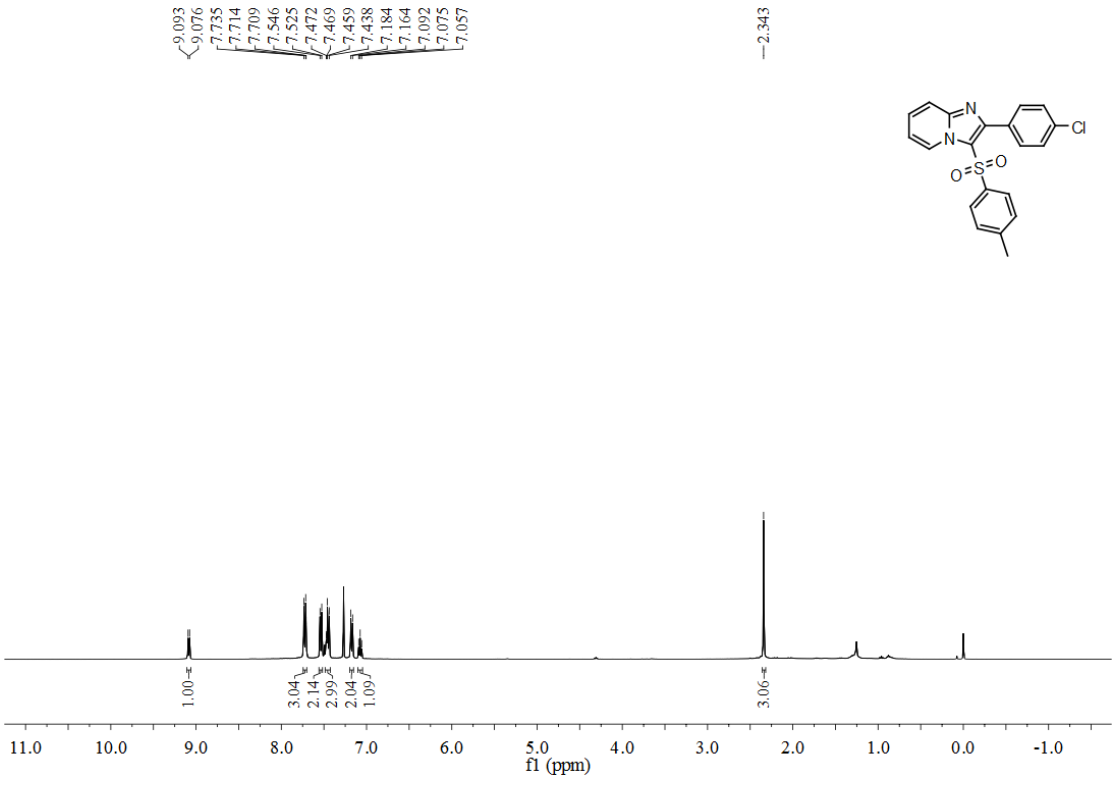
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3c



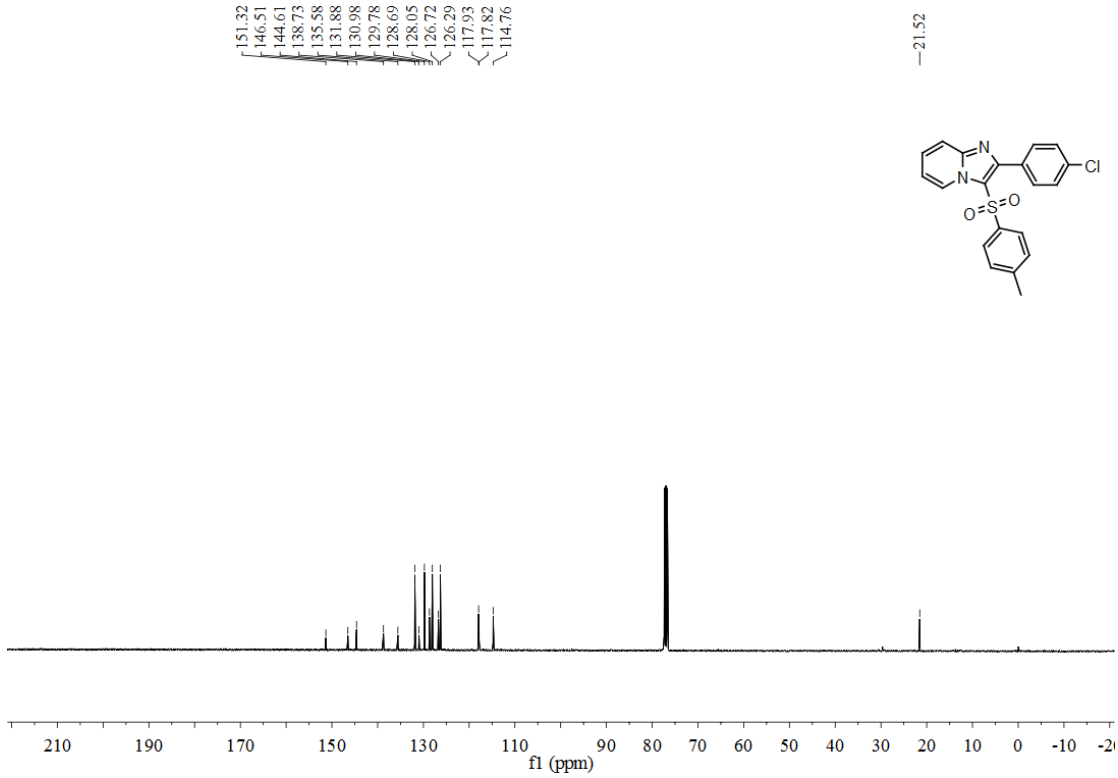
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3c



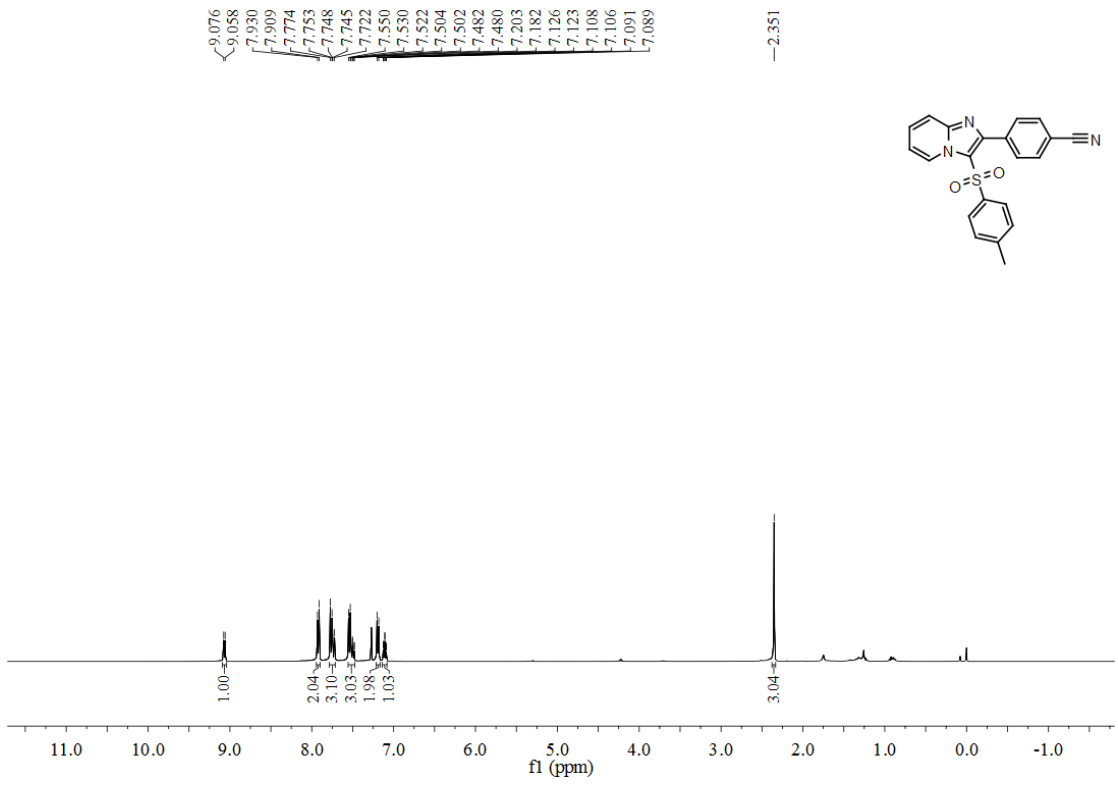
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3d



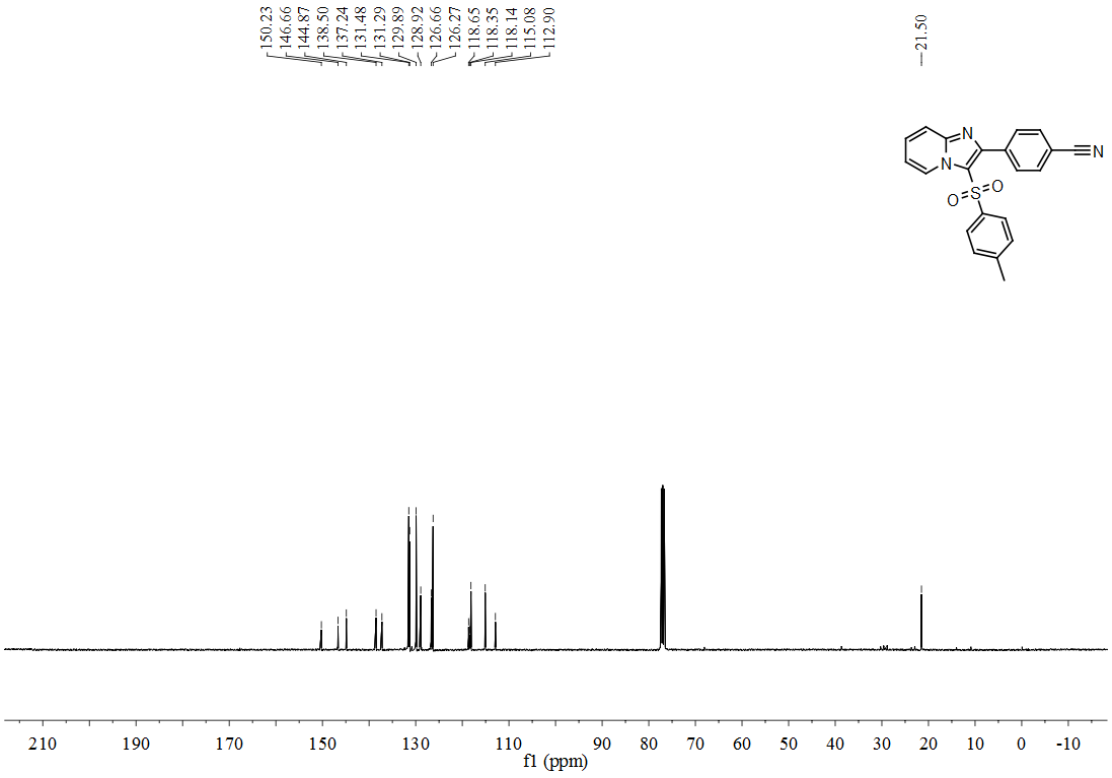
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3d



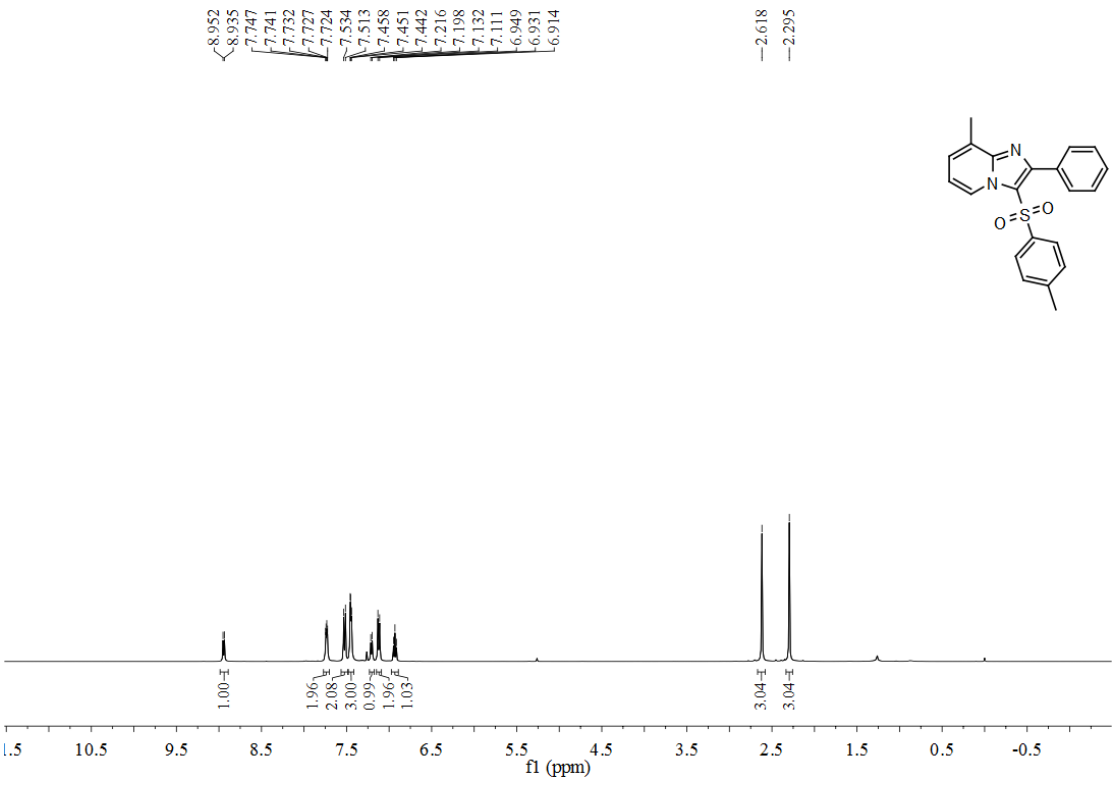
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3e



