Supporting Information

Electrochemical Regioselective C-3 Amination of Imidazo[1,2-a]pyridines with Electron-Deficient Sulfonimides

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1. General information

NMR spectra were recorded with tetramethylsilane (TMS) as the internal standard. ^{1}H NMR spectra were recorded at 400 MHz or 600 MHz, ^{13}C NMR spectra were recorded at 100 MHz or 150 MHz and ^{19}F NMR spectra were recorded at 564 MHz (Bruker Avance). ^{1}H NMR chemical shifts (δ) are reported in ppm relative to tetramethylsilane (TMS) with the solvent signal as the internal standard ($CDCl_3$ at 7.26 ppm, DMSO-d_6 at 2.50 ppm). ^{13}C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$ at 77.1 ppm, DMSO-d_6 at 39.5 ppm). Data are given as: s (singlet), d (doublet), t (triplet), q (quartet), dd (double of doublet) or m (multiplets), coupling constants (Hz) and integration. Flash column chromatography was carried out using silica gel eluting with ethyl acetate, petroleum ether, dichloromethane and methanol. High resolution mass spectra were obtained with the Q-TOF-Premier mass spectrometer. Reactions were monitored by TLC and visualized with ultraviolet light. Cyclic voltammetry experiments were carried out in an equipment of CHI600E. CV curves were recorded using a three-electrode scheme. The working electrode was a glassy carbon electrode, A platinum electrode served as counter electrode. Ag/AgCl (KCl sat'd) was used as the reference electrode. The working electrode was polished before recording each CV curve.

2. General procedure for the synthesis of substrates

2.1 General procedure for synthesis of 1a-1n[1-3]

2-Aminopyridine (112.86 mg, 1.2 mmol) and phenacyl bromide (197.97 mg, 1.0 mmol) were dissolved in absolute ethanol (5 mL). The reaction mixture was stirred for 2 h at room temperature. The progress of the reaction was monitored by thin-layer chromatography (TLC) using an appropriate solvent system. After the reaction was completed, the solvent was removed by vacuum distillation using a rotary evaporator. Alternatively, if a solid precipitates during the reaction, the solid is subjected to vacuum filtration, followed by washing with ethanol and vacuum drying. A solid product is obtained finally (Figure S1); yield: 70%–87%.

2.2 General procedure for synthesis of 1o-1p[1-3]

2-aminobenzothiazole (180.04 mg, 1.2 mmol) and phenacyl bromide (197.97 g, 1 mmol) were dissolved in absolute ethanol (5 mL). The reaction mixture was stirred for 6 h at 80 °C. The progress of the reaction was monitored by thin-layer chromatography (TLC) using an appropriate solvent system. After the reaction was completed, the solvent was removed by vacuum distillation using a rotary evaporator. Alternatively, if a solid precipitates during the reaction, the solid is subjected to vacuum filtration, followed by washing with ethanol and vacuum drying. A solid product is obtained finally (Figure S1); yield: 51%–59%.

2.3 General procedure for synthesis of 2a-2f[4-6]

p-phenylenediamine (1.0 g, 9.2 mmol) was first dissolved in 30 mL of anhydrous ethanol (EtOH) under stirring, followed by the sequential addition of benzenesulfonyl chloride (3.25 g, 18.4 mmol) and triethylamine (Et_3N) (3.85 mL, 27.6 mmol). The reaction mixture was stirred for 12 h at room temperature. Upon completion of the reaction, the precipitated solid was collected by vacuum filtration, washed sequentially with 1 M hydrochloric acid, ethyl acetate and diethyl ether, and finally triturated with acetone to afford an off-white solid (Figure S1); yield: 81%–87%.

2.4 General procedure for synthesis of 2g

To a stirred solution of p-phenylenediamine (1.0 g, 9.2 mmol, 1.0 equiv.) in 30 mL of EtOH was added Et_3N (3.85 mL, 27.6 mmol, 3.0 equiv.), followed by the sequential addition of benzenesulfonyl chloride (3.25 g, 18.4 mmol, 2.0 equiv.). The mixture was stirred at room temperature for 12 h, and the resulting precipitated solid was collected by vacuum filtration, washed with 1 M HCl, ethyl acetate, and diethyl ether, and then triturated with acetone to afford the mono-sulfonamide intermediate as an off-white solid. This intermediate (0.82 g, 2.82 mmol) was then dissolved in a MeOH solvent system in a 100 mL two-necked flask, to which Pd/C (10 wt%) was added. The flask was evacuated and backfilled with H_2 gas, and the mixture was stirred vigorously at room temperature. After completion (monitored by TLC), the mixture was filtered through celite, and the filtrate was concentrated and dried in vacuo to yield the corresponding amino-intermediate (0.52 g). Finally, this amino-intermediate (1.1 g, 1.0 equiv.) was dissolved in 25 mL of pyridine and reacted with 4-(trifluoromethyl)benzenesulfonyl chloride (1.84 g, 1.2 equiv.) under stirring overnight. The reaction mixture was concentrated and transferred into water, and the resulting precipitate was filtered and dried to afford the target compound 2g (59 %) as a white solid.

2.5 General procedure for synthesis of 2h

To an oven-dried round-bottom flask (100 mL) containing a magnetic stir bar, aniline (465.7 mg, 5.0 mmol, 1.0 equiv.) was dissolved in anhydrous DCM (6 mL). Pyridine (791.0 mg, 10.0 mmol, 2.0 equiv.) and TsCl (1.91 g, 10.0 mmol, 2.0 equiv.) were added sequentially at 0 °C. The reaction mixture was allowed to warm to room temperature and stirred for 2 h. Upon completion, the mixture was quenched with saturated aqueous NH_4Cl (15 mL) and extracted with DCM (10 mL). The combined organic layers were washed with water and brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1, v/v) to afford the desired product **2h** (1.24 g, quantitative yield) as a white solid.

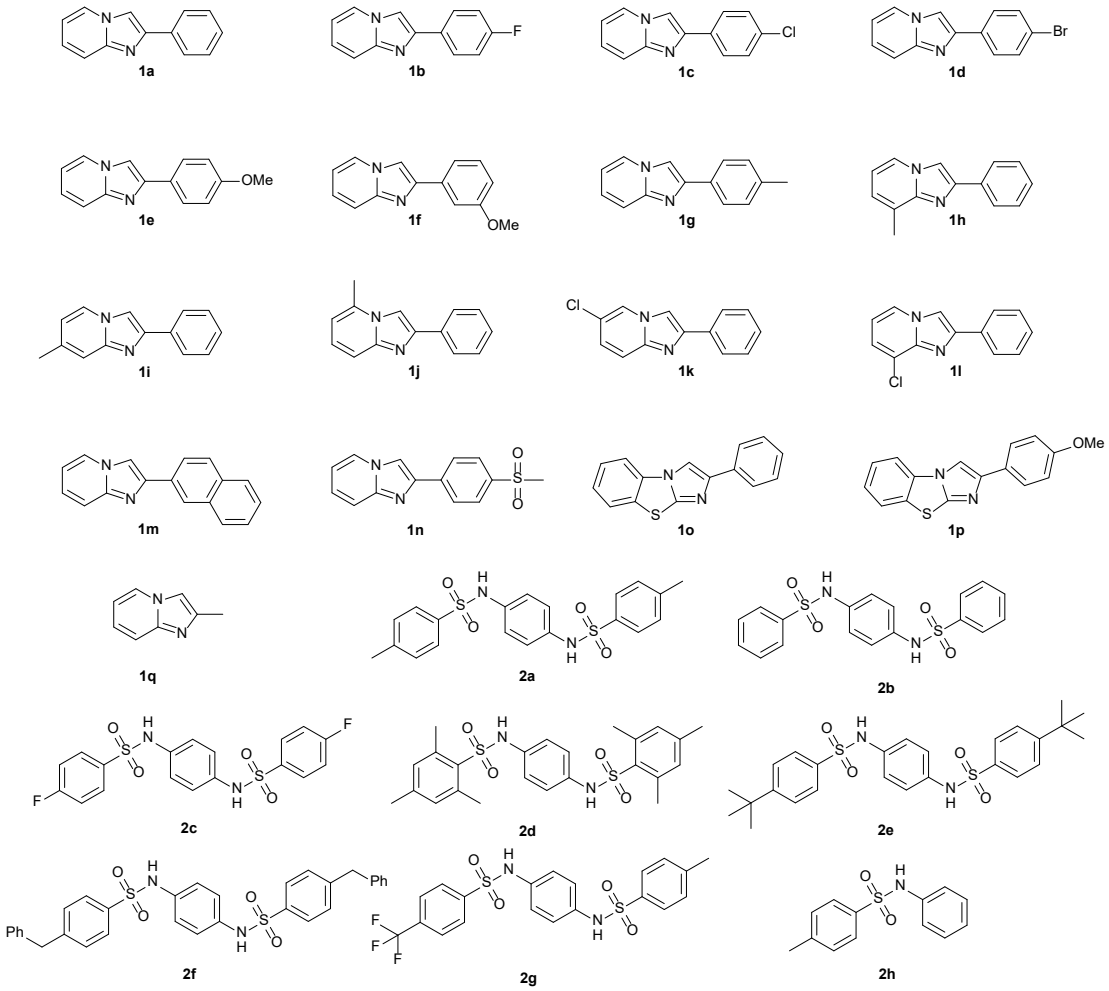
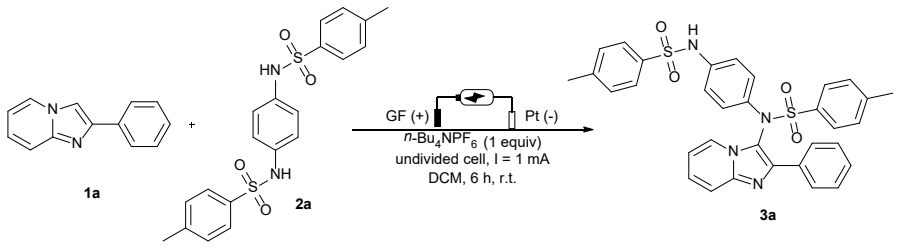


Figure S1. The scope of substrates

3. Optimization of the reaction conditions

Table S1. Optimization of the reaction conditions.*[a]*



Entry	Variation from standard conditions	Yield
1	none	56
2	MeOH instead of DCM	34
3	EtOH instead of DCM	31
4	$CHCl_3$ instead of DCM	54
5	Acetone instead of DCM	26
6	Toluene instead of DCM	42
7	DCE instead of DCM	61

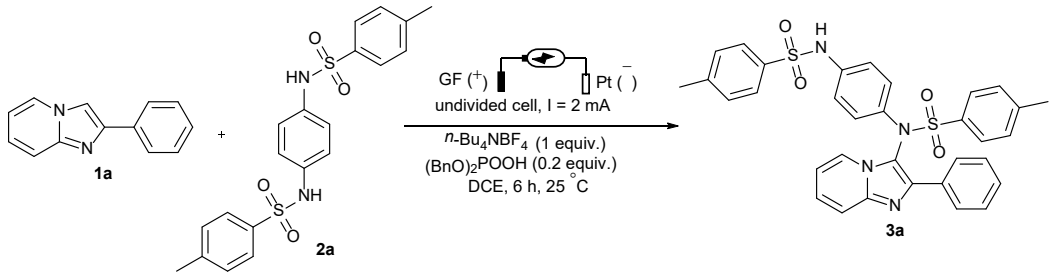
8	0 °C instead of 25 °C	41
9	35 °C instead of 25 °C	45
10	KPF_6 instead of *n*-Bu_4NPF_6	54
11	$LiClO_4$ instead of *n*-Bu_4NPF_6	41
12	*n*-Bu_4NBF_4 instead of *n*-Bu_4NPF_6	62
13	Pt anode	n.d.
14	Graphite felt cathode	n.d.
15	Ni plate cathode	18
16	2 mA, 3 mA	61, 40
17	DCE, *n*-Bu_4NBF_4, 2 mA	65
18[b]	DCE, *n*-Bu_4NBF_4, 2 mA	9
19[c]	DCE, *n*-Bu_4NBF_4, 2 mA	68
20[d]	DCE, *n*-Bu_4NBF_4, 2 mA	31
21[e]	DCE, *n*-Bu_4NBF_4, 2 mA	75
22[f]	DCE, *n*-Bu_4NBF_4, 2 mA	73
23	no electric current	0

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.24 mmol), DCM (6 mL), with 1 equiv. *n*-Bu_4NPF_6 as electrolyte, constant current = 1 mA, undivided cell, GF anode (1.5 cm × 1.0 cm ×0.6 cm) and Pt cathode (1.5 cm × 1.0 cm × 0.6 cm), 25 °C, 6 h. [b] DBU (0.2 equiv.) as an additive. [c] TsOH (0.2 equiv.) as additive. [d] H_3PO_4 (0.2 equiv.) as an additive. [e] $(BnO)_2POOH$ (0.2 equiv.) as an additive. [f] $(BnO)_2POOH$ (0.2 equiv.) as an additive, *n*-Bu_4NBF_4 (0.5 equiv.)

It is demonstrated that 2-phenylimidazo[1,2-a]pyridine **1a** and *N,N′*-1,4-phenylenebis[4-methylbenzenesulfonamide] **2a** were designated as model substrates to optimize the reaction parameters for the C-N cross-coupling reaction. In an undivided electrolysis cell equipped with a carbon rod anode and a platinum plate cathode, the electrolysis was performed under ambient pressure with *n*-Bu_4NFP_6 serving as the electrolyte. The reaction was conducted in a dichloromethane (DCM) medium at a constant current of 1 mA, affording the target product **3a** in 56% isolated yield (Table S1, entry 1). To further optimize this reaction, various reaction conditions were investigated. When solvents such as MeOH, EtOH, $CHCl_3$ and acetone were used to replace DCM, the reaction yield decreased with all these solvents, except that the yield of the target product **3a** was improved when DCE was used as the solvent (Table S1, entries 2-7). Subsequent experiments demonstrated that adjusting the reaction temperature to either 0 °C or 35 °C failed to effectively improve the product yield (Table S1, entries 8-9). As shown in entries 10–12, the yield of the target product increased to 62% when *n*-Bu_4NBF_4 was used as the electrolyte. Meanwhile, the reaction could not proceed smoothly when platinum plates or graphite felt were employed as both the cathode and anode (Table S1, entries 13-15). Furthermore, investigations into the effect of constant current on the reaction in this study revealed that increasing the constant current to 2 mA enhanced the reaction yield to 61%, whereas a further increase in current to 3 mA led to a subsequent decrease in the product yield (Table S1, entries 16).

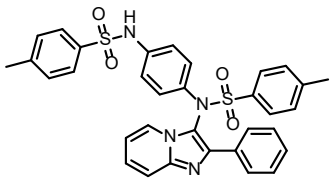
This study also investigated the effects of different additives on the reaction. It was found that in an undivided electrolysis cell with a carbon rod as the anode and a platinum plate as the cathode, under atmospheric pressure, using *n*-Bu_4BF_4 as the electrolyte and conducting the reaction in DCE solution at a constant current of 2 mA, the yield of the target product reached 65%. When DBU (0.2 equiv.) or H_3PO_4 (0.2 equiv.) was used as the additive, the product yield decreased to some extent. In contrast, when TsOH (0.2 equiv.) or $(BnO)_2POOH$ (0.2 equiv.) was employed as the additive, the product yield was improved. Specifically, the highest reaction yield of 75% was achieved when $(BnO)_2POOH$ (0.2 equiv.) was added, and a yield of 73% could still be obtained even when the dosage of the electrolyte n-Bu_4NBF_4 was reduced to 0.5 equivalent (Table S1, entries 17-22). Subsequent control experiments demonstrated that in the absence of an applied electrolysis current, the intended transformation failed to occur entirely under the established reaction parameters (Table S1, entry 23).

4. General procedure for the synthesis of products



Prepare a dry and clean Schlenk tube fitted with a rubber stopper equipped with a carbon rod anode and a platinum plate cathode. Add 2-phenylimidazo[1,2-a]pyridine **1a** (0.2 mmol, 1.0 equiv.), *N,N′*-1,4-phenylenebis[4-methylbenzenesulfonamide] **2a** (0.24 mmol, 1.2 equiv.), *n*-Bu_4NBF_4 (0.2 mmol, 1.0 equiv.), $(BnO)_2POOH$ (0.04 mmol, 0.2 equiv.) and DCE (5 mL) to the Schlenk tube containing a stir bar. Stir the mixture at 25 °C under a constant current of 2 mA for 6 hours. After the reaction is complete, concentrate the reaction solution. Purify the residue by silica gel column chromatography (petroleum ether/EtOAc = 2:1 to 1:1) to obtain the target product **3a**.

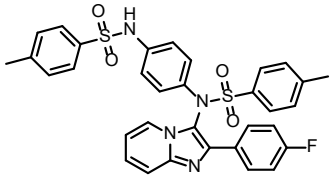
Data of products



4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)-N-(2-phenylimidazo[1,2-a]pyridin-3-yl)benzenesulfonamide (3a)

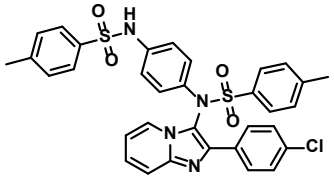
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (38.4 mg, 75% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 8.20 (d, J = 6.4 Hz, 1H), 7.67 (d, J = 9.2 Hz, 1H), 7.63 – 7.58 (m,

2H), 7.57 – 7.49 (m, 4H), 7.42 (t, J = 7.2 Hz, 1H), 7.29 – 7.23 (m, 3H), 7.22 – 7.12 (m, 6H), 7.09 – 7.01 (m, 3H), 2.28 (d, J = 6.0 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.4, 143.7, 143.3, 141.5, 137.2, 136.9, 136.7, 135.7, 132.7, 130.3, 130.1, 128.6, 128.0, 127.3, 127.2, 127.1, 124.1, 123.7, 121.3, 117.9, 117.1, 113.9, 21.5, 21.4. **HRMS (ESI):** calculated for $C_{33}H_{29}N_4O_4S_2^+$ $[M+H]^+$: 609.1625, found: 609.1626.



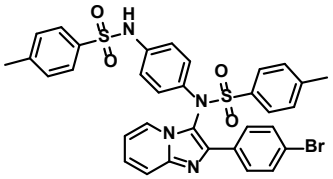
N-(2-(4-fluorophenyl)imidazo[1,2-a]pyridin-3-yl)-4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3b)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (31.5 mg, 72% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.30 (s, 1H), 8.19 (d, J = 7.2 Hz, 1H), 7.66 (d, J = 9.2 Hz, 1H), 7.61 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.0 Hz, 4H), 7.46 – 7.40 (m, 1H), 7.28 (d, J = 8.0 Hz, 2H), 7.20 (d, J = 8.4 Hz, 2H), 7.17 – 7.10 (m, 2H), 7.09 – 6.97 (m, 5H), 2.30 (d, J = 4.8 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 162.5 (d, $J_{C\text{-}F}$ = 244.3 Hz), 145.4, 143.7, 143.5, 140.6, 137.2, 136.8, 136.7, 135.6, 134.5, 130.2 (d, $J_{C\text{-}F}$ = 21.4 Hz), 129.3 (d, $J_{C\text{-}F}$ = 8.3 Hz), 128.0, 127.4, 127.1, 124.2, 123.6, 122.0, 121.3, 117.8, 116.9, 115.5 (d, $J_{C\text{-}F}$ = 21.5 Hz), 114.0, 21.4, 21.4. **^{19}F NMR** (564 MHz, DMSO-d_6) δ -113.4. **HRMS (ESI):** calculated for $C_{33}H_{28}FN_4O_4S_2^+$ $[M+H]^+$: 627.1531, found: 627.1530.



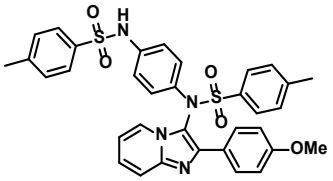
N-(2-(4-chlorophenyl)imidazo[1,2-a]pyridin-3-yl)-4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3c)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (36.5 mg, 75% yield), **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.34 (s, 1H), 8.23 (d, J = 6.6 Hz, 1H), 7.67 (d, J = 9.0 Hz, 1H), 7.61 (d, J = 7.8 Hz, 2H), 7.51 (d, J = 5.6 Hz, 2H), 7.48 – 7.41 (m, 3H), 7.28 (d, J = 7.8 Hz, 2H), 7.22 (d, J = 9.0 Hz, 2H), 7.19-7.16 (m, 4H), 7.10 – 7.04 (m, 3H), 2.30 (d, J = 10.2 Hz, 6H). **^{13}C NMR** (150 MHz, DMSO-d_6) δ 145.5, 143.8, 143.5, 140.2, 137.1, 136.4, 135.6, 133.3, 131.5, 130.3, 130.2, 128.8, 128.6, 128.0, 127.6, 127.1, 124.3, 123.5, 121.3, 117.9, 117.2, 114.1, 21.5, 21.4. **HRMS (ESI):** calculated for $C_{33}H_{28}ClN_4O_4S_2^+$ $[M+H]^+$: 643.1235, found: 643.1238.



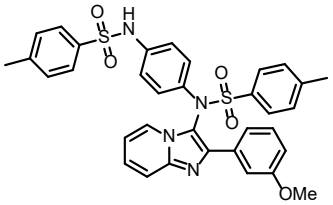
N-(2-(4-bromophenyl)imidazo[1,2-a]pyridin-3-yl)-4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3d)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (32.4 mg, 71% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.15 (s, 1H), 8.24 (d, J = 6.8 Hz, 1H), 7.68-7.61 (m, 3H), 7.50 (d, J = 8.4 Hz, 2H), 7.46 – 7.39 (m, 3H), 7.35 (d, J = 8.8 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 7.17 (dd, J = 8.4, 1.6 Hz, 4H), 7.10 – 7.03 (m, 3H), 2.29 (d, J = 12.8 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.4, 143.5, 143.5, 140.2, 137.5, 137.3, 136.6, 135.6, 131.9, 131.5, 130.3, 130.1, 129.1, 128.0, 127.5, 127.1, 124.3, 123.6, 122.0, 121.3, 117.9, 117.3, 114.1, 21.5, 21.4. **HRMS (ESI):** calculated for $C_{33}H_{28}BrN_4O_4S_2^+$ $[M+H]^+$: 687.0730, found: 687.0728.



N-(2-(4-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)-4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3e)

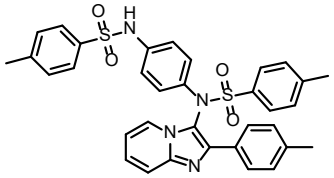
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (33.1 mg, 70% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.38 (s, 1H), 8.15 (d, J = 6.8 Hz, 1H), 7.67 – 7.58 (m, 3H), 7.55 – 7.46 (m, 4H), 7.41 (t, J = 8.8 Hz, 1H), 7.29 (d, J = 8.0 Hz, 2H), 7.21 (d, J = 8.4 Hz, 2H), 7.14 (dd, J = 8.8, 2.0 Hz, 2H), 7.08 – 6.98 (m, 3H), 6.76 (d, J = 8.8 Hz, 2H), 3.76 (s, 3H), 2.31 (d, J = 7.6 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 159.8, 145.3, 143.6, 143.3, 141.4, 137.4, 136.8, 136.8, 135.9, 130.3, 130.1, 128.7, 128.0, 127.1, 127.0, 125.2, 124.0, 123.6, 121.3, 117.6, 116.3, 114.1, 113.7, 55.6, 21.4, 21.4. **HRMS (ESI):** calculated for $C_{34}H_{31}N_4O_5S_2^+$ $[M+H]^+$: 639.1730, found: 639.1733.



N-(2-(3-methoxyphenyl)imidazo[1,2-a]pyridin-3-yl)-4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3f)

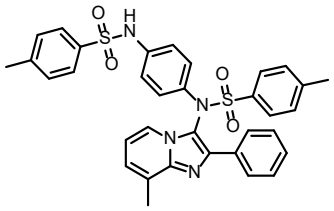
The desired product was purified by silica gel chromatography (petroleum

ether/EtOAc= 2:1) as white solid (42.2 mg, 68% yield). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 8.18 (d, J = 6.4 Hz, 1H), 7.69 (d, J = 8.8 Hz, 1H), 7.61 (d, J = 8.4 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.46 – 7.42 (m, 1H), 7.28 (d, J = 8.0 Hz, 2H), 7.20 – 7.10 (m, 6H), 7.07 – 7.04 (m, 3H), 7.00 (dd, J = 2.4, 1.6 Hz, 1H), 6.84 – 6.81 (m, 1H), 3.52 (s, 3H), 2.30 (d, J = 2.4 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 159.5, 145.3, 143.7, 143.3, 141.2, 137.2, 137.0, 136.4, 135.7, 134.0, 130.4, 130.1, 129.7, 128.0, 127.3, 127.1, 124.1, 123.0, 121.4, 119.8, 117.9, 117.1, 114.8, 114.0, 112.2, 55.3, 21.5, 21.4. **HRMS (ESI)**: calculated for $C_{34}H_{31}N_4O_5S_2^+$ $[M+H]^+$: 639.1730, found: 639.1734.



4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)-N-(2-(p-tolyl)imidazo[1,2-a]pyridin-3-yl)benzenesulfonamide (3g)

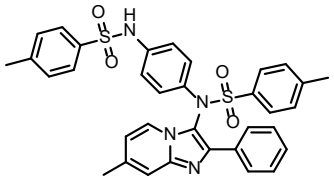
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (45.3 mg, 71% yield). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 8.19 (d, J = 6.8 Hz, 1H), 7.64 (t, J = 10.4 Hz, 3H), 7.53 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 8.0 Hz, 2H), 7.42 – 7.37 (m, 1H), 7.27 (d, J = 8.0 Hz, 2H), 7.18 (dd, J = 8.8, 2.8 Hz, 4H), 7.08 (d, J = 9.2 Hz, 2H), 7.01 (dd, J = 15.2, 6.8 Hz, 3H), 2.28 (d, J = 10.4 Hz, 9H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.3, 143.8, 143.3, 141.6, 138.1, 137.1, 137.1, 136.4, 135.9, 130.3, 130.1, 129.9, 129.2, 128.0, 127.3, 127.1, 124.0, 123.7, 121.3, 117.8, 116.8, 113.8, 21.5, 21.4, 21.2. **HRMS (ESI)**: calculated for $C_{34}H_{31}N_4O_4S_2^+$ $[M+H]^+$: 623.1781, found: 623.1779.