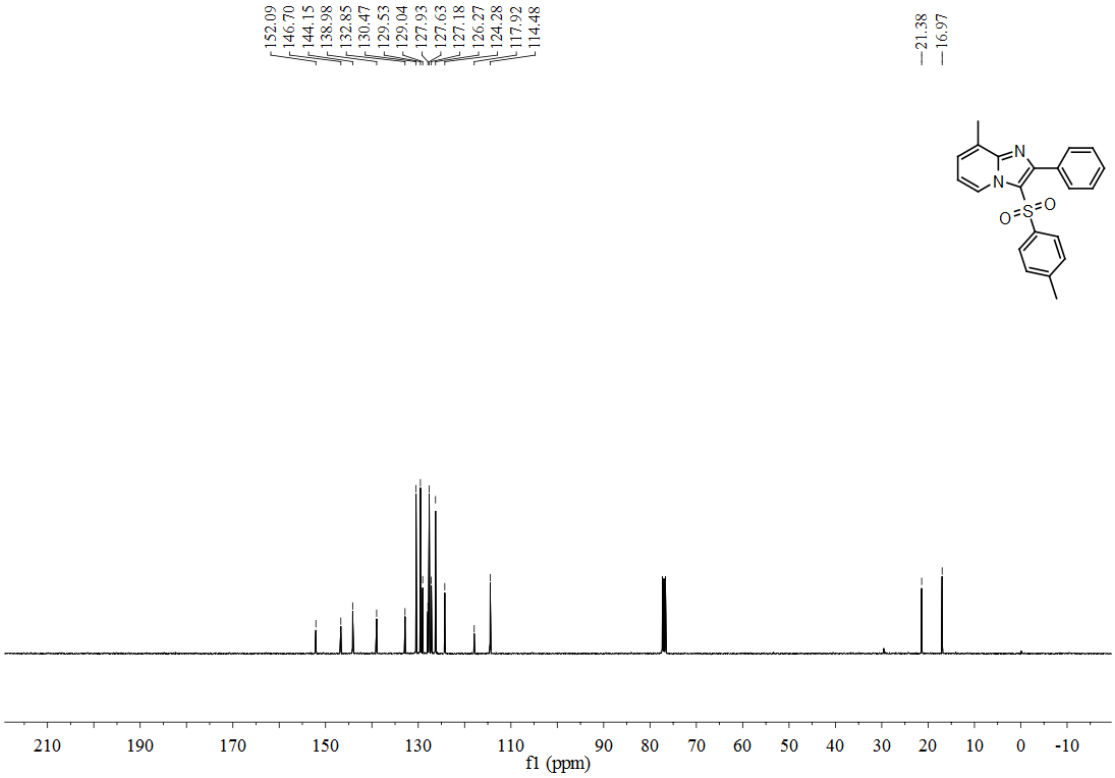
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3e



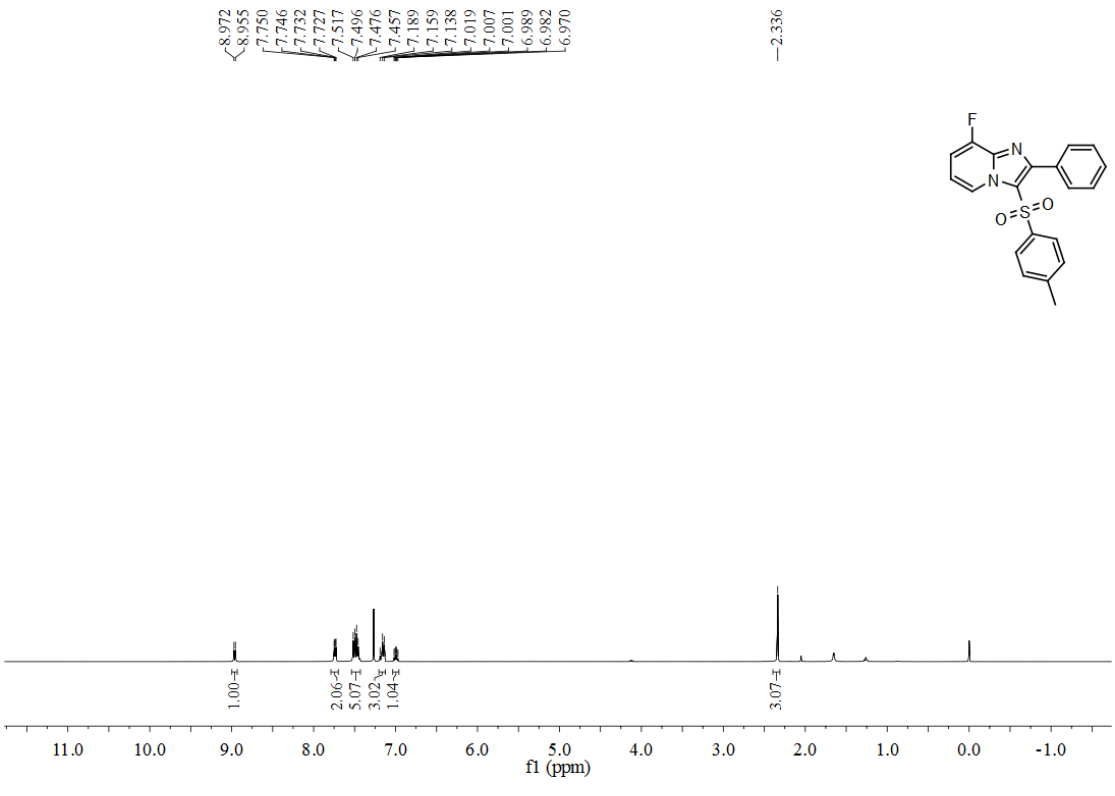
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3f



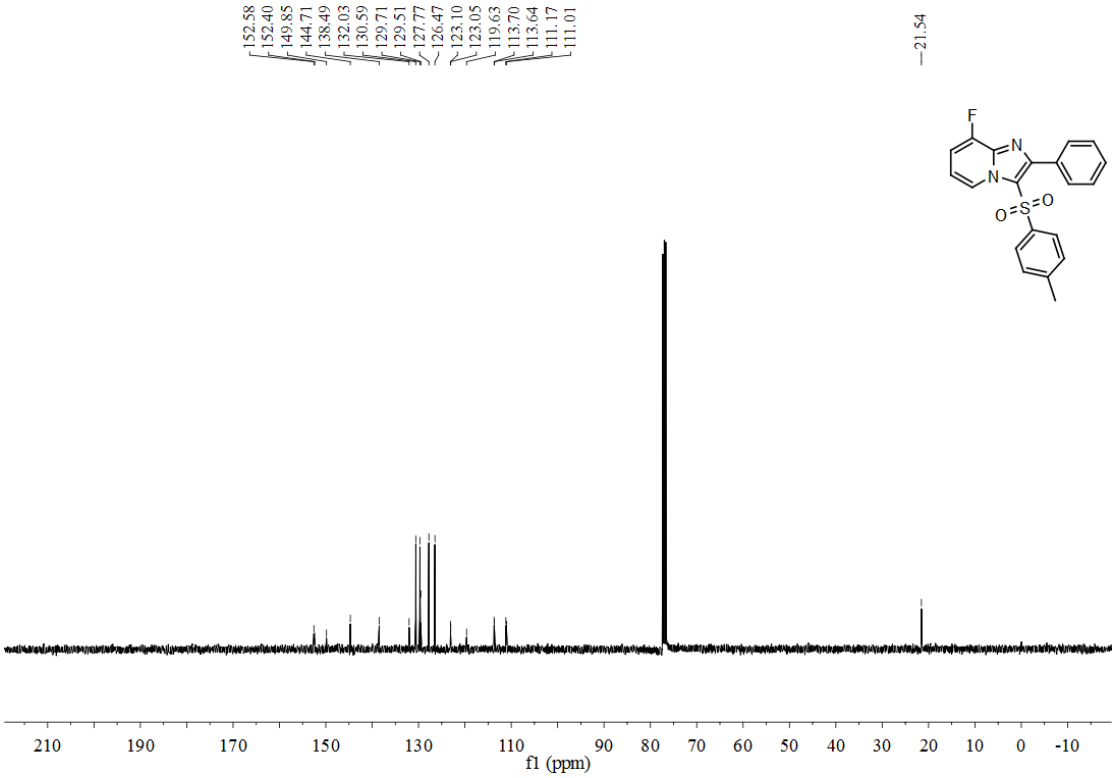
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3f



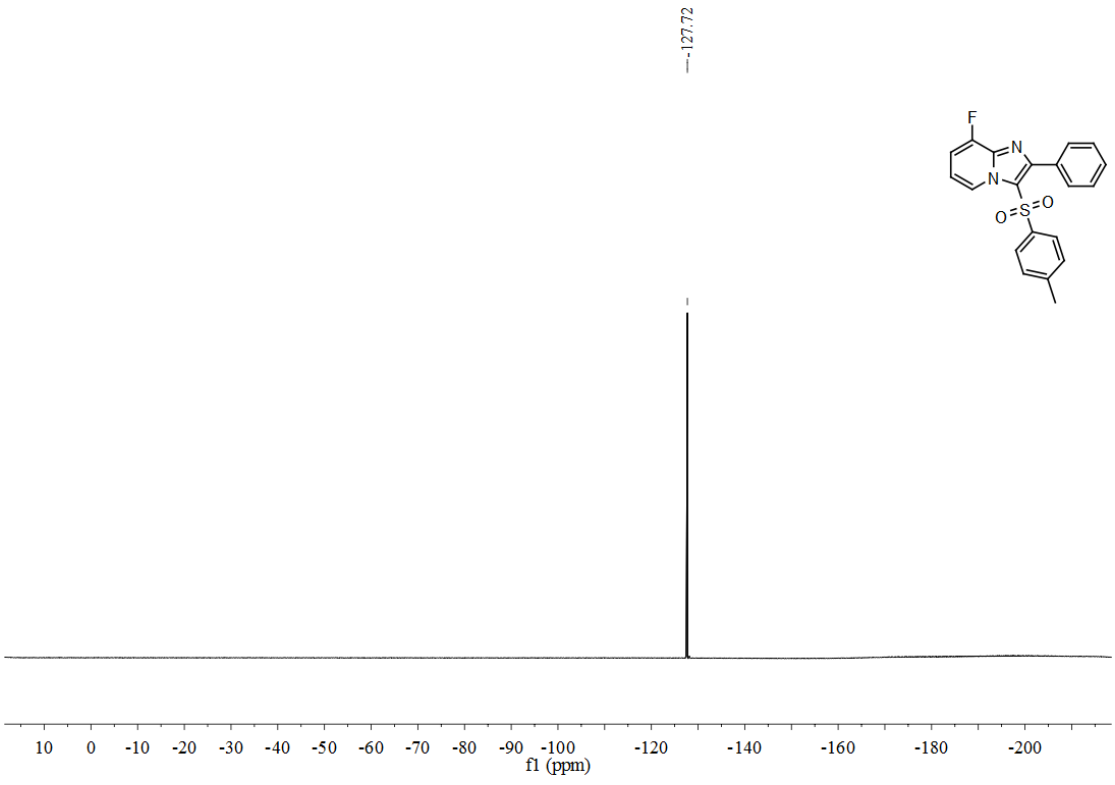
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3g



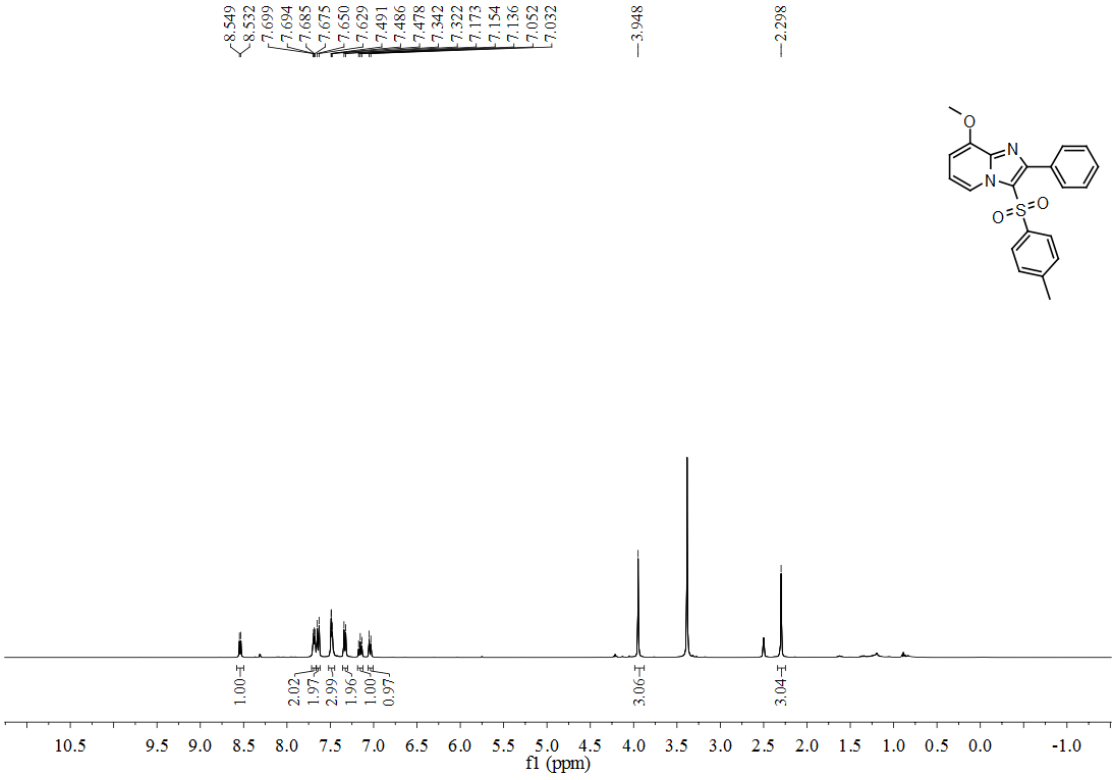
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3g