4-methyl-N-(8-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3h)

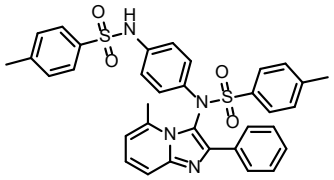
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (37.5 mg, 65% yield). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.33 (s, 1H), 8.02 (d, J = 6.8 Hz, 1H), 7.60 (d, J = 8.0 Hz, 2H), 7.56 – 7.49 (m, 4H), 7.33 – 7.24 (m, 4H), 7.23 – 7.16 (m, 4H), 7.11 (d, J = 8.8 Hz, 2H), 7.03 (d, J = 8.4 Hz, 2H), 7.00 (t, J = 6.8 Hz, 1H), 2.55 (s, 3H), 2.31 (d, J = 6.0 Hz, 6H). **^{13}C NMR** (150 MHz, DMSO-d_6) δ 145.3, 143.8, 143.5, 140.9, 137.1, 137.0, 136.3, 135.8, 132.8, 130.3, 130.2, 128.6, 128.5, 128.0, 127.4, 127.1, 125.7, 123.7, 121.9, 121.3, 117.5, 113.9, 21.5, 21.4, 16.5. **HRMS (ESI)**: calculated for $C_{34}H_{31}N_4O_4S_2^+$ $[M+H]^+$: 623.1781, found:

623.1784.



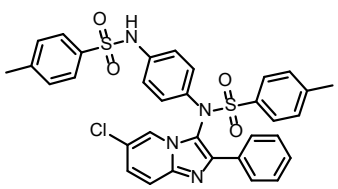
4-methyl-N-(7-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3i)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (29.6 mg, 64% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.35 (s, 1H), 8.04 (d, J = 7.2 Hz, 1H), 7.60 (d, J = 8.0 Hz, 2H), 7.51 (d, J = 8.4 Hz, 4H), 7.43 (s, 1H), 7.30 – 7.22 (m, 3H), 7.21 – 7.15 (m, 4H), 7.12 (d, J = 9.2 Hz, 2H), 7.05 (d, J = 9.2 Hz, 2H), 6.88 (dd, J = 7.2, 4.8 Hz, 1H), 2.39 (s, 3H), 2.29 (d, J = 4.0 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.3, 143.7, 141.2, 137.9, 137.2, 137.0, 136.6, 135.8, 132.8, 130.3, 130.1, 128.5, 128.4, 128.0, 127.2, 127.1, 123.7, 123.4, 121.3, 116.6, 116.3, 116.1, 21.5, 21.4, 21.2. **HRMS (ESI):** calculated for $C_{34}H_{31}N_4O_4S_2^+$ $[M+H]^+$: 623.1781, found: 623.1780.



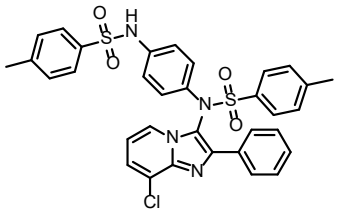
4-methyl-N-(5-methyl-2-phenylimidazo[1,2-a]pyridin-3-yl)-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3j)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (31.4 mg, 68% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.17 (s, 1H), 7.62 – 7.53 (m, 3H), 7.41 (d, J = 8.4 Hz, 2H), 7.39 – 7.33 (m, 1H), 7.27 (d, J = 8.0 Hz, 2H), 7.20 (d, J = 9.2 Hz, 2H), 7.18 – 7.07 (m, 5H), 6.98 – 6.87 (m, 4H), 6.85 (d, J = 6.8 Hz, 1H), 2.70 (s, 3H), 2.29 (s, 3H), 2.20 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.5, 145.0, 143.6, 142.1, 140.4, 137.0, 136.4, 135.5, 134.5, 134.1, 133.0, 130.0, 129.9, 128.3, 128.0, 127.3, 127.1, 122.4, 122.0, 119.5, 116.6, 116.1, 115.6, 21.4, 21.4, 18.6. **HRMS (ESI):** calculated for $C_{34}H_{31}N_4O_4S_2^+$ $[M+H]^+$: 623.1781, found: 623.1780.



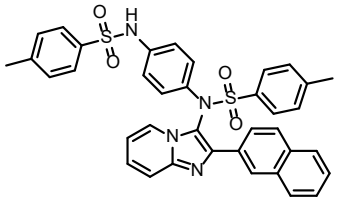
N-(6-chloro-2-phenylimidazo[1,2-a]pyridin-3-yl)-4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3k)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (26.3 mg, 59% yield). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.39 (s, 1H), 8.03 (s, 1H), 7.74 (d, J = 9.6 Hz, 1H), 7.61 (d, J = 8.0 Hz, 2H), 7.55 – 7.47 (m, 5H), 7.32 – 7.26 (m, 3H), 7.25 – 7.15 (m, 6H), 7.06 (d, J = 8.8 Hz, 2H), 2.31 (d, J = 5.6 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.6, 143.8, 142.4, 141.8, 137.0, 136.8, 136.5, 135.6, 132.2, 130.5, 130.2, 128.9, 128.7, 128.2, 127.9, 127.1, 123.8, 121.7, 121.3, 121.0, 117.7, 21.5, 21.4. **HRMS (ESI):** calculated for $C_{33}H_{28}ClN_4O_4S_2^+$ $[M+H]^+$: 643.1235, found: 643.1237.



N-(8-chloro-2-phenylimidazo[1,2-a]pyridin-3-yl)-4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3l)

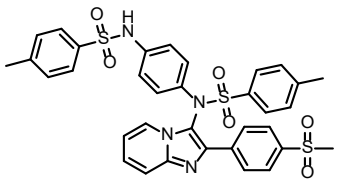
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (31.2 mg, 62% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 8.21 (d, J = 6.8 Hz, 1H), 7.64 (d, J = 7.6 Hz, 1H), 7.59 (d, J = 7.6 Hz, 2H), 7.54-7.50 (m, 4H), 7.33 – 7.24 (m, 3H), 7.20 (t, J = 7.2 Hz, 4H), 7.12 (d, J = 8.8 Hz, 2H), 7.07 – 6.98 (m, 3H), 2.30 (d, J = 6.4 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.5, 143.8, 141.9, 140.3, 137.0, 136.9, 136.4, 135.5, 132.1, 130.4, 130.2, 128.9, 128.7, 128.0, 127.4, 127.1, 126.5, 123.6, 123.5, 122.4, 121.3, 118.6, 113.9, 21.5, 21.4. **HRMS (ESI):** calculated for $C_{33}H_{28}ClN_4O_4S_2^+$ $[M+H]^+$: 643.1235, found: 643.1236.



4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)-N-(2-(naphthalen-2-yl)imidazo[1,2-a]pyridin-3-yl)benzenesulfonamide (3m)

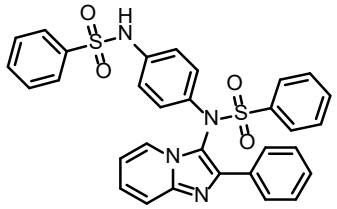
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (30.5 mg, 60% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.34 (s, 1H), 8.37 (d, J = 6.8 Hz, 1H), 7.89 – 7.84 (m, 1H), 7.79 (s, 1H), 7.77 – 7.69 (m, 3H), 7.59 (d, J = 8.0 Hz, 2H), 7.54 (s, 1H), 7.54 – 7.45 (m, 5H), 7.26 – 7.18

(m, 4H), 7.14 – 7.07 (m, 3H), 6.97 (d, *J* = 8.0 Hz, 2H), 2.22 (s, 3H), 1.99 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.2, 143.7, 143.6, 140.9, 137.5, 137.0, 136.3, 135.8, 133.0, 132.9, 130.2, 130.1, 130.0, 128.4, 128.0, 127.9, 127.9, 127.5, 127.1, 126.9, 126.7, 126.2, 125.1, 124.4, 123.3, 121.5, 117.8, 117.6, 114.1, 21.4, 21.2. **HRMS (ESI):** calculated for $C_{37}H_{31}N_4O_4S_2^+$ $[M+H]^+$: 659.1781, found: 659.1780.



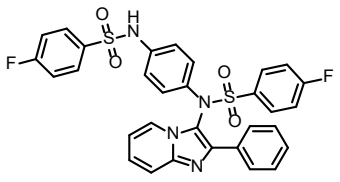
4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)-N-(2-(4-(methylsulfonyl)phenyl)imidazo[1,2-a]pyridin-3-yl)benzenesulfonamide (3n)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (24.6 mg, 61% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.55 (s, 1H), 8.49 (d, *J* = 6.8 Hz, 1H), 7.94 – 7.85 (m, 5H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.72 – 7.66 (m, 3H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 9.2 Hz, 2H), 7.36 – 7.26 (m, 5H), 3.40 (s, 3H), 2.49 (d, *J* = 11.6 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.6, 143.9, 143.7, 140.4, 139.5, 137.3, 137.1, 137.0, 136.4, 135.3, 130.4, 130.2, 128.1, 128.0, 127.7, 127.3, 127.1, 124.5, 123.5, 121.4, 118.1, 118.1, 114.5, 43.9, 21.4, 21.4. **HRMS (ESI):** calculated for $C_{34}H_{31}N_4O_6S_3^+$ $[M+H]^+$: 687.1400, found: 687.1402.



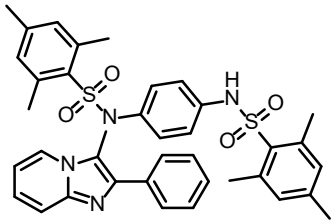
N-(2-phenylimidazo[1,2-a]pyridin-3-yl)-N-(4-(phenylsulfonamido)phenyl)benzenesulfonamide (3o)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (33.9 mg, 71% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.45 (s, 1H), 8.18 (d, *J* = 6.8 Hz, 1H), 7.73 (d, *J* = 7.6 Hz, 2H), 7.70 – 7.63 (m, 3H), 7.60 – 7.54 (m, 3H), 7.52 – 7.46 (m, 2H), 7.42 (t, *J* = 7.6 Hz, 3H), 7.23 – 7.17 (m, 2H), 7.15 (d, *J* = 9.2 Hz, 2H), 7.10 – 7.01 (m, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 143.4, 141.5, 139.9, 138.8, 137.0, 136.5, 134.7, 133.4, 132.7, 130.0, 129.7, 128.8, 128.7, 128.0, 127.3, 127.3, 127.1, 124.1, 123.9, 121.5, 117.9, 117.0, 114.0. **HRMS (ESI):** calculated for $C_{31}H_{25}N_4O_4S_2^+$ $[M+H]^+$: 581.1312, found: 581.1311.



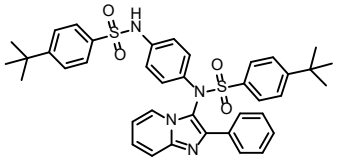
4-fluoro-N-(4-((4-fluorophenyl)sulfonamido)phenyl)-N-(2-phenylimidazo[1,2-a]pyridin-3-yl)benzenesulfonamide (3p)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (28.2 mg, 64% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.44 (s, 1H), 8.26 (d, J = 6.8 Hz, 1H), 7.83 – 7.74 (m, 2H), 7.72 – 7.65 (m, 3H), 7.50 (d, J = 6.8 Hz, 2H), 7.47 – 7.41 (m, 1H), 7.32 (t, J = 8.4 Hz, 2H), 7.25 (d, J = 7.2 Hz, 1H), 7.24 – 7.12 (m, 6H), 7.10 – 7.04 (m, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 166.4 (d, $J_{C\text{-}F}$ = 83.9 Hz), 163.8 (d, $J_{C\text{-}F}$ = 81.3 Hz), 143.46, 141.45, 136.85, 134.8 (d, $J_{C\text{-}F}$ = 2.8 Hz), 134.49, 132.59, 131.3 (d, $J_{C\text{-}F}$ = 9.8 Hz), 130.1 (d, $J_{C\text{-}F}$ = 9.4 Hz), 128.71, 128.62, 127.41, 127.28, 124.24, 123.75, 122.34, 121.66, 117.87, 117.23, 117.0 (d, $J_{C\text{-}F}$ = 4.2 Hz), 116.73, 114.04. **^{19}F NMR** (376 MHz, DMSO-d_6) δ -104.0. **HRMS (ESI):** calculated for $C_{31}H_{23}F_2N_4O_4S_2^+$ $[M+H]^+$: 617.1123, found: 617.1120.



2,4,6-trimethyl-N-(2-phenylimidazo[1,2-a]pyridin-3-yl)-N-(4-((2,4,6-trimethylphenyl)sulfonamido)phenyl)benzenesulfonamide (3q)

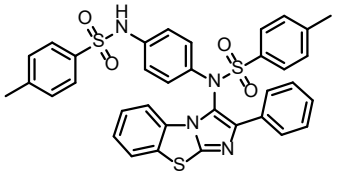
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (26.6 mg, 68% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.31 (s, 1H), 8.19 (d, J = 6.8 Hz, 1H), 7.63 (d, J = 8.8 Hz, 1H), 7.57 (d, J = 6.8 Hz, 2H), 7.38 (t, J = 7.2 Hz,1H), 7.30 – 7.20 (m, 5H), 7.00 – 6.90 (m, 5H), 6.77 (s, 2H), 2.53 (s, 12H), 2.20 (s, 3H), 2.15 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 144.0, 143.2, 142.6, 142.3, 140.0, 139.1, 136.9, 136.8, 134.1, 133.3, 132.6, 132.5, 132.3, 128.6, 128.3, 127.4, 127.2, 125.8, 124.5, 120.6, 117.8, 116.9, 113.7, 23.0, 22.9, 20.9, 20.9. **HRMS (ESI):** calculated for $C_{37}H_{37}N_4O_4S_2^+$ $[M+H]^+$: 665.2251, found: 665.2250.



4-(tert-butyl)-N-(4-((4-(tert-butyl)phenyl)sulfonamido)phenyl)-N-(2-phenylimidazo[1,2-a]pyridin-3-yl)benzenesulfonamide (3r)

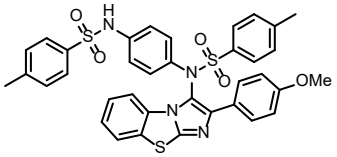
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (25.1 mg, 64% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.41 (s, 1H), 8.23 (d, J = 6.8 Hz, 1H), 7.67 (d, J = 8.8 Hz, 3H), 7.56 (d, J = 8.4 Hz, 2H), 7.50 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 7.2 Hz, 2H), 7.41 (d, J = 8.8 Hz, 1H), 7.36 (d, J = 8.4 Hz, 2H), 7.19-7.16 (m, 3H), 7.13-7.06 (m, 4H), 7.02 (t, J = 6.8 Hz, 1H),

1.20 (d, J = 3.6 Hz, 18H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 157.7, 156.4, 143.4, 141.1, 137.3, 137.3, 136.3, 135.8, 132.6, 128.6, 128.5, 127.9, 127.3, 127.1, 127.0, 126.7, 126.6, 124.2, 123.3, 121.0, 117.8, 117.1, 113.8, 35.3, 35.3, 31.1, 31.1. **HRMS (ESI):** calculated for $C_{39}H_{41}N_4O_4S_2^+$ $[M+H]^+$: 693.2564, found: 693.2563.



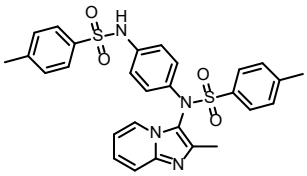
4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)-N-(2-phenylbenzo[d]imidazo[2,1-b]thiazol-3-yl)benzenesulfonamide (3s)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (21.2 mg, 49% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.27 (s, 1H), 8.14 – 8.07 (m, 1H), 7.65 – 7.62 (m, 1H), 7.57 (dd, J = 16.8, 8.4 Hz, 4H), 7.50 – 7.44 (m, 2H), 7.30 – 7.23 (m, 6H), 7.18 (t, J = 7.2 Hz, 1H), 7.12 – 7.03 (m, 6H), 2.27 (d, J = 12.4 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 147.6, 145.3, 143.8, 142.8, 137.9, 137.0, 135.9, 135.4, 132.4, 132.3, 130.2, 130.1, 130.0, 128.6, 128.1, 128.0, 127.1, 127.0, 126.5, 125.77, 125.51, 121.8, 121.6, 119.9, 114.1, 21.4. **HRMS (ESI):** calculated for $C_{35}H_{29}N_4O_4S_3^+$ $[M+H]^+$: 665.1345, found: 665.1346.



N-(2-(4-methoxyphenyl)benzo[d]imidazo[2,1-b]thiazol-3-yl)-4-methyl-N-(4-((4-methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3t)

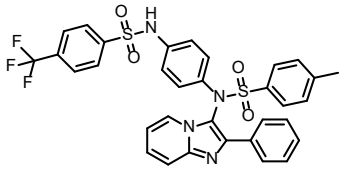
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (18.4 mg, 43% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.24 (s, 1H), 8.11-8.07 (m, 1H), 7.74-7.65 (m, 2H), 7.61-7.52 (dd, J = 18.0, 8.0 Hz, 4H), 7.48-7.32 (m, 2H), 7.36 (d, J = 8.0Hz, 1H), 7.25 (d, J = 15.6 Hz, 4H), 7.16 (d, J = 8.4 Hz, 2H), 7.08 (t, J = 8.0 Hz, 3H), 6.62 (d, J = 8.8 Hz, 1H), 3.71 (s, 3H), 2.27 (d, J = 10.0 Hz, 6H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 159.4, 147.4, 145.2, 143.8, 142.8, 138.0, 137.1, 136.0, 135.3, 132.3, 130.1, 129.9, 129.8, 128.0, 127.8, 127.1, 127.0, 126.1, 125.6, 125.5, 124.9, 121.7, 121.6, 119.1, 114.0, 55.6, 21.4, 21.3. **HRMS (ESI):** calculated for $C_{36}H_{31}N_4O_5S_3^+$ $[M+H]^+$: 695.1451, found: 695.1450.



4-methyl-N-(2-methylimidazo[1,2-a]pyridin-3-yl)-N-(4-((4-

methylphenyl)sulfonamido)phenyl)benzenesulfonamide (3u)

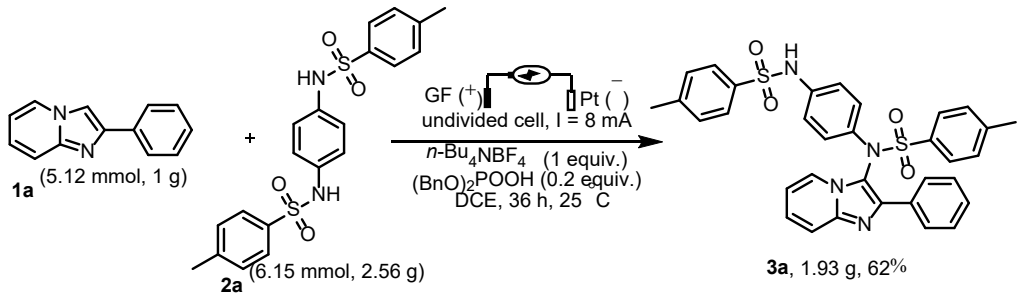
The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (34.3 mg, 70% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.46 (s, 1H), 8.33 (d, J = 7.2 Hz, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.56 (d, J = 8.0 Hz, 2H), 7.48 – 7.39 (m, 3H), 7.35 – 7.26 (m, 5H), 7.09 (d, J = 8.8 Hz, 2H), 6.96 (t, J = 6.8 Hz, 1H), 2.41 (s, 3H), 2.31 (s, 3H), 1.85 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.1, 143.9, 142.8, 141.0, 138.0, 137.2, 136.2, 136.1, 130.6, 130.2, 128.1, 128.0, 127.1, 126.3, 123.8, 120.6, 118.0, 117.0, 113.1, 21.6, 21.4, 13.5. **HRMS (ESI):** calculated for $C_{28}H_{27}N_4O_4S_2^+$ $[M+H]^+$: 547.6675, found: 547.6676.



4-methyl-N-(2-phenylimidazo[1,2-a]pyridin-3-yl)-N-(4-((4-(trifluoromethyl)phenyl)sulfonamido)phenyl)benzenesulfonamide (3v)

The desired product was purified by silica gel chromatography (petroleum ether/EtOAc= 2:1) as white solid (23.4 mg, 43% yield), **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.62 (d, J = 3.6 Hz, 1H), 8.19 (d, J = 6.4 Hz, 1H), 7.98 – 7.85 (m, 4H), 7.74 – 7.60 (m, 2H), 7.56 – 7.47 (m, 4H), 7.46 – 7.40 (m, 1H), 7.22 – 7.14 (m, 6H), 7.11 – 7.04 (m, 3H), 2.30 (d, J = 2.4 Hz, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.4, 143.7, 143.4, 141.5, 136.6 (d, $J_{C\text{-}F}$ = 202.0 Hz), 135.5, 132.6, 130.3, 129.6 (d, $J_{C\text{-}F}$ = 121.9 Hz), 128.6, 128.5,128.1, 128.0, 127.3, 127.2, 127.1, 127.0, 127.0, 124.1, 123.5, 122.0, 117.9, 116.9, 114.0, 21.4. **^{19}F NMR** (376 MHz, DMSO-d_6) δ -61.7. **HRMS (ESI):** calculated for $C_{33}H_{26}F_3N_4O_4S_2^+$ $[M+H]^+$: 663.7097, found: 663.7098.

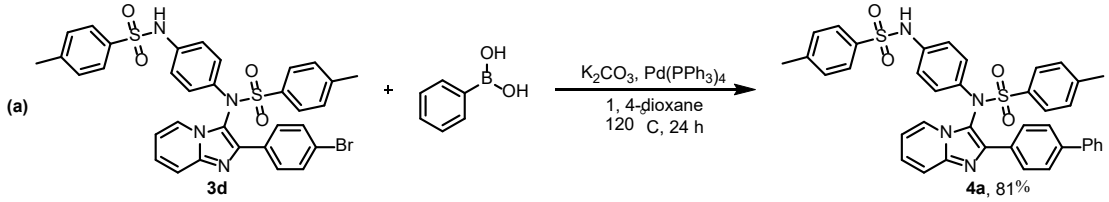
5. Procedure for gram-scale experiment



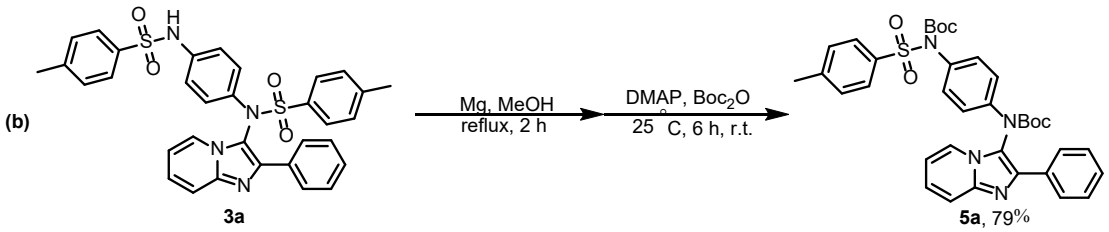
Prepare a dry and clean Schlenk tube fitted with a rubber stopper equipped with a carbon rod anode and a platinum plate cathode. Add 2-phenylimidazo[1,2-a]pyridine **1a** (5.12 mmol, 1 g), *N,N′*-1,4-phenylenebis[4-methylbenzenesulfonamide] **2a** (6.15 mmol, 2.56 g), n-Bu$_4$NBF$_4$ (5.12 mmol, 1.0 equiv.), (BnO)$_2$POOH (1.02 mmol, 0.2 equiv.) and DCE (20 mL) to the Schlenk tube containing a stir bar. Stir the mixture at

25 °C under a constant current of 8 mA for 36 hours. After the reaction is complete, concentrate the reaction solution. Purify the residue by silica gel column chromatography (petroleum ether/EtOAc = 2:1) to obtain the target product **3a** (1.93 g, 62%).

6. Procedure for diversifications



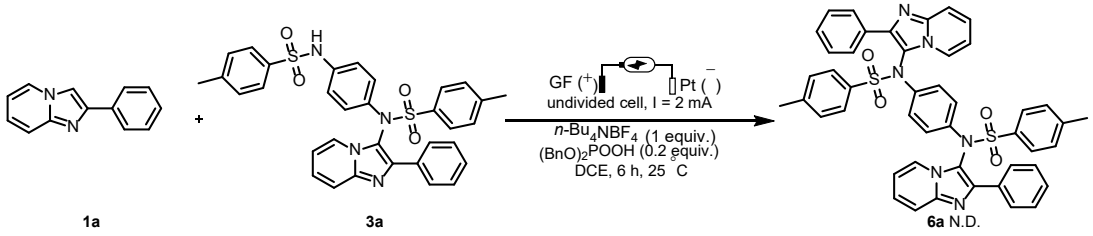
Under a nitrogen atmosphere, compound **3d** (68.60 mg, 0.1 mmol), phenylboronic acid (24.39 mg, 0.2 mmol), $Pd(PPh_3)_4$ (11.56 mg, 0.01 mmol), 1,4-dioxane (2 mL), and K_2CO_3 (55.28 mg, 0.4 mmol) were successively added to a dry pressure tube equipped with a magnetic stir bar. The reaction mixture was stirred at 120 °C in the sealed tube for 24 h. After the starting material was completely consumed as monitored by TLC, the reaction was quenched with water (5 mL), and the majority of the organic solvent was removed under reduced pressure. The aqueous phase was extracted with EtOAc (3 x 10 mL). The combined organic layers were washed with brine, dried over anhydrous $MgSO_4$, filtered, and concentrated in vacuo. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 2:1, v/v) to afford the title compound **4a** as a white solid (55.42 mg, 81% yield). **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.34 (s, 1H), 8.22 (d, J = 6.8 Hz, 1H), 7.73 – 7.64 (m, 3H), 7.62 (d, J = 8.4 Hz, 4H), 7.54 (d, J = 8.4 Hz, 2H), 7.51 – 7.42 (m, 5H), 7.37 (t, J = 7.2 Hz, 1H), 7.27 (d, J = 8.0 Hz, 2H), 7.22 (d, J = 9.2 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 7.12 – 7.02 (m, 3H), 2.25 (s, 3H), 2.17 (s, 3H). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 145.3, 143.8, 143.5, 141.0, 140.1, 139.9, 137.2, 137.1, 136.3, 135.8, 131.7, 130.3, 130.2, 129.4, 128.1, 128.0, 127.8, 127.4, 127.1, 127.0, 126.8, 124.2, 123.4, 121.4, 117.9, 117.1, 114.0, 21.4, 21.4. **HRMS (ESI):** calculated for $C_{39}H_{33}N_4O_4S_2^+$ $[M+H]^+$: 685.1938, found: 685.1939.



The compound **4b** was synthesized according to the reference literature[7].To a dry 50 mL round-bottom flask containing a solution of compound **3a** (60.82 mg, 0.1 mmol) in

anhydrous MeOH (5 mL) were added activated Mg turnings. The mixture was heated to reflux for 2 h. Upon completion as monitored by TLC, the reaction was quenched with saturated aqueous NH_4Cl. The majority of the methanol was removed under reduced pressure. The residue was diluted with water and extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine, dried over anhydrous MgSO4, filtered, and concentrated in vacuo. The resulting crude residue was dissolved in anhydrous THF (5 mL). DMAP (24.43 mg, 0.2 mmol) and Boc_2O (48.02 mg, 0.22 mmol) were added sequentially. The reaction mixture was stirred at room temperature for 6 h. After the solvent was removed under reduced pressure, water (20 mL) was added, and the aqueous phase was extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine, dried over anhydrous MgSO4, filtered, and concentrated. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 5:1, v/v) to afford **5a** as a white solid (51.68 mg, 79% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 6.4 Hz, 1H), 7.70 (d, *J* = 9.2 Hz, 1H), 7.49 – 7.39 (m, 4H), 7.38 – 7.30 (m, 3H), 7.28 (s, 1H), 7.15 (d, *J* = 8.8 Hz, 2H), 6.88 – 6.81 (m, 1H), 2.46 (s, 3H), 1.32 (s, 9H), 1.26 (s, 9H). **^{13}C NMR** (100 MHz, Chloroform-*d*) δ 152.7, 150.8, 144.6, 142.7, 140.6, 139.9, 136.7, 133.2, 132.9, 130.3, 129.4, 128.8, 128.6, 128.3, 126.8, 125.2, 123.1, 121.7, 118.3, 117.9, 112.8, 84.5, 83.0, 27.8, 27.8, 21.7. **HRMS (ESI):** calculated for $C_{36}H_{39}N_4O_6S^+$ $[M+H]^+$: 655.2585, found: 655.2584.

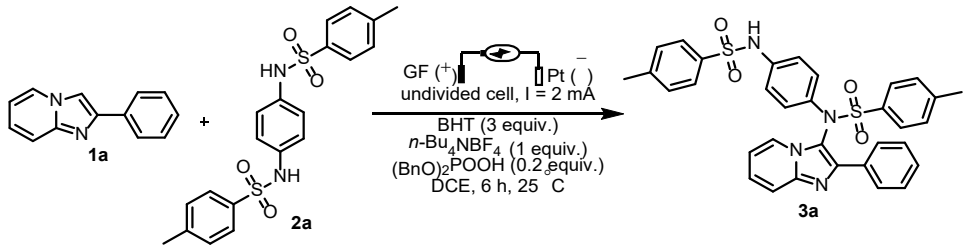
7. Control experiment for over-arylation



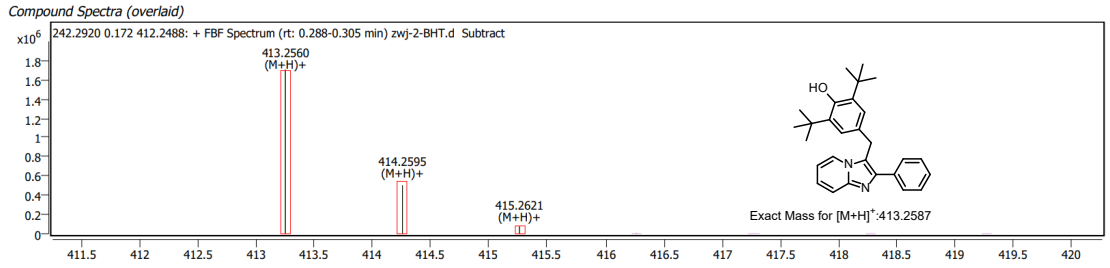
Prepare a dry and clean Schlenk tube fitted with a rubber stopper equipped with a carbon rod anode and a platinum plate cathode. Add **1a** (0.2 mmol, 1.0 equiv.), **3a** (146.1 mg, 0.24 mmol, 1.2 equiv), *n*-Bu_4NBF_4 (0.2 mmol, 1.0 equiv.), $(BnO)_2POOH$ (0.04 mmol, 0.2 equiv.) and DCE (5 mL) to the Schlenk tube containing a stir bar. Stir the mixture at 25 °C under a constant current of 2 mA for 6 hours. No reaction was observed by TLC and LC-MS analysis, and the starting materials were quantitatively recovered.

8. Mechanistic studies

8.1 Radical trapping experiment for the electrochemical oxidative rearrangement of reaction

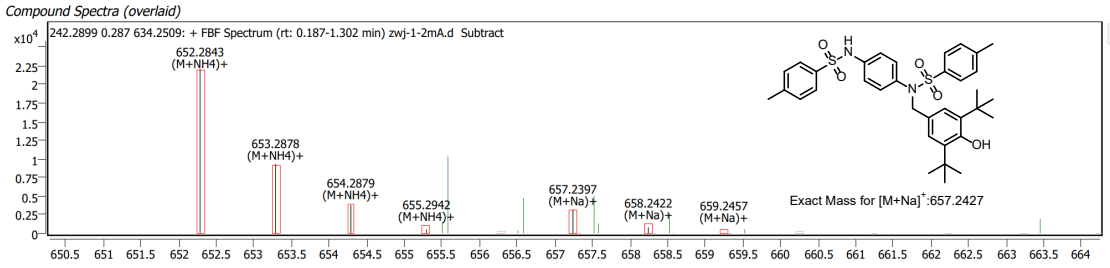


Prepare a dry and clean Schlenk tube fitted with a rubber stopper equipped with a carbon rod anode and platinum plate cathode. Add 2-phenylimidazo[1,2-a]pyridine **1a** (0.2 mmol, 1.0 equiv.), N,N'-1,4-phenylenebis[4-methylbenzenesulfonamide] **2a** (0.24 mmol, 1.2 equiv.), BHT (0.6 mmol, 3 equiv.), *n*-Bu$_4$NBF$_4$ (0.2 mmol, 1.0 equiv.), (BnO)$_2$POOH (0.04 mmol, 0.2 equiv.) and DCE (5 mL) to the Schlenk tube containing a stir bar. Stir the mixture at 25 °C under a constant current of 2 mA for 24 hours.



Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C28 H32 N2 O	(M+H)+	0.172		412.2488		FBF	84.02		84.02

Figure S2 HRMS for 1a



Name	Formula	Species	RT	RT Diff	Mass	CAS	ID Source	Score	Score (Lib)	Score (Tgt)
	C35 H42 N2 O5 S2	(M+NH4)+ (M+Na)+	0.287		634.2509		FBF	87.40		87.40

Figure S3 HRMS for 2a

8.2 Cyclic voltammetry (CV) studies

The cyclic voltammograms were recorded on a CHI 600E instrument using a glassy-carbon working electrode (diameter, 3 mm), a Pt wire auxiliary electrode, an Ag/AgCl reference electrode, and a scan rate of 100 mV/s.

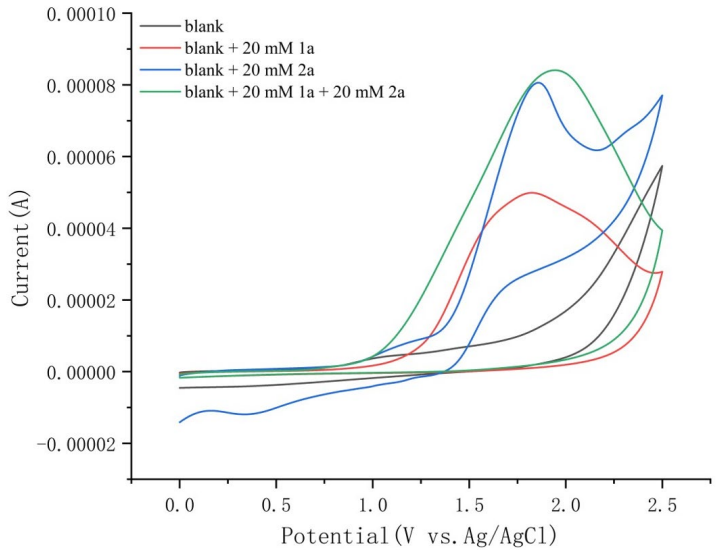


Figure S4 cyclic voltammograms measured in an electrolyte solution of *n*-Bu_4NBF_4 (0.04 M) in DCE. **Conditions**: 20 mM of substrate **1a**, **2a**. A glassy-carbon working electrode (diameter, 3 mm), a Pt wire auxiliary electrode and an Ag/AgCl reference electrode was used. The experiment was conducted in DCE at 25 °C.

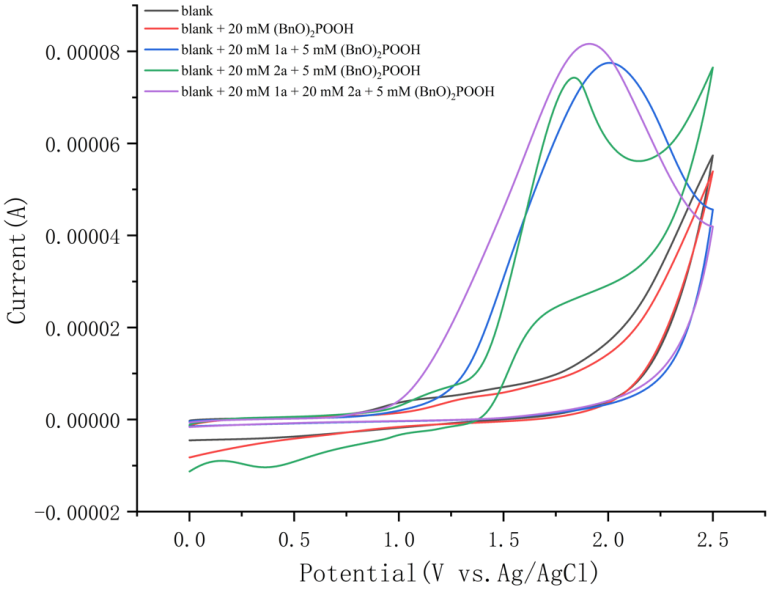


Figure S4 cyclic voltammograms measured in an electrolyte solution of *n*-Bu_4NBF_4 (0.04 M) in DCE. **Conditions**: 20 mM of substrate **1a**, **2a**, 5 or 20 mM of *n*-Bu_4NBF_4. A glassy-carbon working electrode (diameter, 3 mm), a Pt wire auxiliary electrode and an Ag/AgCl reference electrode was used. The experiment was conducted in DCE at 25 °C.

9. Reference

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[2] W. Zhu, Y. Ding, Z. Bian, P. Xie, B. Xu, Q. Tang, W. Wu and A. Zhou, *Adv. Synth. Catal.*, 2017, **359**, 2215–2221.

[3] A. K. Bagdi, M. Rahman, S. Santra, A. Majee and A. Hajra, *Adv. Synth. Catal.*, 2013, **355**, 1741–1747.

[4] R. Adams and A. S. Nagarkatti, *J. Am. Chem. Soc.*, 1950, **72**, 4601–4606.

[5] W.-Y. Ma, C. Gelis, D. Bouchet, P. Retailleau, X. Moreau, L. Neuville and G. Masson, *Org. Lett.*, 2021, **23**, 442.

[6] Y.-Q. Sang, Y.-H. Li and S.-L. You, *Org. Lett.*, 2024, **26**, 4932–4937.

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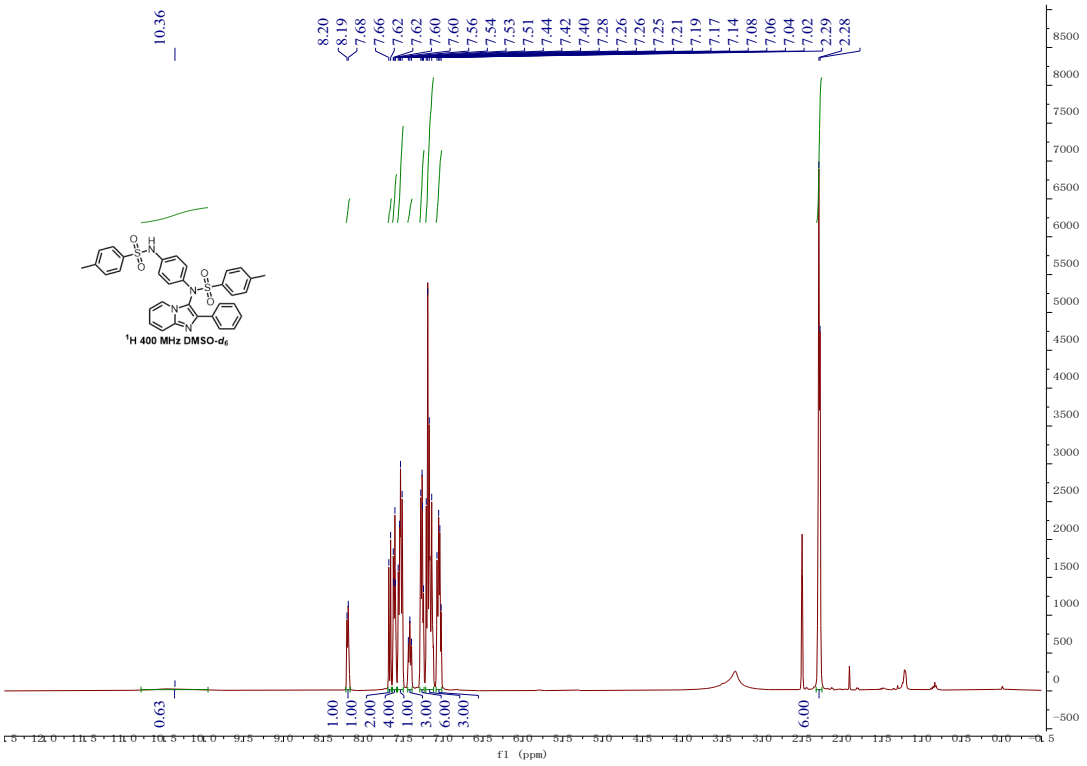
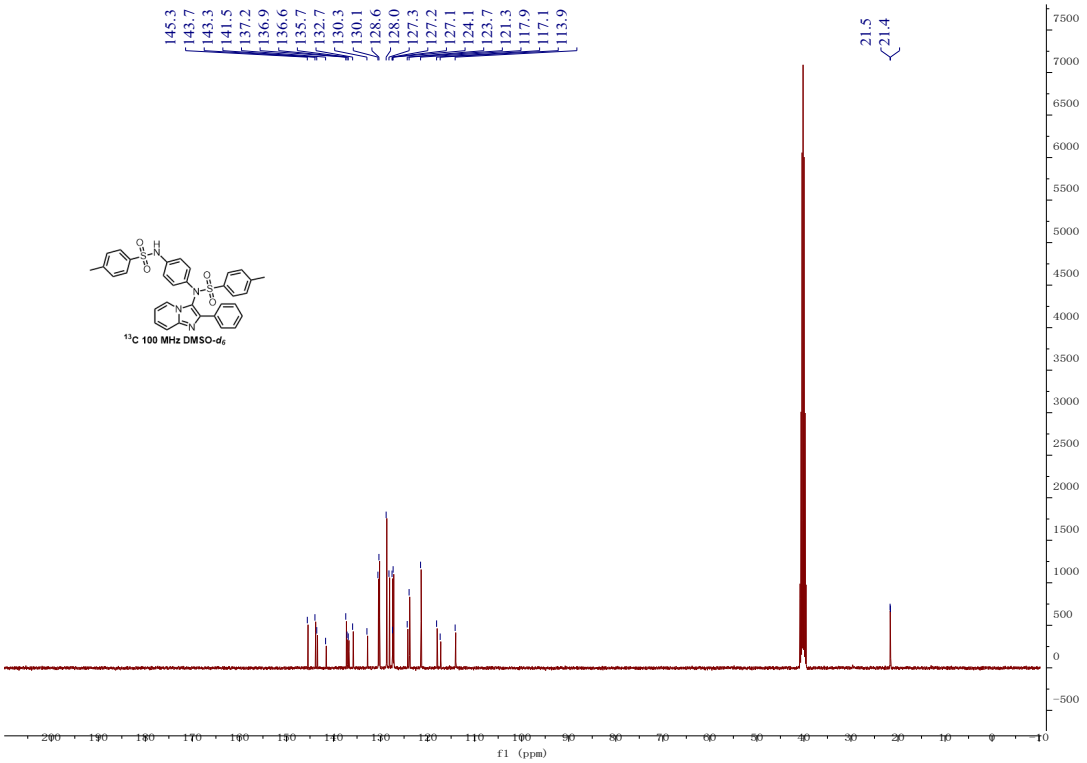
10. NMR spectra

3a





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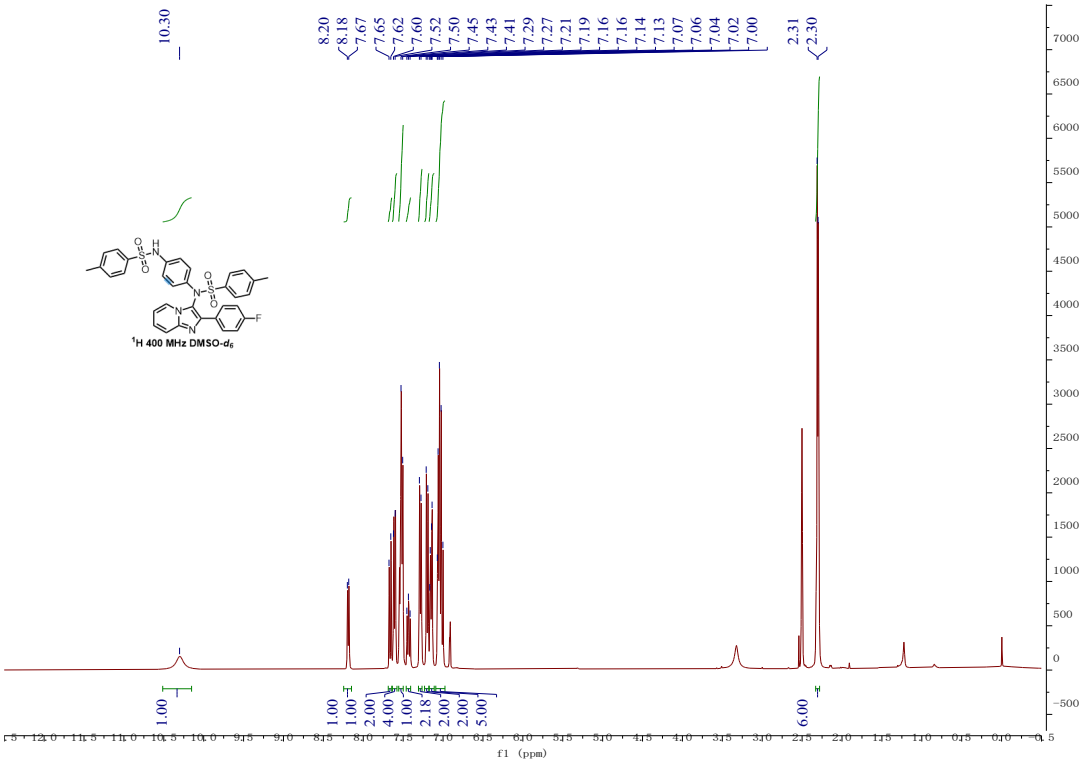
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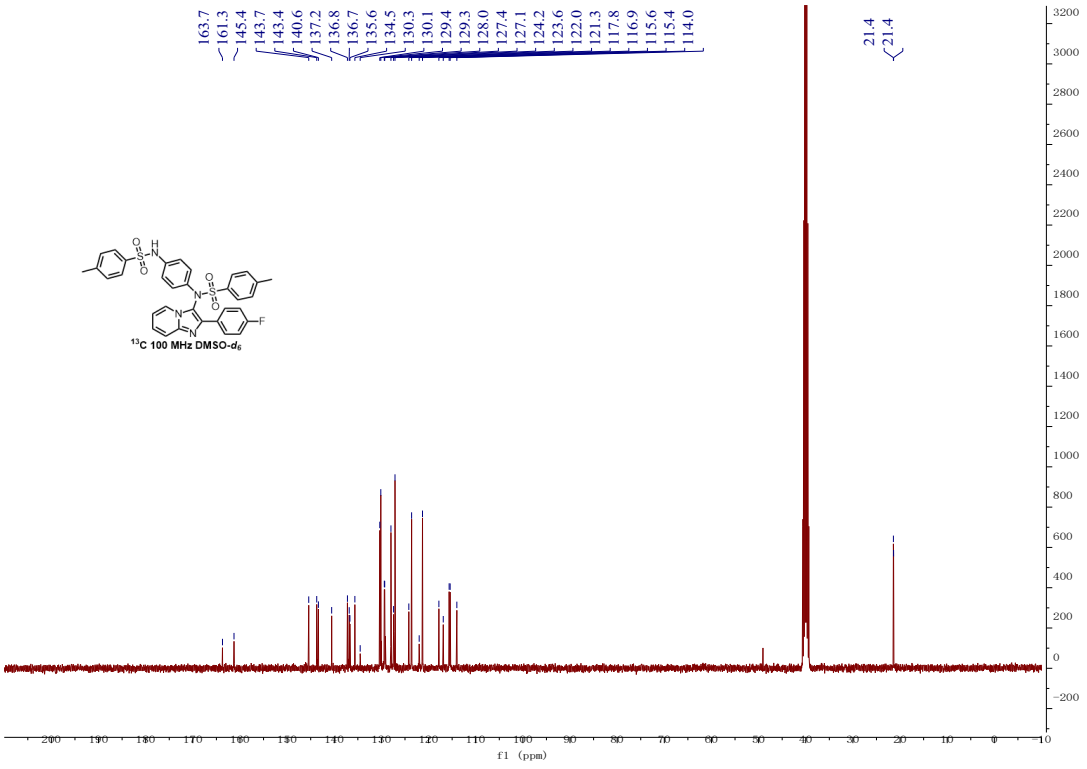
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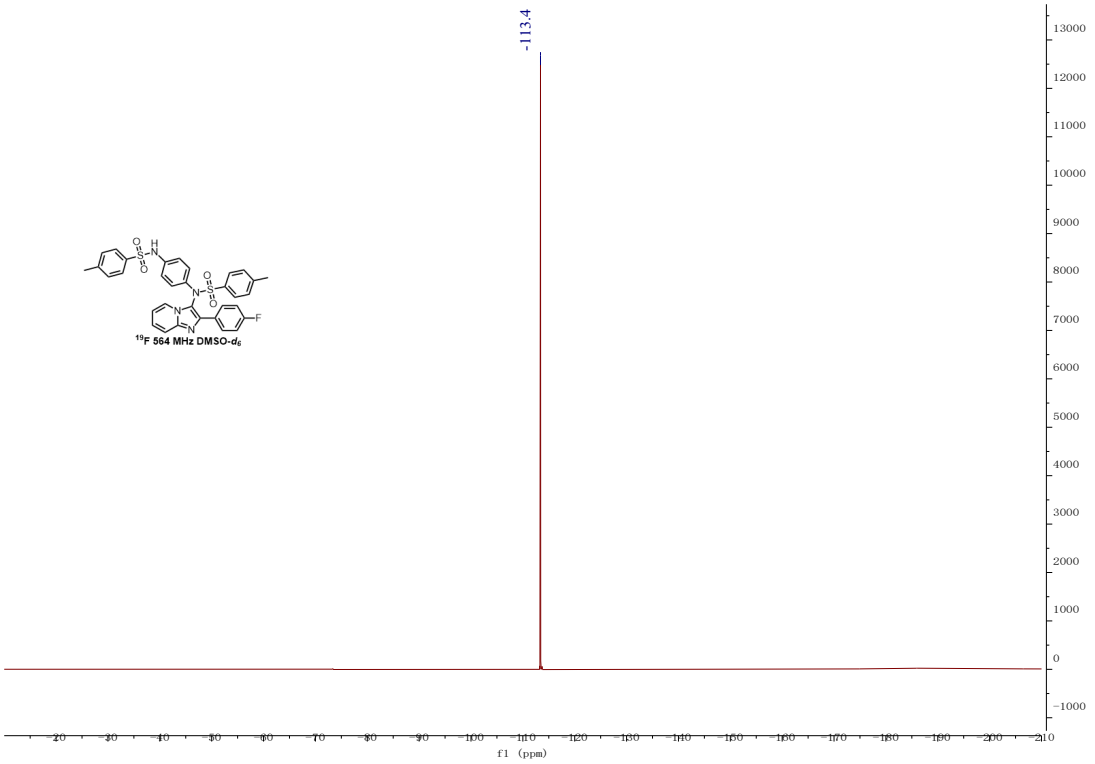
114.0
21.4
21.4
f1 (ppm)
^{13}C 100 MHz DMSO-d_6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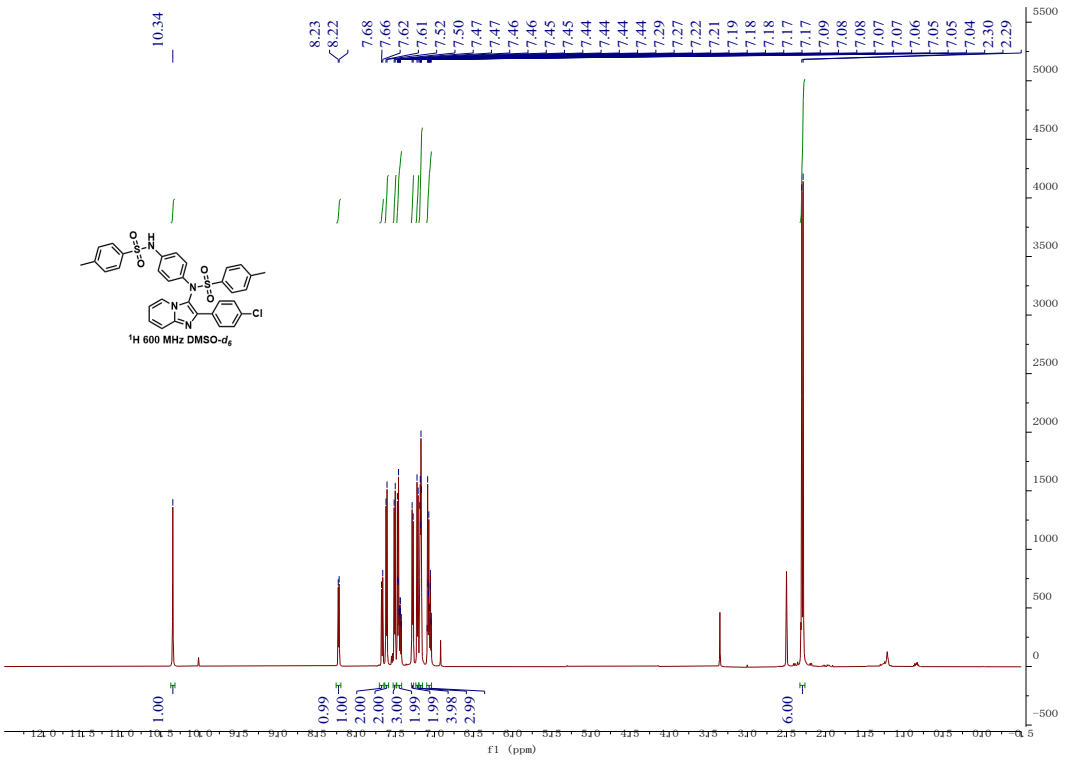
3c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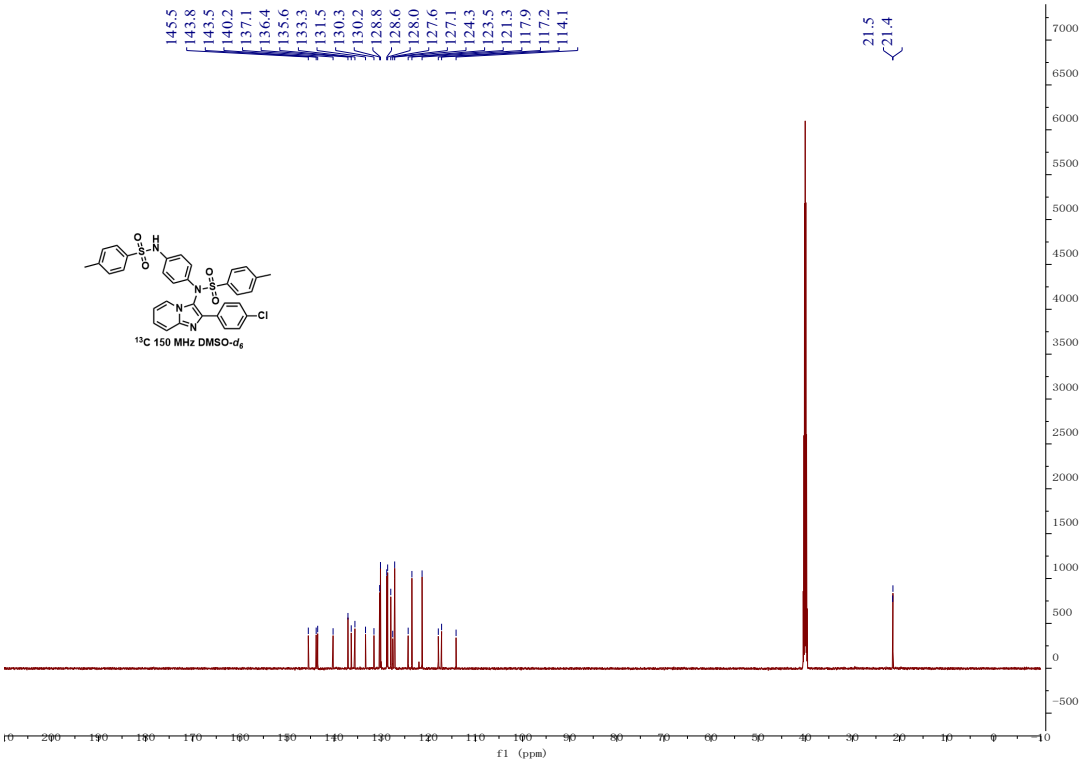
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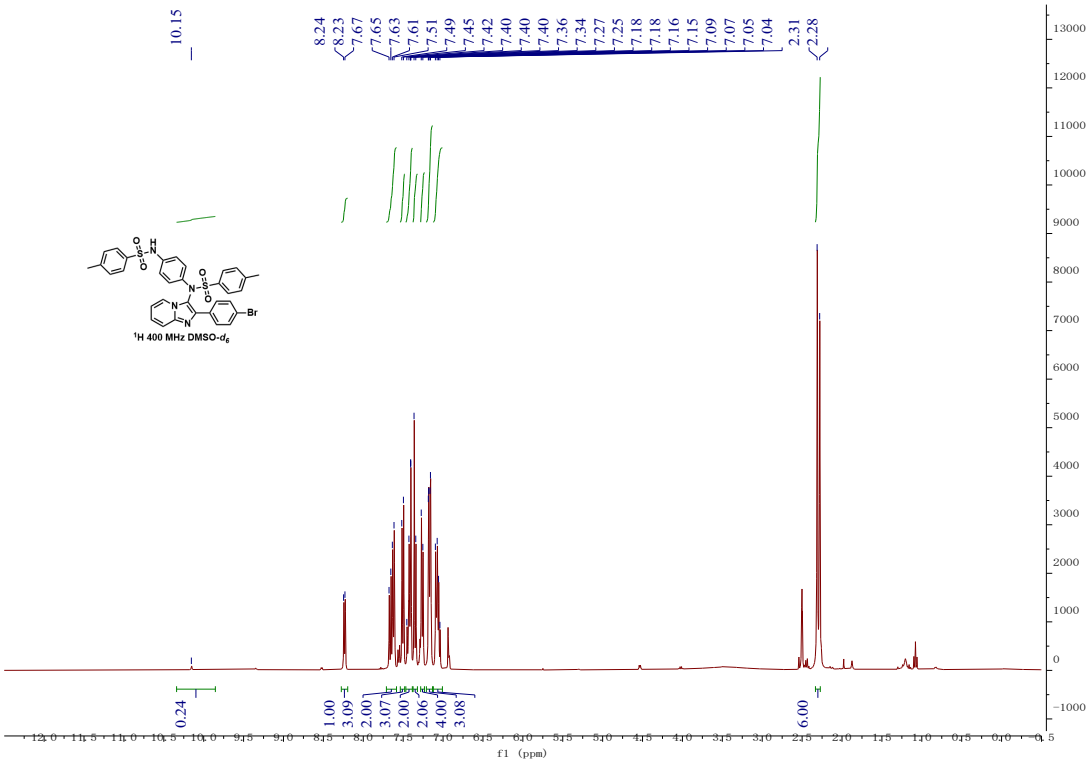
3d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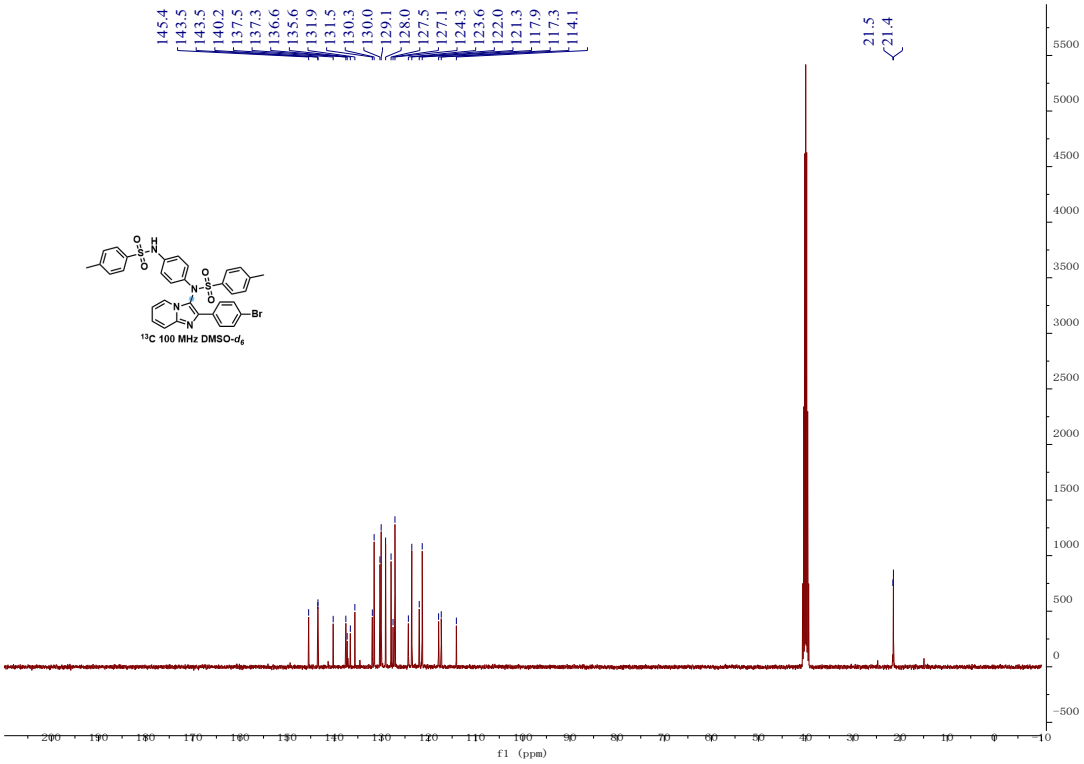
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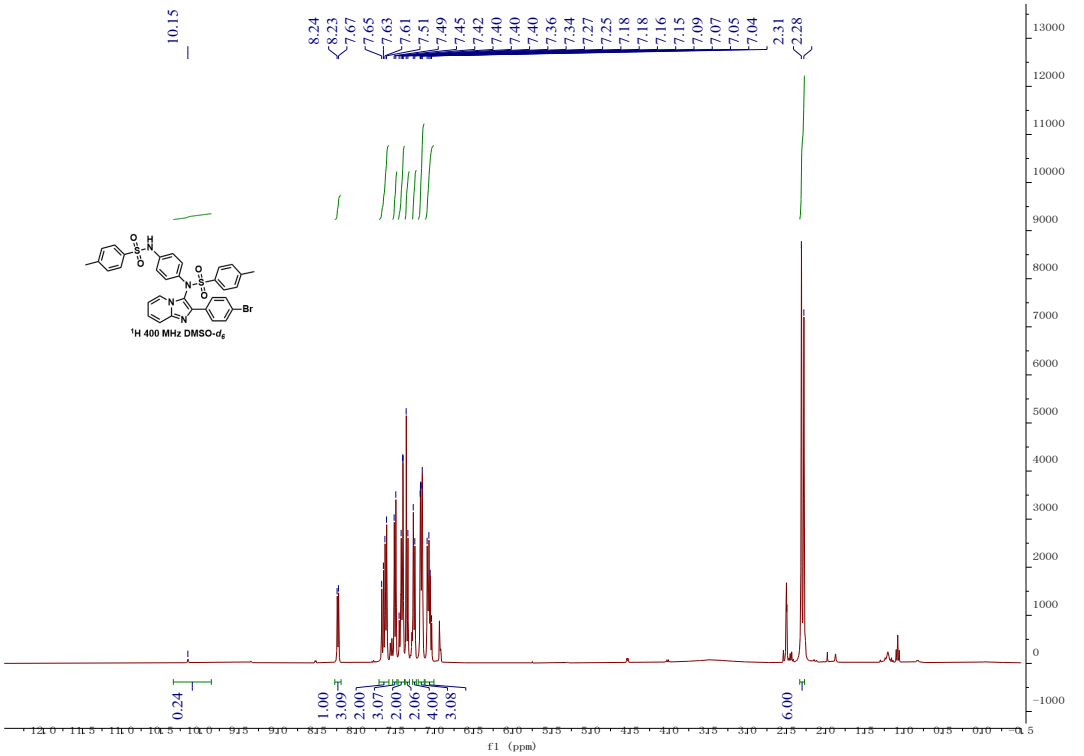
f1 (ppm)