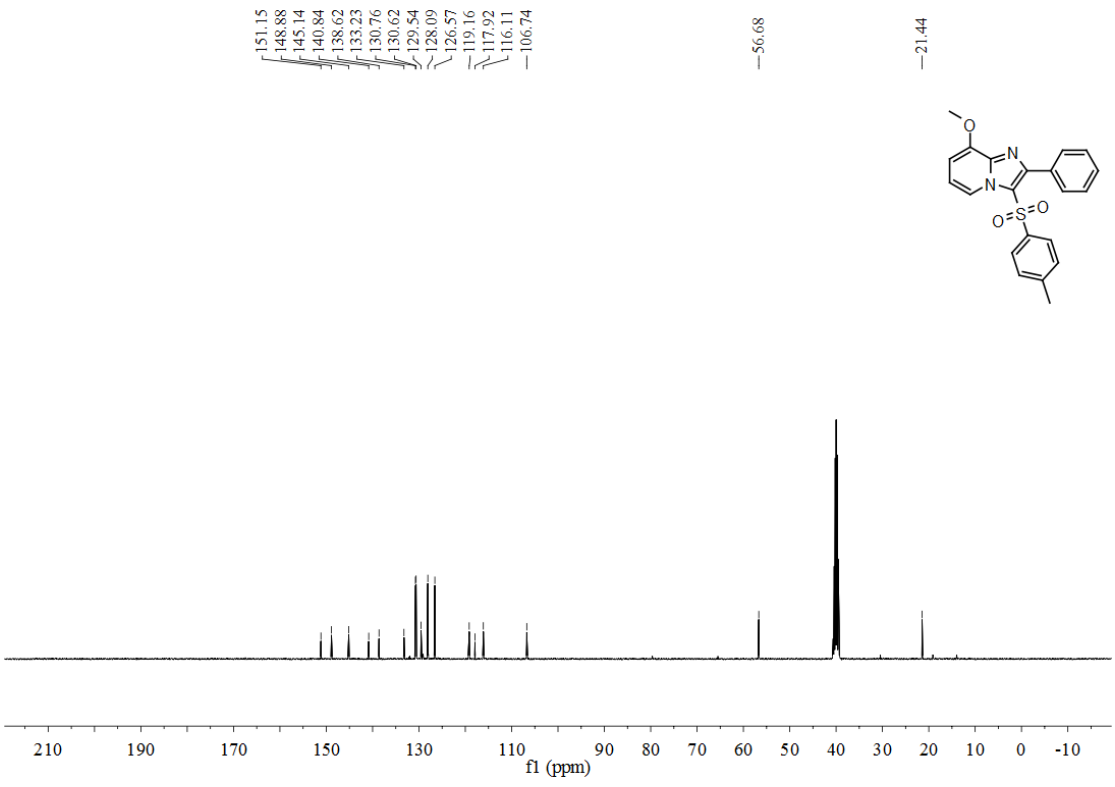
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 3g



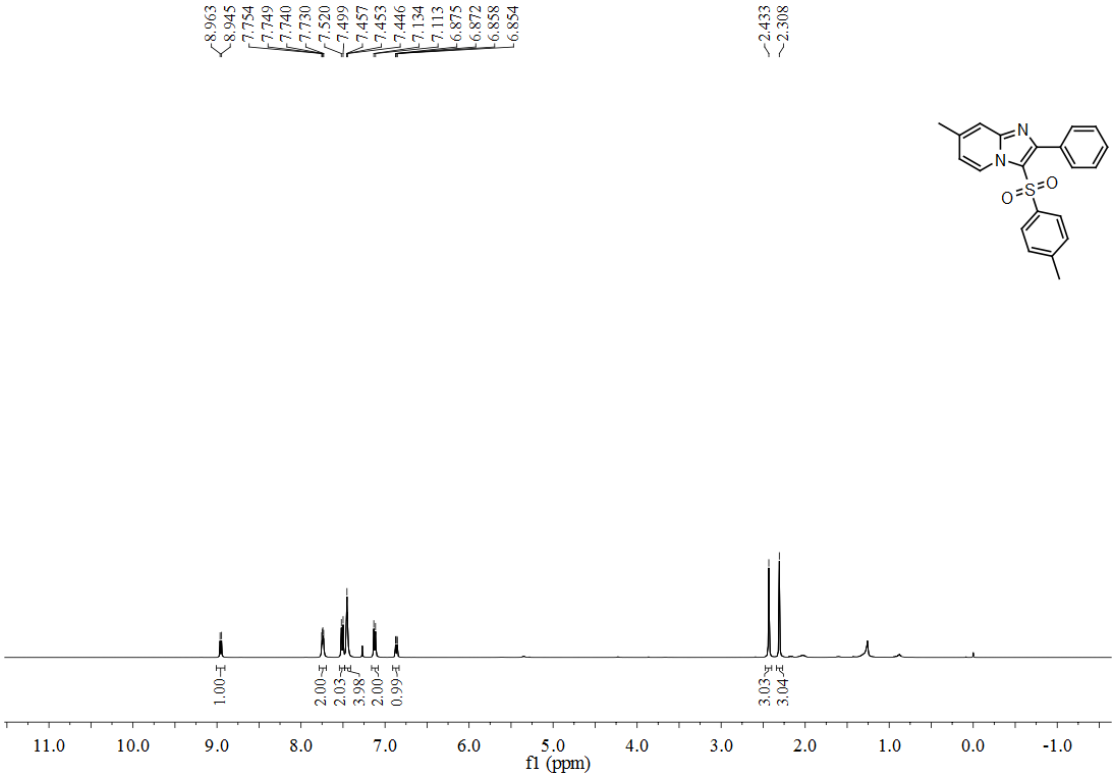
^{1}H NMR (400 MHz, DMSO-D^{6}) spectrum of 3h



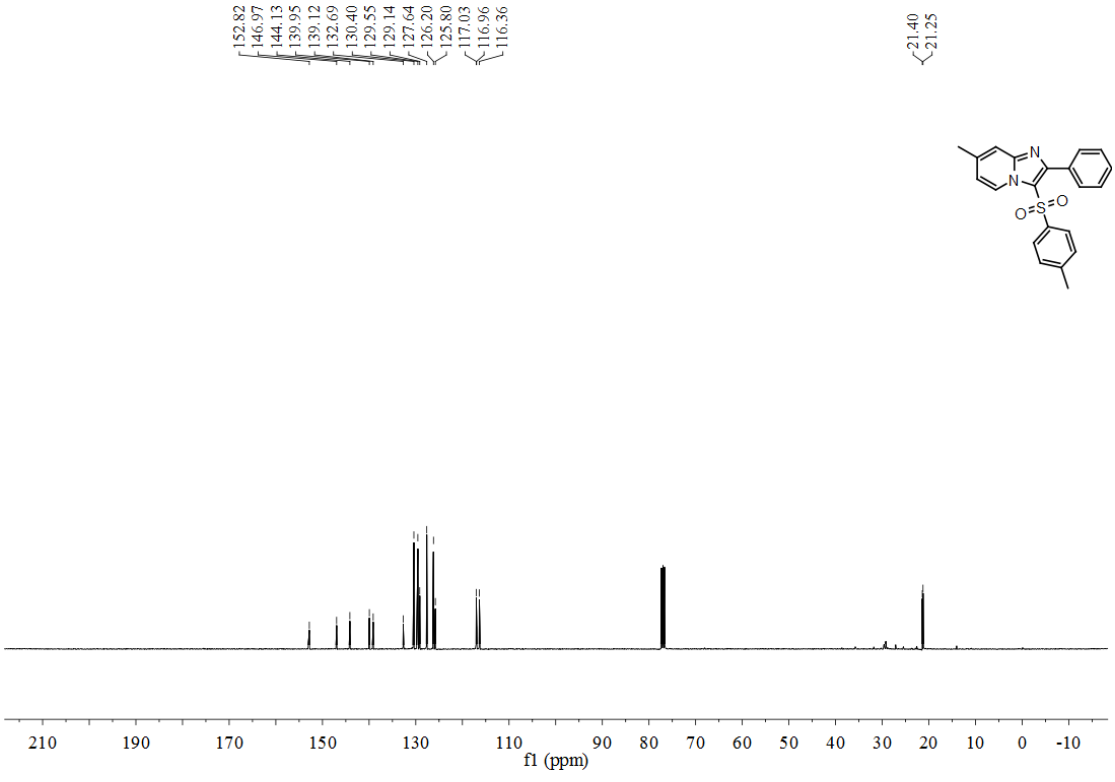
^{13}C NMR (101 MHz, DMSO-D^{6}) spectrum of 3h



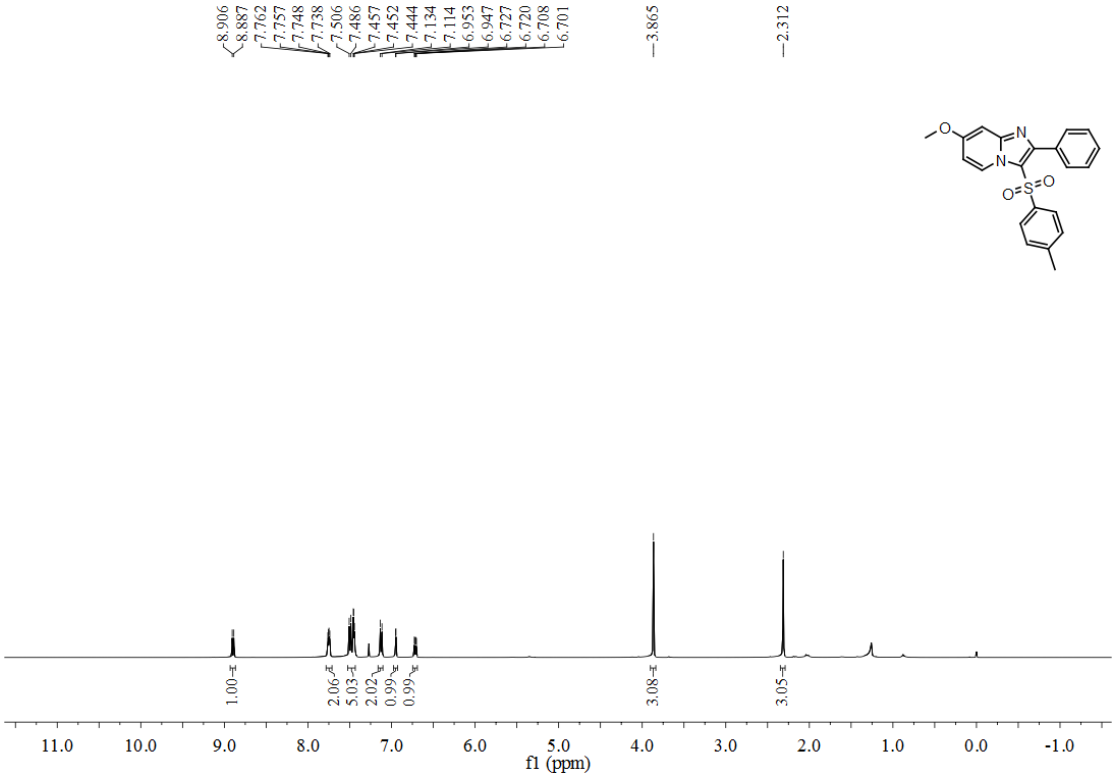
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3i



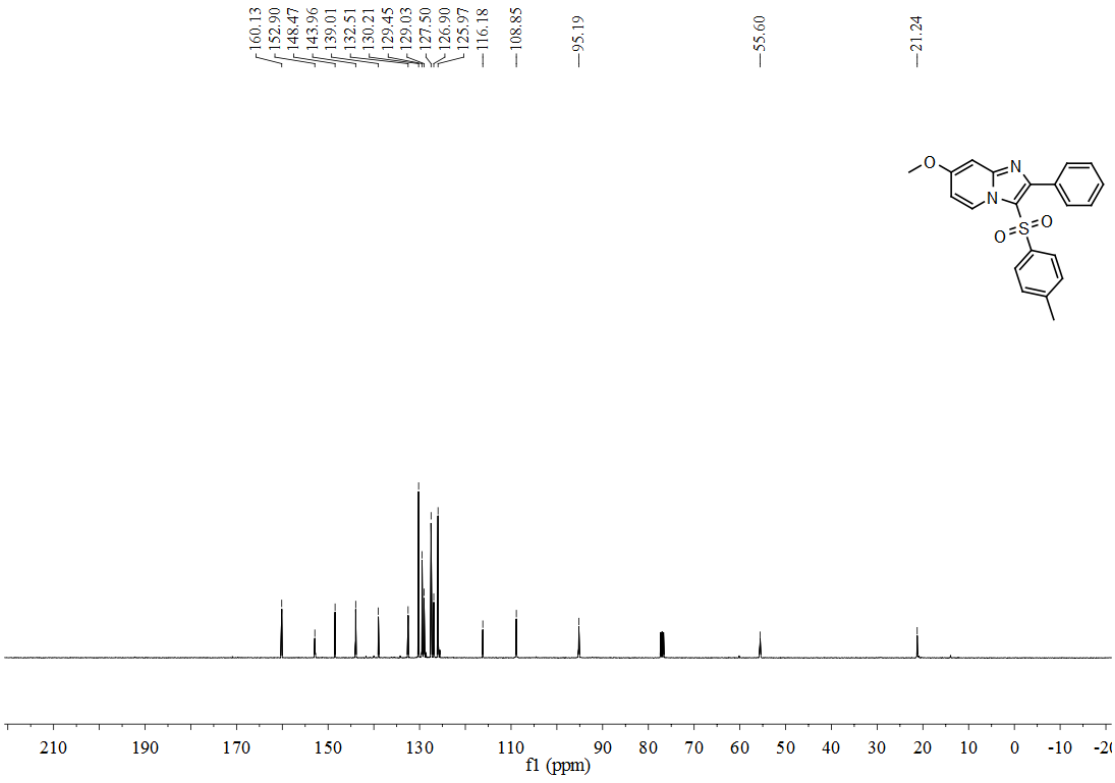
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3i