3e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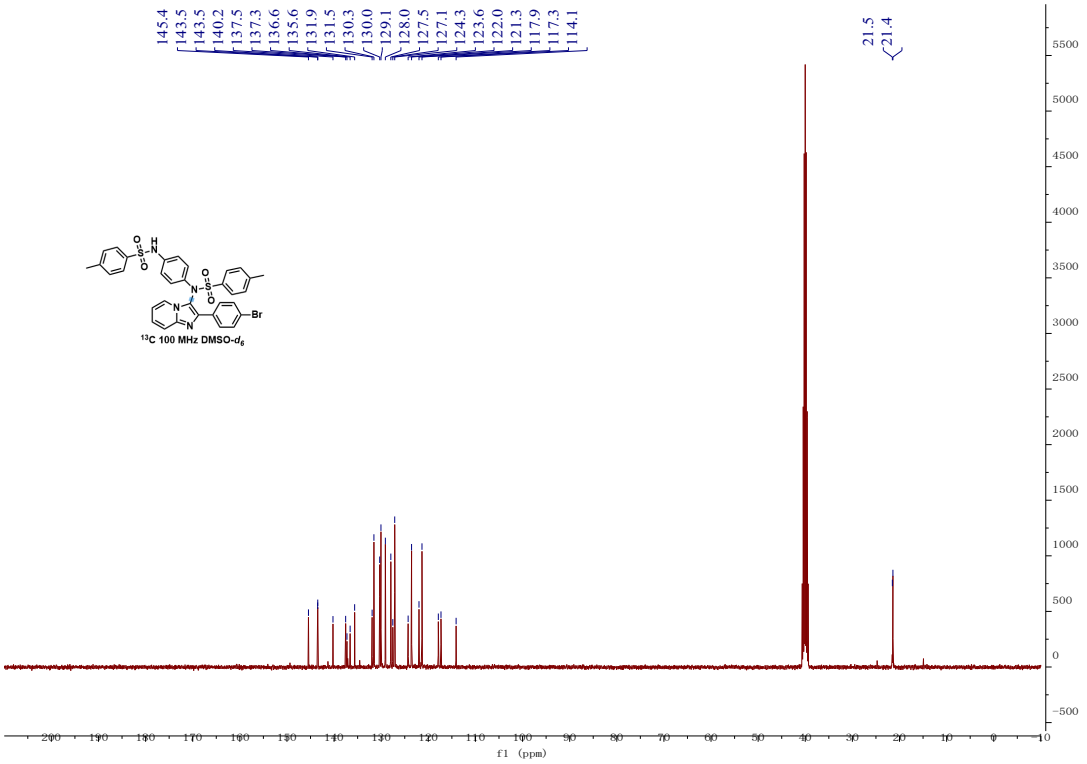
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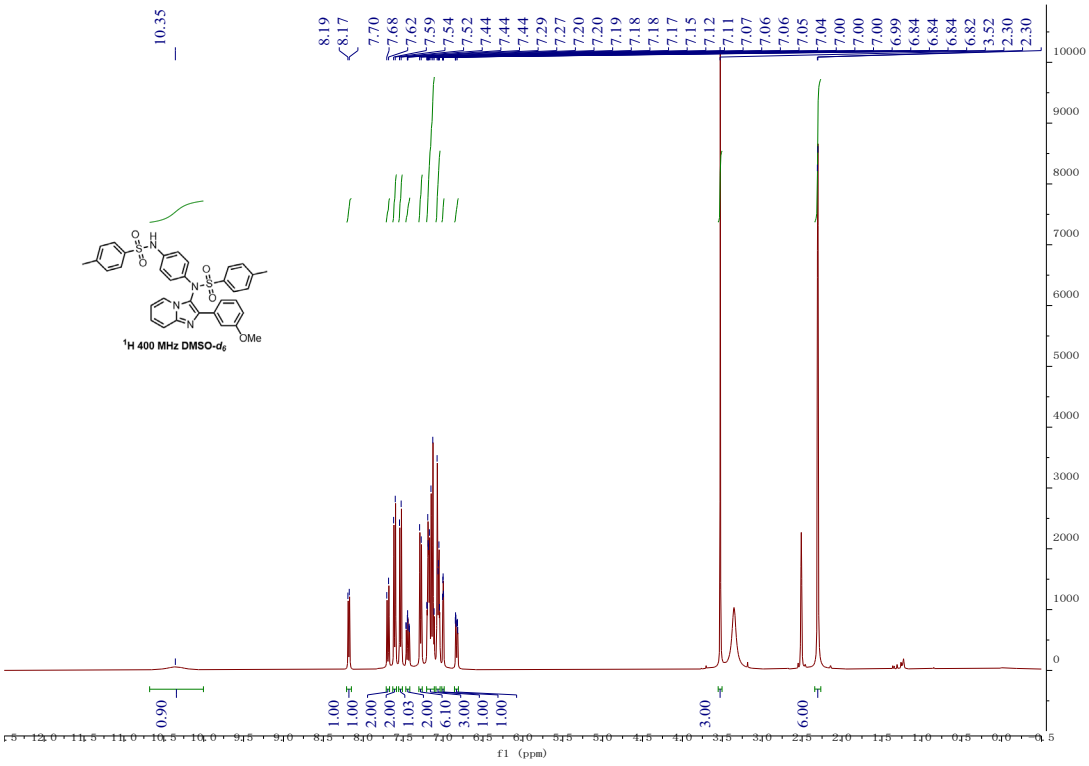
f1 (ppm)

3f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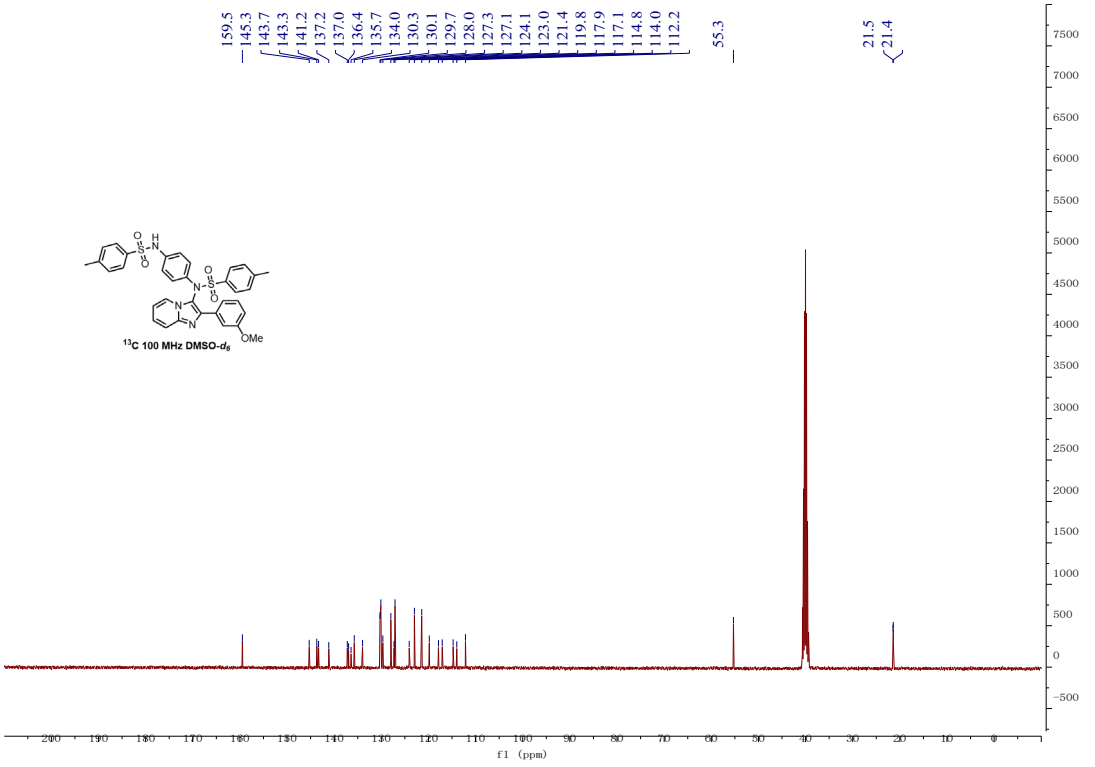
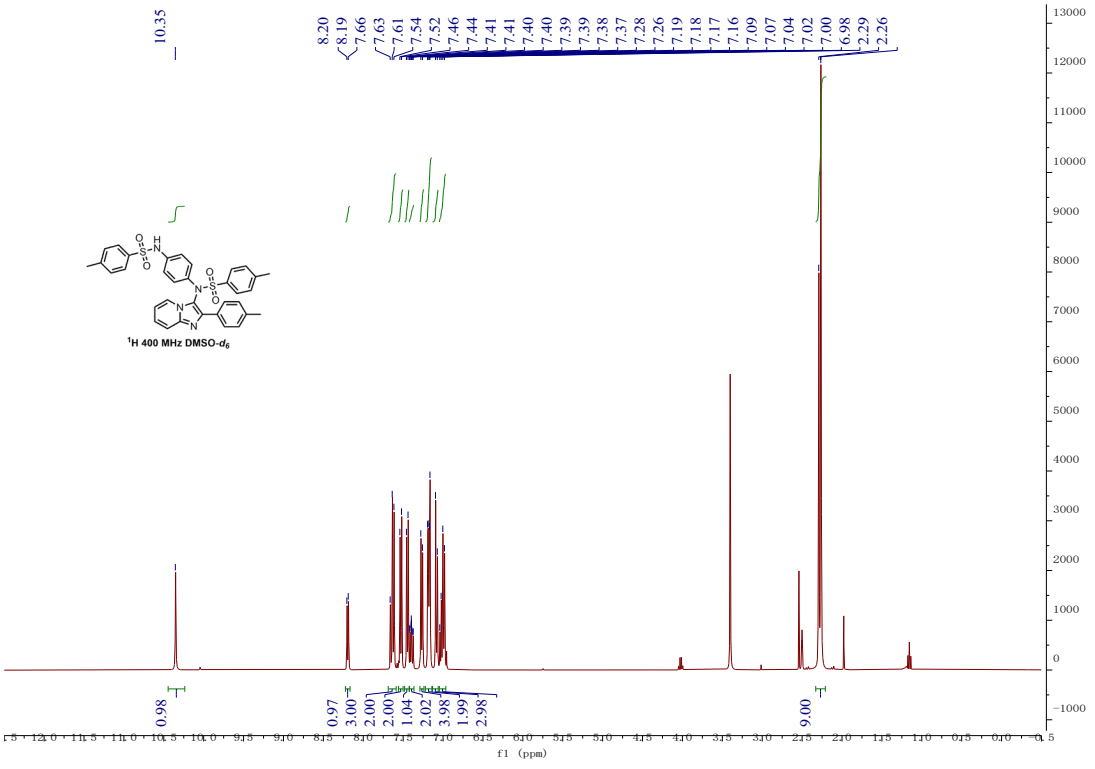
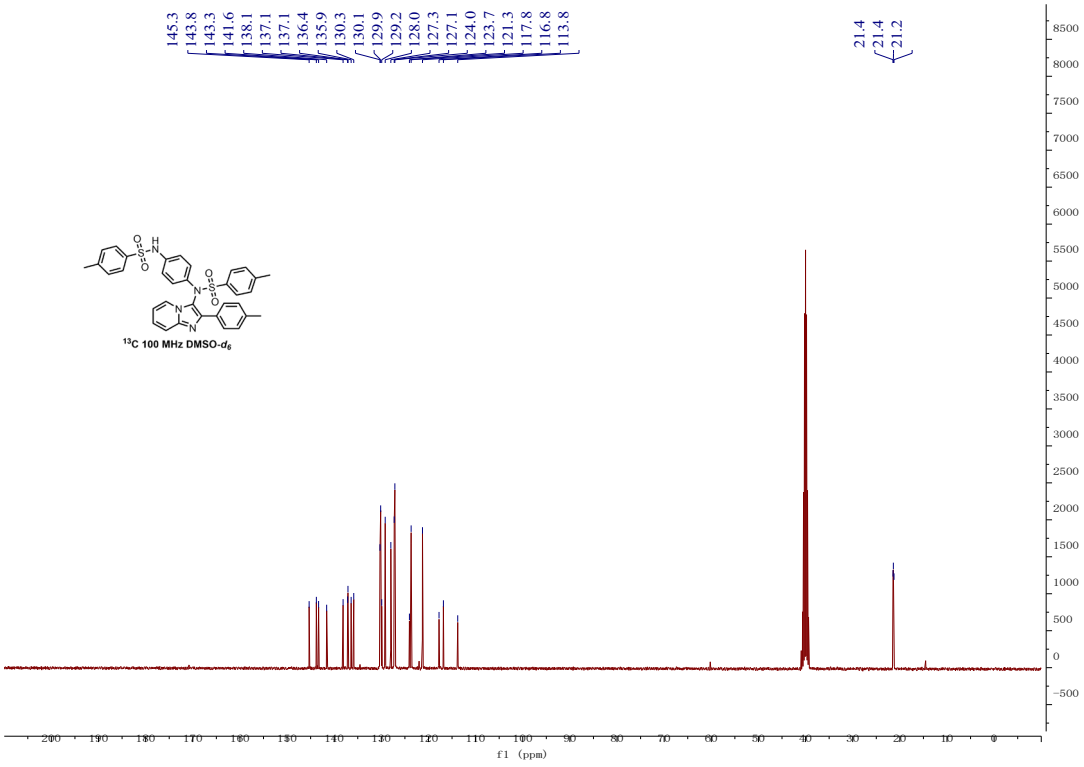
2.30
OMe
1H 400 MHz DMSO-d6
0.90
1.00
1.00
2.00
2.00
1.03
2.00
6.10
3.00
1.00
1.00
3.00
6.00
f1 (ppm)

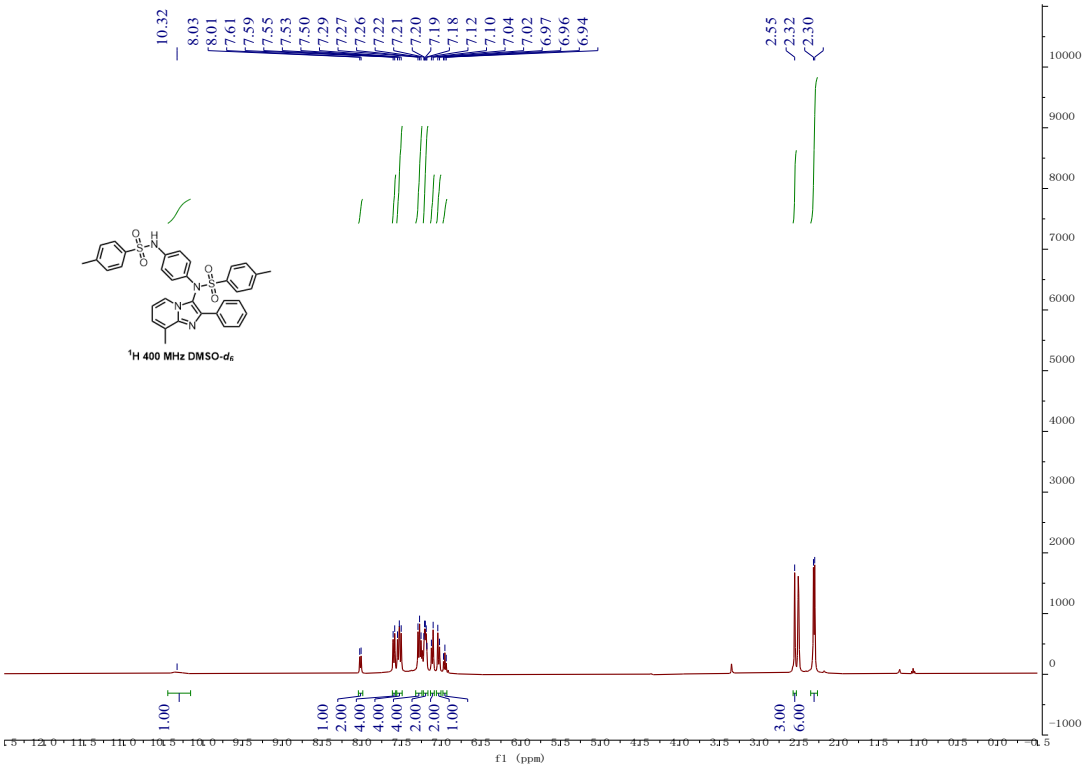

159.5
145.3
143.7
143.3
141.2
137.2
137.0
136.4
135.7
134.0
130.3
130.1
129.7
128.0
127.3
127.1
124.1
123.0
121.4
119.8
117.9
117.1
114.8
114.0
112.2
55.3
21.5
21.4
OMe
13C 100 MHz DMSO-d6
f1 (ppm)

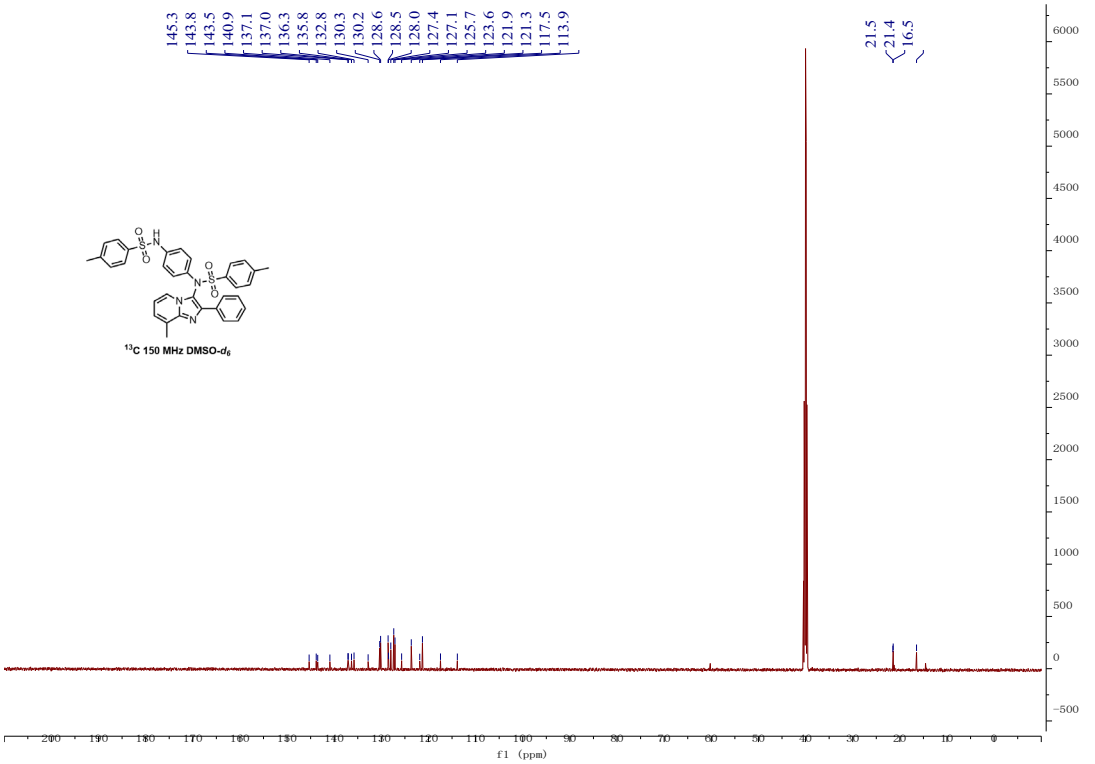
3g


10.35
8.20
8.19
7.66
7.63
7.61
7.54
7.52
7.46
7.44
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.37
7.28
7.26
7.19
7.18
7.17
7.16
7.09
7.07
7.04
7.02
7.00
6.98
2.29
2.26
0.98
0.97
3.00
2.00
2.00
1.04
2.02
3.98
1.99
2.98
9.00
1H 400 MHz DMSO-d6
f1 (ppm)

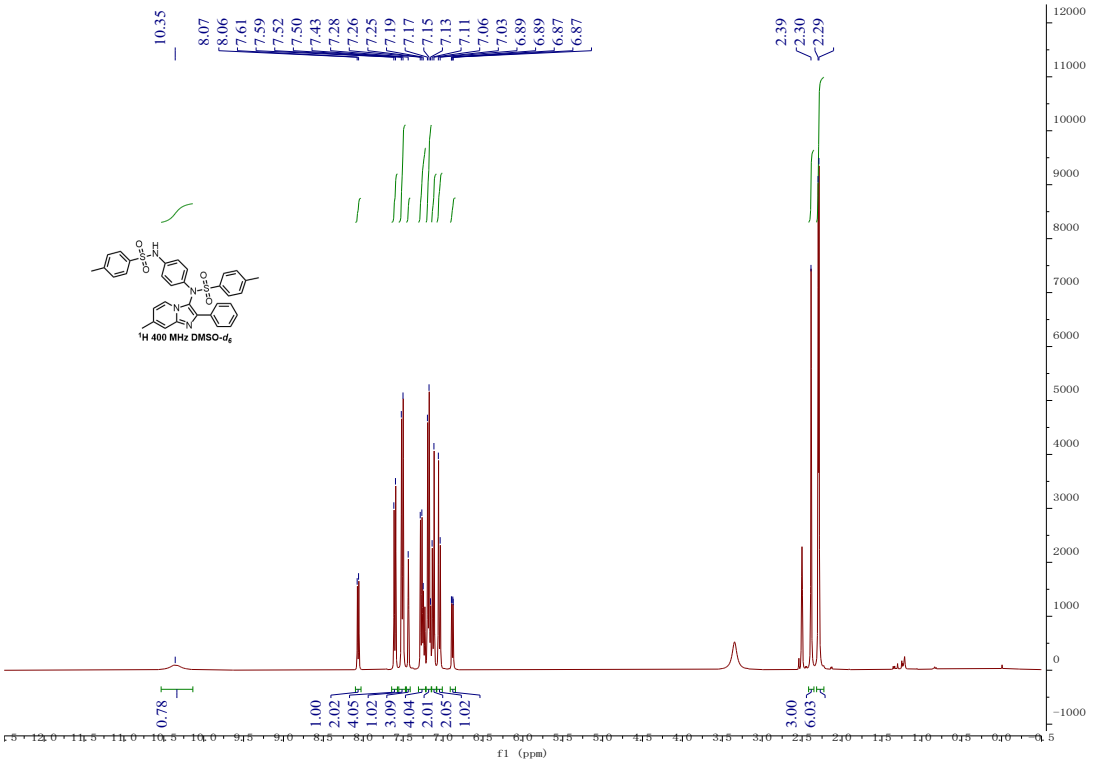

145.3
143.8
143.3
141.6
138.1
137.1
137.1
136.4
135.9
130.3
130.1
129.9
129.2
128.0
127.3
127.1
124.0
123.7
121.3
117.8
116.8
113.8
21.4
21.4
21.2
^{13}C 100 MHz DMSO-d_6
f1 (ppm)

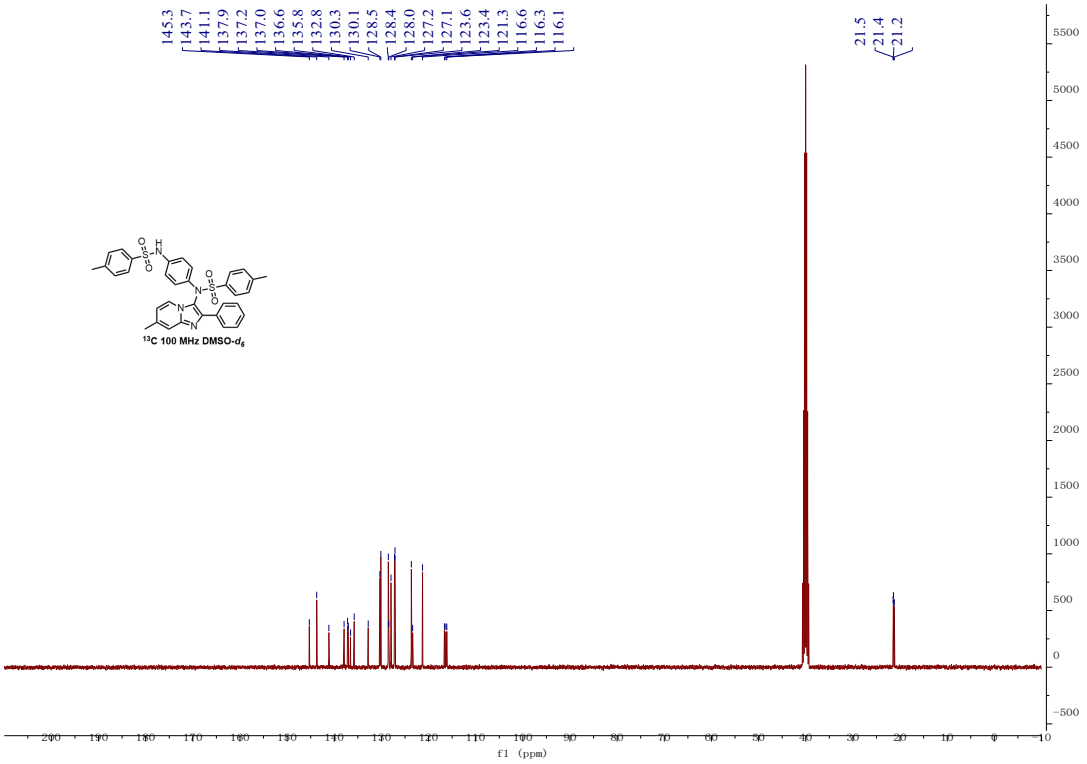
3h


10.32
8.03
8.01
7.61
7.59
7.55
7.53
7.50
7.29
7.27
7.26
7.22
7.21
7.20
7.19
7.18
7.12
7.10
7.04
7.02
6.97
6.96
6.94
2.55
2.32
2.30
1.00
1.00
2.00
4.00
4.00
4.00
2.00
2.00
1.00
3.00
6.00
^{1}H 400 MHz DMSO-d_6
f1 (ppm)

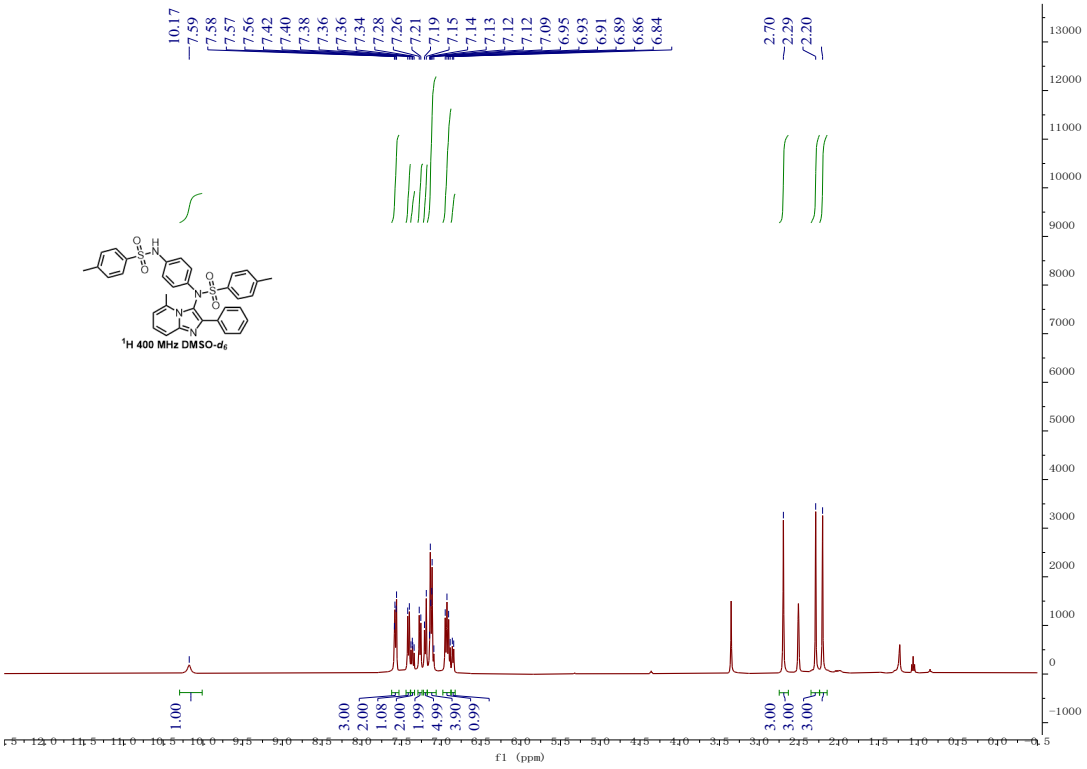

145.3
143.8
143.5
140.9
137.1
137.0
136.3
135.8
132.8
130.3
130.2
128.6
128.5
128.0
127.4
127.1
125.7
123.6
121.9
121.3
117.5
113.9
21.5
21.4
16.5
^{13}C 150 MHz DMSO-d_6
f1 (ppm)

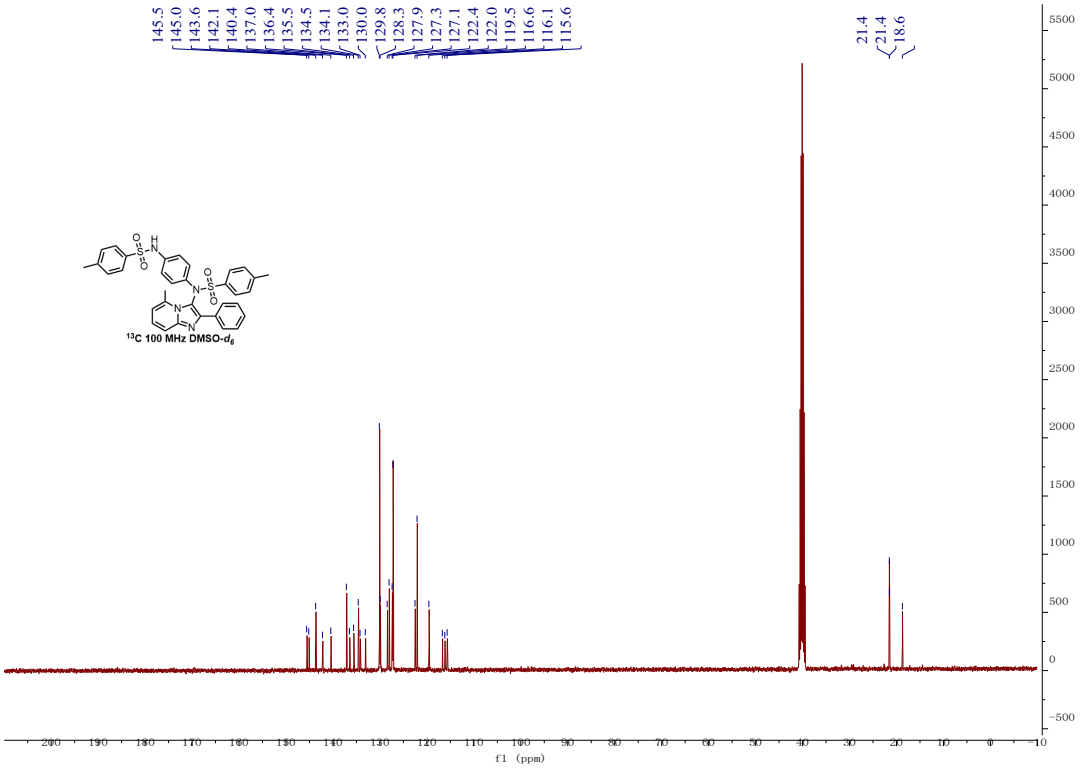
3i


10.35
8.07
8.06
7.61
7.59
7.52
7.50
7.43
7.28
7.26
7.25
7.19
7.17
7.15
7.13
7.11
7.06
7.03
6.89
6.89
6.87
6.87
2.39
2.30
2.29
0.78
1.00
2.02
4.05
1.02
3.09
4.04
2.01
2.05
1.02
3.00
6.03
^{1}H 400 MHz DMSO-d_6
f1 (ppm)

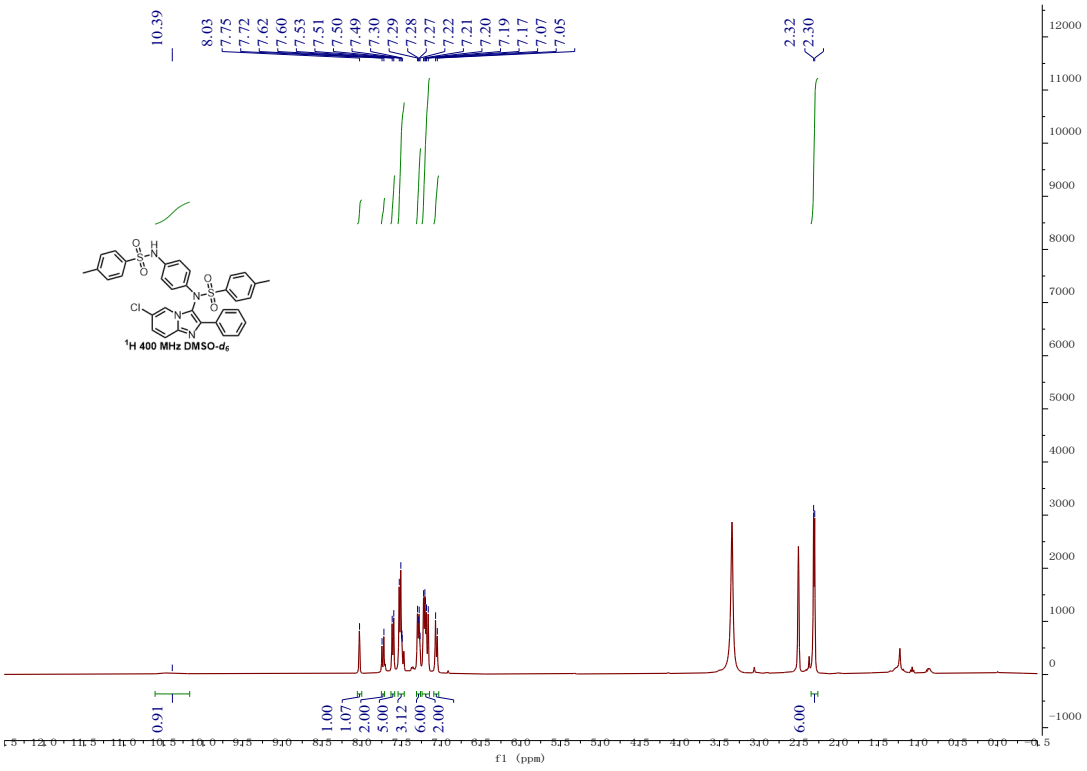

145.3
143.7
141.1
137.9
137.2
137.0
136.6
135.8
132.8
130.3
130.1
128.5
128.4
128.0
127.2
127.1
123.6
123.4
121.3
116.6
116.3
116.1
21.5
21.4
21.2
^{13}C 100 MHz DMSO-d_6
f1 (ppm)

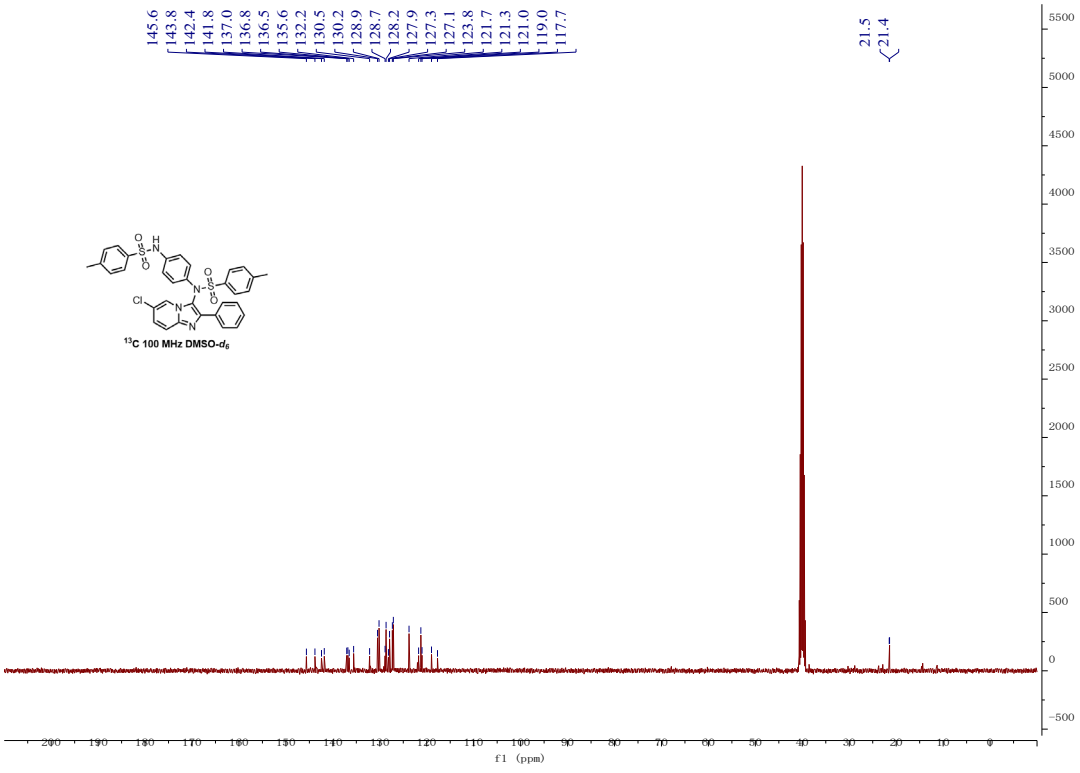
3j


10.17
7.59
7.58
7.57
7.56
7.42
7.40
7.38
7.36
7.36
7.34
7.28
7.26
7.21
7.19
7.15
7.14
7.13
7.12
7.12
7.09
6.95
6.93
6.91
6.89
6.86
6.84
2.70
2.29
2.20
1.00
3.00
2.00
1.08
2.00
1.99
4.99
3.90
0.99
3.00
3.00
3.00
^{1}H 400 MHz DMSO-d_6
f1 (ppm)

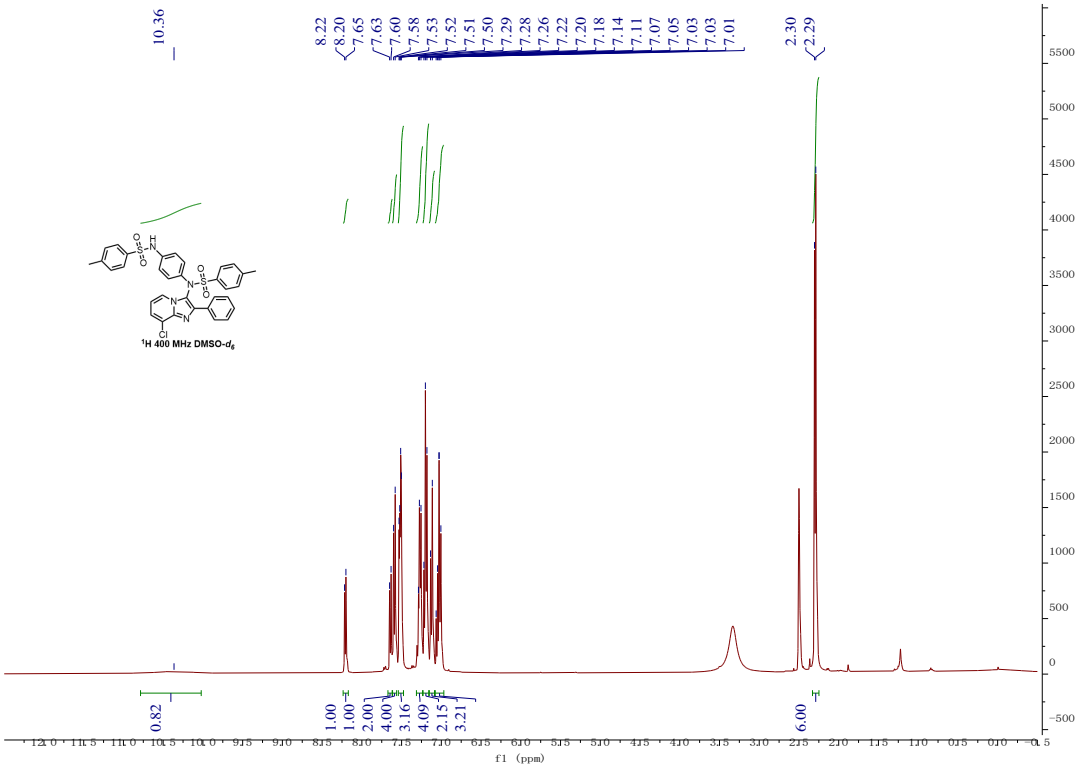

145.5
145.0
143.6
142.1
140.4
137.0
136.4
135.5
134.5
134.1
133.0
130.0
129.8
128.3
127.9
127.3
127.1
122.4
122.0
119.5
116.6
116.1
115.6
21.4
21.4
18.6
13C 100 MHz DMSO-d6
f1 (ppm)

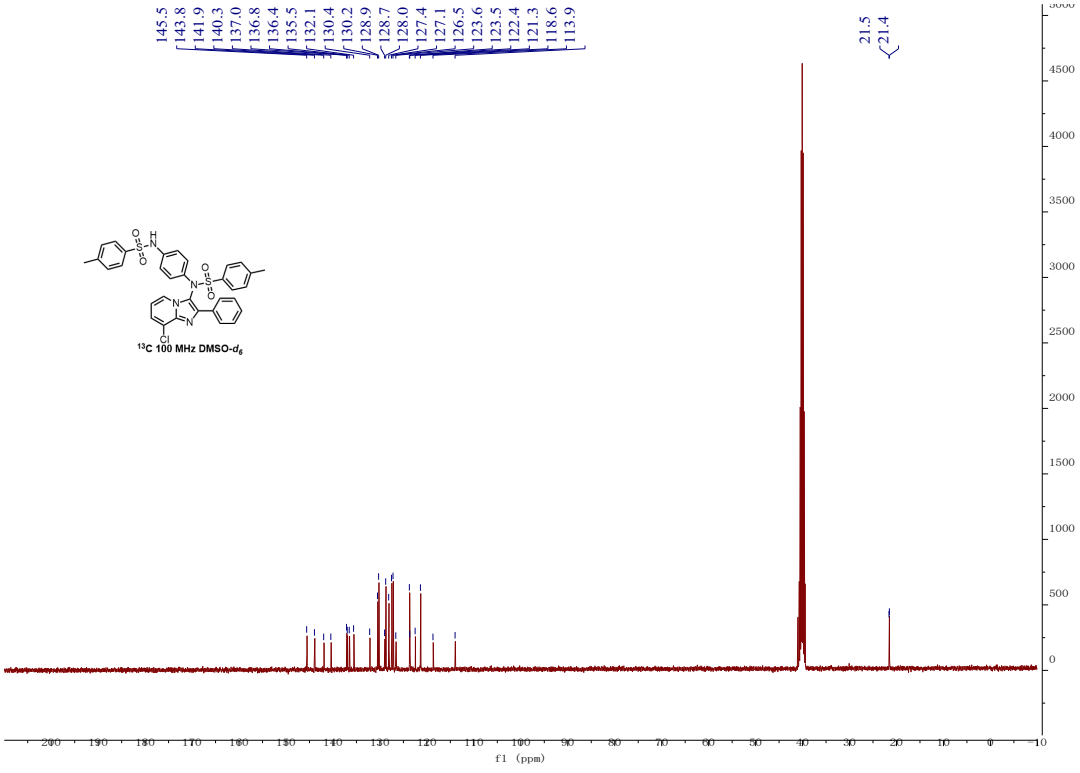
3k


10.39
8.03
7.75
7.72
7.62
7.60
7.53
7.51
7.50
7.49
7.30
7.29
7.28
7.27
7.22
7.21
7.20
7.19
7.17
7.07
7.05
2.32
2.30
0.91
1.00
1.07
2.00
5.00
3.12
6.00
2.00
6.00
1H 400 MHz DMSO-d6
f1 (ppm)