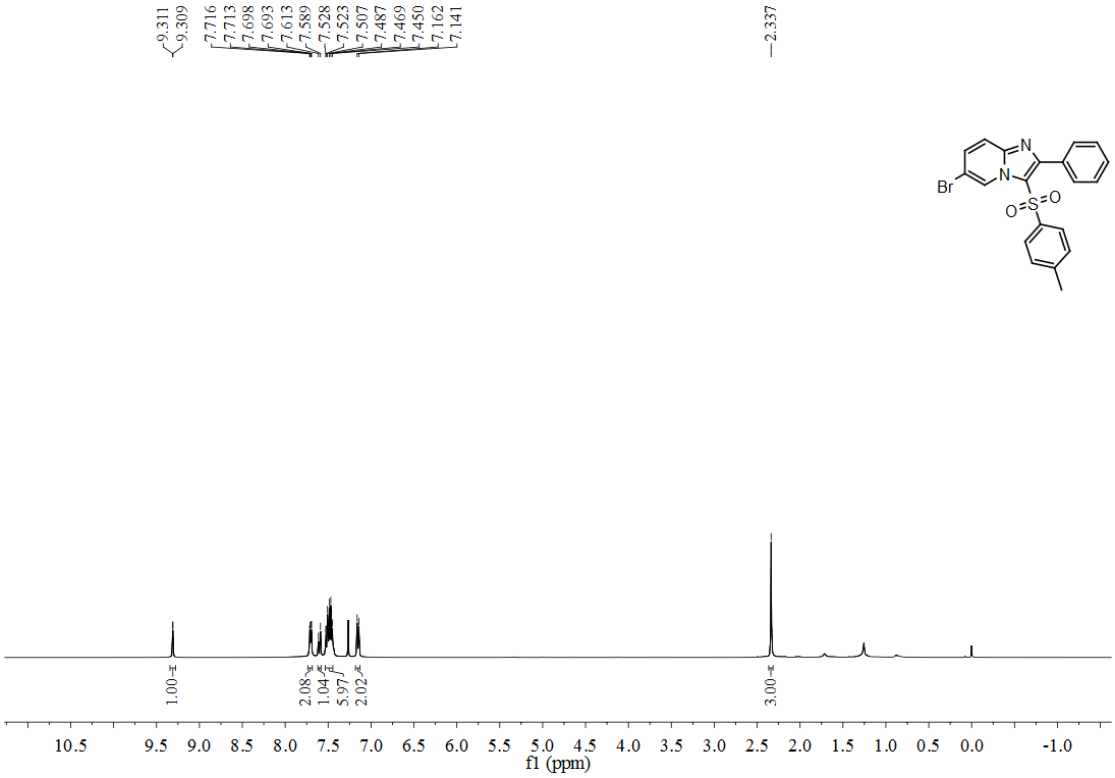
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3j



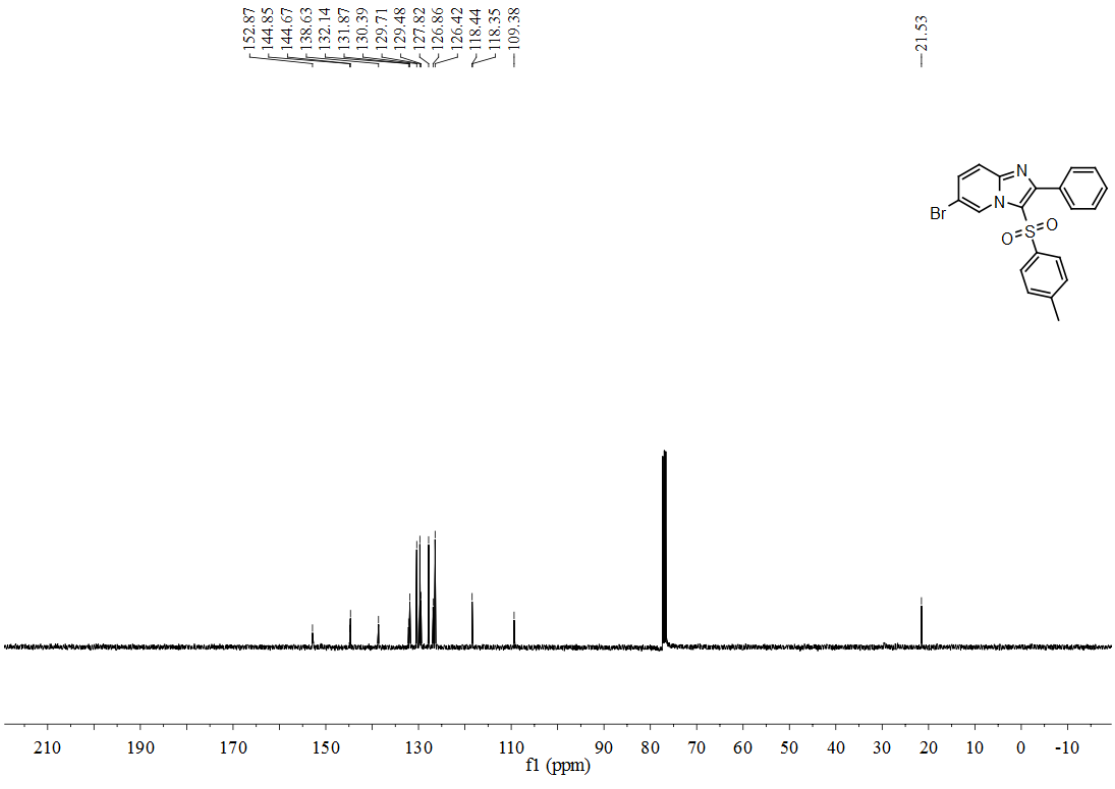
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3j



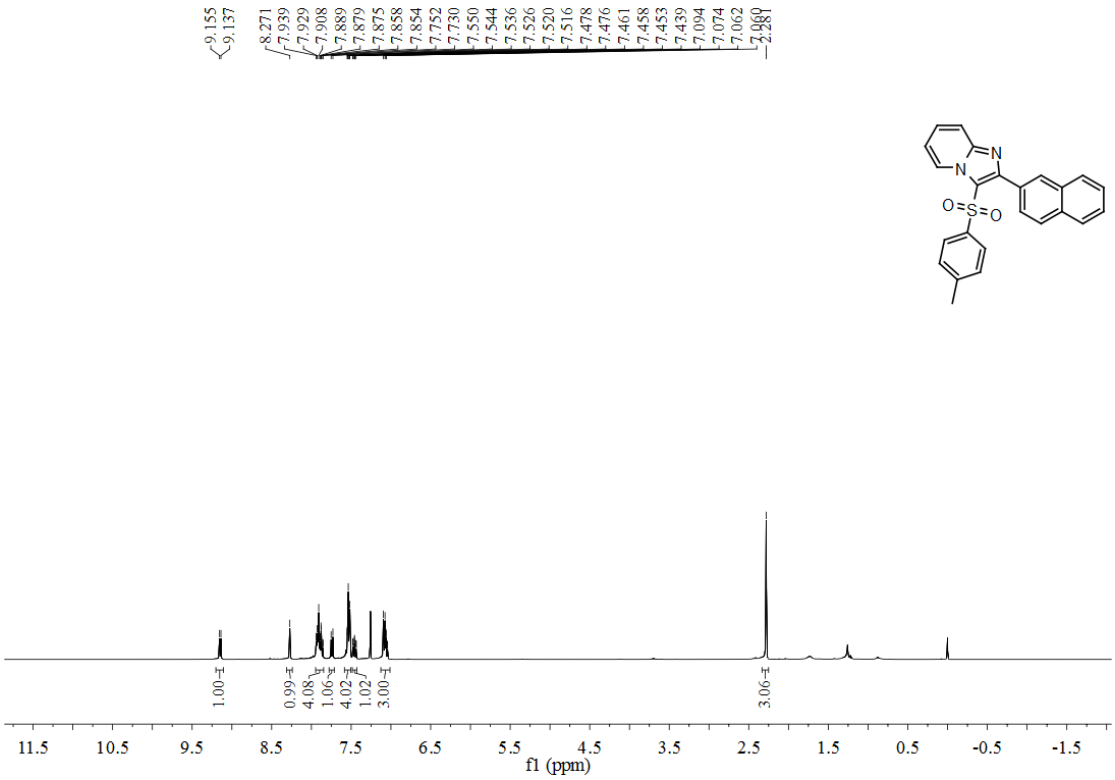
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3k



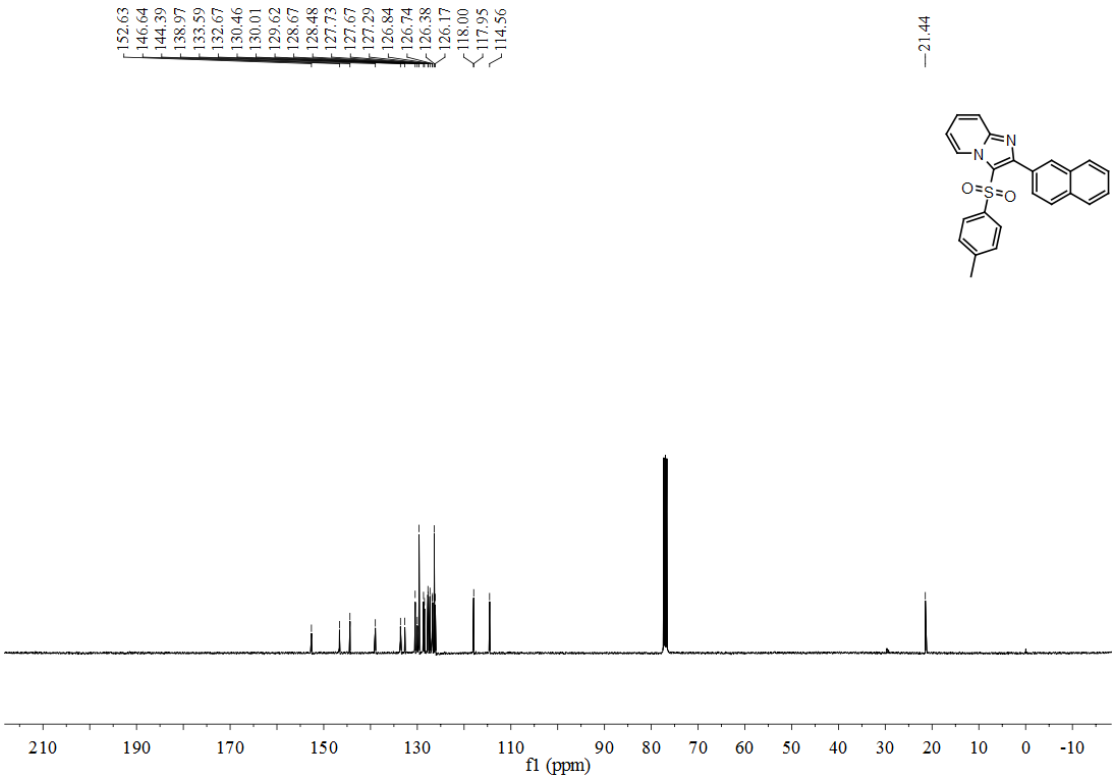
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3k



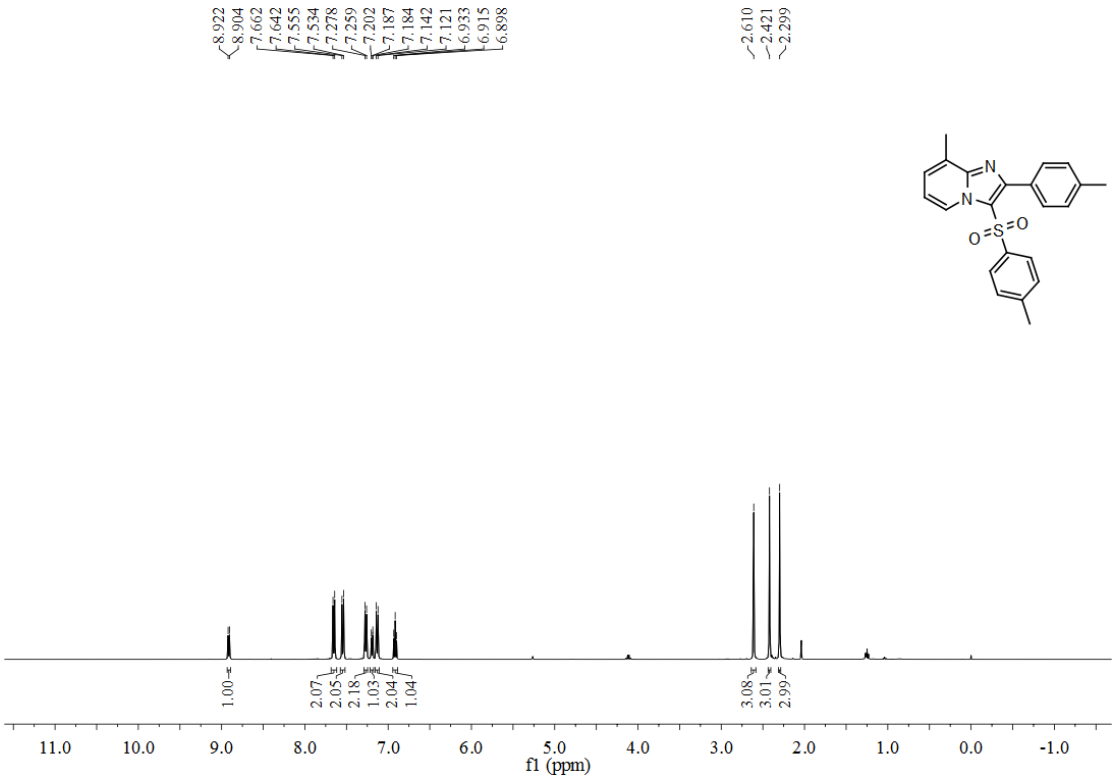
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3l



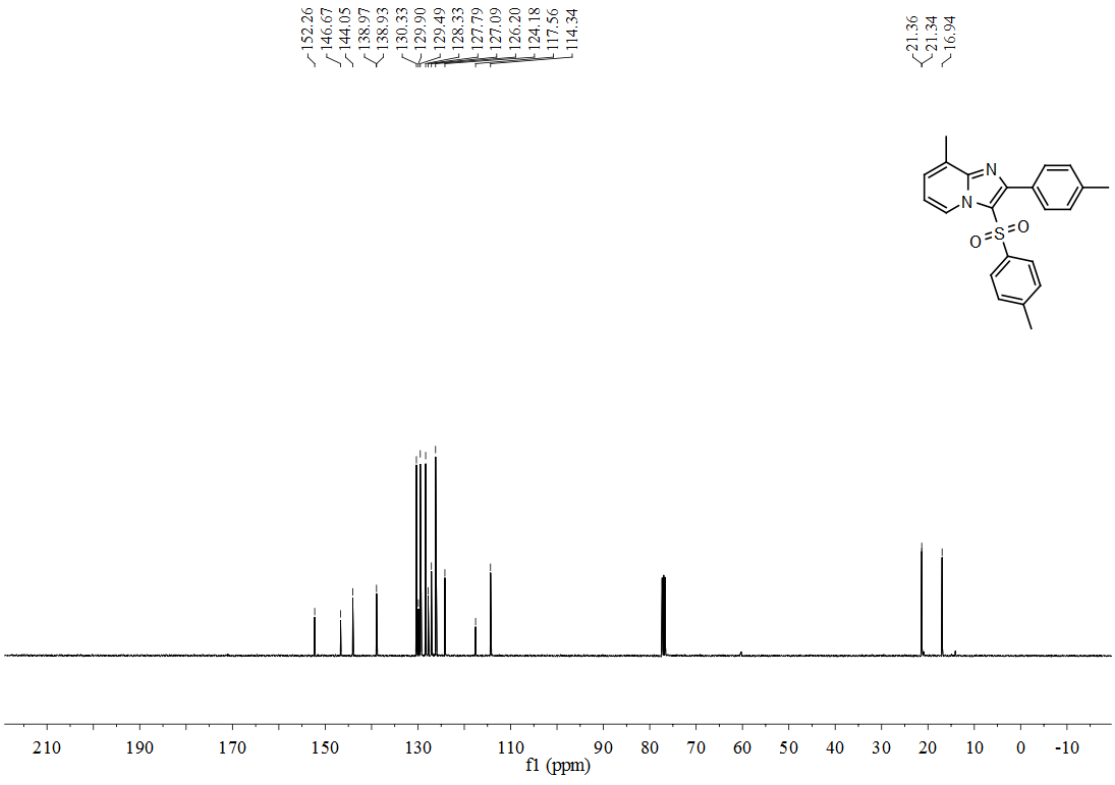
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3l



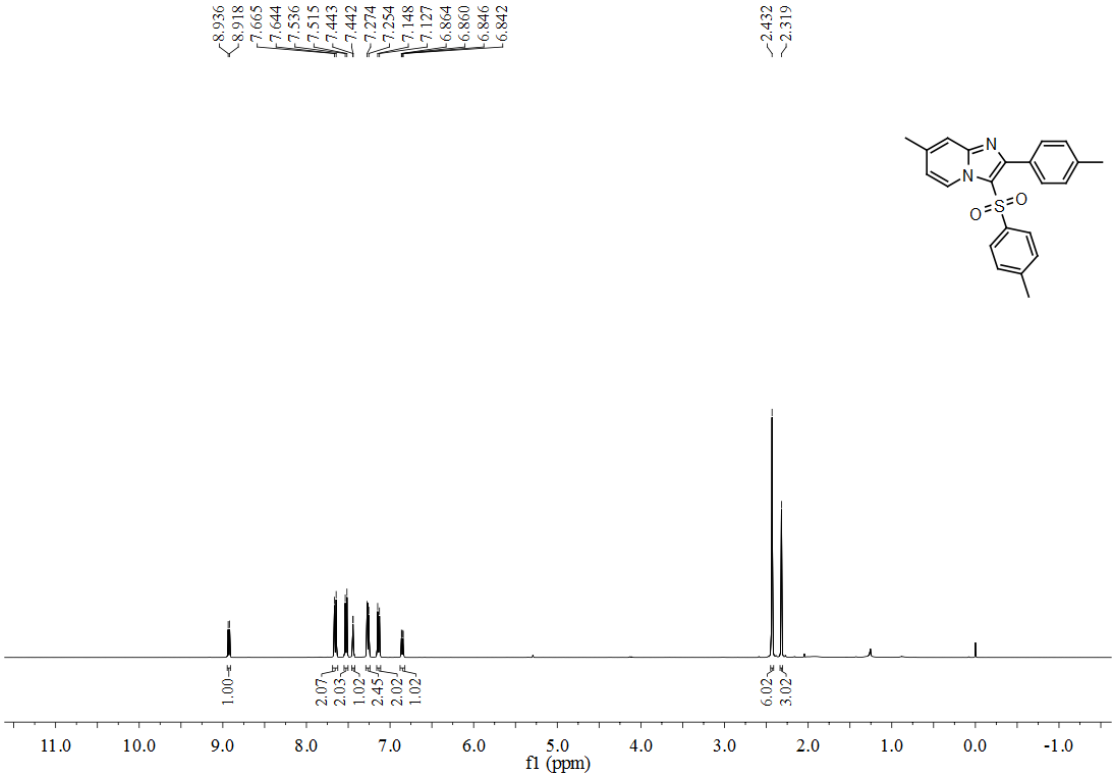
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3m



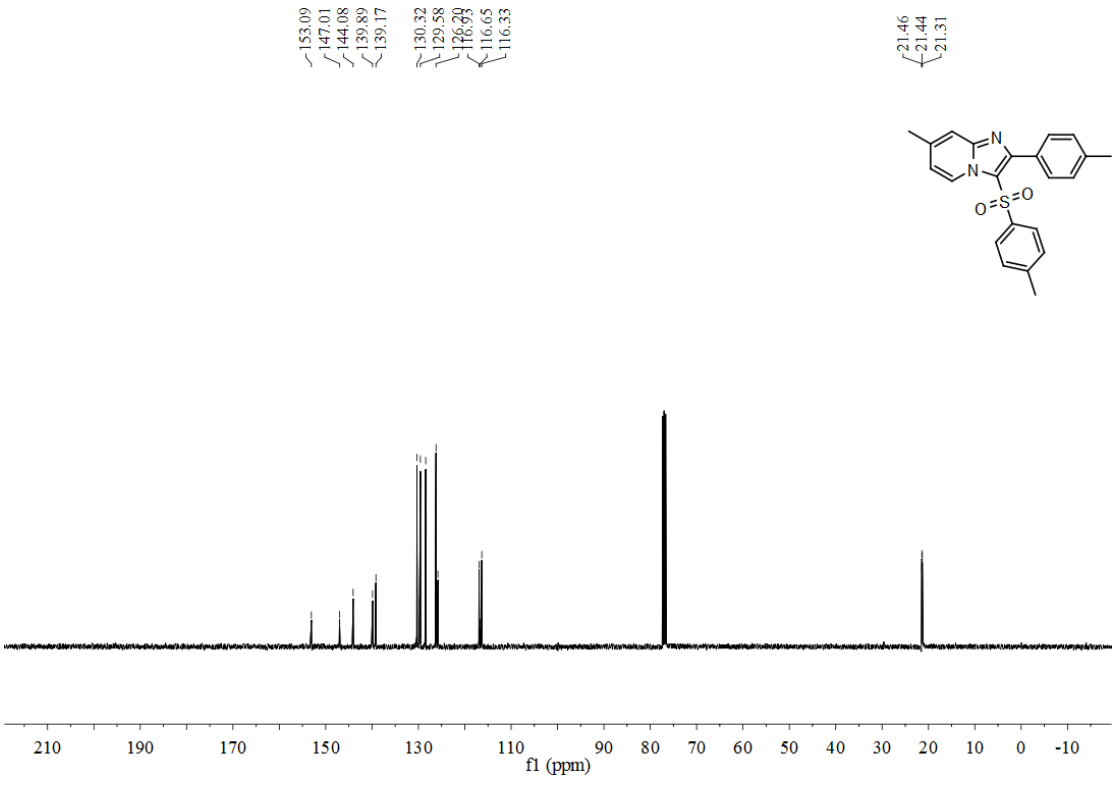
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3m



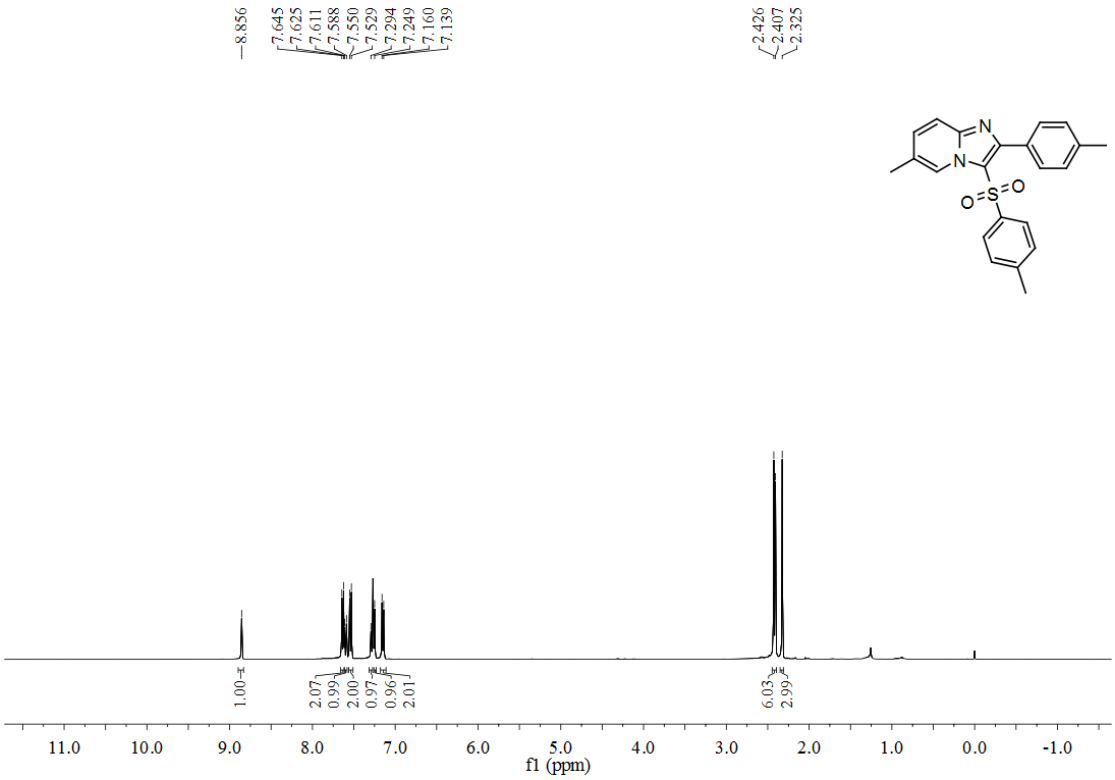
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3n



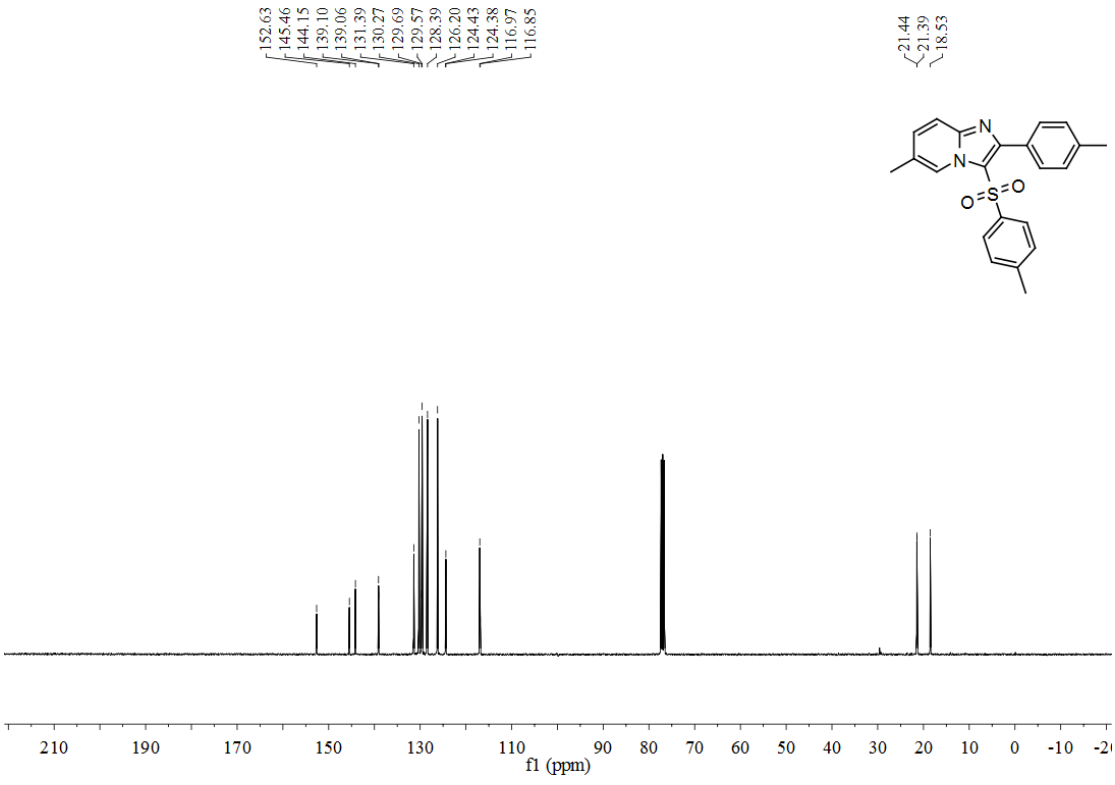
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3n