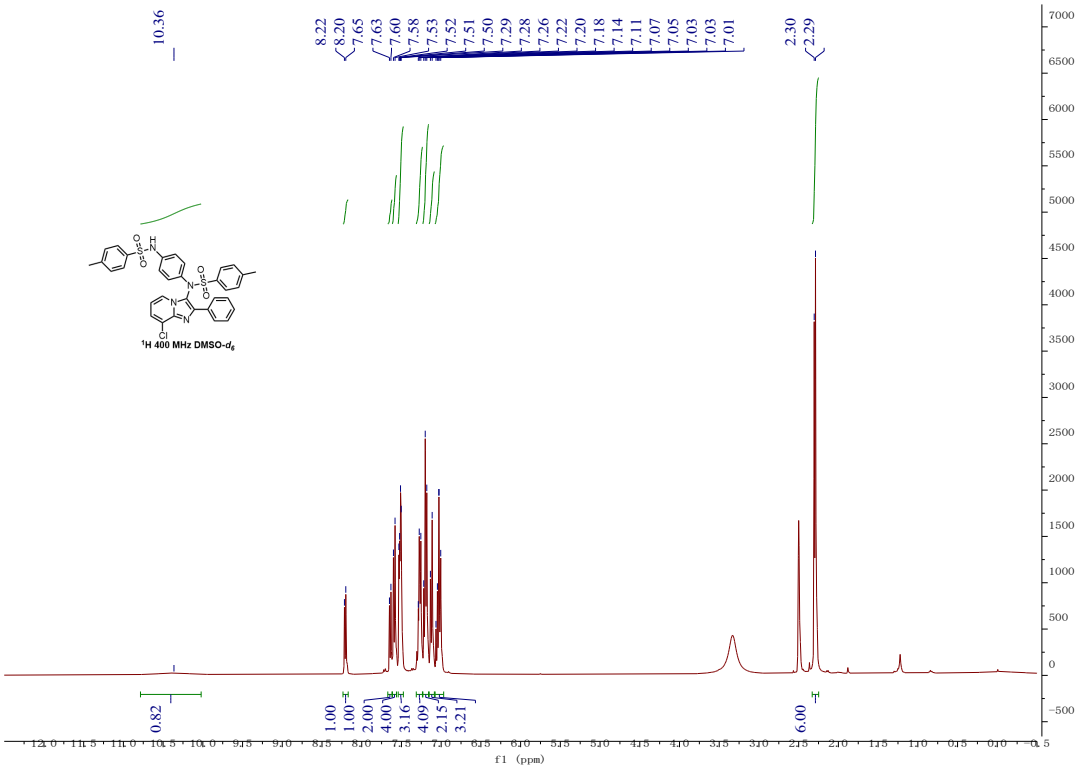

145.6
143.8
142.4
141.8
137.0
136.8
136.5
135.6
132.2
130.5
130.2
128.9
128.7
128.2
127.9
127.3
127.1
123.8
121.7
121.3
121.0
119.0
117.7
21.5
21.4
13C 100 MHz DMSO-d6
f1 (ppm)

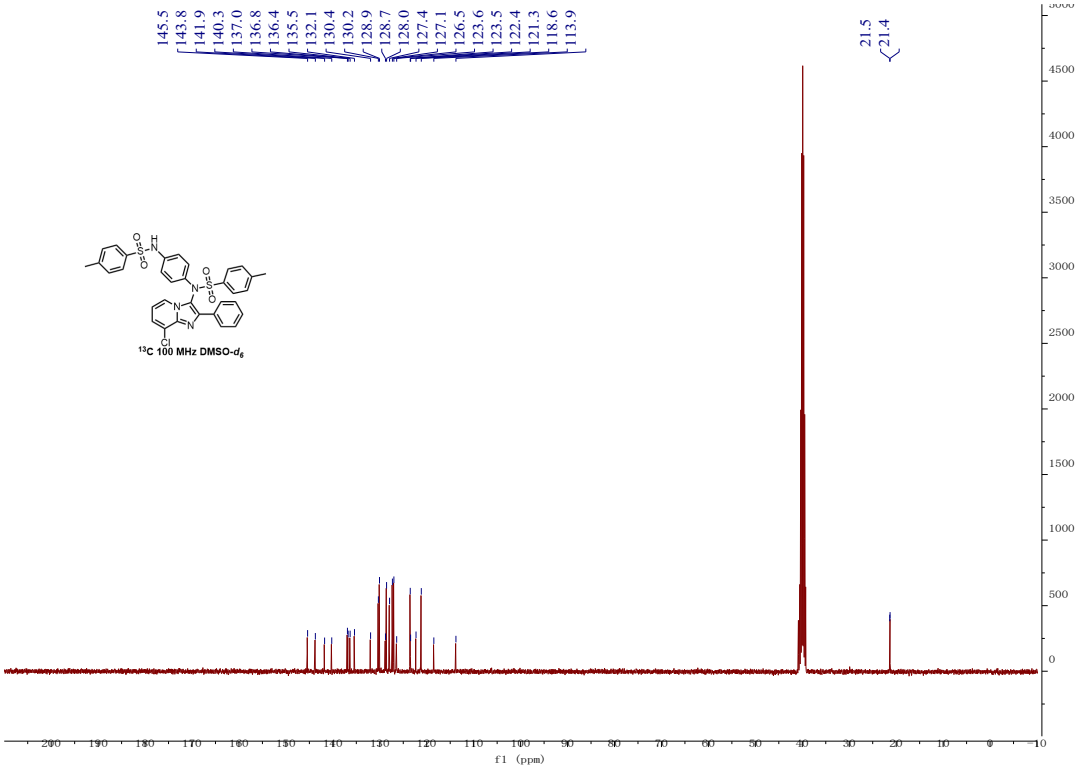
3l


10.36
8.22
8.20
7.65
7.63
7.60
7.58
7.53
7.52
7.51
7.50
7.29
7.28
7.26
7.22
7.20
7.18
7.14
7.11
7.07
7.05
7.03
7.03
7.01
2.30
2.29
1H 400 MHz DMSO-d6
0.82
1.00
1.00
2.00
4.00
3.16
4.09
2.15
3.21
6.00
f1 (ppm)

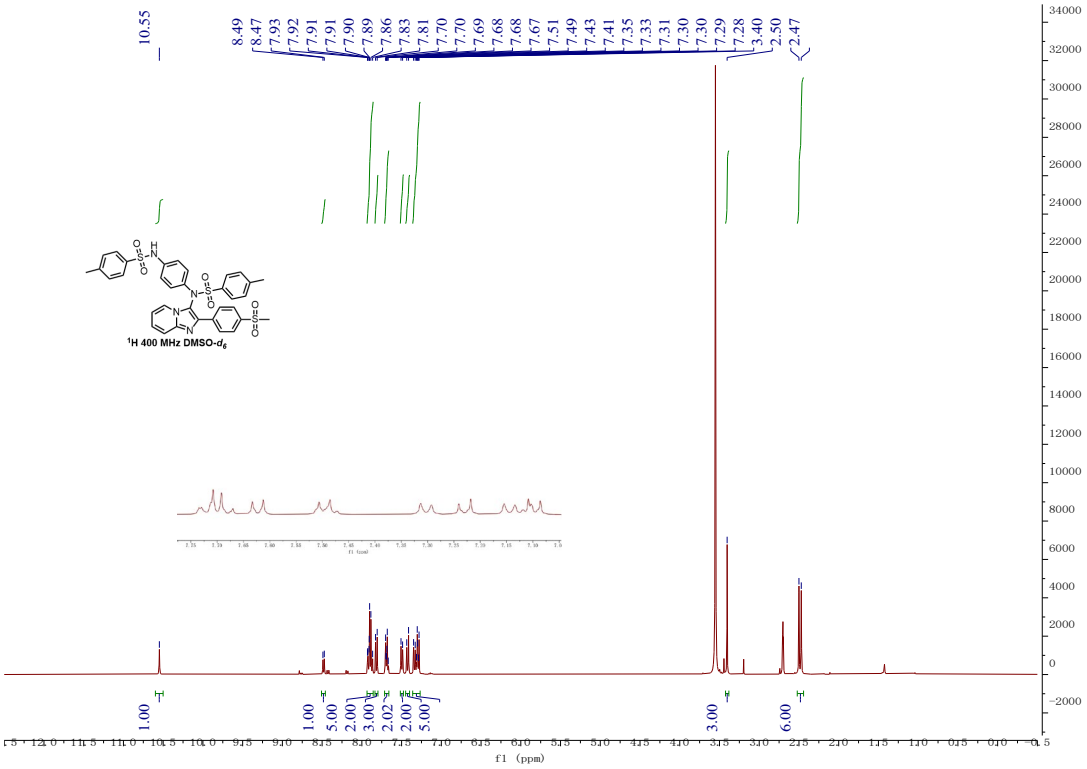

145.5
143.8
141.9
140.3
137.0
136.8
136.4
135.5
132.1
130.4
130.2
128.9
128.7
128.0
127.4
127.1
126.5
123.6
123.5
122.4
121.3
118.6
113.9
21.5
21.4
13C 100 MHz DMSO-d6
f1 (ppm)

3m


10.36
8.22
8.20
7.65
7.63
7.60
7.58
7.53
7.52
7.51
7.50
7.29
7.28
7.26
7.22
7.20
7.18
7.14
7.11
7.07
7.05
7.03
7.03
7.01
2.30
2.29
0.82
1.00
1.00
2.00
4.00
3.16
4.09
2.15
3.21
6.00
1H 400 MHz DMSO-d6
f1 (ppm)


145.5
143.8
141.9
140.3
137.0
136.8
136.4
135.5
132.1
130.4
130.2
128.9
128.7
128.0
127.4
127.1
126.5
123.6
123.5
122.4
121.3
118.6
113.9
21.5
21.4
13C 100 MHz DMSO-d6
f1 (ppm)

3n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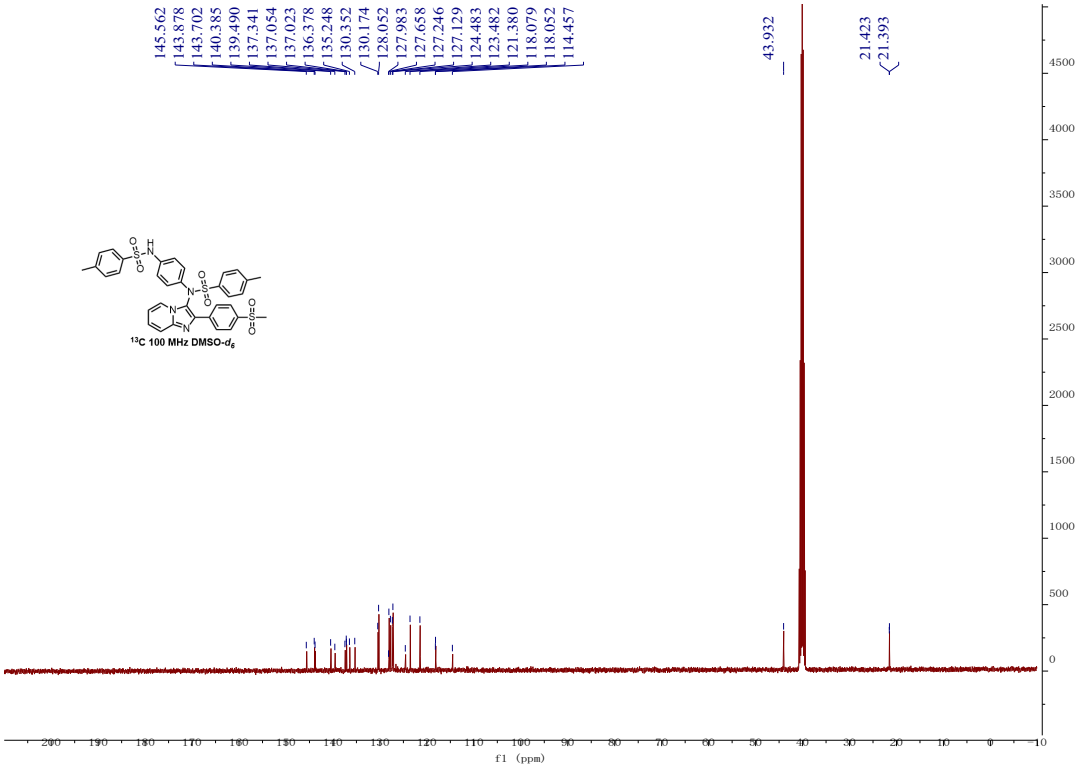
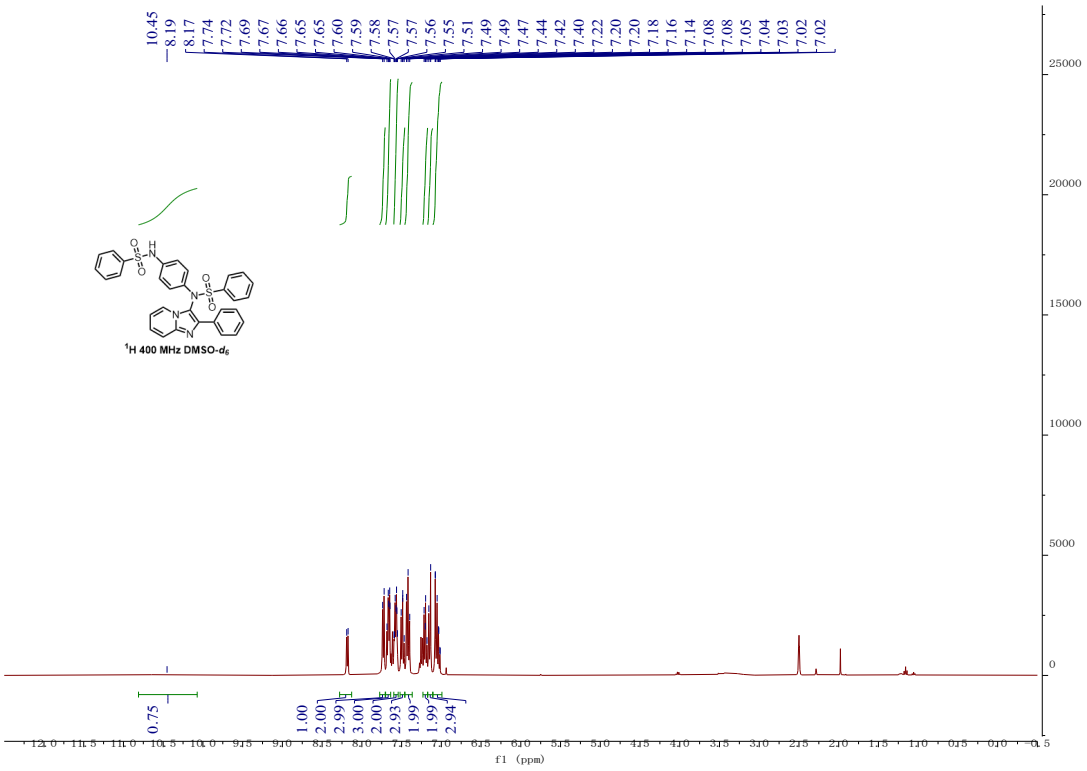
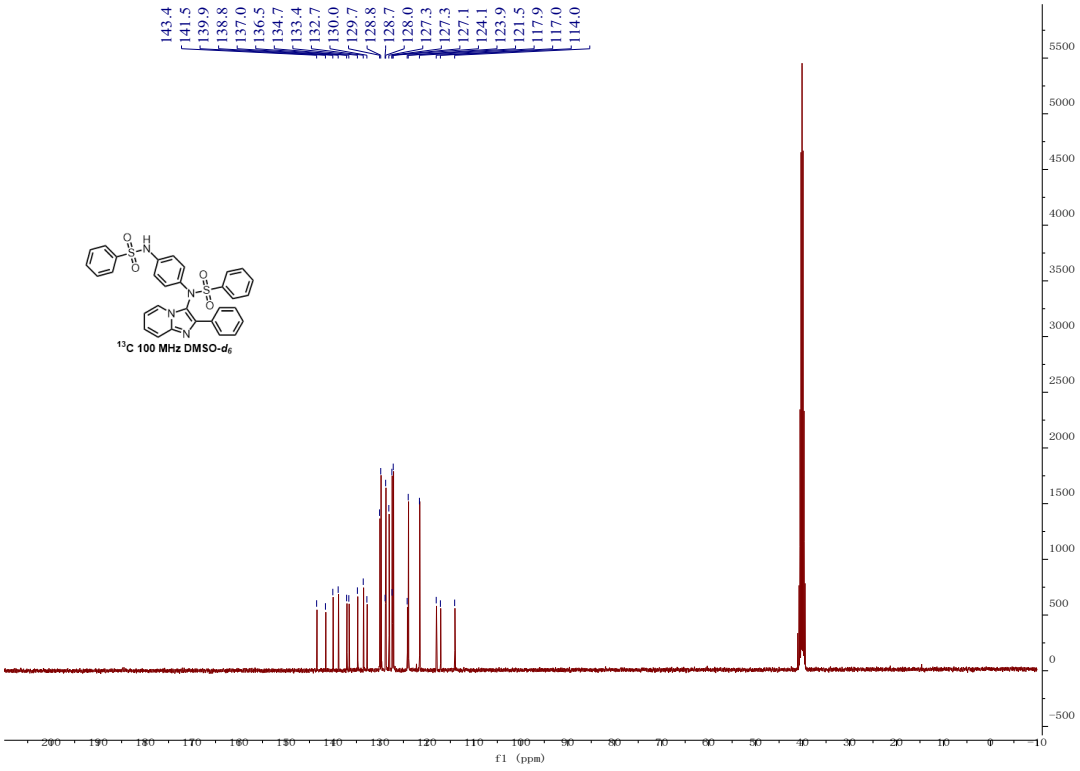
8.47
7.93
7.92
7.91
7.91
7.90
7.89
7.86
7.83
7.81
7.70
7.70
7.69
7.68
7.68
7.67
7.51
7.49
7.43
7.41
7.35
7.33
7.31
7.30
7.30
7.29
7.28
3.40
2.50
2.47
1H 400 MHz DMSO-d6
1.00
1.00
5.00
2.00
3.00
2.02
2.00
5.00
3.00
6.00
f1 (ppm)

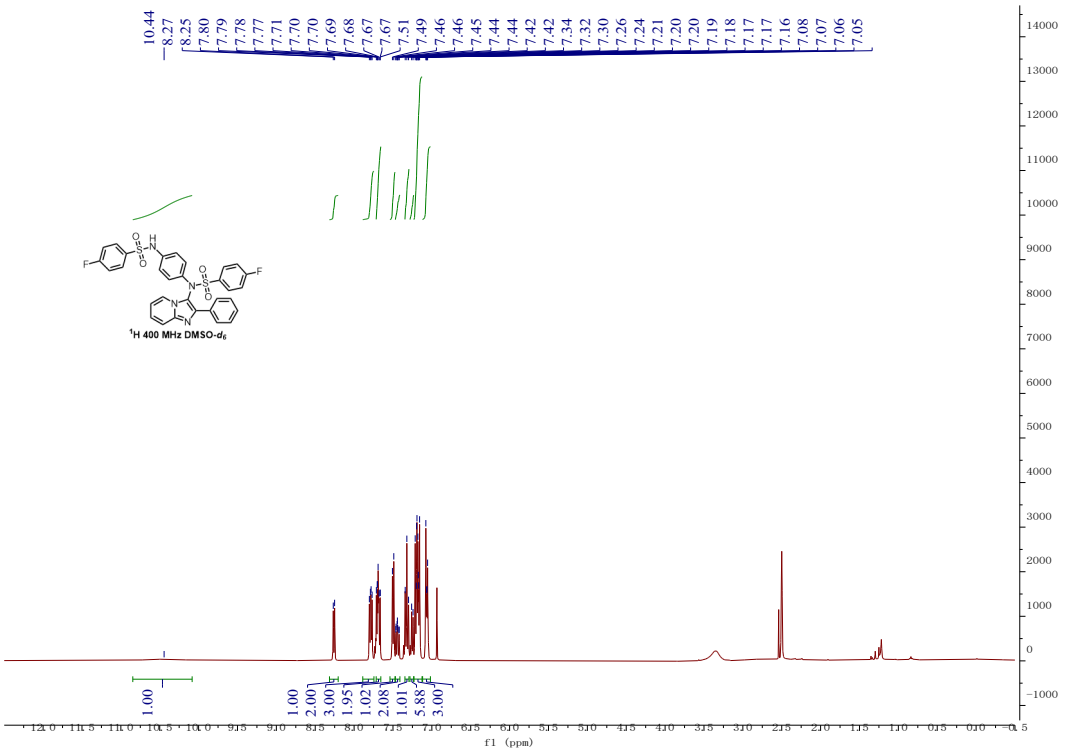

145.562
143.878
143.702
140.385
139.490
137.341
137.054
137.023
136.378
135.248
130.352
130.174
128.052
127.983
127.658
127.246
127.129
124.483
123.482
121.380
118.079
118.052
114.457
43.932
21.423
21.393
13C 100 MHz DMSO-d6
f1 (ppm)

3o


10.45
8.19
8.17
7.74
7.72
7.69
7.67
7.66
7.65
7.65
7.60
7.59
7.58
7.57
7.57
7.56
7.55
7.51
7.49
7.49
7.47
7.44
7.42
7.40
7.22
7.20
7.20
7.18
7.16
7.14
7.08
7.08
7.05
7.04
7.03
7.02
7.02
0.75
1.00
2.00
2.99
3.00
2.00
2.93
1.99
1.99
2.94
1H 400 MHz DMSO-d6
f1 (ppm)


143.4
141.5
139.9
138.8
137.0
136.5
134.7
133.4
132.7
130.0
129.7
128.8
128.7
128.0
127.3
127.3
127.1
124.1
123.9
121.5
117.9
117.0
114.0
13C 100 MHz DMSO-d6
f1 (ppm)