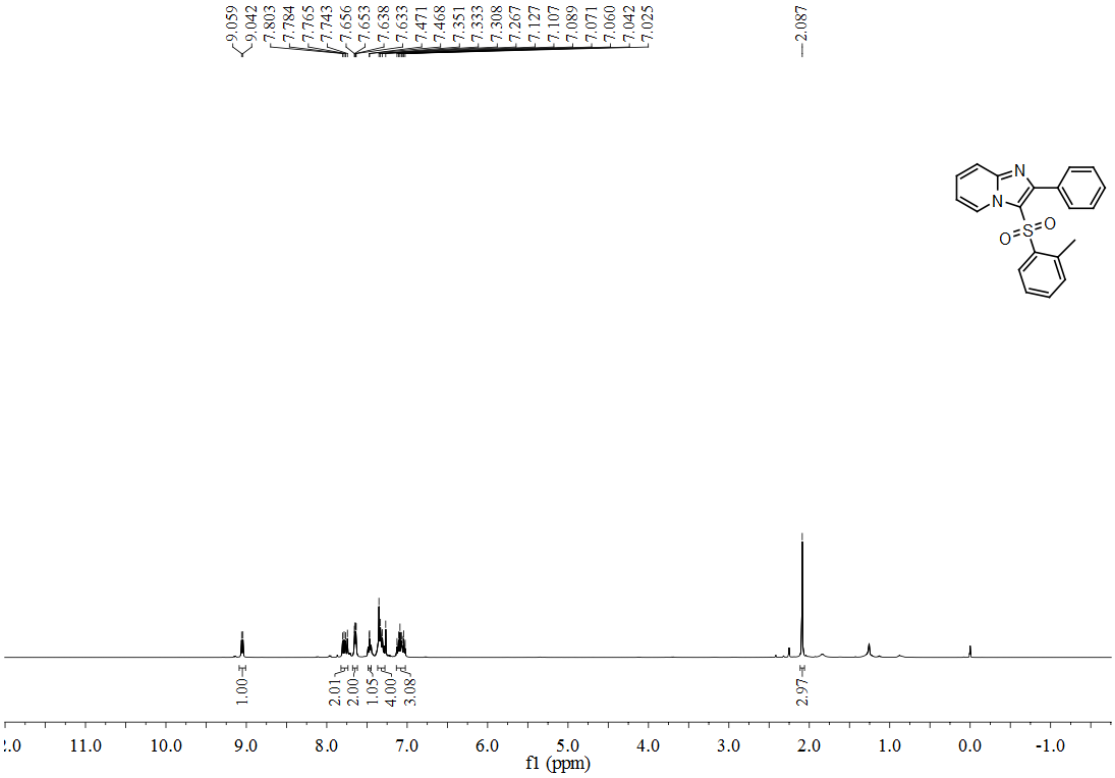
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 3o



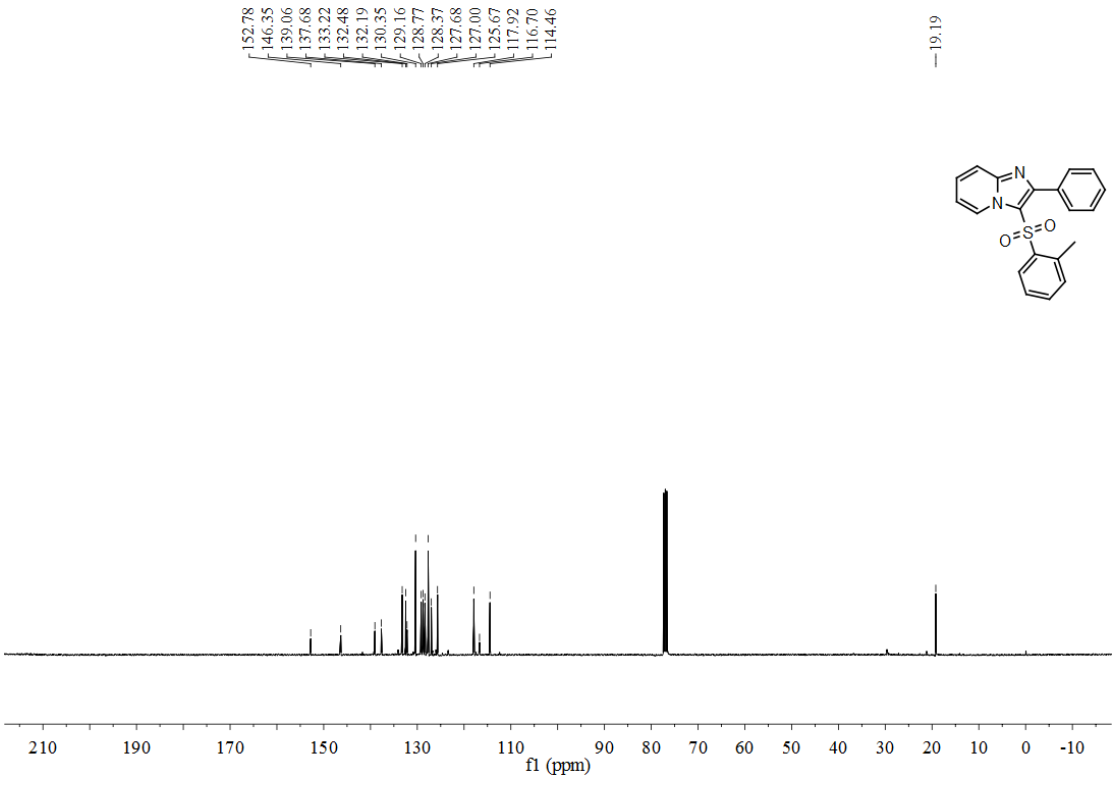
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 3o



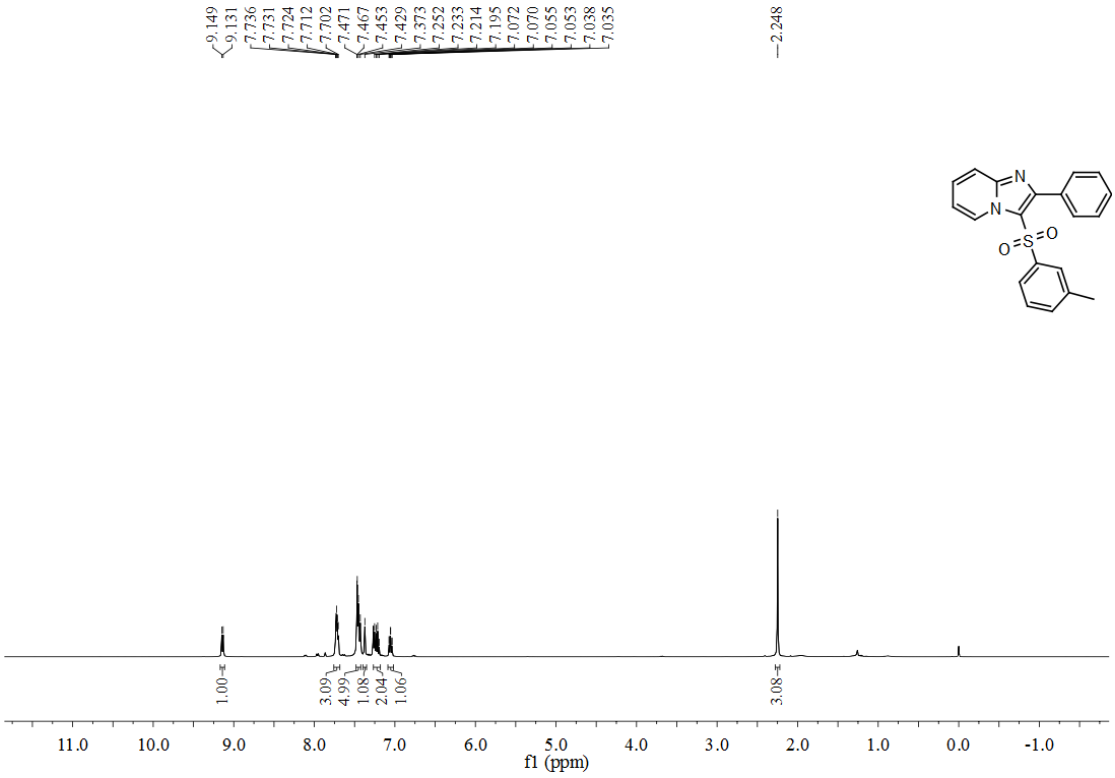
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4a



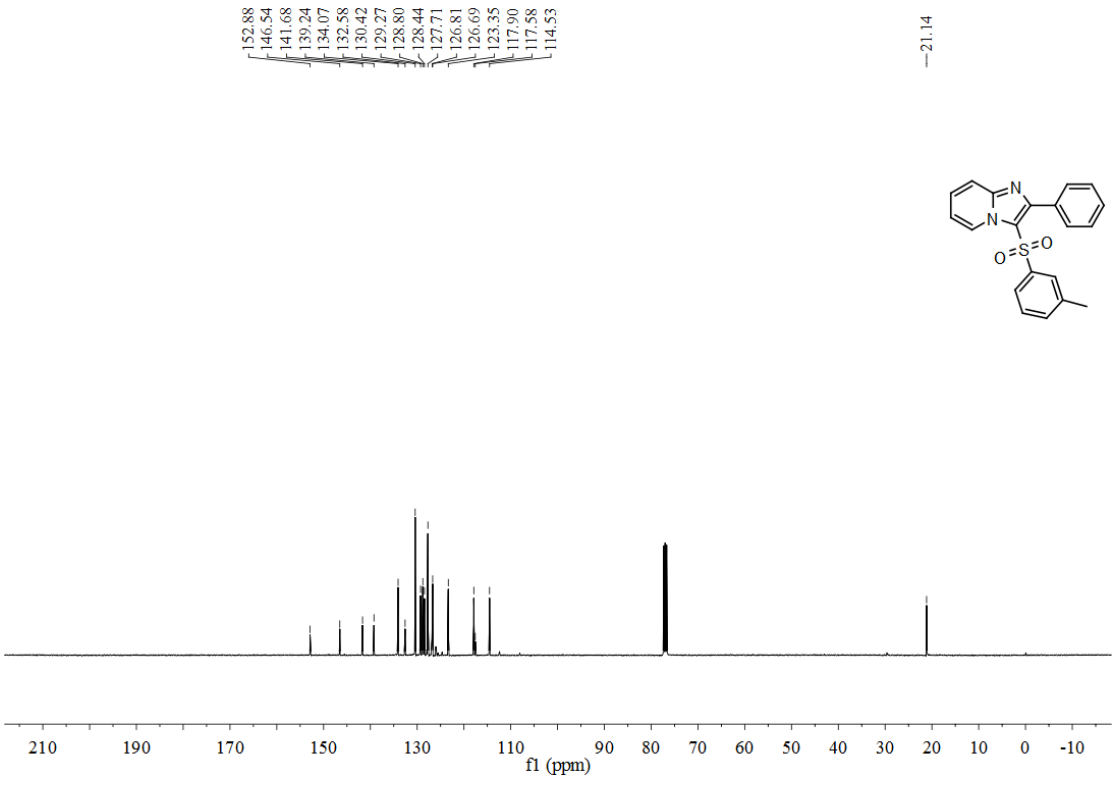
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 4a



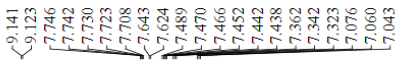
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4b

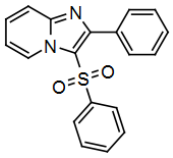


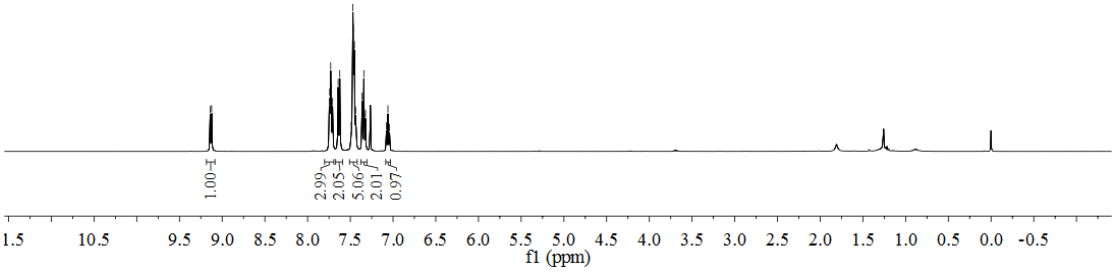
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 4b



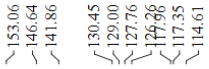
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4c

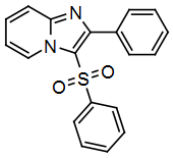


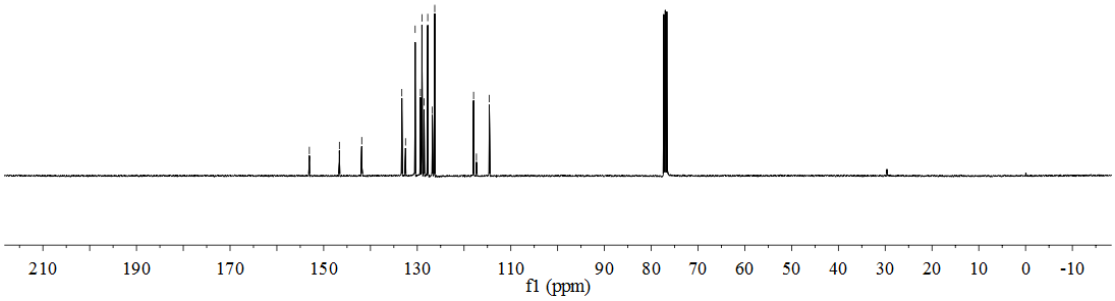




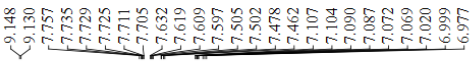
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 4c

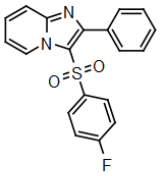


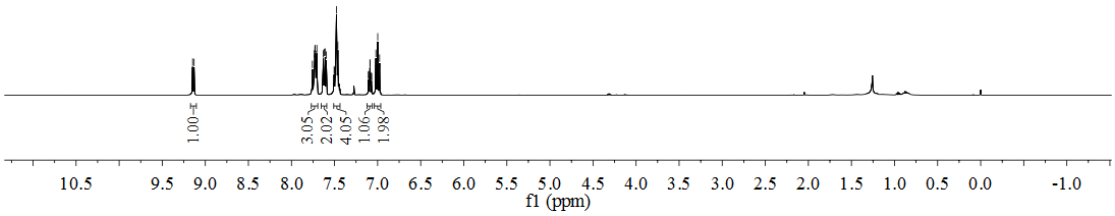




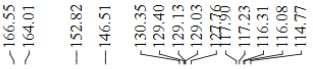
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4d

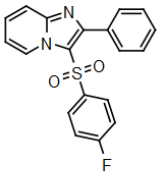


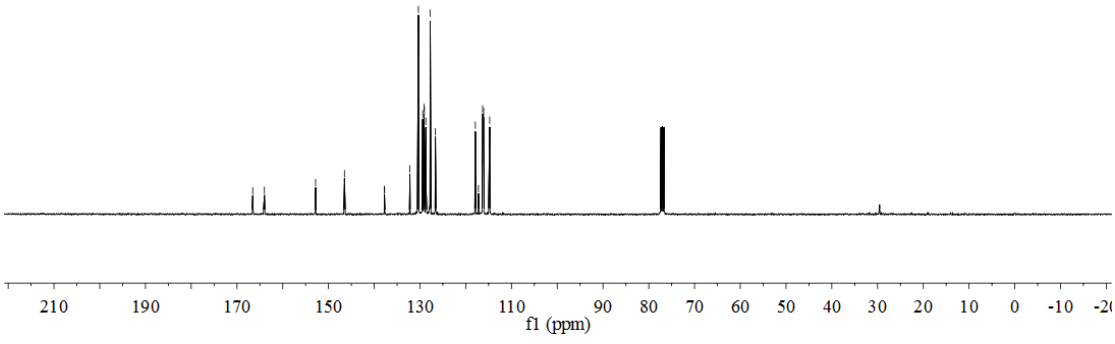




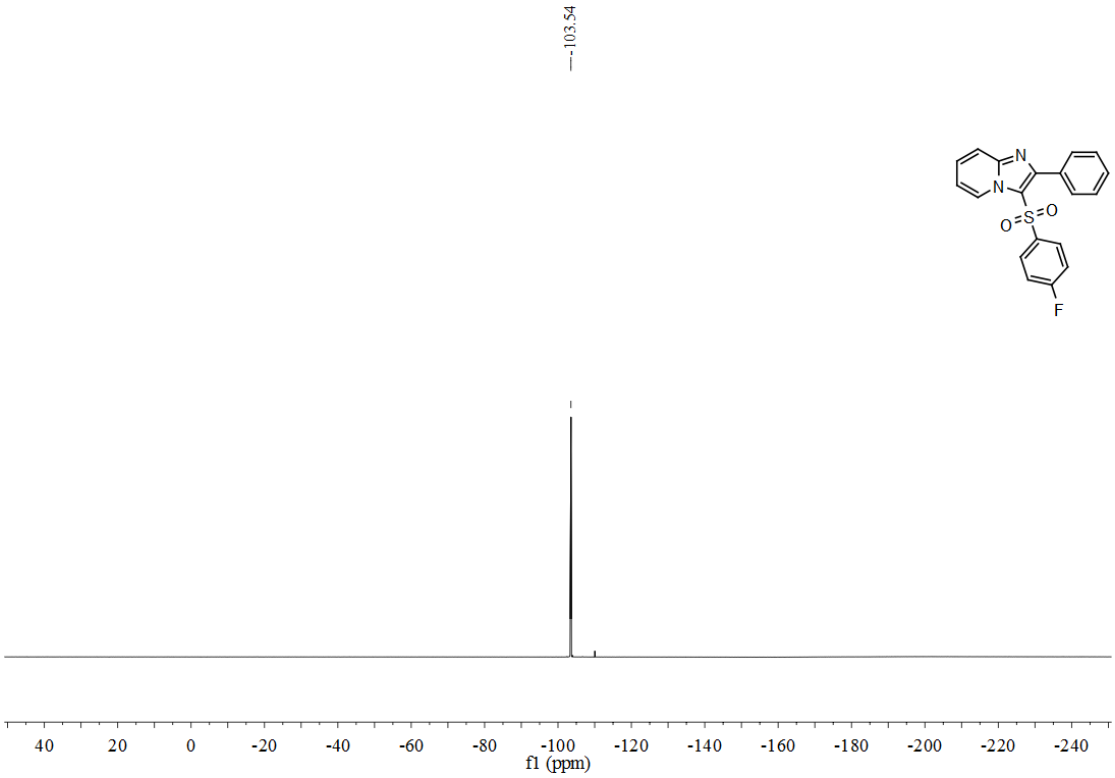
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 4d



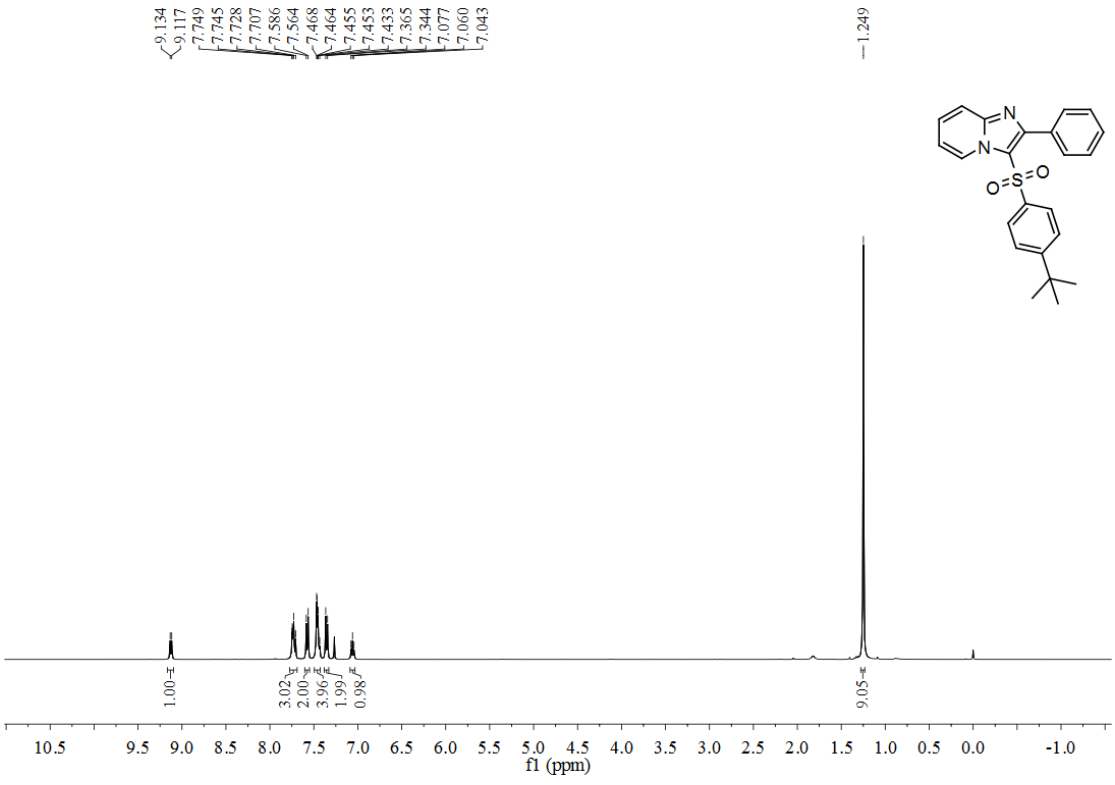




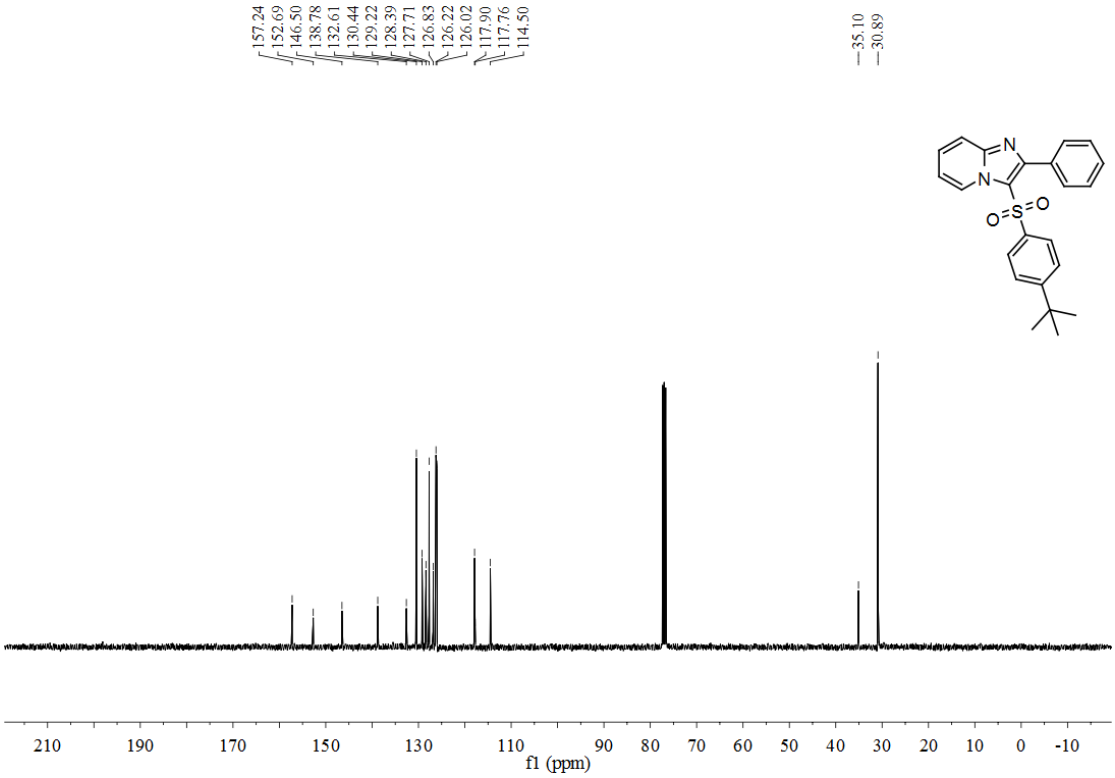
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 4d



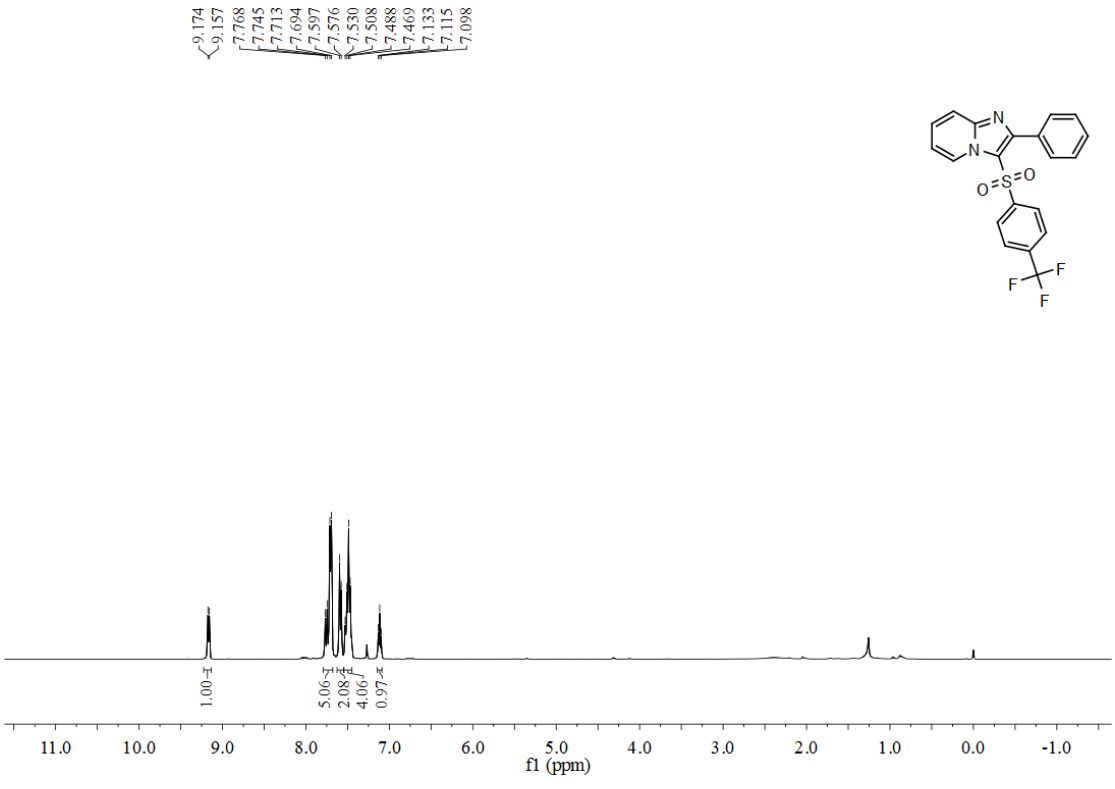
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4e