3p


10.44
8.27
8.25
7.80
7.79
7.78
7.77
7.71
7.70
7.70
7.69
7.68
7.67
7.67
7.51
7.49
7.46
7.46
7.45
7.44
7.44
7.42
7.42
7.34
7.32
7.30
7.26
7.24
7.21
7.20
7.20
7.19
7.18
7.17
7.17
7.16
7.08
7.07
7.06
7.05
1.00
1.00
2.00
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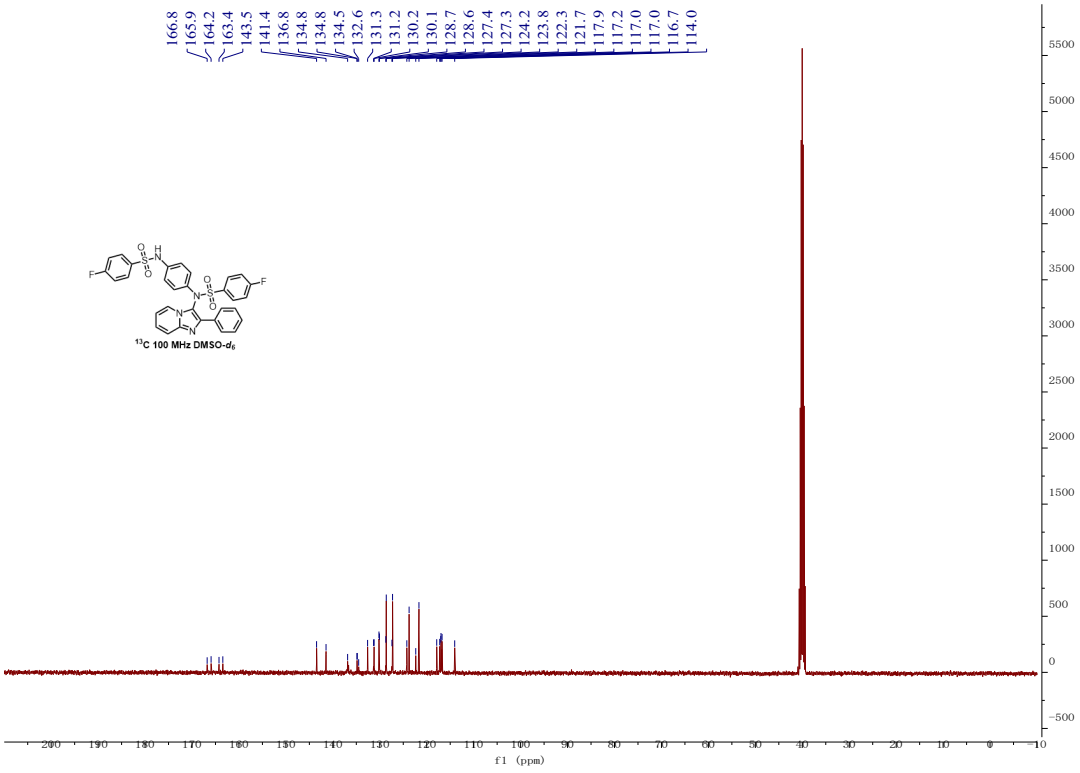
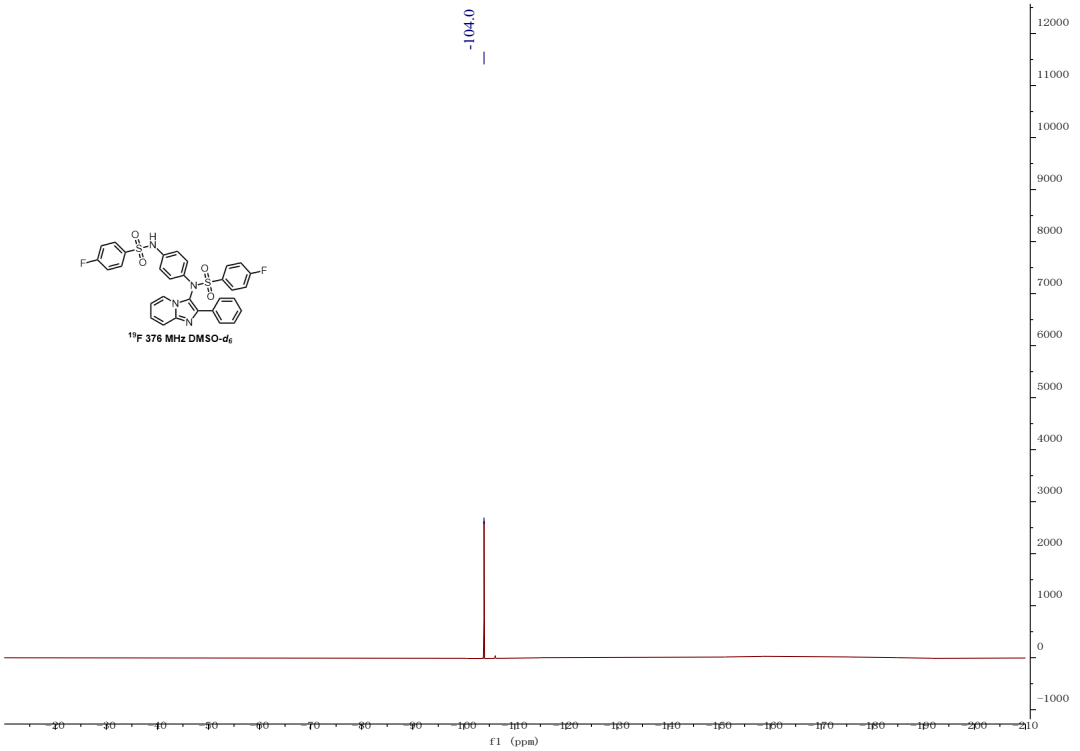
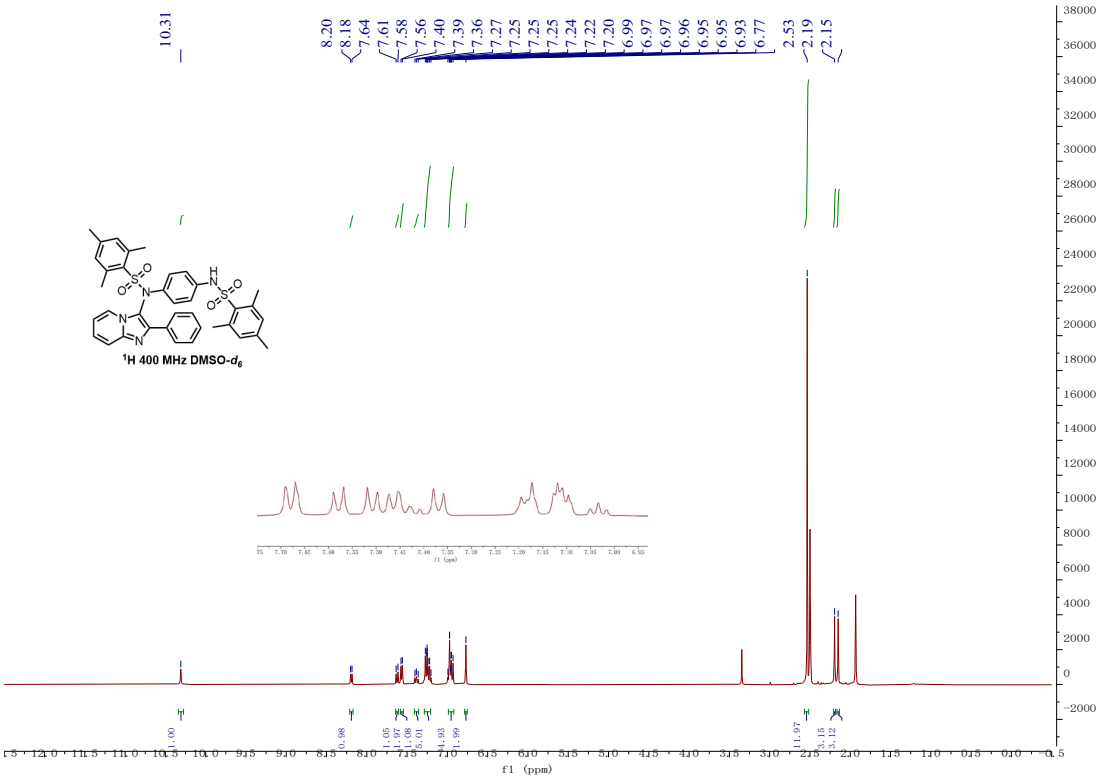
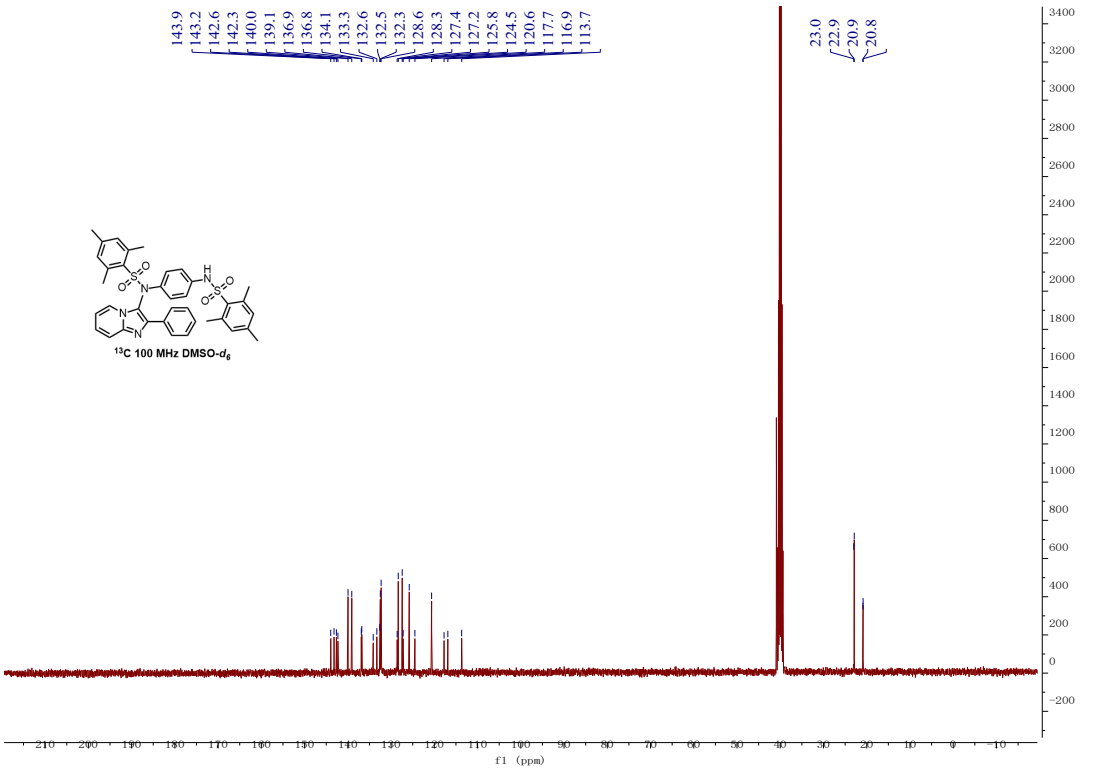
1.95
1.02
2.08
1.01
5.88
3.00
1H 400 MHz DMSO-d6
f1 (ppm)


166.8
165.9
164.2
163.4
143.5
141.4
136.8
134.8
134.8
134.5
132.6
131.3
131.2
130.2
130.1
128.7
128.6
127.4
127.3
124.2
123.8
122.3
121.7
117.9
117.2
117.0
117.0
116.7
114.0
^{13}C 100 MHz DMSO-d_6
f1 (ppm)

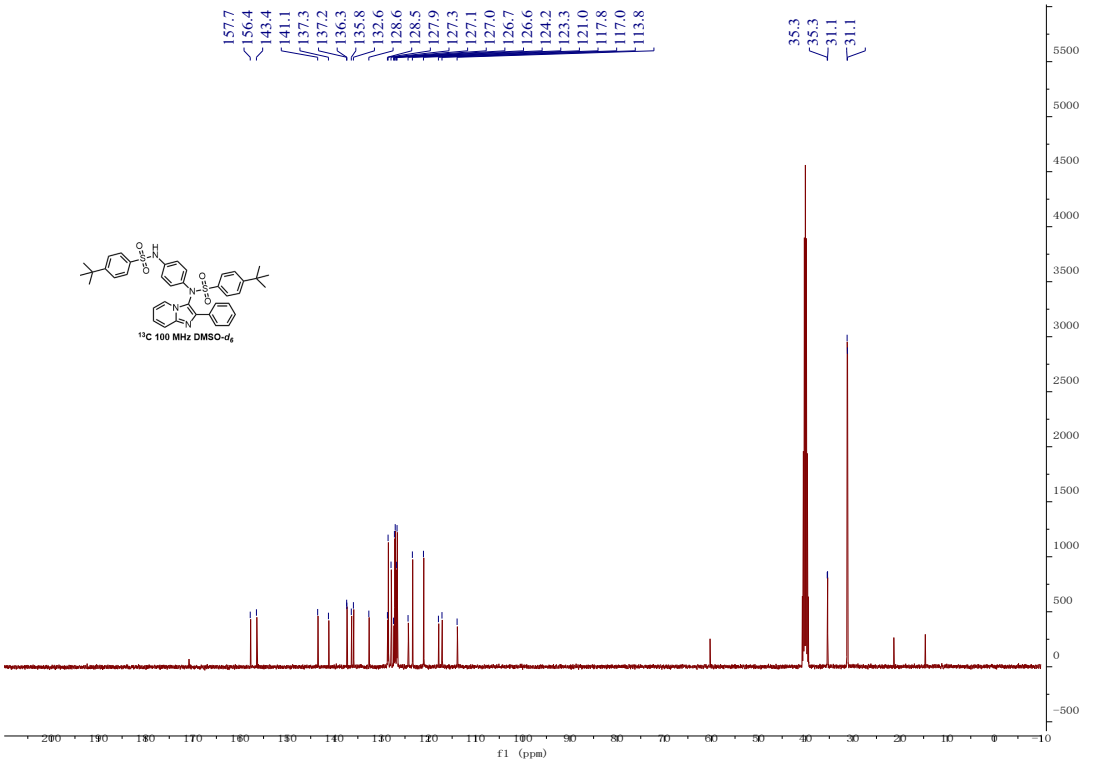

-104.0
^{19}F 376 MHz DMSO-d_6
f1 (ppm)

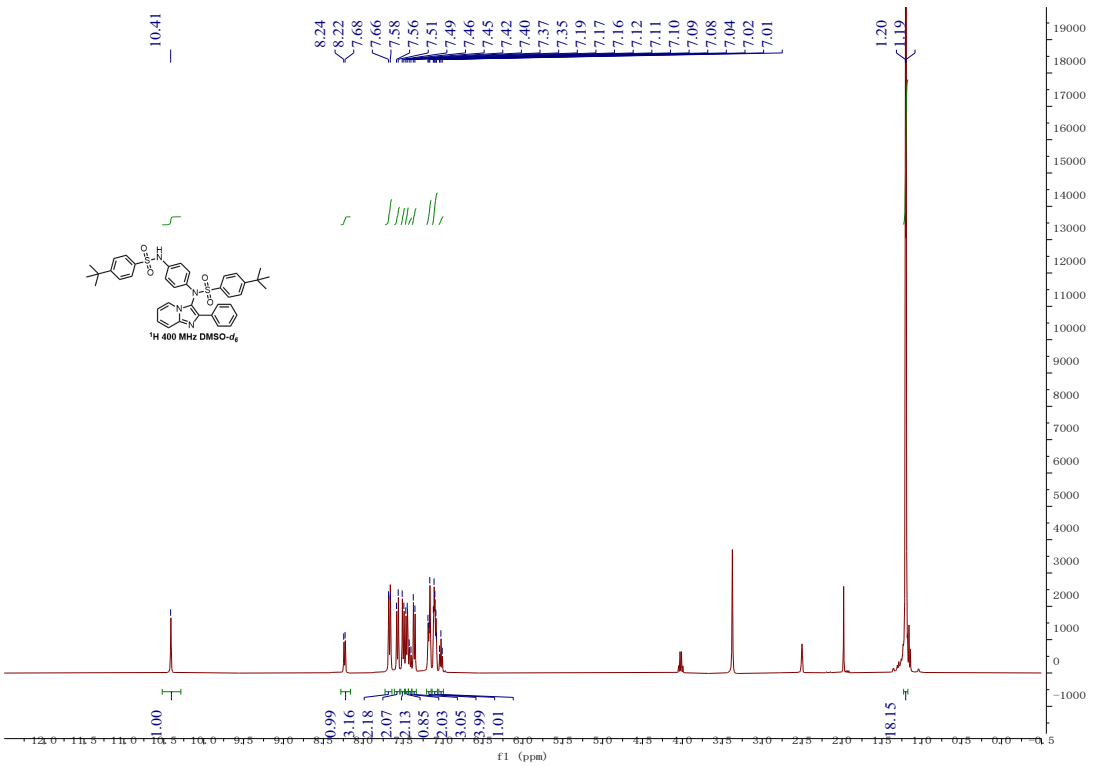
3q


10.31
8.20
8.18
7.64
7.61
7.58
7.56
7.40
7.39
7.36
7.27
7.25
7.25
7.25
7.24
7.22
7.20
6.99
6.97
6.97
6.96
6.95
6.95
6.93
6.77
2.53
2.19
2.15
1.00
0.98
1.05
1.97
0.98
5.01
4.93
1.99
11.97
5.15
5.12
f1 (ppm)
^{1}H 400 MHz DMSO-d_6

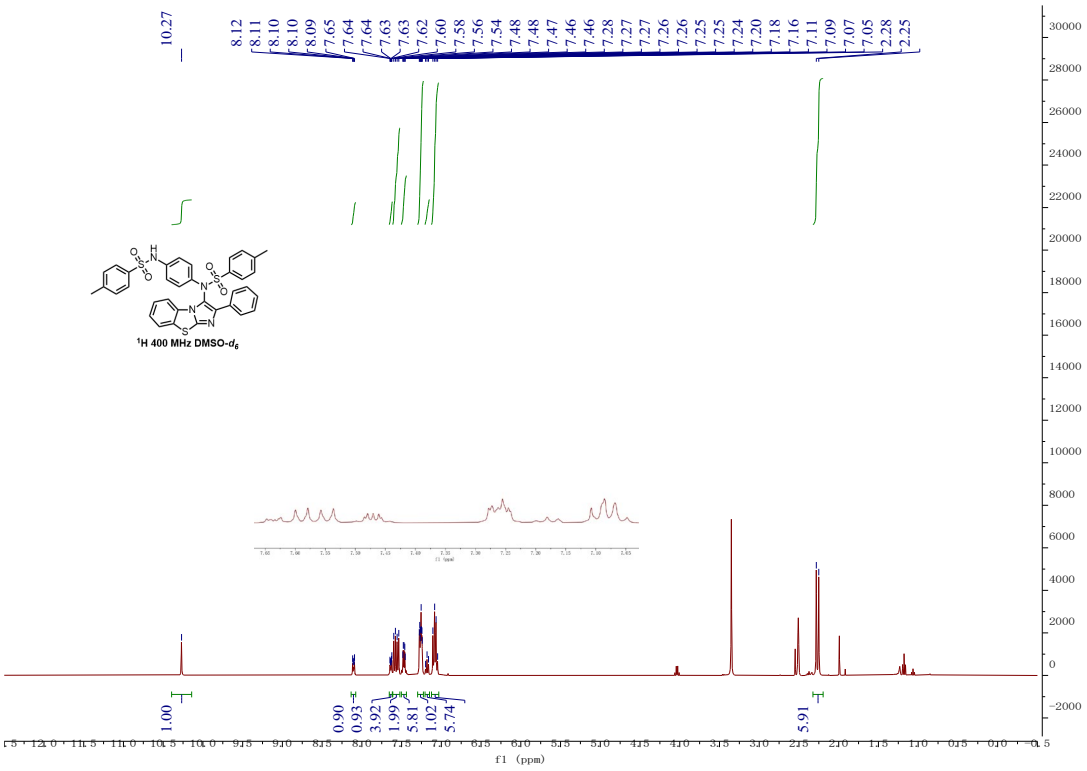

143.9
143.2
142.6
142.3
140.0
139.1
136.9
136.8
134.1
133.3
132.6
132.5
132.3
128.6
128.3
127.4
127.2
125.8
124.5
120.6
117.7
116.9
113.7
23.0
22.9
20.9
20.8
f1 (ppm)
^{13}C 100 MHz DMSO-d_6

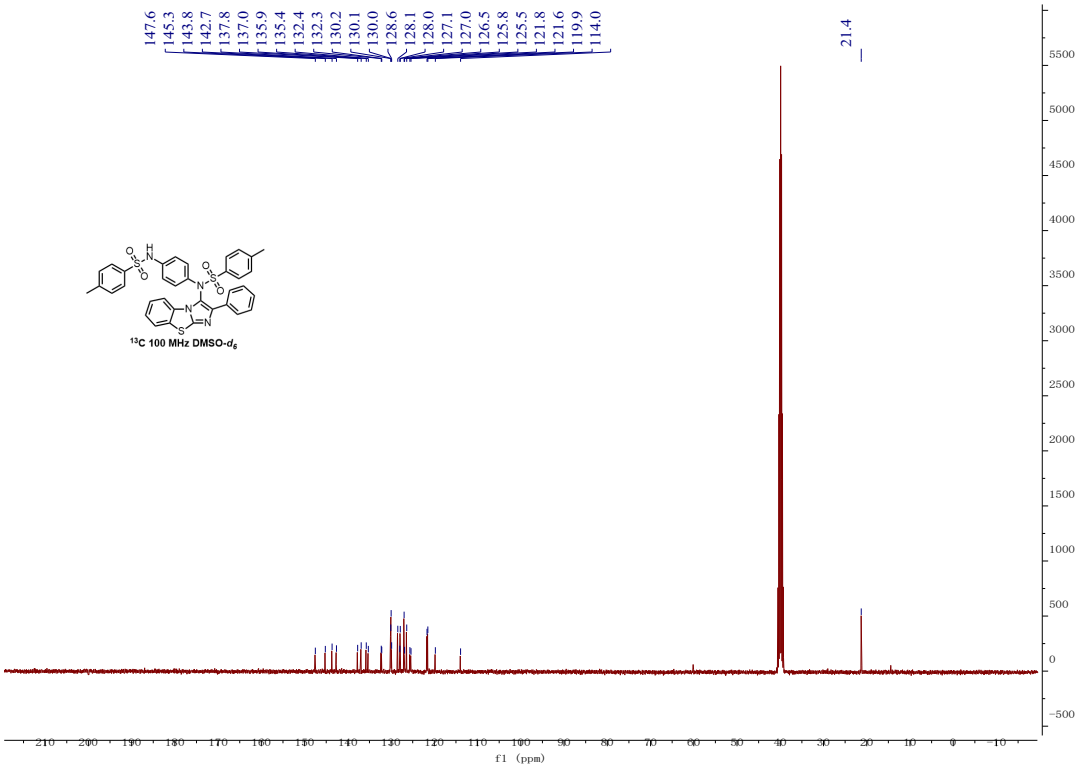
3r


157.7
156.4
143.4
141.1
137.3
137.2
136.3
135.8
132.6
128.6
128.5
127.9
127.3
127.1
127.0
126.7
126.6
124.2
123.3
121.0
117.8
117.0
113.8
35.3
35.3
31.1
31.1
^{13}C 100 MHz DMSO-d_6
f1 (ppm)

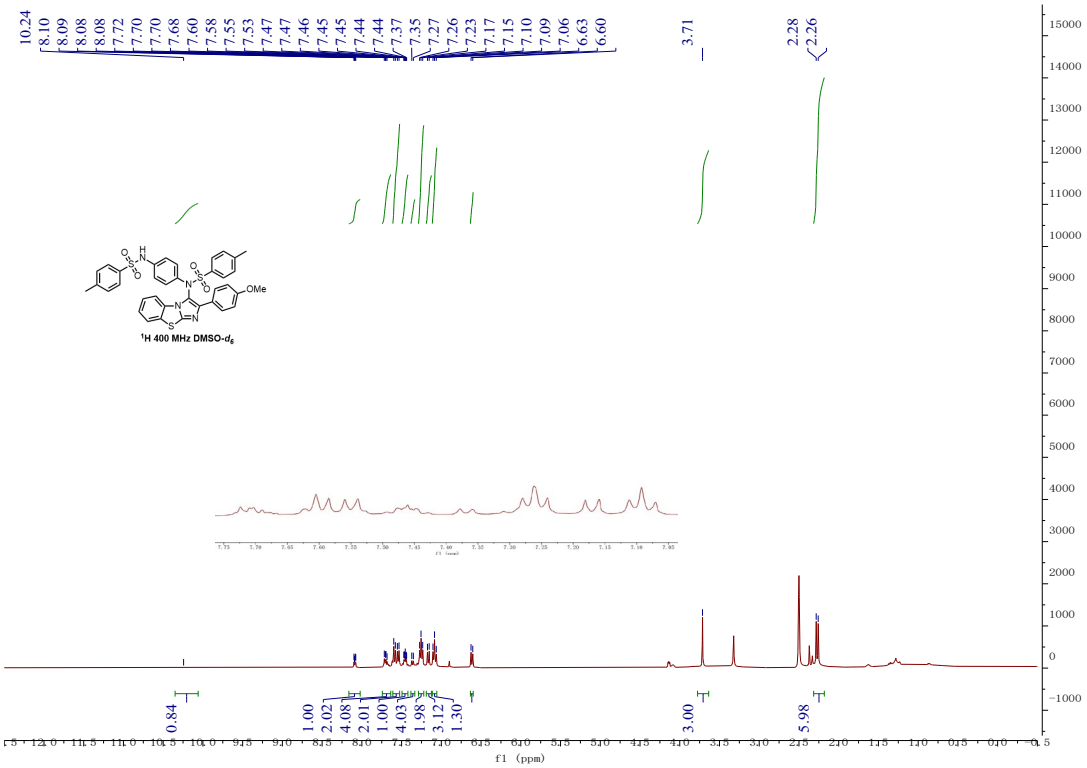

10.41
8.24
8.22
7.68
7.66
7.58
7.56
7.51
7.49
7.46
7.45
7.42
7.40
7.37
7.35
7.19
7.17
7.16
7.12
7.11
7.10
7.09
7.08
7.04
7.02
7.01
1.20
1.19
1.00
0.99
3.16
2.18
2.07
2.13
0.85
2.03
3.05
3.99
1.01
18.15
^{1}H 400 MHz DMSO-d_6
f1 (ppm)

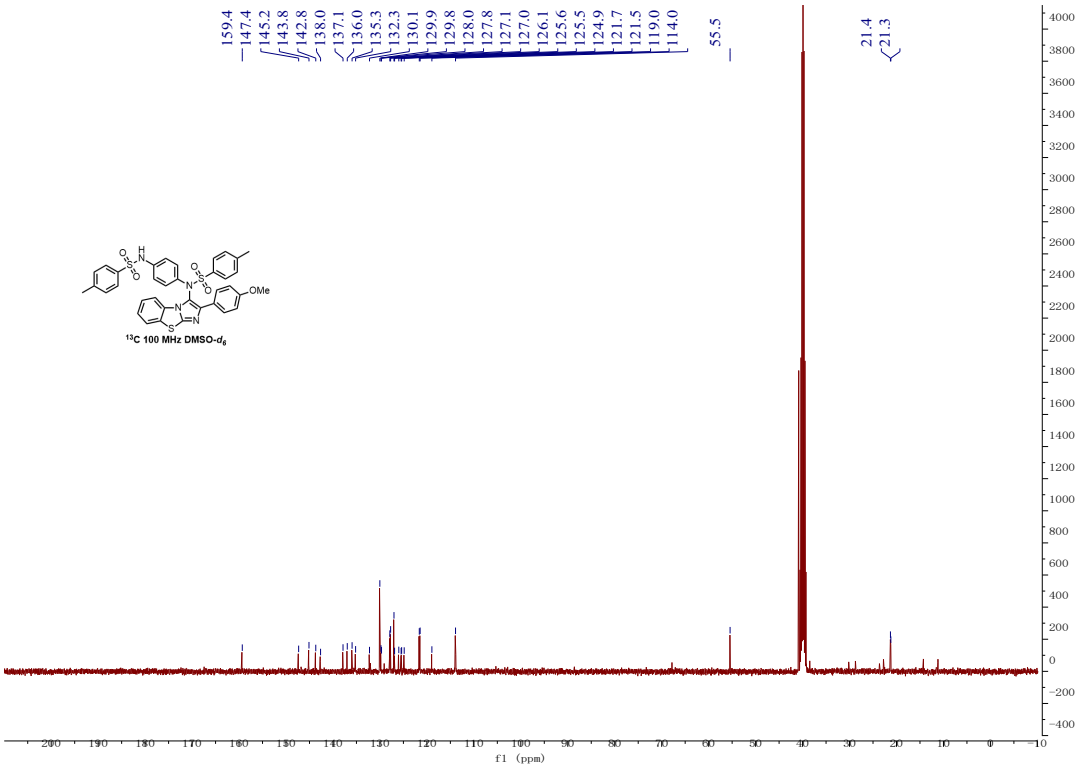
3s


10.27
8.12
8.11
8.10
8.10
8.09
7.65
7.64
7.64
7.63
7.63
7.62
7.60
7.58
7.56
7.54
7.48
7.48
7.47
7.46
7.46
7.28
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.20
7.18
7.16
7.11
7.09
7.07
7.05
2.28
2.25
1.00
0.90
0.93
3.92
1.99
5.81
1.02
5.74
5.91
f1 (ppm)

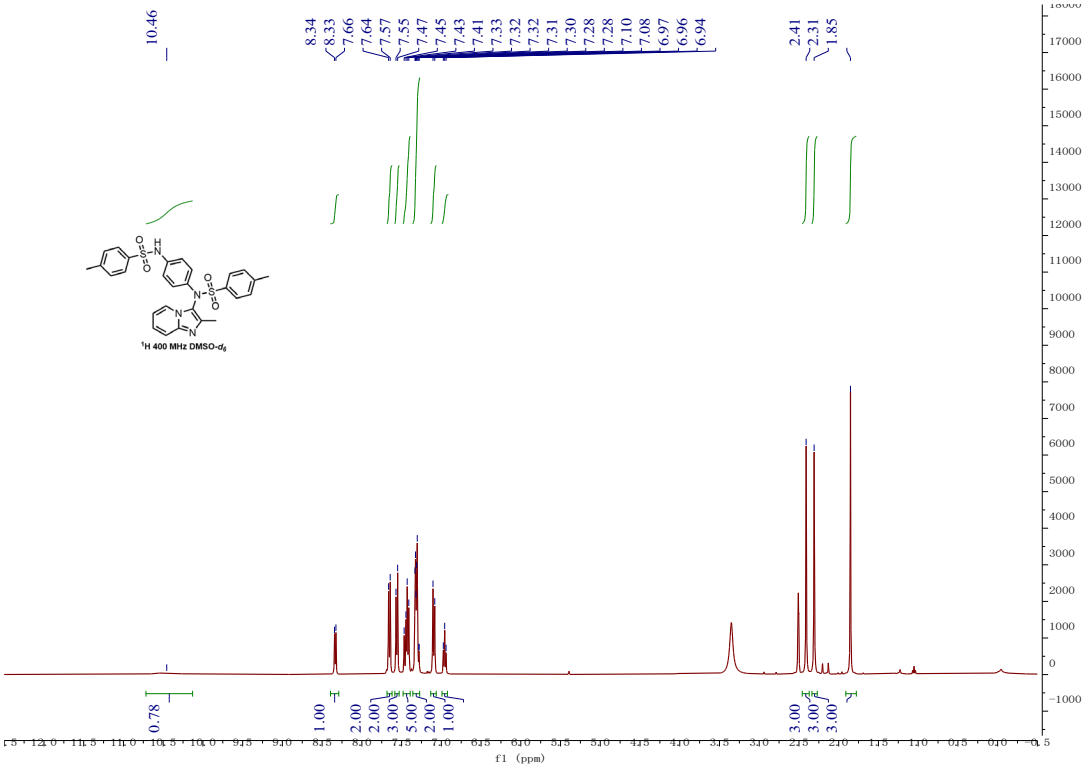

147.6
145.3
143.8
142.7
137.8
137.0
135.9
135.4
132.4
132.3
130.2
130.1
130.0
128.6
128.1
128.0
127.1
127.0
126.5
125.8
125.5
121.8
121.6
119.9
114.0
21.4
f1 (ppm)

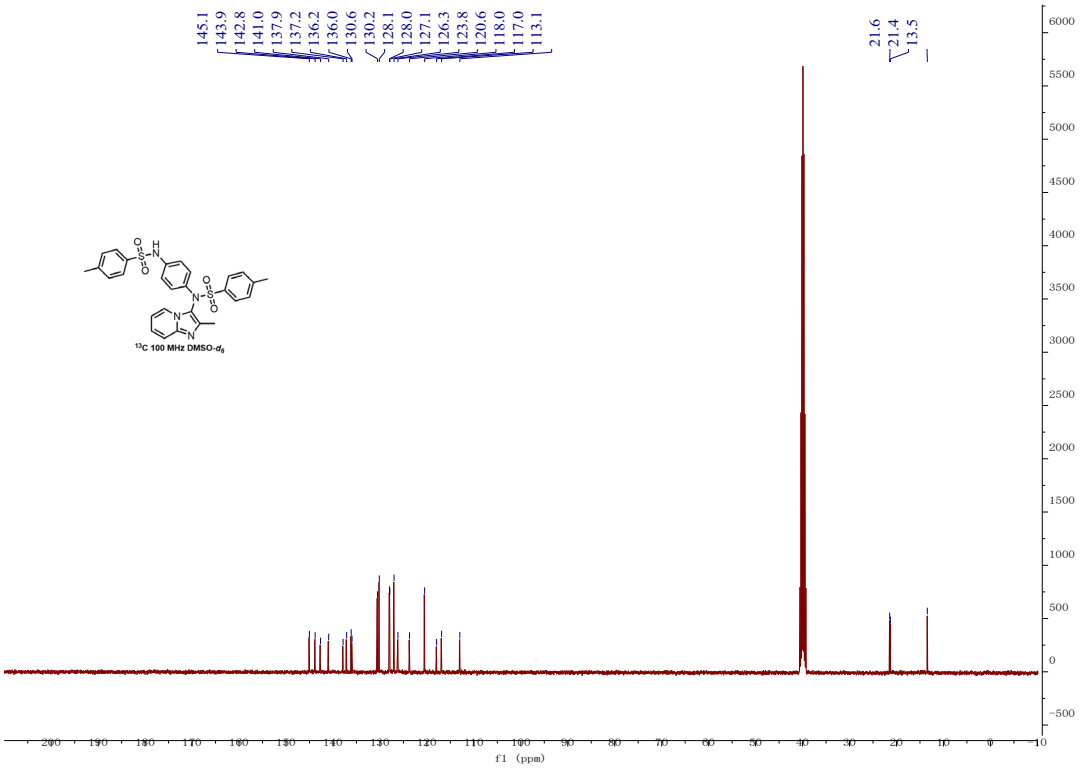
3t


10.24
8.10
8.09
8.08
8.08
7.72
7.70
7.70
7.68
7.60
7.58
7.55
7.53
7.47
7.47
7.46
7.45
7.45
7.44
7.44
7.37
7.35
7.27
7.26
7.23
7.17
7.15
7.10
7.09
7.06
6.63
6.60
3.71
2.28
2.26
OMe
1H 400 MHz DMSO-d6
0.84
1.00
2.02
4.08
2.01
1.00
4.03
1.98
3.12
1.30
3.00
5.98
f1 (ppm)

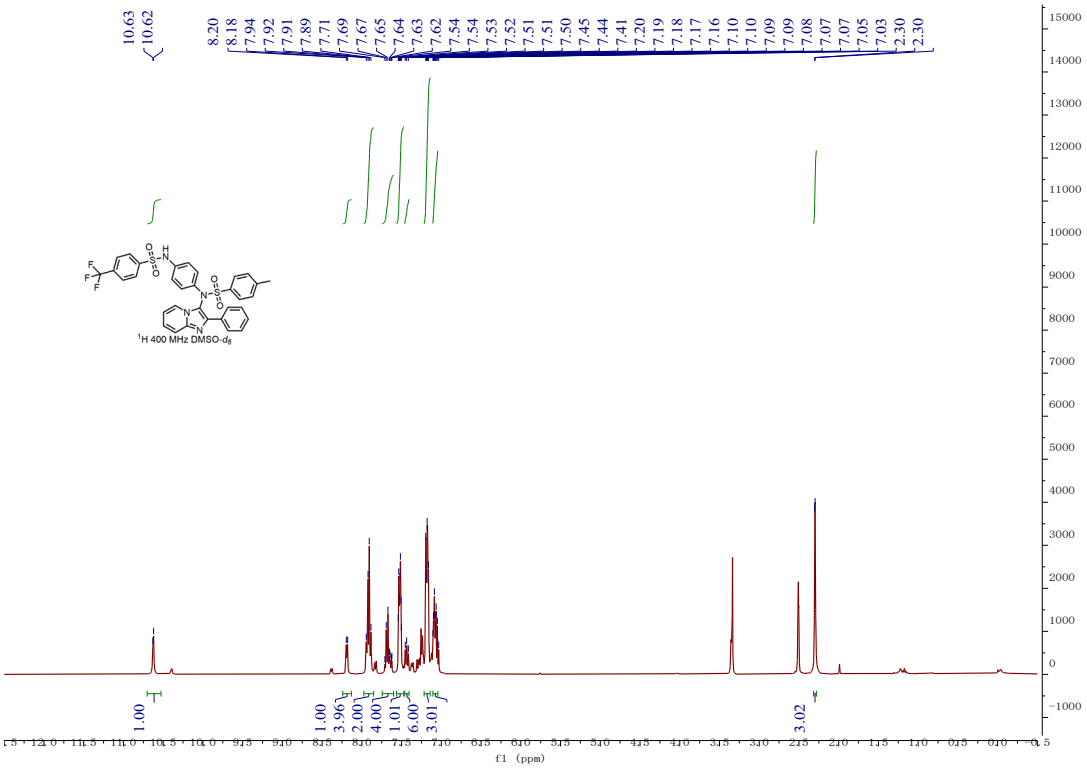

159.4
147.4
145.2
143.8
142.8
138.0
137.1
136.0
135.3
132.3
130.1
129.9
129.8
128.0
127.8
127.1
127.0
126.1
125.6
125.5
124.9
121.7
121.5
119.0
114.0
55.5
21.4
21.3
OMe
13C 100 MHz DMSO-d6
f1 (ppm)

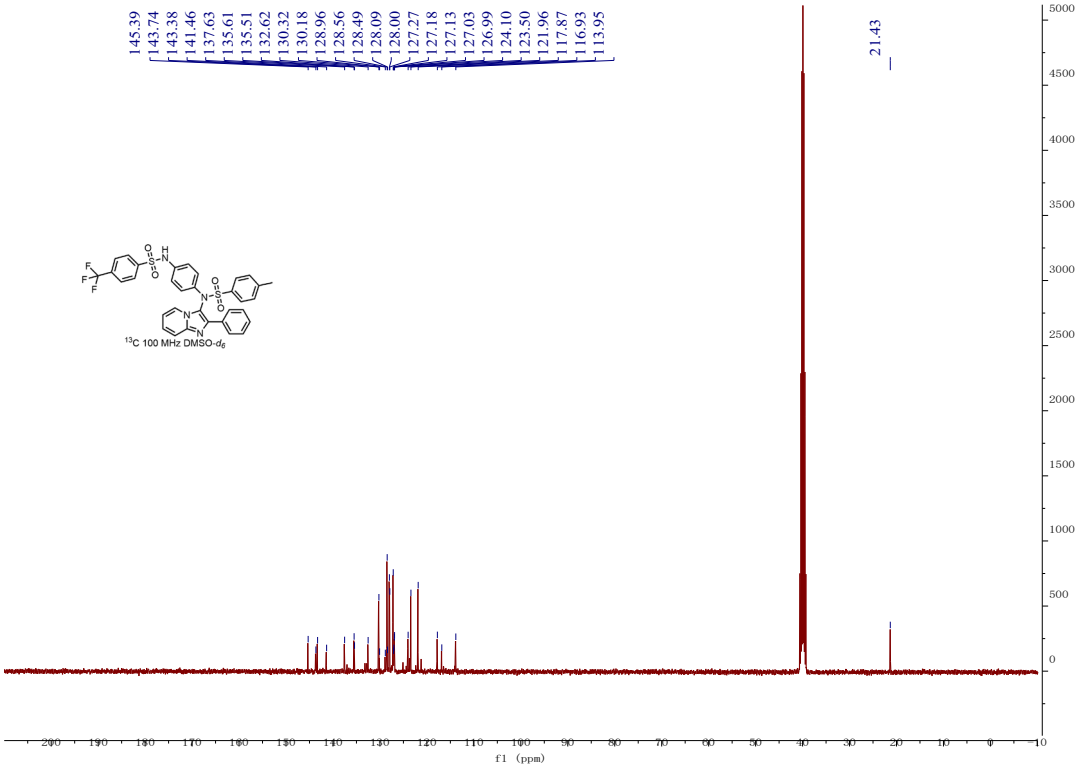
3u

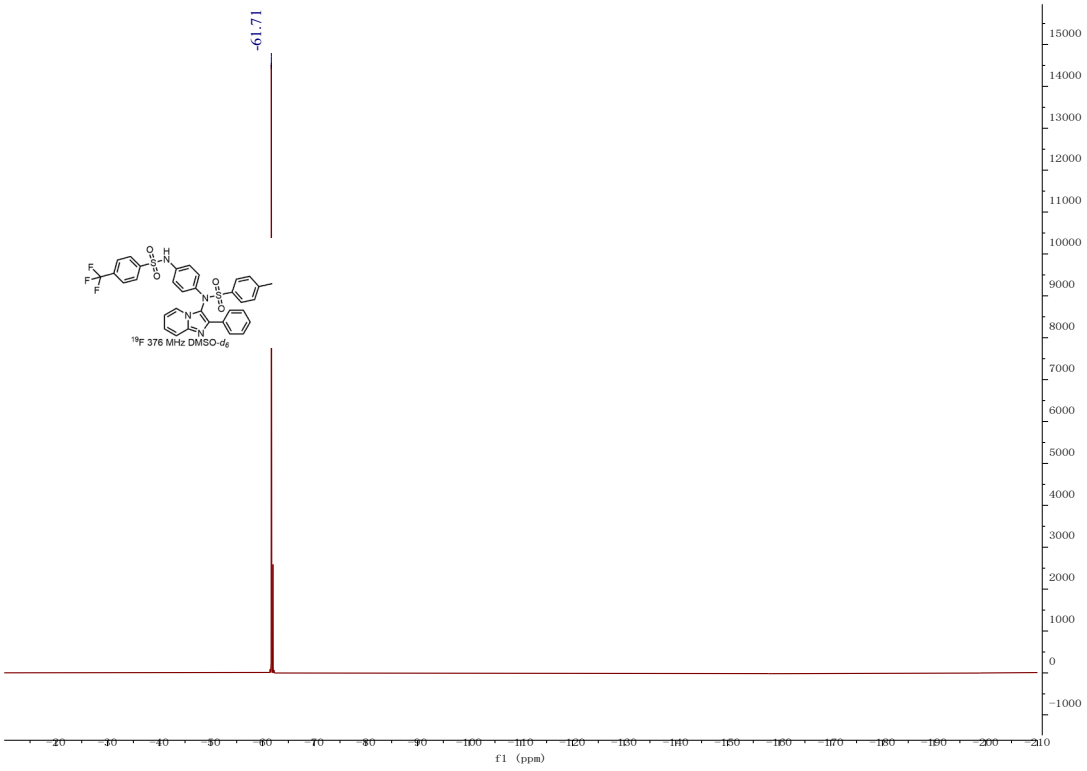

10.46
8.34
8.33
7.66
7.64
7.57
7.55
7.47
7.45
7.43
7.41
7.33
7.32
7.32
7.31
7.30
7.28
7.28
7.10
7.08
6.97
6.96
6.94
2.41
2.31
1.85
0.78
1.00
2.00
2.00
3.00
5.00
2.00
1.00
3.00
3.00
3.00
f1 (ppm)


145.1
143.9
142.8
141.0
137.9
137.2
136.2
136.0
130.6
130.2
128.1
128.0
127.1
126.3
123.8
120.6
118.0
117.0
113.1
21.6
21.4
13.5
f1 (ppm)

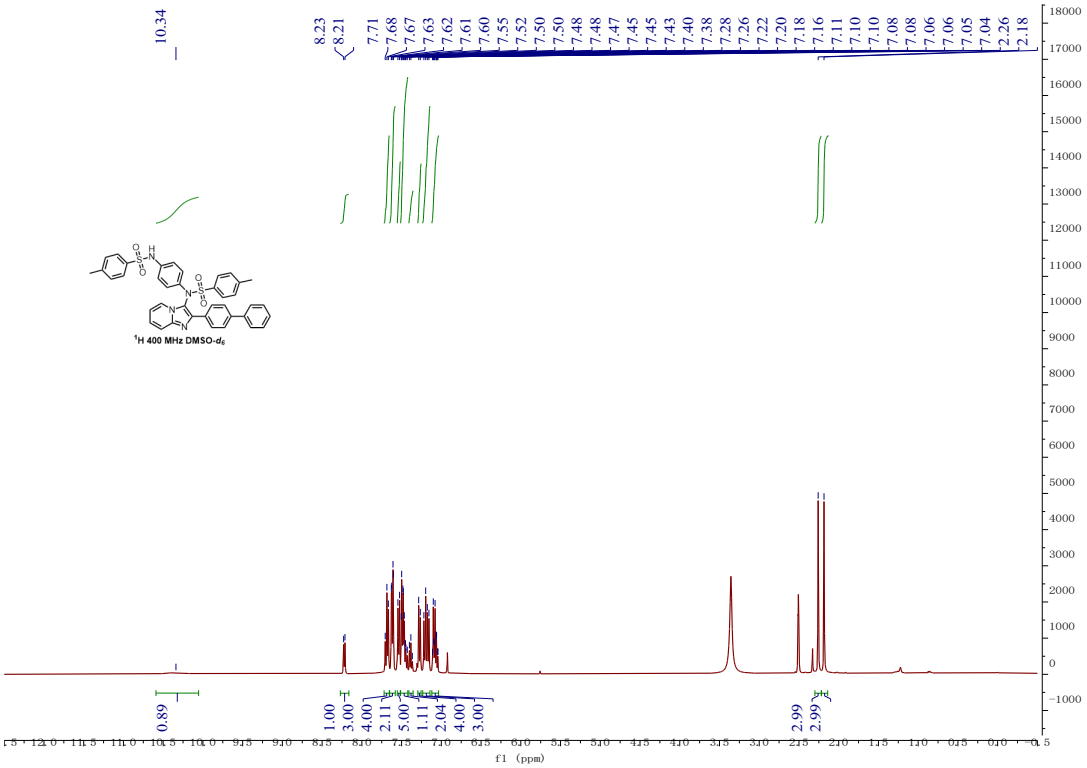
3v

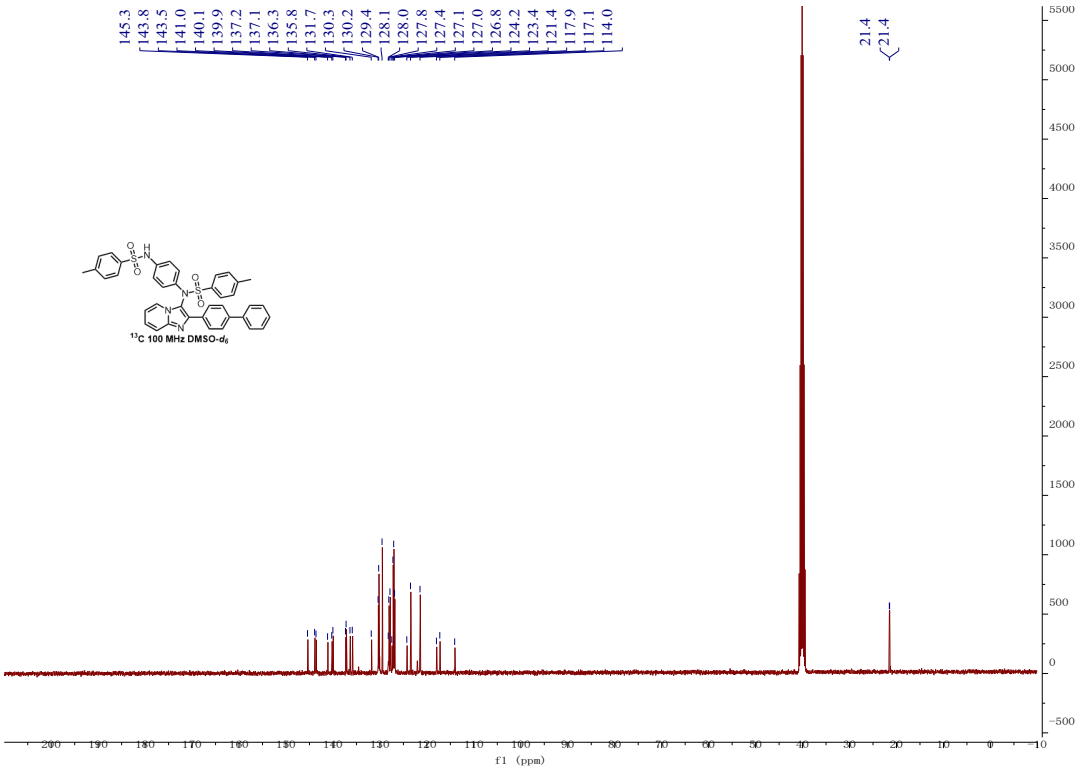

10.63
10.62
8.20
8.18
7.94
7.92
7.91
7.89
7.71
7.69
7.67
7.65
7.64
7.63
7.62
7.54
7.54
7.53
7.52
7.51
7.51
7.50
7.45
7.44
7.41
7.20
7.19
7.18
7.17
7.16
7.10
7.10
7.09
7.09
7.08
7.07
7.07
7.05
7.03
2.30
2.30
1.00
1.00
3.96
2.00
4.00
1.01
6.00
3.01
3.02
f1 (ppm)


145.39
143.74
143.38
141.46
137.63
135.61
135.51
132.62
130.32
130.18
128.96
128.56
128.49
128.09
128.00
127.27
127.18
127.13
127.03
126.99
124.10
123.50
121.96
117.87
116.93
113.95
21.43
f1 (ppm)

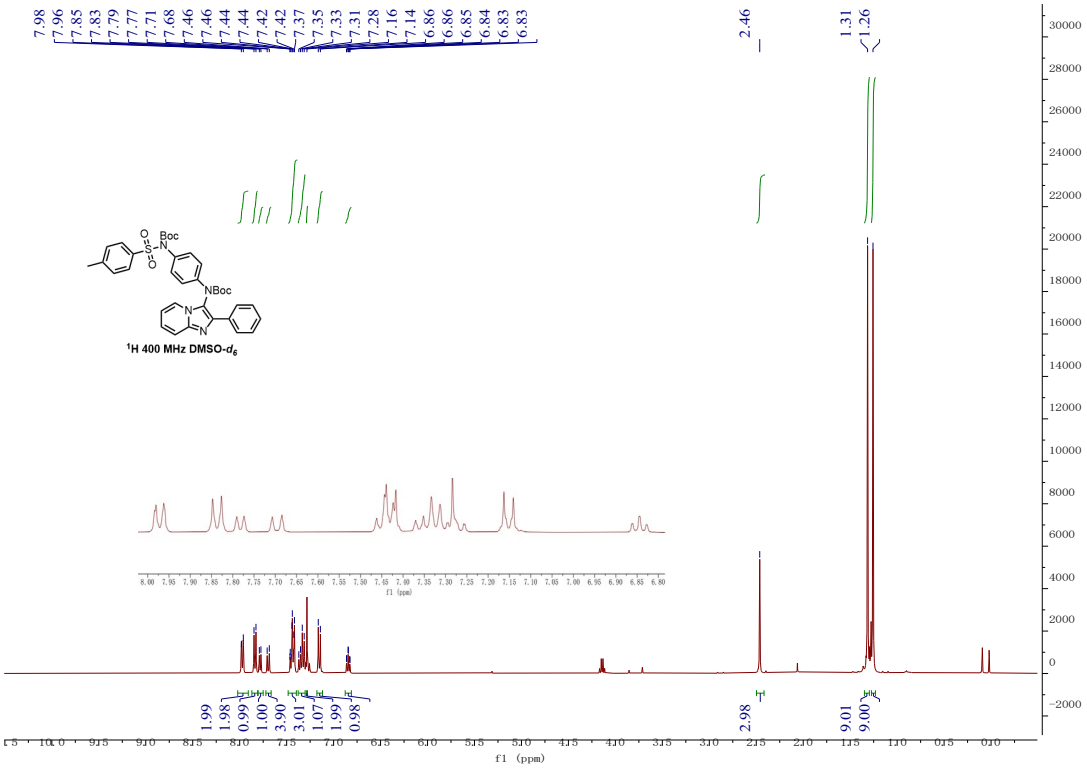

-61.71
^{19}F 376 MHz DMSO-d_6
f1 (ppm)

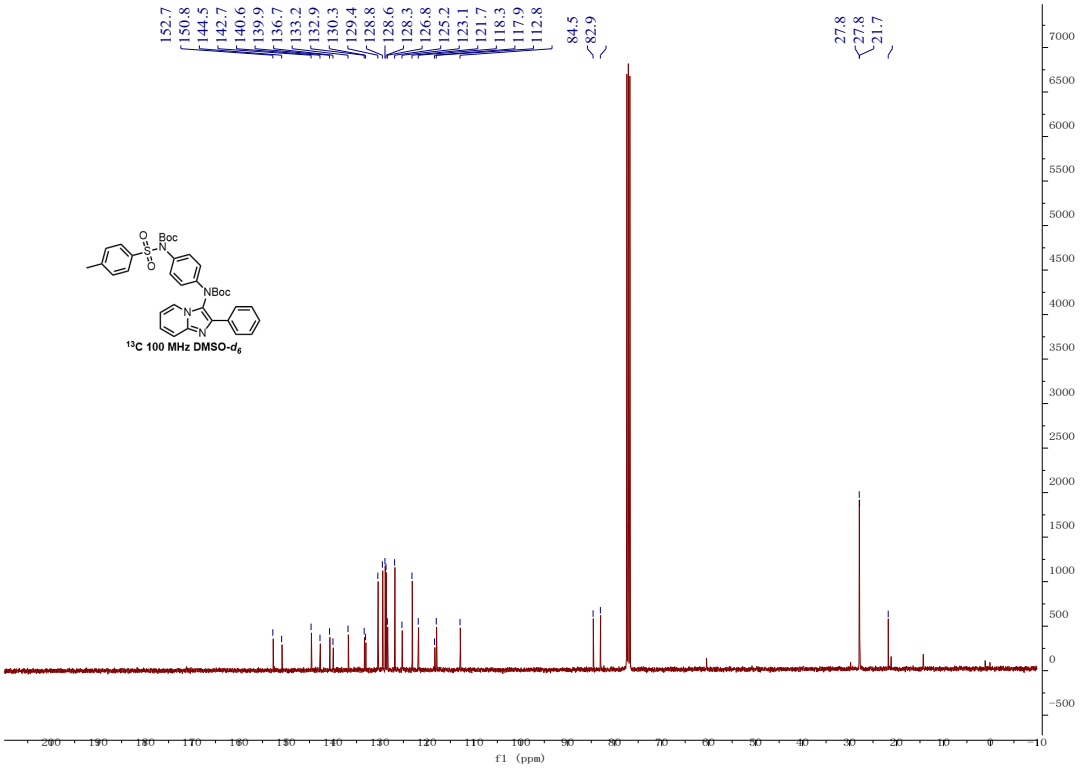
4a


10.34
8.23
8.21
7.71
7.68
7.67
7.63
7.62
7.61
7.60
7.55
7.52
7.50
7.50
7.48
7.48
7.47
7.45
7.45
7.43
7.40
7.38
7.28
7.26
7.22
7.20
7.18
7.16
7.11
7.10
7.10
7.08
7.08
7.06
7.06
7.05
7.04
2.26
2.18
0.89
1.00
3.00
4.00
2.11
5.00
1.11
2.04
4.00
3.00
2.99
2.99
^{1}H 400 MHz DMSO-d_6
f1 (ppm)


145.3
143.8
143.5
141.0
140.1
139.9
137.2
137.1
136.3
135.8
131.7
130.3
130.2
129.4
128.1
128.0
127.8
127.4
127.1
127.0
126.8
124.2
123.4
121.4
117.9
117.1
114.0
21.4
21.4
13C 100 MHz DMSO-d6
f1 (ppm)

5a


7.98
7.96
7.85
7.83
7.79
7.77
7.71
7.68
7.46
7.46
7.44
7.44
7.42
7.42
7.37
7.35
7.33
7.31
7.28
7.16
7.14
6.86
6.86
6.85
6.84
6.83
6.83
2.46
1.31
1.26
Boc
NBoc
1H 400 MHz DMSO-d6
1.99
1.98
0.99
1.00
3.90
3.01
1.07
1.99
0.98
2.98
9.01
9.00
f1 (ppm)


152.7
150.8
144.5
142.7
140.6
139.9
136.7
133.2
132.9
130.3
129.4
128.8
128.6
128.3
126.8
125.2
123.1
121.7
118.3
117.9
112.8
84.5
82.9
27.8
27.8
21.7
Boc
NBoc
13C 100 MHz DMSO-d6
f1 (ppm)