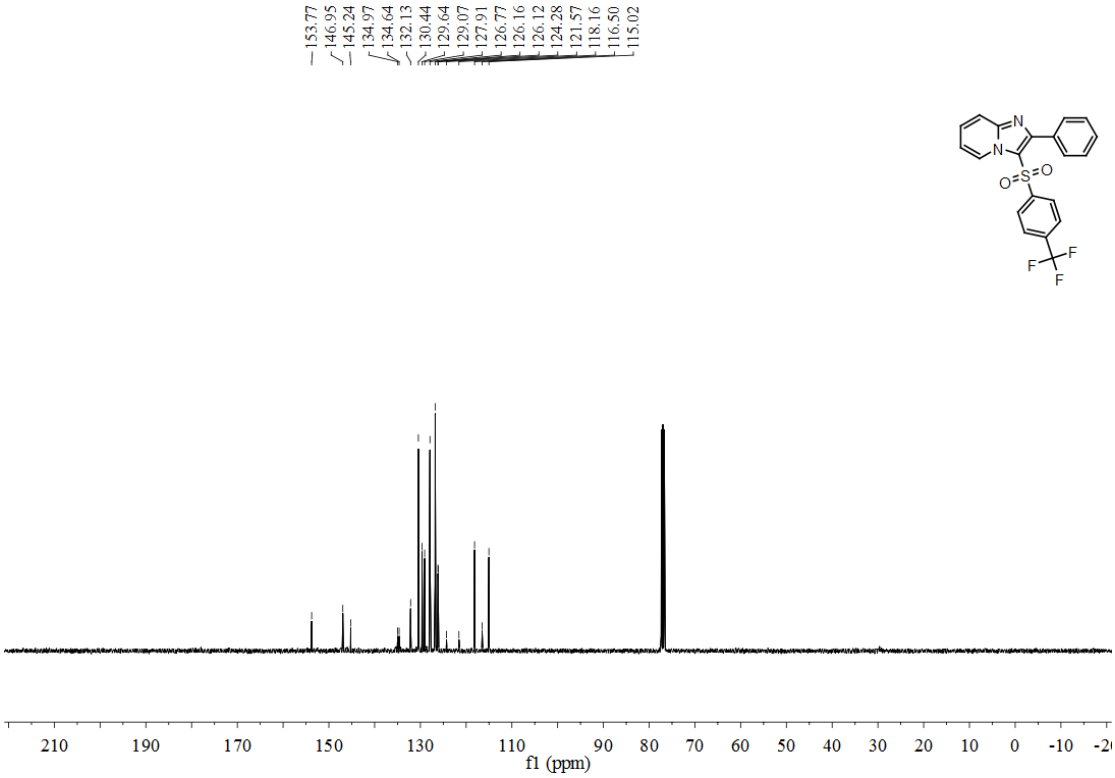
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 4e



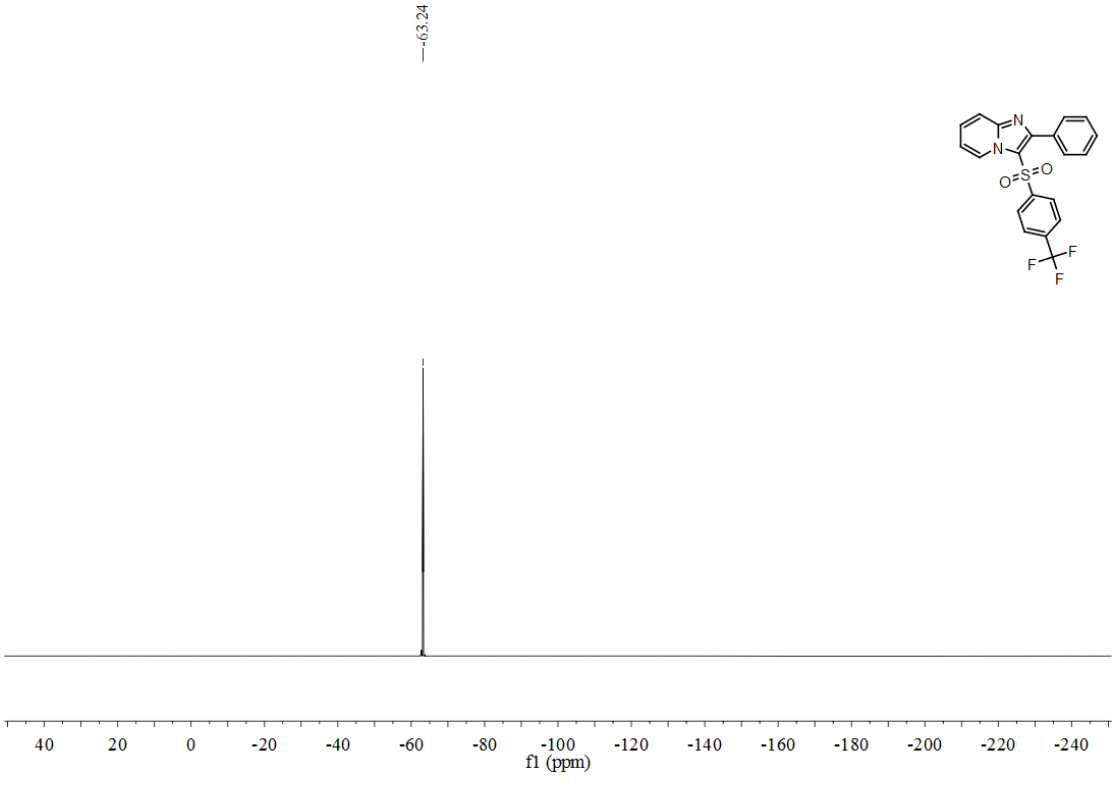
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4f



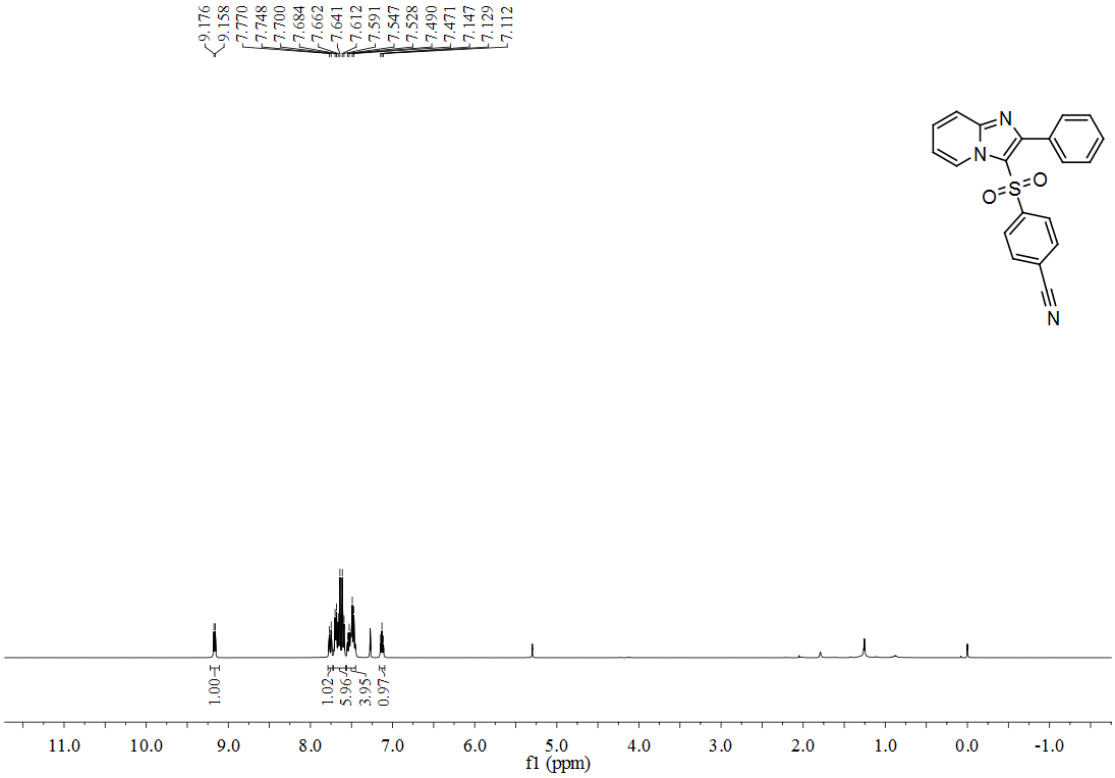
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 4f



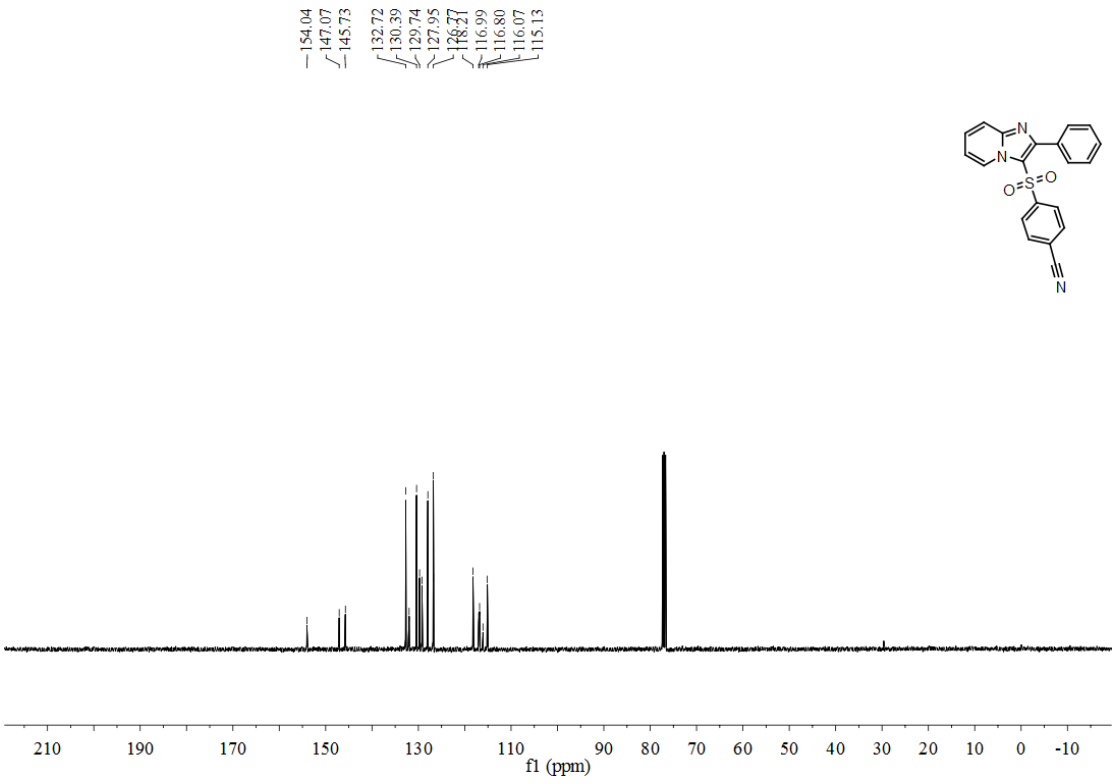
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of 4f



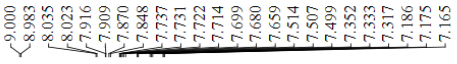
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of 4g

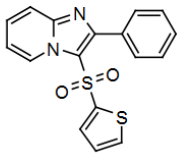


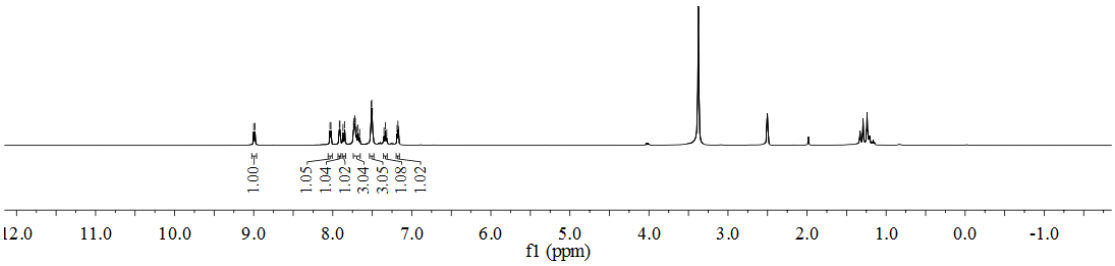
^{13}C NMR (101 MHz, $CDCl_3$) spectrum of 4g



^{1}H NMR (400 MHz, DMSO-D^{6}) spectrum of 4h







^{13}C NMR (101 MHz, DMSO-D^{6}) spectrum of 4h